Quantum information dynamics

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QUANTUM INFORMATION DYNAMICS

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Presented is a study of quantum entanglement from the perspective of the theory of quantum information dynamics. We consider pairwise entanglement and present an analytical development using joint ladder operators, the sum of two single-particle fermionic ladder operators. This approach allows us to write down analytical representations of quantum algorithms and to explore quantum entanglement as it is manifested in a system of qubits.

We present a topological representation of quantum logic that views entangled qubit spacetime histories (or qubit world lines) as a generalized braid, referred to as a super-braid. The crossing of world lines may be either classical or quantum mechanical in nature, and in the latter case most conveniently expressed with our analytical expressions for entangling quantum gates. At a quantum mechanical crossing, independent world lines can become entangled. We present quantum skein relations that allow complicated superbraids to be recursively reduced to alternate classical histories. If the superbraid is closed, then one can decompose the resulting superlink into an entangled superposition of classical links. Also, one can compute a superlink invariant, for example the Jones polynomial for the square root of a knot.

We present measurement-based quantum computing based on our joint number operators. We take expectation values of the joint number operators to determine kinetic level variables describing the quantum information dynamics in the qubit system at the mesoscopic scale. We explore the issue of reversibility in quantum maps at this scale using a quantum Boltzmann equation. We then present an example of quantum information processing using a qubit system comprised of nuclear spins. We also discuss quantum propositions cast in terms of joint number operators.

We review the well known dynamical equations governing superfluidity, with a focus on self-consistent dynamics supporting quantum vortices in a Bose-Einstein condensate (BEC). Furthermore, we review the mutual vortex-vortex interaction and the consequent Kelvin wave instability. We derive an effective equation of motion for a Fermi condensate that is the basis of our qubit representation of superfluidity.

We then present our quantum lattice gas representation of a superfluid. We explore aspects of our model with two qubits per point, referred to as a Q2 model, particularly its usefulness for carrying out practical quantum fluid simulations. We find that it is perhaps the simplest yet most comprehensive model of superfluid dynamics. As a prime application of Q2, we explore the power-law regions in the energy spectrum of a condensate in the low-temperature limit. We achieved the largest quantum simulations to date of a BEC and, for the first time, Kolmogorov scaling in superfluids, a flow regime heretofore only obtainably by classical turbulence models.

Finally, we address the subject of turbulence regarding information conservation on the small scales (both mesoscopic and microscopic) underlying the flow dynamics on the large hydrodynamic (macroscopic) scale. We present a hydrodynamic-level momentum equation, in the form of a Navier-Stokes equation, as the basis for the energy spectrum of quantum turbulence at large scales. Quantum turbulence, in particular the representation of fluid eddies in terms of a coherent structure of polarized quantum vortices, offers a unique window into the heretofore intractable subject of energy cascades.
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- (BROWN) Magnitude of radial amplitude $\phi(r)$.
- (BLUE) Angular momentum number density $\phi(r)^2 v_\theta(r)/a$.
- (THICK BLUE) Amplitude-weighted angular velocity $\phi(r) v_\theta(r)/\sqrt{a}$.
- (BLUE DASHED) Divergent angular velocity $v_\theta(r) = h/(mr)$.
- (RED) $k^{-3}$ spectra occurs within one coherence length, $r \lesssim \xi$.
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x
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6.18 Power spectrum of the quantum fluid’s incompressible kinetic energy (top). There are three regions characterized by differing power laws displayed on the vortex soliton spatial profile (bottom). Numerical data (dots) is from a supercomputer simulation of a quantum lattice gas on a $1024^3$ grid. Kolmogorov (black), transition (green), and core interior (red) regimes are shown.

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7.2 Quantum vortex profiles for $g = 1$ in lattice units with a scale factor $a = 0.02$:
(BROWN) Condensate magnitude $\rho(r)^{\frac{1}{2}}$.
(BLUE) Momentum density $u_{\phi}(r)/a = \rho(r)u_{\phi}(r)/a$.
(BLUE DASHED) Divergent angular velocity $v_{\phi}(r) = \hbar/(m r)$.
(BLACK) Momentum density $\Im[u_{\phi}^a(r)]/a = \rho(r)\Im[u_{\phi}^a(r)]/a$.
(BLACK DASHED) Divergent angular velocity $\Im[u_{\phi}^a(r)]$.
(RED) Kelvin waves extend to the coherence length $\sim \xi$.
(GREEN) Quantum transition region extends out to $\sim \pi \xi$.

7.3 Time development vortex-antivortex reconnection on a 240$^3$ grid. Probability isosurfaces of $|\psi|^2 = |\psi_1 + \psi_1|^2$ are plotted. At $t = 0$ (top), two independent vortex lines, oriented perpendicularly and separated in space (non-intersecting cores). By $t = 24$, the vortex-pair becomes unstable, inducing traveling Kelvin waves along the filamentary core. At $t = 48$, the two vortex cores connect, defined as $t_0$. By $t = 116$ (bottom), the cores are disconnected along the original orientations and reconnected at right angles. Induced quantum Kelvin waves are apparent.

7.4 (LEFT) Quantum vortex is a kink soliton. The flow direction on the left of the center is the opposite from the direction on the right, viz., a phase shift of $\pi$ radians occurs in the condensate wave function as one goes half way around a quantum vortex. (RIGHT) Time development of an analytical kink soliton solution for the velocity field $u = 1 - \rho$ of Burgers equation (run for the case when the kinetic variables are constrained to $\rho = a + b = 1$), shifted vertically for each time increment to avoid overlap. The two the kink solutions are identical. Away from the kink front, the bulk values of the respective fields are $\pm 1$.

7.5 (a) Unperturbed vortex rendered over 160 cyclotron periods. (b) Four wavelengths of a kelvon riding on a larger vortex core, where $\Omega_{\text{cyc}} = \rho c / m$. (c) "Cyclotron" orbit in cross-section view, in units where the core inner radius (coherence length) is $\xi = 1.0$ (brown circle) and the gyration of a trapped quantum particle (small red circle) has a gyro-radius one quarter the core radius. The slow gyration displaces quantum vortex core (blue circle). (d) Quasiparticle trace for 20 cyclotron periods where the gyration frequency is $\Omega_{\text{cyc}}/40$, rendered as a closed world line.

7.6 Simulation of vortex and anti-vortex filaments, originally linear and oriented perpendicularly on a 1024$^3$ grid. Time steps $t = 1200\Delta t$ and $t = 4800\Delta t$ are plotted. Quantum Kelvin waves are seen along the vortex filaments early in the simulation. At the late stages, the filaments bend, reconnect, and exchange vortex rings.
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7.8 The evolution of quantum vortices showing the vortex bending, reconnection and formation of vortex loops on a $1024^3$ grid. Shown are ray traced surfaces of constant number density, $|\varphi| = 0.08|\varphi_{\text{max}}|$, that enclose the nodal lines in the condensate. (a) The initial 12 linear vortex cores (topologically equivalent to 12 vortex rings because of periodic boundaries). (b) At the early time $t = 2500$ large amplitude Kelvin waves have developed. (d) By $t = 55000$ a large number of reconnection events have occurred. (f) At $t = 60200$ the vortex tangle reduces to 12 small vortex rings topologically equivalent to the initial state. (i) The vortex cores at $t = 83600$ (green) closely resembling the initial state, but the Poincaré recurrence time occurs near $t = 167600$ (white). The “bulleyes” are the intersection of the initial vortex cores with the walls at $t = 0$.

7.9 This is a quantum lattice simulation of a BEC superfluid in 3+1 dimensions spontaneously giving rise to turbulent quantum flow. Plotted are ray-traced surfaces of constant probability density showing the cores of tangled vortex solitons (zoom-in online to view the vortex tangles). The most recent quantum lattice gas simulations are run on DoD CRAY XT-5 supercomputers that realize informational substrates with a half trillion qubits and 20 trillion gates. The amount of computational resources needed to simulate quantum turbulence is on the order of 80,000 cycle times, which comprises $10^{18}$ gate operations.

A.1 Quantum circuit diagram using the Deutsch oracle $U_D$. The input lines are “hard-wired.” Measuring the output line deterministically yields a 1 or 0 if the function $f(x)$ is balanced or constant, respectively.

A.2 Quantum circuit diagram whose input and output states are purely classical, having no output lead in superposition. Measuring the top output line deterministically yields $q = 1$ or $q = 0$ when the function $f(x)$ is balanced or constant, respectively.
A.3 Symmetric quantum circuit diagram whose output states contain all the available classical information (two bits), again with no quantum superposition on the output. Measuring the top output line deterministically yields \( q = 1 \) or \( q = 0 \) when the function \( f(x) \) is balanced or constant, respectively. Measuring the bottom output line deterministically yields \( f(1) \), which corresponds to the value of one side of the coin.

C.1 Dispersion relation for He II. The initial slope at small \( k^{-1} \) is linear in the phonon part of the excitation spectrum and the parabolic part of the spectrum is due to roton excitations. The dashed line indicates a solution of \( \varepsilon/p = d\varepsilon/d\rho \) which occurs near the local minimum of the curve, the band gap energy characteristic of superfluids.

E.1 Collisional inversion. The non-equilibrium part of distribution function is shown (black vectors on the left and white on the right). The curved surface is an isentrope and the diagonal plane is a constant mass surface. The incoming \( f \) goes to a point at the intersection of the constant mass and entropy surfaces (black line on left and white line on right view). \( f^{eq} \) is shown (middle black line on left and middle white line on right view). \( f^{eq} \) contacts a lower entropy surface. The ideal (\( \beta = 1 \)) outgoing distribution \( f' = f + \alpha \Delta \) (black line on left and white line on right view) goes to an antipodal point on the curve formed by the intersection of the constant mass and entropy surfaces. Finally for \( \beta = 0.9 \), the outgoing \( f + \alpha \beta \Delta \) (red line on both views) illustrates \( \beta < 1 \) increases the entropy since \( f \) does not contact the original entropy surface.

E.2 Early stage in the development at \( t = 900 \) of the Kelvin-Helmholtz instability modeled with parameters \( \beta = 0.9995 \) and the bare viscosity is \( \nu = 8.3410^{-5} \) (using \( \alpha = 2 \)), on a \( 1024^2 \) grid (only a horizontal strip through the middle of the grid is shown). The 2D model uses a 9-point stencil. Vortex production occurs along the fronts of the braking waves (blue is counterclockwise and red is clockwise rotation). The initial background flow speed is \( u_0 = 0.5 \Delta T \Delta P \), and the Reynolds number \( Re = 9.810^4 \).
E.3 3 stages of symmetric vortex fusion. 1st column ($t < 50K$): Vortices rotate around each other with approximately constant separation distance; the areal size of the vortices grows linearly in time because of viscous diffusion. 2nd column ($50K \leq t < 70K$): Vortices reach a critical size, about 24% of the separation distance. Vortex centers then rapidly merge into a single core. 3rd column ($t \geq 70K$): Vorticity arms roll up around the central pattern, forming a spiral of vorticity, which subsequently spreads and is smoothed by diffusion.

E.4 Streamlines plot of turbulent flow arising from the initial Kida profile.

E.5 The enstrophy (integrated mean square vorticity) decay for bare viscosities ranging from $\nu = 2 \times 10^{-4}$ (for $\beta = 0.9988$) to $\nu = 8 \times 10^{-3}$ (for $\beta = 0.95$) for an initial Kida profile. In the early stages, one sees the effects of vortex stretching with exponential growth in the strength of the vortex filaments. This growth in the enstrophy is independent of viscosity. $\nu$ determines the peak in the enstrophy followed by exponential decay in the inertial range. $Re \approx 6000$ was achieved on the $512^3$ grid.
DEDICATION

I present this dissertation in honor of my wife, Andrea Yepez.
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QUANTUM INFORMATION DYNAMICS
CHAPTER 1

Overview of quantum information dynamics

1.1 Introduction

Quantum information theory is a rapidly emerging field in physics that in recent years has received an abundance of attention from theorists and experimentalists alike. The reason for its rapid development is the hope that quantum information theory will offer us new and profound ways to understand and exploit, for very practical purposes, the mysterious and vast resources contained within entangled quantum systems. Quantum entanglement affords the experimentalist the remarkable ability to alter (e.g. observe) the state of a quantum object that may be located arbitrarily far away in space from his or her nearby quantum device (e.g. measurement apparatus), and this peculiar ability follows when the distant quantum object is perfectly correlated with its counterpart object that is nearby, operated upon or detected by that quantum device. In this thesis, we consider the effects of quantum entanglement by considering quantum information dynamical systems, and thereby
strive to unravel some of the mystery behind this important physical effect.

Einstein, Podolsky and Rosen (EPR) discovered non-local quantum entanglement over three quarters of a century ago [Einstein et al., 1935]. Although their seminal 1935 EPR Physical Review paper, “Can quantum-mechanical description of physical reality be considered complete?” is the most cited physics paper ever, quantum entanglement remains still one of the most mysterious properties of quantum physics. One has to probe particles at high energies that existed a trillionth of a second after the creation of the universe or attempt to probe for the dark energy causing the accelerated cosmic expansion and dark matter to encounter comparable mysteries.

Quantum communication [Bennett and Wiesner, 1992, Bennett et al., 1993] and superdense coding [Schumacher, 1995] are good examples of important applications that exploit the properties of EPR pairs for their efficient operation, and these quantum information protocols can be rendered as physical spacetime diagrams or equivalent quantum information dynamics Feynman diagrams [Cerf and Adami, 1997b]. Yet, the most promising application of quantum entanglement is quantum computing, which theoretically provides a pathway to predict solutions to otherwise intractable problems—efficient quantum simulation of non-perturbative many-body physical systems is its prime application. In a quantum computer, quantum entanglement is created, used, transferred, and destroyed, either with or without any wave function collapse.

Quantum information theory has provided a new paradigm for understanding quantum entanglement. Most work has focused on quantifying and classifying static entangled quantum states, including detection, verification, distillation, and estimation [Braunstein and Caves, 1994],[Vidal, 1999],[Wong and Christensen, 2001],[Eisert and Briegel, 2001, Coffman et al., 2000, Horodecki and Ekert, 2002],[Meyer and Wallach, 2002, Lyons et al., 2008, Horodecki et al., 2005]

1.2 Quantum informational models

Herein we will consider an archetypal quantum informational model of a system of quantum particles in D+1 dimensions. In the prototypical quantum informational model, quantum dynamics is represented on a space made up of an ordered collection of $L^D$ number of points; for example, for $D = 1$, the set of points $\{x_1, x_2, \ldots, x_L\}$ say. Information is measured in unit of bits, and fractions of bits are physically allowed in quantum logic.

A basic property of a point (as represented in the model) is that it may contain a fixed amount of information and any two (correlated) points may contain a fixed amount of joint information. The simplest case, a Q2 quantum lattice gas model, has each point comprising two quantum bits (qubits). Several mathematical representations of qubits are presented in Sec. 2.1—they are two-level objects, so two qubits encode four distinct states, $|\alpha\rangle$ say, for $\alpha = 0, 1, 2, 3$, and $n$ qubits encode $2^n$ states. Each of the four states at a point in a Q2 model represents the amplitude
for a particular configuration of particle occupancy at that point; for example,

\[
\begin{align*}
|0\rangle &= |00\rangle, & \nu_0 & \text{(empty or pair hole)} \\
|1\rangle &= |01\rangle, & \nu_1 & \text{(plus or spin-up)} \\
|2\rangle &= |10\rangle, & \nu_1 & \text{(minus or spin-down)} \\
|3\rangle &= |11\rangle, & \nu_{11} & \text{(double or pair)}
\end{align*}
\]

(1.1)

is a typical encoding at each point. Regarding information contained in a pair of qubits, the Deutsch problem is one of the earliest examples of how a quantum circuit can be used to efficiently extract joint information. Appendix A gives a simple quantum circuit demonstration of how quantum superposition is used to speedup the solution of the Deutsch problem for determining whether a binary function is balanced or constant.

In the case of the Q2 model, one can think of one qubit storing the amplitude of a spin-up particle occupying some point and the other storing the amplitude of a spin-down particle at that point, directly associating a qubit to a container for a particle with a particular spin. The terms “qubit” and “particle” are sometimes used interchangeably, blurring the distinction between a container and its contents. This occurs when a qubit is identified with the spin-degree of freedom of a spin-$\frac{1}{2}$ particle. Yet, this identification is not the one we use in quantum information dynamics. Instead of thinking of a qubit as a particle per se (i.e. since it has no mass or charge nor an intrinsic dynamics), we suggest a fundamental definition of a qubit: it is a logical container allowing either zero or one fermion to occupy a point, and the type of Fermi particle represented at that point depends on the number of qubits per point and the choice of encoding. The Pauli exclusion principle derives directly from the qubit representation of a point of space and otherwise is not intrinsic to the encoded particles per se. This is in contradistinction with the common practice of attributing the exclusion property (or the associated short-range repulsive exchange force) to the chiral matter itself and not to the space that
contains the chiral matter.

Furthermore, the Bose-Einstein or Fermi-Dirac quantum statistics of the system of particles represented in the qubit system derive from how the points are stitched together, so to speak. Two points are neighbors because their respective qubits are coupled, viz., one qubit from a point is coupled to a qubit from another point by a quantum gate. It is the quantum gate that connects two points together and that gives rise to the quantum statistics of the modeled system of quantum particles. Thus, the quantum statistics of the modeled fermions are not intrinsic to the particles per se. Again, this is in contradistinction with the common practice of attributing the quantum statistics of a system of particles to particles themselves and not to the space that contains them.

With regards to coupling a pair of qubits (which need not reside at the same point), let us denote the first qubit by $|q_\alpha\rangle$ and the second one by $|q_\beta\rangle$. A quantum gate is supposed to represent the most basic of informational transformations that can occur. Denoting the combined state of two qubits by $|q_\alpha q_\beta\rangle$, every quantum gate is generated by a hermitian operator, $N_{\alpha\beta}$ say, for example as follows

$$|q_\alpha q_\beta\rangle' = e^{i\zeta N_{\alpha\beta}}|q_\alpha q_\beta\rangle,$$

where $\zeta$ is a real parameter called the gate angle. A thorough presentation of quantum gates is given in Chapter 2 where we introduce a powerful analytical technique—Chapter 2 is the foundational chapter upon which all the subsequent ones depend.\footnote{For example, the Bogoliubov quasiparticles and their governing equations of motion are derived in Chapter 5 and their representation in terms of mode entangled quantum states is treated in Sec. 5.4, which is devoted to the superfluid dynamics of a Fermi condensate.} It is the behavior of a large collection of quantum gates that is the subject of this work, yet for now let us begin by considering a small number of them.

There are two archetypal cases of interest:

1. $N_{\alpha\beta}^2 = N_{\alpha\beta}$, and
2. $N_{\alpha\beta}^3 = N_{\alpha\beta}$ but $N_{\alpha\beta}^2 \neq N_{\alpha\beta}$.

A quantum gate $e^{i\zeta N_{\alpha\beta}}$ is the fundamental logical construct for building up more general quantum dynamics over a field of qubits. For example, four qubits could be coupled together by three quantum gates as follows

$$|q_{\alpha}q_{\beta}q_{\gamma}q_{\delta}\rangle' = e^{i\zeta N_{\alpha\beta}}e^{i\zeta N_{\alpha\gamma}}e^{i\zeta N_{\gamma\delta}}|q_{\alpha}q_{\beta}q_{\gamma}q_{\delta}\rangle. \quad (1.3)$$

The composite unitary transformation

$$e^{i\zeta N_{\alpha\beta\gamma\delta}} \equiv e^{i\zeta N_{\alpha\beta}}e^{i\zeta N_{\alpha\gamma}}e^{i\zeta N_{\gamma\delta}} \quad (1.4)$$

is an example of a quantum circuit. Information is weaved together according to some particular sequence of quantum gates. That is, in quantum information theory, one specifies the quantum gate configuration comprising a quantum circuit (e.g. first $e^{i\zeta N_{\gamma\delta}}$ then $e^{i\zeta N_{\beta\gamma}}$ and then $e^{i\zeta N_{\alpha\beta}}$ on the right-hand side of 1.4), and one does not specify the generator of the transformation (e.g. $N_{\alpha\beta\gamma\delta}$ on the left-hand side of 1.4). For large qubit systems, $N_{\alpha\beta\gamma\delta}$ is hard to analytically determine because the respective quantum gates do not in general commute with one another. This is one of the features that makes the quantum circuit representation of quantum dynamics so powerful—a quantity that is analytically difficult (and in fact intractable for large qubit systems) is represented in a direct unitary way that is practical for quantum simulation purposes.

1.2.1 Quantum circuits: pathways for information flow

The quantum informational approach of specifying quantum dynamics, which is originally due to Feynman [Feynman, 1960, Feynman, 1982], is a rather new approach in the history of physics. Traditionally, one uses a Hamiltonian (in condensed matter physics) or a Lagrangian (in high-energy physics) to specify the quantum
dynamics of a system of particles, a practice that dates back to the earliest formu-
lation of quantum field theory in the first half of the 20th century and that in
turn follows in the tradition of Lagrangian and Hamiltonian classical mechanics of
many-body classical dynamics in the late 18th and early 19th centuries.

In the quantum informational approach of specifying quantum dynamics, one
uses wiring diagrams to represent quantum circuits schematically, somewhat similar
to well known electrical wiring diagrams. With the advent of topological quantum
computing and quantum algorithms for computing knot invariants such as the
Jones polynomial, it is fitting to use diagrammatic conventions from knot theory.
Yet, there are no well established conventions for diagrammatically representing
quantum circuits in this context, at least as far as I know. The diagrams I will use
are intended to help make the presentation clearer by graphically representing vari-
ous concepts, albeit they are otherwise cumbersome to use to specify complicated
quantum algorithms that do not have a regular pattern of interconnections.\(^2\)

One usually weaves a braid out of a number of pliable strands of string. In
the context of a quantum circuit, the strands that comprise a braid are thought of
as quantum wires, \textit{i.e.} directed pathways for the transfer of quantum information.
A quantum wire carries the quantum state of a single particle that in general is
entangled with the quantum information "flowing" in the other quantum wires of
the circuit. So a wire induces a directed world-line trajectory in spacetime of a
particle encoded on that wire and correlated with the other qubit states in the
modeled system.

In our wiring diagram, the intersection of any two wires represents a quantum
gate operation. Letting \(|\psi\rangle \equiv |g_\alpha g_\beta g_\gamma g_\delta\rangle\), the time-histories of individual qubit

\(^2\)Although quantum algorithm protocols are specified using operator notation, it is often help-
ful to also keep in mind the equivalent wiring diagram. Exploiting symmetries in the quantum
circuit diagram helps to improve the quantum algorithm, \textit{e.g.} giving it a high-order numerical
convergence when used for modeling many-body dynamics. This was the case for the Q2 model in
3+1 dimensions used for simulating a quantum gas, for example.
states coupling via the three quantum gates in the above example circuit can be represented as the following sub-circuits

\[ |\psi'\rangle = e^{i\kappa N_{\alpha\beta}} |\psi\rangle \quad \leftrightarrow \quad |q_\alpha q_\beta q_\gamma q_\delta\rangle \quad (1.5a) \]

\[ |\psi'\rangle = e^{i\kappa N_{\alpha\gamma}} |\psi\rangle \quad \leftrightarrow \quad |q_\alpha q_\beta q_\gamma q_\delta\rangle \quad (1.5b) \]

\[ |\psi'\rangle = e^{i\kappa N_{\alpha\delta}} |\psi\rangle \quad \leftrightarrow \quad |q_\alpha q_\beta q_\gamma q_\delta\rangle \quad (1.5c) \]

In Chapter 3, we will “zoom in” on an intersection point, so to speak, to describe its behavior in more detail; viewed at high resolution, the world lines do not actually ever intersect\(^3\). Yet, it is sufficient to consider the low-resolution diagrams such as (1.5) to make a number of preliminary observations. In (1.5b) the wires connecting \(|q_\alpha\rangle\) to \(|q'_\alpha\rangle\) and \(|q_\gamma\rangle\) to \(|q'_\gamma\rangle\) each cross \(|q_\delta\rangle\). Such crossings are classical braids, either a negative \((-1)\) crossing \(\chi\) or a positive \((+1)\) crossing \(\chi\). When using a quantum circuit model of a fermionic system of particles, the final “scattering” outcome of two qubit states (encoded in \(|q_\alpha\rangle\) with \(|q'_\alpha\rangle\) in this example) depends on the state of all preceding qubits (\(|q_\beta\rangle\) in this example) but does not depend on any qubits that follow (\(|q_\delta\rangle\) in this example). In practice (and without loss of generality), every quantum gate operation should be thought of as a local operation and any intermediate strand in the way needs to be appropriately braided so as to make the

\(^3\)This is a principle well known in quantum field theory, for example where one may use the (low resolution) Fermi theory of beta decay versus the (higher resolution) Glashow-Salam-Weinberg theory of the weak interaction with intermediate gauge matter.
quantum gate strictly local. And it does not matter whether one chooses to cross over or under an intermediate strand so long as the braid itself is represented by a local quantum swap gate, which is a nonentangling quantum gate that in matrix representation, respectively, has the form

\[
\text{SWAP}_\pm = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & \pm1 & 0 \\
0 & \pm1 & 0 \\
0 & 0 & 0 & -1
\end{pmatrix} = e^{\pm i\pi \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & \frac{1}{2} & -\frac{1}{2} & 0 \\
0 & -\frac{1}{2} & \frac{1}{2} & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}}. \tag{1.6}
\]

This convention avoids any ambiguity in interpreting a quantum circuit diagram with braided wires.

In this type of quantum circuit construction, the speed at which information flows from the top to the bottom, projected along the vertical, is taken to be a constant. Therefore, if all the wires going from the top to the bottom have equal lengths, \textit{viz.} not as drawn in (1.5), then the speed of information moving along the wires would be constant too. Yet, it is not necessary to render the diagram with equal length strands; what is necessary is that the speed with which information moves in the vertical direction be constant. The most important distinction to make is which qubits the quantum gates act upon, and in what order. Given a particular quantum circuit, so long as no wires are cut and all the intersection points are maintained in the diagram’s original ordering, the actual positioning of the quantum wires in the diagram can be changed; the circuit is topologically invariant with respect to the isotopy of the embedding space.

So far we have discussed the shape of the wires, or their topological properties. Another important property of quantum wires is the direction of the flow of information along a wire—a quantum wire behaves like an oriented strand. With time advancing along the vertical axis going from top to bottom, the convention we use renders a bit 0 (hole) moving forward in time as an upward oriented strand (\dagger) and
a bit 1 (particle) moving forward in time as a downward oriented strand (↓):

\[
\begin{align*}
0_0 & \equiv \uparrow \\
1_1 & \equiv \downarrow.
\end{align*}
\] (1.7)

Consequently, a bit that reverses its motion in time necessarily complements its value; for example, the four flow reversal diagrams

\[
\begin{array}{cccc}
1 & 0 & \circlearrowleft & 0 \\
1 & 0 & \circlearrowleft & 1
\end{array}
\] (1.8)

follow from (1.7).

Now, if you are not already familiar with the skein relation

\[
\begin{array}{c}
|0\rangle \\
|1\rangle
\end{array}
\xrightarrow{\text{time}}
\begin{array}{c}
\{0\} \\
\{1\}
\end{array}
\] (1.10a)

from knot theory, you can nevertheless interpret it from a quantum informational viewpoint simply by applying the convention (1.7). For instance, we know that the \(A\) parameter here must represent the amplitude for the exchange of two bits of information within a quantum state

\[
|\ldots 0 \ldots 1 \ldots \rangle \xrightarrow{A_{\text{time}}} |\ldots 1 \ldots 0 \ldots \rangle,
\] (1.10b)

whereas its inverse \(A^{-1}\) represents the amplitude for no exchange

\[
|\ldots 0 \ldots 1 \ldots \rangle \xrightarrow{A^{-1}_{\text{time}}} |\ldots 0 \ldots 1 \ldots \rangle.
\] (1.10c)

Now consider the diagrammatic mirror image of (1.10a), where we also take \(A \xrightarrow{\text{parity}} A^{-1}\), so that the skein relation becomes

\[
\begin{array}{c}
|0\rangle \\
|1\rangle
\end{array}
\xrightarrow{\text{time}}
\begin{array}{c}
\{0\} \\
\{1\}
\end{array}
\] (1.11a)

\footnote{Using complement notation \(\bar{0} \equiv 1\) and \(\bar{1} \equiv 0\), we can also write (1.8) as

\[
\begin{array}{cccc}
\bar{1} & \bar{1} & \circlearrowleft & \bar{1} \\
\bar{1} & 1 & \circlearrowleft & 1
\end{array}
\] (1.9)

which is akin the Feynman diagrammatic convention for fermion lines, and (complement) anti-fermion lines, used in quantum field theory to represent pair creation or destruction.}
Here, we find another interpretation of the $A$ parameter. Now the $A^{-1}$ parameter necessarily represents the amplitude for the exchange of two bits of information within a quantum state

$$|\ldots 0\ldots 1\ldots \rangle \xrightarrow{A^{-1}_{\text{time}}} |\ldots 1\ldots 0\ldots \rangle,$$  \hspace{1cm} (1.11b)

while its inverse $A$ represents the amplitude for no exchange

$$|\ldots 0\ldots 1\ldots \rangle \xleftarrow{A_{\text{time}}} |\ldots 0\ldots 1\ldots \rangle.$$ \hspace{1cm} (1.11c)

Comparing (1.10) with (1.11), if $A$ represents the amplitude for a transition in time, then $A^{-1}$ represent the time-reversed transition. So, for example, the skein relations (informational transitions) are invariant with respect to the product of a parity operation and time-reversal (that is, $PT = 1$). Quantum mechanically entangled qubit world lines and tangled strands are closely related, and we explore this connection in Chapter 3. We find, for example, that when $A$ is complex unimodular, its phase has the physical interpretation of an internal e-bit phase angle; that is, $A = e^{i(\xi - \frac{\pi}{2})}$.

**Feynman’s 1982 conjecture**

Now, let us move on to an important conjecture originally due to Feynman [Feynman, 1982] regarding the existence of a universal quantum simulation that may be stated as follows: The dynamical properties of a system of quantum particles can be exactly modeled with quantum circuits. In the scaling limit, when the number of qubits becomes large, the long wavelength behavior of the system of qubits can accurately approximate a physical quantum field theory (in its low-energy representation). If Feynman’s conjecture holds, then all non-local quantum effects, including those normally associated with the ordering of quantum particles whose dynamical operators satisfy nonabelian gauge groups, are ultimately reducible to a collection of the kind of archetypal quantum gates embedded at the intersection points within a patchwork of quantum wires.
There are conventional quantum gates [Barenco et al., 1995], such as the controlled-NOT quantum gate, and it has been known for a while that 2-qubit gates are computationally universal [DeVincenzo, 1995, Barenco, 1995]. Quantum gates are customarily described using matrix or algebraic representations. For our purposes an analytical representation of quantum gates decomposed into ladder operators is most useful.

Although a qubit is parameterized by two real-valued internal angles it can contain no more than a single bit of information. A joint information theoretic operator, such as an entanglement operator (or joint number operator) denoted $N_{\Delta \alpha \beta}(\vartheta, \xi)$, can generate a pairwise entangled state that contains anywhere from zero up to one bit of entangled information, an e-bit. $N_{\alpha \beta} = N_{\alpha \beta}^2$ is our prototypical joint informational operator. Like a qubit, an e-bit is also parameterized by two real-valued angles, which are a gate angle $\zeta$ (herein the variable $\vartheta$ is most often used as a gate angle) and an internal phase angle $\xi$. The gate angle $\zeta$ in (1.2) parameterizes the strength of the e-bit, whereby the e-bit's content ranges from 0 to 1 bit of shared information as $\zeta$ goes from 0 to $\pi/2$.

Bennett et al., in the context of quantum teleportation [Bennett and Wiesner, 1992, Bennett et al., 1993], have explored how a system of e-bits with entanglement $< 1$ can be concentrated into an informationally equivalent system of fewer maximally entangled e-bits [Bennett et al., 1996]. To quantify the amount of entanglement in a partly entangled pure state of a bipartite qubit state, say between the $\alpha$th and $\beta$th qubits, one determines the partial traces of density matrix

$$\rho_{\alpha} = \text{Tr}_{\beta}|q_{\alpha}q_{\beta}\rangle\langle q_{\alpha}q_{\beta}| \quad (1.12a)$$
$$\rho_{\beta} = \text{Tr}_{\alpha}|q_{\alpha}q_{\beta}\rangle\langle q_{\alpha}q_{\beta}|. \quad (1.12b)$$

Reduced density matrices were proposed by Yang as a means to quantify long-range order in superconductors [Yang, 1962]. If the entangled states are shared between
spatially remote locations, one qubit by Alice and the other by Bob say, then the von Neumann entropy is determined by either party [Schumacher, 1995]

\[ E = -\text{Tr}\rho_\alpha \log_2 \rho_\alpha = -\text{Tr}\rho_\beta \log_2 \rho_\beta. \]  

(1.13)

An e-bit is a bi-directional shared informational resource indeed. Now, let us return to our small quantum circuits.

To make a composite quantum circuit, we simply “solder” together the respective output and input leads of the sub-circuits, e.g. (1.4) becomes

\[
\begin{align*}
|q_\alpha q_\beta q_\gamma q_\delta\rangle \\
|q'_\alpha q'_\beta q'_\gamma q'_\delta\rangle
\end{align*}
\]

(1.14)

Now let us consider a quantum circuit with closed-loop feedback. Such a circuit is fashioned by connecting, with a quantum wire, each output qubit to the respective input qubit. For example, with 4 qubits this is

\[
\begin{align*}
|q_\alpha q_\beta q_\gamma q_\delta\rangle \\
|q'_\alpha q'_\beta q'_\gamma q'_\delta\rangle
\end{align*}
\]

(1.15)
Closing (1.14) gives

\[ \text{extra dimension} \]

We refer to this kind of link of quantum wires as an informational substrate. It is a network of closed quantum wires on which entangled information cyclically flows. It is convenient to use an internal extra dimension that is orthogonal to the spatial dimensions represented by the ordered qubit field. In Fig. 1.16 this extra dimension is the vertical direction. The dynamics of this type of qubit system can be specified analytically by the following map

\[ |\psi'\rangle = e^{iC N_{\alpha\beta\gamma\delta}} |\psi\rangle \rightarrow |\psi\rangle. \] (1.17)

A basic construct in the model, as mentioned above, is that all bits of information move with constant unit speed in the extra dimension. That is, the time it takes for a bit of information to complete one full cycle in the extra substrate dimension is a characteristic unit of time, \(\Delta t\) say, and this time is independent of the pathway the bit takes.

As mentioned earlier, when the number of qubits \(|q_\alpha, q_\beta, q_\gamma, q_\delta, \ldots\) becomes large, analytically calculating the eigenvalues and eigenvectors of \(N_{\alpha\beta\gamma\delta} \ldots\) becomes intractable in general. For a system with \(Q\) qubits, there are \(2^Q\) eigenvalues. An interesting case is when these invariants derive only from the regular structure of the substrate, viz., for quantum algorithms where the only free input parameters are a very small number of local gate angles (an important class of quantum algorithmic models we shall discuss later on). Similarly, a link with \(Q\) strands has \(2^Q\)
knot invariants, of which the Jones polynomial and the Alexander polynomial are examples.

If $N_{\alpha\beta\gamma\delta\ldots}$ represents the Hamiltonian of a physical system of interest, then one wants to know at least the smallest eigenvalue and its corresponding eigenstate, the ground state of the system. There is a branch of quantum information theory entirely dedicated to this task due to Farhi et al. [Farhi et al., 2000, Childs et al., 2001, Steffen et al., 2003]. The method is called adiabatic quantum computing. It has been proven that an adiabatic quantum computer is universal, although in the worst case some quantum algorithms may suffer slowing down [Aharonov et al., 2008]. The universality proof by Kempe, Kitaev, and Regev follows from showing that the 2-local Hamiltonian problem is quantum Merlin-Arthur complete (QMA-complete) [Kempe et al., 2006].

There are a number of premises in the adiabatic approach to quantum computing: (1) the Hamiltonian of interest has a free part and an interaction part with a scalar coupling strength and solutions are known to the free part of the Hamiltonian; (2) the ground state of the free Hamiltonian can be accurately prepared on the quantum computer; (3) the quantum gates within the quantum circuit that represent the Hamiltonian can be tuned while the circuit is running (i.e. controlled time-dependence) so that the initial zero coupling strength of the interaction Hamiltonian can be slowly ramped up over the course of the quantum computation gradually activating the nonlinear interaction (i.e. consistent with the quantum adiabatic theorem); (4) the time to ramp up to the full interaction is not too long; and (5) errors that occur along the way can be corrected as they occur.

If there is a gap between the ground state and all other higher spectral energy levels, at the end of the quantum computation, the system resides in the

\footnote{The QMA complexity class is the quantum analog of the classical NP (non-polynomial) complexity class.}
ground state of the perturbed system. The time it takes to ramp up the coupling strength to the desired (nonperturbative) value scales as a polynomial of the inverse of the gap energy [Schaller et al., 2006]. After running for this amount of time, one uses a quantum algorithm for phase estimation due to Abrams and Lloyd to measure the ground state energy eigenvalue and eigenvector of the qubit system [Abrams and Lloyd, 1999]. The probability of obtaining the correct ground state energy is equal to $|\langle \Psi_{\text{adiab}} | \Psi_{\text{exact}} \rangle|^2$, which in the case of a flawless adiabatic quantum computation is 1. Of course a long adiabatic quantum computational cycle would be subject to many errors, so error-correction has been worked out by Jordan, Farhi, and Shor to stabilize the developing ground states against independent qubit errors [Jordan et al., 2006]. The pathway in time from the initial Hamiltonian to the desired one may vary, with the final eigenstate invariant with respect to topological changes in the pathway so long as any unwanted excitations do not exceed the gap energy.

1.2.2 Quantum lattice gas

In the scaling limit as the number of qubits become large, one can use quantum circuits with closed-loop feedback as an analog simulator, e.g. a qubit system can represent the dynamical behavior of another quantum system. Here the resolution of the spatial dimensions becomes large while the resolution in the extra dimension, as shown in (1.16), remains fixed and is rather low. This is because the size of the extra dimension is determined only by the quantum algorithm, which has a regular repeated structure of quantum gates.

For practical implementation reasons, one is basically forced to consider quantum circuit configurations like this where the quantum gates couple qubits within a local neighbor of relatively small size compared to the overall size of the circuit.
The size of the regularly repeating local structure of quantum gates depends on the numerical accuracy one requires—a larger stencil covering a greater number of qubits is required to achieve better numerical convergence. The size of the local neighborhood is exactly the characteristic size of the extra dimension that we first encountered in (1.16).

For simulations of 1+1 dimensional quantum dynamics, the substrate tends to look like a long narrow tube, or a torus for the case of periodic spatial boundary conditions as shown in the top of Fig. 1.1. The collection of bits that flow within the substrate behaves like a gas on a lattice. Such a quantum circuit with closed-loop feedback is called a quantum lattice gas.

It is one of the earliest quantum algorithms devised [Riazanov, 1958, Feynman, 1946, Feynman and Hibbs, 1965, 't Hooft, 1988, 't Hooft, 1997, Yepez, 1996d, Yepez, 1996c, Bialynicki-Birula, 1994, Benioff, 1996, Meyer, 1997, Boghosian and Taylor, 1998a]. If the local gate structure (i.e. quantum algorithmic protocol) is chosen appropriately, then the flow of quantum information can emulate, in the long wavelength limit, a quantum wave function governed by an equation of motion such as the Weyl, Dirac, or Schroedinger wave equation [Yepez, 2007]. A time history of a quantum lattice gas emulating a quantum wave packet of a massive, nonrelativistic, charge-neutral, spinless, scalar quantum particle in 1+1 dimensions is shown in the bottom of Fig. 1.1. The algorithmic protocol is 16 gates deep and is based on a $\sqrt{\text{SWAP}}$ gate; more details about this particular algorithm is given in Ref. [Yepez, 2007], including a derivation of the Schroedinger wave equation as the effective field theory in the long wavelength limit. A derivation for the simplest version of the quantum algorithm for 3+1 dimensional simulations is given in Sec. 6.3.1. The $\sqrt{\text{SWAP}}$ gate when applied twice results in a swap operation. So the $\sqrt{\text{SWAP}}$ is like the swap
operation but it only goes "half way" so to speak. In matrix form it is
\[
\sqrt{\text{SWAP}} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{2} + \frac{i}{2} & \frac{1}{2} - \frac{i}{2} & 0 \\
0 & \frac{1}{2} - \frac{i}{2} & \frac{1}{2} + \frac{i}{2} & 0 \\
0 & 0 & 0 & i
\end{pmatrix} = e^{i\frac{\pi}{2}} \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & \frac{1}{2} & -\frac{1}{2} & 0 \\
0 & -\frac{1}{2} & \frac{1}{2} & 0 \\
0 & 0 & 0 & i
\end{pmatrix}.
\] (1.18)

That squaring (1.18) yields a \text{SWAP} gate is easily verified.\textsuperscript{6} The smallest time step \(t = 1\) is the unit of time it takes for the bits to flow once around the small dimension of the toroidal substrate.

A quantum gate, along with the quantum wires leading to and from it, can be thought of as the essence of a "scattering pathway" for two particles; and even though a gate scatters only 2 bits many qubits can be affected. If the two incoming qubits are independent, the outgoing qubits are are entangled by action of the gate. Also, if the incoming qubits are entangled, it is possible they become separated (i.e. unentangled) by the action of the gate.

1.3 Organization

Our basic approach, presented in Chapter 2, focuses on pairwise entanglement and uses an analytical development based on two types of fundamental joint ladder operators, each type the sum of two single-particle fermionic ladder operators. As

\textsuperscript{6} For \(\Delta\) as a boolean number with value either 0 or 1 (i.e. \(\Delta^2 = \Delta\)), it is easy to see that

\[
\sqrt{1 - 2\Delta} = 1 + (i - 1)\Delta,
\]

which is the positive root. Similarly, (1.18) is generated by \(N = N^2\). To see this, do the Taylor expansion

\[
e^{zN} = 1 + zN + \frac{1}{2!}(zN)^2 + \frac{1}{3!}(zN)^3 + \cdots
\]

(1.19)

\[
e^{zN} = 1 + (e^z - 1)N,
\]

(1.20)

from which \(\text{SWAP} = e^{i\pi N} = 1 - 2N\) follows. In turn the positive root of this is

\[
\sqrt{\text{SWAP}} = e^{i\frac{\pi}{2}N} = \sqrt{1 - 2N} = 1 + (i - 1)N.
\]

(1.21)
FIG. 1.1: (Top) An example of a simple closed-loop quantum circuit (informational substrate of a Q2 model) representing a space of size $L = 64$ by using a field of 128 qubits (total of 1024 quantum gates). (Bottom) Time history (measured in cycle time) of a modeled wave packet, with initial width $L/10$, of a massive scalar particle. The analytical solution of the linear Schrödinger wave equation (curve) and the prediction (dots) from the Q2 model agree. The spatial resolution is 64 points. [For simulation details see Yepez and Boghosian, 2002.]
one would expect, joint number operators are constructed as a product of a joint creation and a joint destruction operator. These joint number operators (generators of entangling quantum gates) are used in a number of ways to analyze quantum entanglement in quantum systems. There are two ladder operators, a raising operator $a_\alpha^+$ and a lowering operator $a_\alpha$, that act on one qubit $|q_\alpha\rangle$. Representations of qubits and these singleton operators are given in Sections 2.1 and 2.2, respectively. There are four joint ladder operators that act on two qubits $|q_\alpha\rangle$ and $|q_\beta\rangle$, for $\alpha \neq \beta$, and these are

$$
a_{\alpha\beta}^+ \equiv \frac{1}{\sqrt{2}} \left( a_\alpha^+ - e^{-i\xi} a_\beta^+ \right), \quad a_{\alpha\beta} \equiv \frac{1}{\sqrt{2}} \left( a_\alpha - e^{i\xi} a_\beta \right), \quad (1.22a)
$$

$$
a_{\alpha\beta}^+ \equiv \frac{1}{\sqrt{2}} \left( a_\alpha + e^{-i\xi} a_\beta^+ \right), \quad a_{\alpha\beta} \equiv \frac{1}{\sqrt{2}} \left( a_\alpha^+ + e^{i\xi} a_\beta \right), \quad (1.22b)
$$

where $\xi$ is a real-valued angle that parametrizes an e-bit’s internal phase. In general, there are $2^n$ joint ladder operators that act on $n$ different qubits.

In Chapter 3 we present our a topological representation of quantum logic (outlined above) that views entangled qubit spacetime histories (or qubit world lines) as a generalized braid, referred to as a superbraid [Yepez, 2010]. The crossing of world lines may be either classical or quantum mechanical in nature, and in the latter case most conveniently expressed with analytical expressions for entangling quantum gates using (1.22a). At a quantum mechanical crossing, independent world lines become entangled and this process may be depicted by curvy lines representing the spacetime histories of qubits. Using our convention whereby the time axis is oriented vertically (advancing from top to bottom with two qubit entering the top legs of each diagram and existing from the bottom legs) and the space axis is horizontal, a quantum mechanical crossing is

$$
\text{qubit world lines in a superbraid: } A^{-1} \left[ \frac{(e^{i\xi} - 1)}{A - e^{i\xi}} \right] = A \bigg| \overline{\text{crossed}} \bigg| - A \bigg| \overline{\text{uncrossed}} \bigg|, \quad (1.23a)
$$
for $d = -A^2 - A^{-2}$. For $e^z - 1 = A^{-2}d$, (1.23a) reduces to $A\{\gamma\gamma\} = \chi = A^{-1}\gamma + A\chi$, which is a classical braid. Remarkably, the entangling gate operation (1.23a) is the fundamental (information-theoretic) mechanism underlying quantum vortex reconnection occurring within a quantum gas.

Quantum vortices in a superfluid:

If we move the last term in (1.23a) over to the left-hand side, then the quantum gate is more readily seen as a superposition of the classical alternatives $\gamma\gamma$ and $\gamma\chi$. We use the ordering of diagrams in (1.23a) to match the time evolution in (1.23b). The condensate in (1.23b) is represented by a large collection of qubits locally evolving according to (1.23a). This connection between the quantum gate scale and the scale of topological defects is basically why (1.23a) (the basis of a quantum lattice gas) can be used to faithfully simulate mutually interacting quantum vortices. As a side note, on the right-hand side of (1.23b), the remnant Kelvin waves due to Bogoliubov quasiparticle excitations in the vortex core are easily seen (the emitted phonons are not rendered). For applications to future quantum computing, we suggest a candidate role for controlled quantum vortices (qubits) and mutual vortex-vortex interactions (entangling quantum gates) in spinor superfluids regarding quantum information processing, topologically protected quantum memories (with effectively infinite $T_2$ decoherence time) and superbraids as entangling quantum gates [Yepez, 2010].

Pure quantum logic is strictly unitary whereas, in general, braiding is a nonunitary operation. The quantum skein relation (1.23a) reduces to a classical skein relation when $e^z = A^{-4}e^{i\pi}$, as mentioned above. In experimental (real-world) systems, the quantum dynamics occurring within the system is not strictly unitary because
one must necessarily consider the effects of decoherence which causes long-range entanglement to become progressively localized in space over time and projective (Von Neumann) measurement which causes localization by destroying entanglement in the system via wave function collapse. With these practical constraints in mind, we have pioneered measurement-based quantum computing using entangled clusters [Yepez, 1998, Yepez, 1999b, Yepez, 2001a, Yepez, 2007, Yepez, 2001c, Yepez, 2001b, Yepez, 2002b, Berman et al., 2002a], and in Chapter 4 we provide a brief review of our progress over the past decade. We take expectation values of these joint number operators to determine kinetic-level variables that describe the quantum information dynamics in the qubit system at the mesoscopic scale [Yepez, 2001a]. We explore the issue of reversibility in quantum maps at this scale (associated with a quantum Boltzmann equation [Yepez, 2006]). We then present a pioneering experimental result in quantum information processing, testing the predicted behavior (at the large scale) of a qubit system comprised of nuclear spins [Pravia et al., 2002, Pravia et al., 2003, Chen et al., 2006]. To explain why measurement-based quantum computing is efficient, consider a quantum lattice gas model with \( Q \) per point where the number of encoded particles at that point is \( N=2 \) (number of incoming particles scattering at a point). In this case, we need only consider zero-momentum pair states. Hence, the entangled cluster state (in momentum-space) has the form

\[
|\text{entangled cluster state}\rangle = \frac{1}{\sqrt{|\text{E.C.}|}} \left( \frac{k}{-k} + \frac{k'}{-k'} + \cdots + \frac{-k''}{-k''} \right),
\]

where the right-hand side is a quantum superposition of over the equivalence class (E.C.) of configurations of two-body configurations with the same momentum and energy [Yepez, 1996a, Boghosian et al., 1997, Yepez, 1999b, Yepez, 1999a, Yepez, 2007].
The entangled cluster state (1.24) is generated by a local interaction Hamiltonian $H'$ [Yepez, 2007]. The Hilbert space is partitioned into E.C. blocks with equal numbers of particles, total momentum, and total kinetic energy since $H'$ commutes with the total number and momentum operators and conserves energy. The number of terms, $|\text{E.C.}|$, that appear on the right-hand side of (1.24) depends on the value of $Q$ and is straightforward to calculate using a generating function method [Yepez, 2007]. If one performs a measurement of a single qubit (say encoding momentum state $k$) within the entangled cluster and obtains the output $|1\rangle$, then one knows conclusively that the entire cluster has collapsed into a unique classical state. That is, in our $N = 2$ example, the qubit encoding $-k$ necessarily has also collapsed and so a subsequent measurement of this qubit’s state deterministically yields $|1\rangle$ since the qubits were paired. The property of quantum entanglement allows one to compute an outgoing configuration from a scattering event by wave function collapse induced by measurement of an entangled qubit.\footnote{In general, in a quantum lattice gas simulation, the number of particles per point is $N \in [0, Q]$, where $N$ is the sum of the particles that participated in the local collision plus the spectator particles that did not participate in the collision, so one needs to measure $Q/2$ number of qubits to ensure an entangled qubit is measured to guarantee that the cluster state is collapsed into a unique classical state (fully separated over all the qubits).} The characteristic feature of a measurement-based quantum lattice gas model is that the entangled cluster states are local to each point in the system. It turns out that this feature is also characteristic of the Bose-Einstein condensate (BEC) phase of low-temperature superfluids. The quantum state of the superfluid is fully separated over all the points of the system. Hence, a localized quantum lattice gas is a representative model of a BEC, where instead of by projective measurement, quantum state localization occurs unitarily by independent phase rotations locally generated by $V_{\text{BEC}}[\varphi(x)] = \mu|\varphi(x)|^2 - \frac{g}{4}|\varphi(x)|^4$ at every spacetime point $x$ in the system, where $\varphi$ is the complex scalar condensate field, $\mu$ is the chemical potential, and $g$ is the coupling strength of the nonlinear Hartree interaction.
As a prelude to presenting our quantum lattice gas model of a BEC, we treat the theory of superfluidity of dynamical Bose and Fermi condensates in Chapters 5. We first review effective field theories governing Bose condensate dynamics, and review the subject of nodal topological defects in the Bose condensate, which are filamentary quantum vortices. Their mutual interaction leads to the Kelvin wave instability. We then present a derivation of the nonrelativistic effective field theory of a Fermi condensate and derive its governing equation of motion

\[ i\hbar \partial_t \psi = -\frac{\hbar^2}{2m} \sigma_x \nabla^2 \psi + \left[ V_{\text{H}}(\rho) + \rho \frac{\partial V_{\text{H}}(\rho)}{\partial \rho} - \mu \right] \sigma_x \psi, \]  

(1.25)

where \( \psi \) is a spinor field and \( \mu \) is the chemical potential. The ansatz is that local Hartree potential \( V_{\text{H}}(\rho) \) is a nonlinear function of the condensate number density \( \rho \).

In Chapter 6, we present a quantum lattice gas representation of the dynamics of a superfluid condensate governed as lowest order by the Gross-Pitaevskii equation

\[ i\hbar \partial_t \varphi = -\frac{\hbar^2}{2m} \nabla^2 \varphi + \left[ V_{\text{H}}(\rho) + \rho \frac{\partial V_{\text{H}}(\rho)}{\partial \rho} - \mu \right] \varphi, \]  

(1.26)

where \( \varphi \) represents a field of Cooper pairs, its value at each point being a sum of the amplitudes of \( \psi \), in (1.25), at that point. This quantum lattice gas representation explores some aspects of the Q2 model, particularly its usefulness for carrying out practical computational quantum fluid dynamics simulations. We find that it is perhaps the simplest yet most comprehensive expression of the quantum dynamics that occurs within a nonlinear superfluid with a scalar condensate field [Yepez, 1996b, Vahala et al., 2004, Yepez et al., 2009b]. As an application of Q2, we explore the power-law regions in the kinetic energy spectrum of the condensate. We have been able to achieve the largest quantum simulations to date of a BEC (on massively parallel supercomputers) and have explored for the first time Kolmogorov scaling in superfluids, a flow regime heretofore only obtainably by classical turbulence models [Yepez et al., 2009c].
In Chapter 7, we provide some final remarks on the subject of turbulence in regard to the information conservation on the small scales (both mesoscopic and microscopic) underlying the flow dynamics on the large hydrodynamic (macroscopic) scale [Boghosian et al., 2001, Boghosian et al., 2003, Boghosian et al., 2004a] [Keating et al., 2007]. To make the connection between classical turbulence and quantum turbulence, we derive the hydrodynamic-level moment equation which have the exact form of a viscous Navier-Stokes equation (effective viscous dissipation occurs even in an ultracold quantum gas or low-temperature superfluid because of vortex instabilities that couple to acoustic waves). These viscous fluid equations, originally derived by Harvey [Harvey, 1966] for the hydrodynamic variables $\rho$ (number density or quantum probability density) and $v$ (flow velocity or quantum probability current), are

\begin{align}
\partial_t \rho + \partial_j (\rho v_j) &= 0 \\
\partial_t (m \rho v_i) + \partial_j (m \rho v_i v_j) &= -\partial_i P + \partial_j \sigma'_{ij},
\end{align}

(1.27a) \hspace{1cm} (1.27b)

where the viscous stress tensor is

\begin{equation}
\sigma'_{ij} = \eta (\partial_i w_j + \partial_j w_i),
\end{equation}

(1.27c)

the velocity field supporting shear within a quantum vortex is

\begin{equation}
w \equiv \frac{\hbar}{m} \frac{\nabla \sqrt{\rho}}{\sqrt{\rho}},
\end{equation}

(1.27d)

and the shear viscosity is the fundamental quantity

\begin{equation}
\eta \equiv \frac{\hbar \rho}{4}.
\end{equation}

(1.28)

The set of equations (1.27) provide a basis for the $k^{-5/3}$ Kolmogorov kinetic energy spectrum in quantum turbulence at large scales. Quantum turbulence in superfluids, in particular the representation of fluid eddies in terms of a coherent structure of polarized quantum vortices, offers a unique window into the heretofore nearly intractable subject matter of kinetic energy cascades.
CHAPTER 2

Quantum logic in analytical form

2.1 Introduction

Let us begin by introducing some notation:

1 state (called “minus” on the Bloch sphere)

\[ |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ the alternate symbol is } |-\rangle \]

0 state (called “plus” on the Bloch sphere)

\[ |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ the alternate symbol is } |+\rangle. \]

In the Bloch sphere representation (discussed below), the alternate symbols \(|+\rangle\) and \(|-\rangle\) are used to denote logical states.\(^1\) A qubit is the fundamental quantum state representing the smallest unit of quantum information containing one bit of classical information accessible by measurement. A qubit is a mathematical object (an abstraction of a two-state quantum object) with a “one” state and a “zero”

\(^1\)The names “up” and “down,” and the respective symbols \(|\uparrow\rangle\) and \(|\downarrow\rangle\), are reserved for spin-\(\frac{1}{2}\) particles, encoded using 2 qubits.
state:
\[ |q⟩ = α|0⟩ + β|1⟩ = α \begin{pmatrix} 1 \\ 0 \end{pmatrix} + β \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \]
where $α$ and $β$ are complex numbers. These complex numbers are called amplitudes.

The basis states are orthonormal
\[
\begin{align*}
⟨0|0⟩ &= ⟨1|1⟩ = 1 \\
⟨0|1⟩ &= ⟨1|0⟩ = 0.
\end{align*}
\]

In general, the qubit $|q⟩$ in (2.1) is said to be in a superposition state of the two logical basis states $|0⟩$ and $|1⟩$. If $α$ and $β$ are complex, it would seem that a qubit should have four free real-valued parameters (two magnitudes and two phases):
\[
|q⟩ = \begin{pmatrix} α \\ β \end{pmatrix} = \begin{pmatrix} φ₀ e^{iθ₀} \\ φ₁ e^{iθ₁} \end{pmatrix}. \tag{2.3}
\]

Yet, for a qubit to contain only one classical bit of information, a qubit needs to be unimodular (normalized to unity)
\[
α^*α + β^*β = 1. \tag{2.4}
\]

Hence it lives on the complex unit circle, depicted on the top of Fig. 2.1. (2.4) constrains the value of the magnitudes, so we can write a qubit as
\[
|q⟩ = \begin{pmatrix} \sqrt{1-f} \\ \sqrt{f} e^{iφ} \end{pmatrix}, \tag{2.5}
\]
where $0 ≤ f ≤ 1$ and where an irrelevant overall phase is factored out. So, as required, the length (or norm) of the qubit is an invariant quantity
\[
⟨q|q⟩ = |α|^2 + |β|^2 = |\sqrt{1-f}|^2 + |\sqrt{f}|^2 = 1. \tag{2.6}
\]

Why is an overall phase irrelevant for a single qubit? The quantum property of measurement follows from identifying the moduli squared of the amplitudes as occupation probabilities $f$ and $1 - f$ for the qubit to occupy its logical states $|1⟩$ and
\[ f = |\beta|^2 \]  
\[ 1 - f = |\alpha|^2. \]  

There are only two relevant free parameters to specify the state of a qubit, but upon measurement, the qubit originally in the superposition state \( |2.5\rangle \) is found to occupy only one of its logical states

\[ |q\rangle_{\text{measure}} \begin{cases} 
|1\rangle, \text{ with probability } f, \\
|0\rangle, \text{ with probability } 1 - f. 
\end{cases} \]  

Thus, upon a single measurement, \( |q\rangle \) is found to be in either the state \( |0\rangle \) or \( |1\rangle \), an outcome that is said to be specified by a single classical bit \( \{0, 1\} \). Thus in actual experiments, the occupation probability \( f \) equals the frequency of occurrence of the result 1 obtained from many repeated measurements. So, a qubit is embodied by a physical object that contains one bit of information that also nonlinearly couples to a measuring device (a projection operator), through which that bit of information is extracted according to (2.9).

**Time-dependent qubits states**

The state \( |q(t)\rangle \) of a time-dependent qubit, as a two-energy level quantum mechanical entity, is governed by the Schrödinger wave equation

\[ i \frac{\partial}{\partial t} |q(t)\rangle = \omega \sigma_z |q(t)\rangle, \]  

with \( \hbar = 1 \). The time-dependent qubit is just like the spin-degree of freedom of a spin-1/2 particle in a uniform background magnetic field. The energy eigenvalues are \( \pm \omega \), and the energy eigenstates are

\[ |0\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \]
where $|0\rangle$ is the ground state and $|1\rangle$ is the excited state of the qubit, say. In terms of the angular frequency $\omega$ (e.g., Rabi frequency), the time-dependent qubit state is

$$|q(t)\rangle = A_0 e^{-i\omega t}|0\rangle + A_1 e^{i\omega t}|1\rangle,$$  

where the complex probability amplitudes satisfy $|A_0|^2 + |A_1|^2 = 1$ since the qubit resides on the complex circle in Hilbert space (or the Bloch sphere in spin space).

Now, we can explicitly write out qubit basis states of the Bloch sphere with $\hat{u} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$ as

$$|+\rangle_u = \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\frac{\varphi}{2}} \\ \sin \frac{\theta}{2} e^{i\frac{\varphi}{2}} \end{pmatrix} = \cos \frac{\theta}{2} e^{-i\frac{\varphi}{2}}|0\rangle + \sin \frac{\theta}{2} e^{i\frac{\varphi}{2}}|1\rangle,$$

(2.13a)

$$|-\rangle_u = \begin{pmatrix} -\sin \frac{\theta}{2} e^{-i\frac{\varphi}{2}} \\ \cos \frac{\theta}{2} e^{i\frac{\varphi}{2}} \end{pmatrix} = -\sin \frac{\theta}{2} e^{-i\frac{\varphi}{2}}|0\rangle + \cos \frac{\theta}{2} e^{i\frac{\varphi}{2}}|1\rangle.$$

(2.13b)

One can write 2-spinor basis states, $\xi(\uparrow)$ and $\xi(\downarrow)$ say, in terms of qubit states

$$\xi(\uparrow) \equiv e^{i\frac{\varphi}{2}}|+\rangle = \begin{pmatrix} \cos \frac{\theta}{2} \\ e^{i\varphi} \sin \frac{\theta}{2} \end{pmatrix} = \cos \frac{\theta}{2}|0\rangle + \sin \frac{\theta}{2} e^{i\varphi}|1\rangle,$$

(2.14a)

$$\xi(\downarrow) \equiv e^{-i\frac{\varphi}{2}}|-\rangle = \begin{pmatrix} -e^{-i\varphi} \sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix} = -\sin \frac{\theta}{2} e^{-i\varphi}|0\rangle + \cos \frac{\theta}{2}|1\rangle.$$

(2.14b)

2.1.1 Qubit representations

The space of all possible orientations of $|q\rangle$ on the complex unit circle is called its Hilbert space. In the logical basis, the two degrees of freedom of the qubit are
often expressed as two angles $\theta$ and $\varphi$, where $f = \sin^2 \left( \frac{\theta}{2} \right)$. So without any loss of generality the Hilbert space representation of a qubit (2.1) can be written as

$$|q\rangle = \cos \left( \frac{\theta}{2} \right) |0\rangle + \sin \left( \frac{\theta}{2} \right) e^{i\varphi} |1\rangle. \quad (2.15)$$

These angles have a well known geometrical interpretation as Euler angles.

**SU(2) and O(3) representations**

For a geometrical interpretation of a qubit, consider a three-dimensional space with "unit vectors" $\sigma_x$, $\sigma_y$, and $\sigma_z$ chosen as an orthonormal basis. In quantum information theory, one sometimes represents each basis element by a $2 \times 2$ matrix, a traceless hermitian generator of two-dimensional special unitary group, SU(2). To do so, one defines the symmetric product (dot product) as

$$\sigma_i \cdot \sigma_j \equiv \frac{1}{2} \left( \sigma_i \cdot \sigma_j + \sigma_j \cdot \sigma_i \right). \quad (2.16a)$$

Furthermore, one defines the anti-symmetric product (cross product) as

$$\sigma_i \times \sigma_j \equiv -\frac{i}{2} \left( \sigma_i \cdot \sigma_j - \sigma_j \cdot \sigma_i \right). \quad (2.16b)$$
Note that the centered dot symbol on the right-hand side of (2.16) denotes matrix multiplication. Thus, a basis that is orthonormal satisfies the following conditions

\[
\sigma_i \cdot \sigma_j = \begin{cases} 
1, & \text{for } i = j \text{ (normal)}, \\
0, & \text{otherwise (orthogonal)},
\end{cases} \tag{2.17a}
\]

and

\[
\sigma_i \times \sigma_j = \begin{cases} 
0, & \text{for } i = j, \\
\sigma_k, & \text{for cyclic indices}.
\end{cases} \tag{2.17b}
\]

A fundamental matrix representation that satisfies (2.17) is the well known Pauli basis

\[
\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.18}
\]

The Pauli matrices (2.18) satisfy the orthonormality conditions (2.17) which is just the structure equation for the SU(2) group

\[
[S_i, S_j] = i \epsilon_{ijk} S_k,
\]

where \( S_i \equiv \sigma_i \) and the structure constant \( \epsilon_{ijk} \) is the anti-symmetric Levi-Civita symbol.

Now we can express the qubit (2.15) in vector form (i.e. with three real components) as follows:

\[
\vec{q} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta). \tag{2.19}
\]

(2.19) is a representation of a qubit on the Bloch sphere where \( \theta \) is the elevation angle and \( \varphi \) is the azimuthal angle. In this representation, depicted on the right-hand side of Fig. 2.1, the qubit is considered as a vector element of the three-dimensional orthogonal group, O(3). Defining the Pauli spin vector (which has matrix components)

\[
\vec{\sigma} \equiv (\sigma_1, \sigma_2, \sigma_3), \tag{2.20}
\]
a qubit can also be expressed in matrix form

\[
M_q \equiv \vec{q} \cdot \vec{\sigma}
\]  
\[
= \sin \theta \cos \varphi \sigma_1 + \sin \theta \sin \varphi \sigma_2 + \cos \theta \sigma_3
\]  
\[
\approx \begin{pmatrix}
\cos \theta & e^{-i\varphi} \sin \theta \\
e^{i\varphi} \sin \theta & -\cos \theta
\end{pmatrix}
\]

In this representation, the qubit is considered as an element of the SU(2) group.

In quantum information, usually 2 \times 2 unitary matrices are considered single-qubit quantum gates, but such matrices can themselves represent qubits too. Table 2.1 gives a summary of the three common qubit representations.

<table>
<thead>
<tr>
<th>Representations</th>
<th>QUBIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hilbert space</td>
<td>(</td>
</tr>
<tr>
<td>O(3) group</td>
<td>(\vec{q} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta))</td>
</tr>
</tbody>
</table>
| SU(2) group    | \(M_q = \begin{pmatrix}
\cos \theta & e^{-i\varphi} \sin \theta \\
e^{i\varphi} \sin \theta & -\cos \theta
\end{pmatrix}\) |

TABLE 2.1: Qubit representations.

### 2.2 Singleton ladder operators

There are two basic operators from which all other quantum operator are constructed. These operators are \(\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\) and \(\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\), which by matrix multiplication generate \(\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\) and \(\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\). A one in each slot—what could be simpler? Each of these four operators carries physical significance. They are named for their function.

Raising ladder operator:

\[
a^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{1}{2} (\sigma_1 - i\sigma_2)
\]  
\[
(2.22a)
\]
Lowering ladder operator:

\[
a = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{1}{2} (\sigma_1 + i \sigma_2). \quad (2.22b)
\]

1 number (particle) operator:

\[
n = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = a^\dagger a = \frac{1}{2} (1 - \sigma_3). \quad (2.22c)
\]

0 number (hole) operator:

\[
h = \bar{n} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = a a^\dagger = \frac{1}{2} (1 + \sigma_3). \quad (2.22d)
\]

Operating on logical states, the singleton ladder operators give

\[
\begin{align*}
a^\dagger |0\rangle &= |1\rangle & \text{Raise 0 to 1} \\
a^\dagger |1\rangle &= \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \text{Exclusion of 1's} \\
a|0\rangle &= \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \text{Exclusion of 0's} \\
a|1\rangle &= |0\rangle & \text{Lower 1 to 0},
\end{align*}
\]

where the state \( \begin{pmatrix} 0 \\ 0 \end{pmatrix} \) is called oblivion. Furthermore, operating on the logical states, the singleton number operators give

\[
\begin{align*}
n|0\rangle &= \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \text{Exclusion of 0’s} \\
n|1\rangle &= |1\rangle & \text{Counts 1’s} \\
h|0\rangle &= |0\rangle & \text{Counts 0’s} \\
h|1\rangle &= \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \text{Exclusion of 1’s}.
\end{align*}
\]

From the simple identity

\[
n + h = 1_2
\]

follows the anticommutation relation algebraically expressing the local exclusion principle

\[
a^\dagger a + a a^\dagger = 1_2.
\]
TABLE 2.2: Summary of individual operators acting on a qubit and joint operators acting on a qubit pair in the second-quantized representation.

Finally, The observable number “1” (our fundamental unit of information) is implicitly defined as the eigenvalue of \( n \):

\[
n|1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} = 1 \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} = |1\rangle.
\]

(2.27)

The singleton number operator is the simplest representation of a polarizer.

### 2.3 Joint ladder operators

Let us consider entangling two fermionic quantum bits, say, \(|q_\alpha\rangle\) and \(|q_\beta\rangle\), in a system comprised of \( Q \geq 2 \) qubits and where the integers \( \alpha \) and \( \beta \in [1, Q] \) are not equal, \( \alpha \neq \beta \). Pair creation and pair annihilation operators (herein generically referred to as joint ladder operators) act on a qubit pair [Yepez, 2001a, Yepez, 2010].

There are two distinct types of such joint ladder operators, defined in terms of the individual fermionic ladder operators \( a_\alpha^\dagger \) and \( a_\alpha \), that act on a state \( |\ldots q_\alpha \ldots q_\beta \ldots \rangle \).
with a pair of qubits located at positions \( \alpha \) and \( \beta \):

\[
\begin{align*}
a_{\alpha \beta}^\dagger & \equiv \frac{1}{\sqrt{2}} \left( a_{\alpha}^\dagger - e^{-i\xi a_{\beta}^\dagger} \right), & a_{\alpha \beta} & \equiv \frac{1}{\sqrt{2}} \left( a_{\alpha} - e^{i\xi a_{\beta}} \right), \\
a_{\alpha \beta}^\dagger & \equiv \frac{1}{\sqrt{2}} \left( a_{\alpha} + e^{-i\xi a_{\beta}^\dagger} \right), & a_{\alpha \beta} & \equiv \frac{1}{\sqrt{2}} \left( a_{\alpha}^\dagger + e^{i\xi a_{\beta}} \right).
\end{align*}
\]  

(2.28a)  
(2.28b)

So we denote a pair by grouping together two integers \( (\alpha/3) \). Let us consider a second pair \( (\alpha'/3') \) that is specified with respect to the first pair in the following way: if \( \alpha = \alpha' \) then \( \beta = \beta' \), and if \( \alpha \neq \alpha' \) then \( \beta \neq \beta' \). That is, if \( \alpha = \alpha' \) then the pairs are identical, and if \( \alpha \neq \alpha' \) then the pairs are nonoverlapping.\(^2\) Since the qubit creation operator \( a_{\alpha}^\dagger \) and annihilation operator \( a_{\alpha} \) satisfy the anticommutation relations

\[
\{a_{\alpha}, a_{\beta}^\dagger\} = \delta_{\alpha\beta}, \quad \{a_{\alpha}, a_{\beta}\} = 0, \quad \{a_{\alpha}^\dagger, a_{\beta}^\dagger\} = 0,
\]

(2.29)

similar anticommutation relations follows for the joint ladder operators:

\[
\begin{align*}
\{a_{\alpha\beta}, a_{\alpha'\beta'}^\dagger\} & = \delta_{\alpha\alpha'}, \quad \{a_{\alpha\beta}, a_{\alpha'\beta'}\} = 0, \quad \{a_{\alpha\beta}^\dagger, a_{\alpha'\beta'}^\dagger\} = 0; \\
\{a_{\alpha\beta}, a_{\alpha'\beta'}^\dagger\} & = \delta_{\alpha\alpha'}, \quad \{a_{\alpha\beta}, a_{\alpha'\beta'}\} = 0, \quad \{a_{\alpha\beta}^\dagger, a_{\alpha'\beta'}^\dagger\} = 0.
\end{align*}
\]  

(2.30a)  
(2.30b)

In (2.30) the Boolean Kronecker delta on the right-hand side of the annihilation/creation anticommutator could also have been written as \( \delta_{\alpha\alpha'} = \delta_{\beta\beta'} = \delta_{\alpha\alpha'} \delta_{\beta\beta'} \) because of the pairing condition we imposed: either \( (\alpha\beta) = (\alpha'\beta') \) or \( (\alpha\beta) \neq (\alpha'\beta') \).

In turn, the two joint number operators are

\[
\begin{align*}
n_{\alpha\beta} & = a_{\alpha\beta}^\dagger a_{\alpha\beta} = \frac{1}{2} \left( n_{\alpha} + n_{\beta} - e^{i\xi a_{\beta}^\dagger} a_{\beta} - e^{-i\xi a_{\alpha}^\dagger} a_{\alpha} \right), \\
n_{\alpha\beta} & = a_{\alpha\beta} a_{\alpha\beta} = \frac{1}{2} \left( h_{\alpha} + n_{\beta} - e^{-i\xi a_{\beta}^\dagger} a_{\beta}^\dagger - e^{i\xi a_{\alpha}^\dagger} a_{\alpha}^\dagger \right)
\end{align*}
\]  

(2.31a)  
(2.31b)

where the individual qubit number and hole operators are \( n_{\alpha} = a_{\alpha}^\dagger a_{\alpha} \) and \( h_{\alpha} = a_{\alpha} a_{\alpha}^\dagger \), respectively. The joint number operators are both idempotent\(^3\), \( n_{\alpha\beta}^2 = n_{\alpha\beta} \) and

\(^2\)As mentioned above, a pair \( (\alpha/\beta) \) is constructed on the condition \( \alpha \neq \beta \). Thus, if the pairs \( (\alpha/\beta) \) and \( (\alpha'/\beta') \) are nonoverlapping, then we are assured that their indices satisfy \( \alpha \neq \beta' \) and \( \beta \neq \alpha' \).

\(^3\)Later in this chapter we will encounter a tri-idempotent entanglement number operator, \( n_{\alpha\beta}^3 = n_{\alpha\beta} \). However, for now to make the presentation simpler, we will not deal with this case.
Finally, one finds entanglement number operators

\[ e_{\Delta \alpha \beta} = n_{\alpha \beta} + (\Delta - 1)n_{\alpha}n_{\beta} \quad (2.32a) \]
\[ e_{\Delta \alpha \beta} = n_{\alpha \beta} + (\Delta - 1)h_{\alpha}n_{\beta}, \quad (2.32b) \]

where \( \Delta \) is a Boolean variable, 0 for the commuting case and 1 for the anti-commuting (fermionic) case. The entanglement number operators (2.32) are idempotent as well. The reason for the appearance of the term \((\Delta - 1)n_{\alpha}n_{\beta}\) in (2.32a) follows from the fact that the quantum mode entanglement number operator is idempotent; Appendix B.1 presents a derivation that leads to the occurrence of this term when we require \(e_{\Delta \alpha \beta}^2 = e_{\Delta \alpha \beta}\). By a similar line of reasoning, \((\Delta - 1)h_{\alpha}n_{\beta}\) appears in (2.32b).

The shorthand convention where two subscripts attached to a large quantum state specify the locations of two qubits of interest in that state \(|qq\rangle_{\alpha \beta} \equiv |\ldots q_\alpha \ldots q_\beta \ldots \rangle\) is convenient here. This convention is useful since the joint operators act strictly on a qubit pair, regardless of the pair’s location within the larger system of \(Q\) qubits. In the \(\alpha \beta\)-subspace, let us denote the singlet substate as

\[ |\Phi^-\rangle_{\alpha \beta} = \frac{1}{\sqrt{2}} \left( |01\rangle - |10\rangle \right)_{\alpha \beta} \quad (2.33a) \]

and the triplet substates as

\[ |\Phi^\pm\rangle_{\alpha \beta} = \frac{1}{\sqrt{2}} \left( |01\rangle + |10\rangle \right)_{\alpha \beta}, \quad |\Psi^\pm\rangle_{\alpha \beta} = \frac{1}{\sqrt{2}} \left( |11\rangle \pm |00\rangle \right)_{\alpha \beta}. \quad (2.33b) \]

The quantum substates (2.33) constitute the set of pairwise entangled Bell states in the \(\alpha \beta\) subspace that is a \(2^2\) dimensional slice of the full Hilbert space of dimension \(2^Q\). For added specificity, the symbols \(\perp\) and \(\parallel\) are applied as superscripts on the Bell states. The convention used here is that a ket \(|qq\rangle_{\alpha \beta}\) will be said to be perpendicular with respect to its constituent qubits \(|q\rangle_{\alpha}\) and \(|q\rangle_{\beta}\) when \(q \neq q'\) and parallel when \(q = q'\). Example perpendicular and parallel two-qubit states are
FIG. 2.2: Example of perpendicular and parallel two-qubit substates. The perpendicular substate |10⟩ (top pair) and the parallel substate |00⟩ (bottom pair) are depicted with qubits as unit vectors on the complex circle.

depicted in Fig. 2.2. Continuing with this convention, it is natural to define the following pairwise entangled quantum states

\[
|\Phi_\perp\rangle_{\alpha\beta} \equiv \frac{1}{\sqrt{2}} \left( |01\rangle - e^{i\xi} |10\rangle \right)_{\alpha\beta},
\]

\[
|\Psi_\parallel\rangle_{\alpha\beta} \equiv \frac{1}{\sqrt{2}} \left( |11\rangle - e^{i\xi} |00\rangle \right)_{\alpha\beta},
\]

by introducing a real-valued angle \( \xi \), which is physically interpreted as the internal phase of an entangled bit (e-bit). The four Bell states (2.33) are just special cases of (2.34) for angles \( \xi = \pi \) and \( \xi = 0 \). Applying the entanglement operators to the perpendicular and parallel pairwise entangled states, one finds some rather simple relations:

\[
e_\Delta |\Phi_\perp\rangle_{\alpha\beta} = |\Phi_\perp\rangle, \quad e_\Delta |\Psi_\parallel\rangle_{\alpha\beta} = \Delta |11\rangle.
\]

\[
e_\Delta |\Psi_\perp\rangle_{\alpha\beta} = \Delta |01\rangle, \quad e_\Delta |\Phi_\parallel\rangle_{\alpha\beta} = |\Psi_\parallel\rangle.
\]

\( |\Phi_\perp\rangle \) is an eigenket of \( e_\Delta \) and \( |\Psi_\parallel\rangle \) is an eigenket of \( e_\Delta \). In the \( \Delta = 0 \) case, the pairwise entangled states (2.34) are the eigenkets of the entanglement operators:

\[
e_0 |\Phi_\perp\rangle_{\alpha\beta} = |\Phi_\perp\rangle, \quad e_0 |\Psi_\parallel\rangle_{\alpha\beta} = 0
\]

\[
e_0 |\Psi_\perp\rangle_{\alpha\beta} = |\Psi_\parallel\rangle, \quad e_0 |\Phi_\parallel\rangle_{\alpha\beta} = 0.
\]

\(^4\)As a matter of notational shorthand, in (2.35) the \( \alpha\beta \) indices are dropped as subscripts from the entanglement operators and are also dropped on the right-hand side of an equation since avoiding redundancy in this way does not introduce any ambiguity.
That is, for the $\Delta = 0$ case, $|\Phi_\perp\rangle$ and $|\Psi_\parallel\rangle$ are eigenkets of $\varepsilon_\Delta$, with eigenvalues 1 and 0, respectively. Also, $|\Phi_\perp\rangle$ and $|\Psi_\parallel\rangle$ are both eigenkets of $\varepsilon_\Delta$, with eigenvalues 0 and 1, respectively. As a special case of (2.36), the Bell states are the eigenvectors of $\varepsilon^+_0$ and $\varepsilon^-_0$ for the particular internal $e$-bit angles $+ = \pi$ and $- = 0$, respectively.

### 2.4 Analytical quantum logic

Let us pursue an analytical approach to quantum computation based on second-quantized operators that is useful for numerical implementations. We will construct universal two-qubit quantum gates that can create (or destroy) pairwise entanglement between previously independent (or correlated) qubits. The basic approach associates entangling quantum gates with the unitary transformations generated by (2.31)

\[
U_{\alpha\beta} = e^{i\theta}e^{\Delta_{\alpha\beta}} = 1 + (e^{i\theta} - 1)e^{\Delta_{\alpha\beta}} \tag{2.37a}
\]

\[
\Omega_{\alpha\beta} = e^{i\theta}e^{\Delta_{\alpha\beta}} = 1 + (e^{i\theta} - 1)e^{\Delta_{\alpha\beta}}. \tag{2.37b}
\]

We may distinguish between two fundamentally different types of classical operations, $|01\rangle \leftrightarrow |10\rangle$ and $|00\rangle \leftrightarrow |11\rangle$. The former operation is a swap and the latter is pair creation/destruction. Equation set (2.37) is the quantum mechanical generalization of these perpendicular (swapping) and parallel (pairing) operations. $U$ and $\Omega$ behave as quantum phase gates when acting on the perpendicular and parallel entangled states:

\[
U |\Phi_\perp\rangle_{\alpha\beta} = e^{i\theta} |\Phi_\perp\rangle \quad \Omega |\Psi_\parallel\rangle_{\alpha\beta} = e^{i\theta} |\Psi_\parallel\rangle. \tag{2.38}
\]

A general class of joint operators can be found by using the joint number operators (2.31) to affect a similarity transformation of all the other joint operators
FIG. 2.3: Example of perpendicular and parallel entangling gates for the case when 
\( \xi = \frac{\pi}{2} \). The initial perpendicular substate \(|10\rangle\) is rotated by \( e^{-i \frac{\vartheta}{2} U} \) through the angle \( \vartheta \) (top) and the parallel substate \(|11\rangle\) similarly rotated by \( e^{-i \frac{\vartheta}{2} U} \) (bottom). These qubit-pair states are depicted as unit vectors on a circle for the cases: \( \vartheta = 0, \frac{\pi}{2}, \pi, \frac{3\pi}{2} \).

defined above. That is, for some operator \( O \), the generalization of \( O \) is obtained by either \( O'(\vartheta) \equiv e^{i\theta n_\alpha n_\beta} O e^{-i\theta n_\alpha n_\beta} \) or \( \mathcal{D}'(\vartheta) \equiv e^{i\theta n_\alpha n_\beta} O e^{-i\theta n_\alpha n_\beta} \). Thus, a similarity transformation of the number operators \( n_\alpha \) and \( n_\beta \) yields

\[
n'_\alpha(\vartheta, \xi) \equiv e^{i\theta n_\alpha n_\beta} n_\alpha e^{-i\theta n_\alpha n_\beta}
\]

\[
= \cos^2 \left( \frac{\vartheta}{2} \right) n_\alpha + \sin^2 \left( \frac{\vartheta}{2} \right) n_\beta + \frac{i \sin \vartheta}{2} \left( e^{i\xi a_\alpha^\dagger a_\beta} - e^{-i\xi a_\beta^\dagger a_\alpha} \right) \tag{2.39b}
\]

\[
n'_\beta(\vartheta, \xi) \equiv e^{i\theta n_\alpha n_\beta} n_\beta e^{-i\theta n_\alpha n_\beta}
\]

\[
= \sin^2 \left( \frac{\vartheta}{2} \right) n_\alpha + \cos^2 \left( \frac{\vartheta}{2} \right) n_\beta - \frac{i \sin \vartheta}{2} \left( e^{i\xi a_\alpha^\dagger a_\beta} - e^{-i\xi a_\beta^\dagger a_\alpha} \right) \tag{2.39c}
\]

and

\[
n'_\alpha(\vartheta, \xi) \equiv e^{i\theta n_\alpha n_\beta} n_\alpha e^{-i\theta n_\alpha n_\beta}
\]

\[
= \cos^2 \left( \frac{\vartheta}{2} \right) n_\alpha + \sin^2 \left( \frac{\vartheta}{2} \right) h_\beta + \frac{i \sin \vartheta}{2} \left( e^{-i\xi a_\alpha^\dagger a_\beta^\dagger} + e^{i\xi a_\alpha a_\beta} \right) \tag{2.39f}
\]

\[
n'_\beta(\vartheta, \xi) \equiv e^{i\theta n_\alpha n_\beta} n_\beta e^{-i\theta n_\alpha n_\beta}
\]

\[
= \sin^2 \left( \frac{\vartheta}{2} \right) h_\alpha + \cos^2 \left( \frac{\vartheta}{2} \right) n_\beta + \frac{i \sin \vartheta}{2} \left( e^{-i\xi a_\alpha^\dagger a_\beta^\dagger} + e^{i\xi a_\alpha a_\beta} \right) \tag{2.39g}
\]

Thus, the joint number operators (2.39) continuously rotate starting from \( n'_\alpha(0, \xi) = n'_\alpha(0, \xi) = n_\alpha \) and \( n'_\beta(0, \xi) = n'_\beta(0, \xi) = n_\beta \) to the number and hole operators
They are also idempotent. That information is conserved by this similarity transformation is seen by the conservation laws that follow directly from (2.39)

\[ n'_\alpha(\vartheta, \xi) + n'_\beta(\vartheta, \xi) = n_\alpha + n_\beta \]  
\[ n'_\alpha(\vartheta, \xi) - n'_\beta(\vartheta, \xi) = n_\alpha - n_\beta, \]

where (2.40a) is bit number conservation and (2.40b) is number velocity conservation. The left-hand side counts the information in its quantum mechanical (entangled) form whereas the right-hand side counts information in its classical (separable) form. In any case, the total information content in the \( \alpha \beta \) subspace is conserved. Conservation of perpendicular entanglement is related to particle number (mass) conversation whereas conservation of parallel entanglement is related to number velocity (momentum) conservation. In a quantum informational system comprising a large number of qubits, the microscopic conservation laws (2.40) give rise to effective nonlinear equations of motion at the macroscopic scale.\(^5\)

We may also construct generalized joint ladder operators:

\[ a'_\alpha = e^{i\vartheta n_{\alpha \beta}} a_\alpha e^{-i\vartheta n_{\alpha \beta}} \quad a'^\dagger_\alpha = e^{i\vartheta n_{\alpha \beta}} a_\alpha^\dagger e^{-i\vartheta n_{\alpha \beta}} \]  
\[ a'_\alpha = e^{i\vartheta n_{\alpha \beta}} a_\alpha e^{-i\vartheta n_{\alpha \beta}} \quad a'^\dagger_\alpha = e^{i\vartheta n_{\alpha \beta}} a_\alpha^\dagger e^{-i\vartheta n_{\alpha \beta}}. \]

After some algebraic manipulation, these can be expressed explicitly just in terms of the original ladder operators

\[ a'_\alpha = e^{-i\vartheta \frac{3}{2}} \left[ \cos \left( \frac{\vartheta}{2} \right) a_\alpha + i e^{i\xi} \sin \left( \frac{\vartheta}{2} \right) a_\beta \right] \]  
\[ a'^\dagger_\alpha = e^{i\vartheta \frac{3}{2}} \left[ \cos \left( \frac{\vartheta}{2} \right) a_\alpha^\dagger - i e^{-i\xi} \sin \left( \frac{\vartheta}{2} \right) a_\beta^\dagger \right] \]

\(^5\)As a concrete illustration of this principle, the pairs of joint number operators (2.39b) and (2.39d), obeying the microscopic conservation law (2.40a), served as the basis of the first experimental demonstration of measurement-based (type-II) quantum computation used to numerically predict the time-dependent solutions of a nonlinear hydrodynamic equation [Chen et al., 2006, Yepez, 2006].
and

\[ a'_\alpha = e^{i\frac{\mathcal{G}}{2}} \left[ \cos \left( \frac{\vartheta}{2} \right) a_\alpha + ie^{-i\xi} \sin \left( \frac{\vartheta}{2} \right) a_\beta^\dagger \right] \quad (2.42c) \]

\[ a'^\dagger_\alpha = e^{-i\frac{\mathcal{G}}{2}} \left[ \cos \left( \frac{\vartheta}{2} \right) a_\alpha^\dagger - ie^{i\xi} \sin \left( \frac{\vartheta}{2} \right) a_\beta \right]. \quad (2.42d) \]

The product of the joint ladder operators (2.42),

\[ n'_\alpha = a'^\dagger_\alpha a'_\alpha \quad n'_\beta = a'^\dagger_\beta a'_\beta, \quad (2.43) \]
yields the joint number operators (2.39), as expected. Noting that \( n_\alpha n_\beta \) is invariant under the similarity transformation, we can also write a generalization of (2.32) as

\[ N_{\Delta\alpha\beta} = e^{i\vartheta n_{\alpha\beta}} [n_\alpha + (\Delta - 1)n_\alpha n_\beta] e^{-i\vartheta n_{\alpha\beta}} \quad (2.44a) \]

\[ = \cos^2 \frac{\vartheta}{2} n_\alpha + \sin^2 \frac{\vartheta}{2} n_\beta + \frac{i}{2} \left( e^{i\xi} a_\alpha^\dagger a_\beta - e^{-i\xi} a_\beta^\dagger a_\alpha \right) + (\Delta - 1)n_\alpha n_\beta \quad (2.44b) \]

\[ \mathfrak{N}_{\Delta\alpha\beta} = e^{i\vartheta n_{\alpha\beta}} [n_\alpha + (\Delta - 1)\mathfrak{N}_\alpha n_\beta] e^{-i\vartheta n_{\alpha\beta}} \quad (2.44c) \]

\[ = \cos^2 \frac{\vartheta}{2} n_\alpha + \sin^2 \frac{\vartheta}{2} n_\beta + \frac{i}{2} \left( e^{i\xi} a_\alpha^\dagger a_\beta + e^{-i\xi} a_\alpha a_\beta \right) + (\Delta - 1)\mathfrak{N}_\alpha n_\beta. \quad (2.44d) \]

Equation set (2.44) are e-bit number operators where the rotation angle \( \vartheta \) determines the extent of pairwise entanglement in the \( \alpha\beta \)-subspace. The entanglement number operators (2.44) satisfy \( N_{\Delta\alpha\beta}^2 = N_{\Delta\alpha\beta} \) and \( \mathfrak{N}_{\Delta\alpha\beta}^3 = \mathfrak{N}_{\Delta\alpha\beta} \), so they are idempotent and tri-idempotent (but not an involution), respectively.\(^6\) We may also associate entangling quantum logic gates with the unitary transformations generated by (2.44)

\[ W_{\alpha\beta} = e^{i\Theta_\alpha N_{\Delta\alpha\beta}} = 1 + (e^{i\Theta_\alpha} - 1)N_{\Delta\alpha\beta} \quad (2.45a) \]

\[ \mathfrak{W}_{\alpha\beta} = e^{i\Theta_\alpha \mathfrak{N}_{\Delta\alpha\beta}} = 1 + i \sin \Theta_\alpha \mathfrak{N}_{\Delta\alpha\beta} + (\cos \Theta_\alpha - 1) \mathfrak{N}_{\Delta\alpha\beta}^2 \quad (2.45b) \]

where \( \Theta_\alpha \) is a real-valued gate angle. We can physically interpret the entanglement operators (2.44) as Hamiltonians by introducing a triangle relation \( E_{\alpha}^2 = E_{\alpha}^2 + |\Delta_\alpha|^2 \),

\(^6\)Actually, it is the \( \Delta = 0 \) parallel operator that a tri-idempotent \( \mathfrak{N}_{\Delta\alpha\beta}^3 = \mathfrak{N}_{\Delta\alpha\beta} \) whereas the fermionic parallel operator is simply idempotent \( \mathfrak{N}_{\Delta\alpha\beta}^2 = \mathfrak{N}_{\Delta\alpha\beta} \).
where we define three real-valued quantities: the pairing energy $E_\alpha$, the single particle kinetic energy $\epsilon_\alpha$, and the gap energy magnitude $|\Delta_\alpha|$. The names of these quantities, and their respective symbols, are taken from the theory of superconductivity.

Letting the rotation angle in (2.44) be qubit dependent, $\vartheta \rightarrow \vartheta_\alpha$, the triangle relation relates this angle to the energies as follows: $\cos \vartheta_\alpha = \frac{\epsilon_\alpha}{E_\alpha}$ and $\sin \vartheta_\alpha = \frac{|\Delta_\alpha|}{E_\alpha}$. We will need the half-angle identities: $\cos^2 \frac{\vartheta_\alpha}{2} = \frac{1}{2} \left( 1 + \frac{\epsilon_\alpha}{E_\alpha} \right)$ and $\sin^2 \frac{\vartheta_\alpha}{2} = \frac{1}{2} \left( 1 - \frac{\epsilon_\alpha}{E_\alpha} \right)$.

Finally, taking the gap function to be complex, we are free to choose to write it as $\Delta_\alpha = |\Delta_\alpha| e^{-i\xi}$. In the new energy variables, and setting the Boolean variable $\Delta$ (not to be confused with the gap function) equal to 1 (for the case of fermionic entangling gates), we can rewrite (2.44) as

$$N_{1\alpha\beta} \overset{(2.46b)}{=} \frac{1}{2} \left( 1 + \frac{\epsilon_\alpha}{E_\alpha} \right) a_\alpha^\dagger a_\alpha + \frac{1}{2} \left( 1 - \frac{\epsilon_\alpha}{E_\alpha} \right) a_\beta^\dagger a_\beta - \frac{\Delta_\alpha^*}{2E_\alpha} a_\beta^\dagger a_\alpha - \frac{\Delta_\alpha}{2E_\alpha} a_\beta a_\alpha$$

$$\mathcal{H}_{1\alpha\beta} \overset{(2.46d)}{=} \frac{1}{2} \left( 1 + \frac{\epsilon_\alpha}{E_\alpha} \right) a_\alpha^\dagger a_\alpha + \frac{1}{2} \left( 1 - \frac{\epsilon_\alpha}{E_\alpha} \right) a_\beta a_\beta^\dagger + \frac{\Delta_\alpha}{2E_\alpha} a_\alpha a_\beta^\dagger + \frac{\Delta_\alpha^*}{2E_\alpha} a_\beta a_\alpha$$

where in the last term we made use of the anticommutation relation $a_\alpha a_\beta = -a_\beta a_\alpha$ for $\alpha \neq \beta$. Now if we multiply through by the pair energy $E_\alpha$ and sum over all pairings, denoted as $\langle \alpha\beta \rangle$ (in the situation where there are no unpaired qubits), then the energy-weighted sums over the entanglement operators (2.46) are

$$H_{\perp} \equiv \sum_{\langle \alpha\beta \rangle} E_\alpha N_{1\alpha\beta} \overset{(2.46a)}{=} \sum_{\alpha} E_\alpha a_\alpha^\dagger a_\alpha - \frac{1}{2} \sum_{\langle \alpha\beta \rangle} \left( \Delta_\alpha^* a_\beta^\dagger a_\alpha + \Delta_\alpha a_\beta a_\alpha^\dagger \right)$$

$$H_{\parallel} \equiv \sum_{\langle \alpha\beta \rangle} E_\alpha \mathcal{H}_{1\alpha\beta} \overset{(2.46b)}{=} \sum_{\alpha} \epsilon_\alpha a_\alpha^\dagger a_\alpha + \frac{1}{2} \sum_{\langle \alpha\beta \rangle} \left( \Delta_\alpha a_\alpha^\dagger a_\beta^\dagger + \Delta_\alpha^* a_\beta a_\alpha \right) + \frac{1}{4} \sum_{\alpha} (E_\alpha - \epsilon_\alpha).$$

These are total energy operators, respectively counting perpendicular and parallel pairwise entanglement, of the qubit system.\(^7\)

\(^7\)We recognize (2.47) from condensed matter theories of strongly correlated fermions: (A) Hamiltonian (2.47a) has the form of the single-band Hubbard Hamiltonian in the tight-binding limit [Hubbard, 1963] with $\Delta_\alpha^*/2$ serving as the hopping parameter with just a self-energy $E_\alpha$, and (B) Hamiltonian (2.47b) has the form of the BCS Hamiltonian in the theory of superconductivity [Schrieffer, 1988].
CHAPTER 3

Superbraids of entangled qubit world lines

3.1 Introduction

In topological quantum computing [Zanardi and Lloyd, 2003, Nayak et al., 2008], a quantum gate operation derives from braiding quasiparticles, for example, two Majorana zero-energy vortices made of entangled Cooper-pair states in a $p + ip$ superconductor where the vortex-vortex phase interaction has a non-Abelian SU(2) gauge group [Ivanov, 2001, Tewari et al., 2007]. Dynamically braiding such quantum vortices (point defects in a planar cross section of the condensate) induces phase shifts in the quantum fluid's multiconnected wave function. Local nonlinear interactions between deflects (vortex-vortex straining) is otherwise neglected; that is, the separation distance $\delta$ of the zero-mode vortices is much greater then the vortex core size, which scales as the coherence length $\xi \ll \delta$ in quantum fluids. The braiding occurs adiabatically so the quantum fluid remains in local equilibrium and the number of deflects (qubits) remains fixed. For implementations, the usual question is
how can quantum logic gates, and in turn quantum algorithms, be represented by braiding defects, quasiparticles with a non-Abelian gauge group.

This chapter addresses the related fundamental question about the relationship between quantum entanglement, tangled strands, quantum logic, and quantum information theory [Heydari, 2007, Zhang et al., 2005, Kauffman and Lomonaco, 2004, Asoudeh et al., 2004, Kauffman and Jr, 2002, Dye, 2003, Kauffman, 2005]. How can a quantum logic gate, and in turn a quantum algorithm, be decomposed into a linear combination (entangled superposition) of classical braid operators? The goal is to comprehend and categorize quantum information topologically. This is done by first viewing a quantum gate as a braid of two qubit spacetime histories or world lines. Qubit-qubit interaction associated with a quantum gate is rendered as a tree-level scattering diagram, a form of ribbon graph. A quantum algorithm may be represented as a weave of such graphs, a superbraid of qubit world lines. Finally, one closes a superbraid to form a superlink. In fact, quantum lattice gas algorithms, for example, those employed for the simulation of superfluids themselves [Yepez et al., 2009c], are a good superlink archetype; hence the shared nomenclature.

With this technology we can calculate superlink invariants. In principle, each quantum circuit has its own unique invariant (associated with a Laurent polynomial); for example two competing quantum circuit implementations of a particular algorithm can be judged equivalent, irrespective of circuit schemes and the placement of gates and wires. If two quantum algorithms, first- and second-order accurate, are topologically equivalent, then the simpler one can be used for analytical predictions of their common effective theory while the latter can be used for faster simulations with fewer resources.

In short, presented is a quantum generalization of the Temperley-Lieb algebra $TL_Q$ and Artin braid group $B_Q$: a superbraid and its closure, a superlink, is formed
out of the world lines of $Q$ qubits (strands) undergoing dynamics generated by quantum gates. Furthermore, the superbraid representation of quantum dynamics works naturally for fermionic quantum simulations. There exists a classical limit where the generalized Temperley-Lieb algebra and the superbraid group, defined later in this chapter, reduce to the usual Temperley-Lieb algebra and braid group. There also exists a purely quantum mechanical limit where superbraids reduce to conservative quantum logic operators. Thus, the superbraid is the progenitor of the braid operator and quantum gate operator.

This chapter is organized as follows. A condensed review of knot theory sufficient to define the Jones polynomial and a condensed review of qubit ladder operators sufficient to define quantum logic operators and superbraid operators are given in Sec. 3.2. A diagrammatic representation of quantum logic, a hybrid between the usual quantum circuit diagrams and Feynman diagrams, is given in Sec. 3.3. A generalization of the Temperley-Lieb algebra (that includes fermionic particle dynamics) is presented in Sec. 3.4. The superbraid group relations are given in terms of this generalized algebra in Sec. 3.5, whereby the superbraid operator is cast in three different mathematical forms. The first (exponential form) illustrates how a superbraid is an amalgamation of a classical braid operator and a quantum gate. The second (knot theory form) illustrates the very close connection to the well-known classical braid operator. The third (product form) illustrates the physics of pairwise quantum entanglement as the braiding of two qubit world lines through a particular quantum gate Euler angle. Novel quantum skein relations are given in Sec. 3.6 and calculations of superlink invariants, for example for the square-root knots introduced here, are given in Sec. 3.7. Thus, using the superbraid formalism, quantum knots such as the square-root of unknot or the square-root of the trefoil knot are well-defined topological objects and each have their own knot invariant. Finally, a brief summary and some final remarks are given in Sec. 3.8.
3.2 Links, ladders, and logic

Classical braid operators (nearest-neighbor permutations), represented in terms of Temperley-Lieb algebra [Temperley and Lieb, 1971], were originally discovered in six-vertex Potts models and statistical mechanical treatments of two-dimensional lattice systems [Baxter, 1982, Levy, 1990]. The quantum algorithm to compute the Jones polynomial [Aharonov et al., 2006, Kauffman and Samuel J. Lomonaco, 2007] employs unitary gate operators that are mapped to unitary representations of the braid group, this is, generated by Hermitian representations of the Temperley-Lieb algebra. To prepare for our presentation of superbraids as a topological representation of the quantum logic underlying quantum information dynamics, let us first briefly mention some basics of knot theory and some basic quantum gate technology using qubit ladder operators.

A link comprising $Q$ strands, denoted by $L$, say, is the closure of a braid. The Jones polynomial $V_L(A)$ is an invariant of $L$ [Jones, 1985], where $A$ is a complex parameter associated with the link whose physical interpretation will be presented later in this chapter. $V_L(A)$ is a Laurent series in $A$. The Jones polynomial is defined for a link embedded in three space—an oriented link. One projects $L$ onto a plane. In the projected image, in general crossing of strands occurs but is disambiguated by its sign $\pm 1$; that is, one assigns overcrossings the sign of $+1$ and undercrossings $-1$. The writhe $w(L)$ is sum of the signs of all the crossings, that is, the net sign of a link’s planar projection. The Jones polynomial is computed as follows

$$V_L(A) = (-A^3)^{-w(L)} \frac{K_L(A)}{d},$$

where $K_L(A)$ is the Kauffman bracket of the link. $K_L(A)$ is determined from a planar projection of $L$, for example, using the skein relations below. In the simplest
case of an unknotted link (or unknot), the Kauffman bracket is

$$
\bigcirc = K_\bigcirc(A) = d = -A^2 - A^{-2}.
$$

(3.2)

The Kauffman bracket of a disjoint union of \( n \) unknots has the value \( d^n \), for example, \( \bigcirc \bigcirc = d^2 \).

\( KL(A) \) for a link with crossings can be computed recursively using a skein relation that equates it to the weighted sum of two links, each with one less crossing:

\[
\begin{align*}
\text{(3.3a)} & \quad \bigotimes = A \bigotimes + A^{-1} \bigotimes, \\
\text{(3.3b)} & \quad \bigotimes = A \bigotimes + A^{-1} \bigotimes,
\end{align*}
\]

where \( A \) and its inverse are the weighting factors. As an example, let us recursively apply (3.3) to prove an intuitively obvious link identity \( \bigotimes \bigotimes \bigotimes = \bigcirc \). One reduces the relevant braid as follows

\[
\begin{align*}
\text{(3.3a)} & \quad \bigotimes \bigotimes \bigotimes = A \bigotimes \bigotimes + A^{-1} \bigotimes \bigotimes, \\
\text{(3.3b)} & \quad = A^2 \bigotimes \bigotimes + A \bigotimes \bigotimes + A^{-1} \bigotimes \bigotimes, \\
\text{(3.3b)} & \quad = A^2 \bigotimes \bigotimes + A \bigotimes \bigotimes + A^{-1} \bigotimes \bigotimes + A^{-2} \bigotimes \bigotimes, \\
\text{(3.2)} & \quad = A^2 \bigotimes \bigotimes + A \bigotimes \bigotimes + d \bigotimes + A^{-2} \bigotimes \bigotimes, \\
\text{(3.2)} & \quad = \bigotimes + (d + A^2 + A^{-2}) \bigotimes, \\
\text{(3.2)} & \quad = \bigcirc.
\end{align*}
\]

(3.4)

A quantum gate represents the qubit-qubit coupling that occurs at the crossing of world lines of a pair of qubits, say \( |q_\alpha \rangle \) and \( |q_\gamma \rangle \) in a system of \( Q \) qubits. Every quantum gate is generated by a Hermitian operator, \( \mathcal{E}_{\alpha \gamma} \) say, and whose action on the quantum state may be expressed as

$$
| \ldots q_\alpha \ldots q_\gamma \ldots \rangle' = e^{i \mathcal{E}_{\alpha \gamma}} | \ldots q_\alpha \ldots q_\gamma \ldots \rangle,
$$

(3.5)
where $\zeta$ is a real parameter. The archetypal case considered here is $E^{2}_{\alpha \gamma} = E_{\alpha \gamma}$; the generator is idempotent.

Suppose the system of qubits is employed to model the quantum dynamics of fermions or bosons. Is there an analytical form of the generator $E_{\alpha \gamma}$ that allows one to easily distinguish between the two cases? It is natural to begin by treating Fermi statistics. With the logical one state of a qubit $|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, notice that $\sigma_{z}|1\rangle = -|1\rangle$, so one can count the number of preceding bits that contribute to the overall phase shift due to fermionic bit exchange involving the $\gamma$th qubit with tensor product operator, $\sigma_{z}^{\otimes \gamma-1}|\psi\rangle = (-1)^{N_{\gamma}}|\psi\rangle$. The phase factor is determined by the number of bit crossings $N_{\gamma} = \sum_{k=1}^{\gamma-1} n_{k}$ in the state $|\psi\rangle$ and where the Boolean number variables are $n_{k} \in [0, 1]$. Hence, an annihilation operator is decomposed into a tensor product:

$$a_{\gamma} = \sigma_{z}^{\otimes \gamma-1} \otimes a \otimes 1^{\otimes Q-\gamma}$$

(3.6)

for integer $\gamma \in [1, Q]$ and here the singleton operator is $a = \frac{1}{2}(\sigma_{x} + i\sigma_{y})$, where $\sigma_{i}$ for $i = x, y, z$ are the Pauli matrices. See page 17 of Ref. [Fetter and Walecka, 1971] for a typical way of determining $N_{\gamma}$. The destruction (lowering) operator (3.6) and its transpose, the creation (raising) operator $a_{\gamma}^\dagger = a_{\gamma}^{T}$, satisfy the anticommutation relations

$$\{a_{\gamma}, a_{\beta}^\dagger\} = \delta_{\gamma\beta}, \quad \{a_{\gamma}, a_{\beta}\} = 0, \quad \{a_{\gamma}^\dagger, a_{\beta}^\dagger\} = 0.$$

(3.7)

The Hermitian generator of a quantum gate can be analytically expressed in terms of qubit creation and annihilation operators. A novel generator that is manifestly Hermitian is the following:

$$E_{\Delta \alpha \gamma} = d^{-1}\left[-A^{2} n_{\alpha} - A^{-2} n_{\gamma}ight.$$

$$- A a_{\alpha}^\dagger a_{\gamma} - A^{-1} a_{\gamma} a_{\alpha} + d (\Delta - 1) n_{\alpha} n_{\gamma}\right],$$

(3.8)
where $d = -A^2 - A^{-2}$ is real. The parameter $\Delta$ is Boolean, and it allows one to select between Fermi anticommuting ($\Delta = 1$) or commuting ($\Delta = 0$) statistics of the modeled quantum particles. The operator generated by $E_{\Delta \alpha \gamma}$ is

$$e^{z}E_{\Delta \alpha \gamma} = 1^{\otimes q} + (e^{z} - 1)E_{\Delta \alpha \gamma},$$

which is a unitary quantum state interchange for the case when $z$ is pure imaginary. That is, (3.9) is a conservative quantum logic gate for $z = i\zeta$. For the case when $z$ is complex, (3.9) is proportional to a superbraid operator.

The coefficients in (3.8) can be parametrized by a real angle $\vartheta$: $E_{\Delta \alpha \gamma} = E_{\Delta \alpha \gamma}(\vartheta)$ with

$$A^2 = -\frac{\cos \vartheta + 1}{\sin \vartheta}$$

and $d = -A^2 - A^{-2} = 2 \csc \vartheta$. Then, (3.8) takes the form

$$E_{\Delta \alpha \gamma} = \cos^2 \frac{\vartheta}{2} n_{\alpha} + \sin^2 \frac{\vartheta}{2} n_{\gamma} - \frac{1}{2} \sin \vartheta \left( A a_{\alpha}^\dagger a_{\gamma} + A^{-1} a_{\gamma}^\dagger a_{\alpha} \right) + (\Delta - 1) n_{\alpha} n_{\gamma}.$$  

(3.11a)

Let us take a moment to explain the origin of (3.11a). The perpendicular joint entanglement operator (2.44b) that we derived in Sec. 2.4 is

$$N_{\Delta \alpha \beta} = \cos^2 \left( \frac{\vartheta}{2} \right) n_{\alpha} + \sin^2 \left( \frac{\vartheta}{2} \right) n_{\beta} + \frac{i \sin \vartheta}{2} \left( e^{i\xi} a_{\alpha}^\dagger a_{\beta} + e^{-i\xi} a_{\beta}^\dagger a_{\alpha} \right) + (\Delta - 1) n_{\alpha} n_{\beta}.$$  

(3.11b)

We have the freedom to choose $A = -ie^{i\xi}$, and thus we recovered the mathematical form of (3.11a) for $E_{\Delta \alpha \beta}(A) \equiv N_{\Delta \alpha \beta}[\vartheta(A), \xi(A)]$. Remember that $E_{\Delta \alpha \beta}(A)$ is a hermitian generator of the Temperley-Lieb algebra. Since the braiding operation it generates may be nonunitary for certain values of $A$, it should be distinguished from a hermitian generator of entanglement for those particular values of $A$. 
### 3.3 Diagrammatic quantum logic

The state evolution (3.5) by the quantum logic gate (3.9) can be understood as scattering between two qubits

\[
|\psi\rangle = e^{i\xi E_{\Delta} \gamma} |\psi\rangle \quad \Longleftrightarrow \quad \begin{array}{c} |q_{\alpha}\rangle \ |q_{\gamma}\rangle \\
|\delta_{\alpha}\rangle \ |q_{\gamma}\rangle \\
|q_{\alpha}\rangle \ |q_{\gamma}\rangle \\
|\delta_{\alpha}\rangle \ |q_{\gamma}\rangle 
\end{array} \tag{3.12a}
\]

\[
|\psi\rangle = e^{-i\xi E_{\Delta} \gamma} |\psi\rangle \quad \Longleftrightarrow \quad \begin{array}{c} |\delta_{\alpha}\rangle \ |q_{\gamma}\rangle \\
|q_{\alpha}\rangle \ |q_{\gamma}\rangle \\
|\delta_{\alpha}\rangle \ |q_{\gamma}\rangle \\
|q_{\alpha}\rangle \ |q_{\gamma}\rangle 
\end{array} \tag{3.12b}
\]

where the "gauge field" that couples the external qubit world lines is represented by an internal double wavy line (or ribbon). The external lines either overcross or undercross and are assigned +1 and −1 multiplying the action, that is, \(\pm \xi E_{\Delta}\). This sign disambiguates between a quantum gate and its adjoint, respectively, as shown in (3.12a) and (3.12b). Let us denote a qubit graphically \(|q_{\alpha}\rangle \equiv u_{\alpha} \uparrow + d_{\alpha} \downarrow\), with complex amplitudes constrained by conservation of probability \(|u_{\alpha}|^2 + |d_{\alpha}|^2 = 1\).

Starting, for example, with a separable input state \(|\psi\rangle = |q_{\alpha}\rangle |q_{\gamma}\rangle\), a scattering diagram is a quantum superposition of four oriented graphs:

\[
\begin{array}{c}
|q_{\alpha}\rangle \ |q_{\gamma}\rangle \\
\end{array} = u_{\alpha}u_{\gamma} \begin{array}{c}
\uparrow \uparrow \\
\hline
\hline
\hline
\hline
\downarrow \downarrow
\end{array} + u_{\alpha}d_{\gamma} \begin{array}{c}
\uparrow \uparrow \\
\hline
\hline
\hline
\hline
\downarrow \downarrow
\end{array} +

\begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} + d_{\alpha}d_{\gamma} \begin{array}{c}
\uparrow \uparrow \\
\hline
\hline
\hline
\hline
\downarrow \downarrow
\end{array}. \tag{3.13}
\]

Each oriented scattering graph can be reduced to a quantum superposition of classical graphs, or just a single classical graph, as the case may be. There are four **quantum skein relations** representing dynamics generated by (3.8):

\[
\begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} = \begin{array}{c}
\uparrow \uparrow \\
\hline
\hline
\hline
\hline
\downarrow \downarrow
\end{array} \tag{3.14a}
\]

\[
\begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} = \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} + \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} \tag{3.14b}
\]

\[
\begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} = \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} + \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} \tag{3.14c}
\]

\[
\begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} = \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} + \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} \tag{3.14d}
\]

\[
\begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} = \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} + \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} \tag{3.14e}
\]

\[
\begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} = \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} + \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} \tag{3.14f}
\]

\[
\begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} = \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} + \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} \tag{3.14g}
\]

\[
\begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} = \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} + \begin{array}{c}
\hline
\hline
\hline
\hline
\uparrow \uparrow \\
\downarrow \downarrow
\end{array} \tag{3.14h}
\]
These are the quantum analog of (3.3). Adjoint quantum skein relations are obtained simply by taking $\zeta \rightarrow -\zeta$ in the amplitudes in the diagrams in (3.14). All superbraids can be reduced to a quantum superposition of classical braids. The closure of a superbraid forms a superlink. Hence, a superlink can be reduced to a quantum superposition of classical links and, consequently, for each superlink one can compute an associated invariant, for example a superposition of Jones polynomials. An example calculation of such invariants is presented in Sec. 3.7.

In the context of quantum information dynamics, a physical interpretation of the parameter $A$ can be rendered as follows. If the strands in $L$ are considered closed spacetime histories of $Q$ qubits (e.g. qubit states evolving in a quantum circuit with closed-loop feedback), then the left-hand-side of (3.14) represents a trajectory configuration within a piece of the superlink where entanglement is generated by a qubit-qubit coupling that occurs at a quantum-gate (i.e. generalized crossing point). For the one-body cases (3.14b) and (3.14c), the right-hand side represents classical alternatives in quantum superposition: $d^{-1}e^{i\xi}(A^{2}e^{i\xi}-A^{-2}e^{\pm i\xi})$ is the amplitude for no interaction (nonswapping of qubit states) whereas the amplitude of a SWAP interaction (interchanging of qubit states) goes as $d^{-1}A^{\mp 1}(e^{i\xi} - 1)$.

As a first example of reducing a superbraid, let us recursively apply (3.14) to prove an obvious evolution identity: the composition of a quantum gate with its adjoint is the identity operator, that is, $UU^\dagger = 1$. For simplicity, let us start with $|q_0\rangle = \uparrow$ and $|q_\pi\rangle = \downarrow$, so the initially oriented superbraid is reduced to a superposition of classical braids as follows:

\[
\begin{array}{c}
\begin{array}{c}
\text{(3.14b)}
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
= \frac{-A^2 - A^{-2}e^{i\xi}}{d} \begin{array}{c}
\text{(3.15)}
\end{array}
\end{array}
\end{array}
\end{array}
\end{array}
\end{array}
\[
\begin{align*}
(3.14b) & \equiv \frac{-A^2 - A^{-2} e^{i\zeta}}{d} \left( -A^2 - A^{-2} e^{-i\zeta} \right) \\
& + \frac{-A^2 - A^{-2} e^{i\zeta}}{d} \left( A^{-1} \left( e^{-i\zeta} - 1 \right) \right) \\
& + \frac{A^{-1} \left( e^{i\zeta} - 1 \right)}{d} \\
(3.14c) & \equiv \frac{A^4 + A^{-4} + 2 \cos \zeta}{d^2} \left( -A^{-1} \left( A^2 + A^{-2} e^{i\zeta} \right) \right) \\
& + \frac{A^{-1} \left( e^{-i\zeta} - 1 \right)}{d^2} \\
& = \frac{A^4 + A^{-4} + 2 \cos \zeta}{d^2} \left( -A^{-1} \left( A^2 e^{i\zeta} - A^{-2} e^{-i\zeta} - A^2 + A^{-2} \right) \right) \\
& + \frac{2 - 2 \cos \zeta}{d^2} \\
& = \chi.
\end{align*}
\]

It is easy to verify that the same result occurs for inputs \(|q_\alpha\rangle = \downarrow\) and \(|q_\gamma\rangle = \uparrow\). Furthermore, the identity trivially follows for \(|q_\alpha\rangle = \uparrow\) and \(|q_\gamma\rangle = \uparrow\) and for \(|q_\alpha\rangle = \downarrow\) and \(|q_\gamma\rangle = \downarrow\) since \(\Delta\) is Boolean.

### 3.4 Generalization of TLQ(d)

With adjacent indices, for example, \(\gamma = \alpha + 1\) in (3.9), we need write the first index only (i.e. suppress the second indice), \(E_{\Delta \alpha} \equiv E_{\Delta \alpha, \alpha+1}\). Using this compressed notation, (3.8) satisfies the following generalized Temperley-Lieb algebra

\[
E_{\Delta \alpha}^2 = E_{\Delta \alpha}, \quad \alpha = 1, 2, \ldots, Q - 1,
\]

\[
E_{\Delta \alpha} E_{\Delta \alpha \pm 1} E_{\Delta \alpha} - E_{\Delta \alpha \pm 1} E_{\Delta \alpha} E_{\Delta \alpha \pm 1} = d^{-2} E_{\Delta \alpha} - d^{-2} E_{\Delta \alpha \pm 1},
\]

\[
E_{\Delta \alpha} E_{\Delta \beta} = E_{\Delta \beta} E_{\Delta \alpha}, \quad |\alpha - \beta| \geq 2.
\]

To help understand this algebra, we may write (3.16b) as follows

\[
E_{\Delta \alpha} E_{\Delta \alpha+1} E_{\Delta \alpha} - d^{-2} E_{\Delta \alpha} = d^{-2} X_{\alpha, \alpha+1}
\]

\[
E_{\Delta \alpha+1} E_{\Delta \alpha} E_{\Delta \alpha+1} - d^{-2} E_{\Delta \alpha+1} = d^{-2} Y_{\alpha, \alpha+1},
\]
where $X_{a,a+1}$ and $Y_{a,a+1}$ are introduced solely for the purpose of separating (3.16b) into two equations. For (3.17) to be equivalent to (3.16b), one must demonstrate that $X_{a,a+1} = Y_{a,a+1}$. Inserting (3.8) into the left-hand side of (3.17), after considerable ladder operator algebra, one finds that the difference of the right-hand side of (3.17) is

$$X_{a,a+1} - Y_{a,a+1} = \Delta(\Delta - 1)[(A^4 - A^{-4})n_\alpha n_{\alpha+1}n_{\alpha+2} - A^4n_\alpha n_{\alpha+1} + A^{-4}n_{\alpha+1}n_{\alpha+2}], \quad (3.18)$$

vanishing for Boolean $\Delta$. Thus, (3.16b) follows from (3.8).

As one finds that $X$ and $Y$ are proportional to $\Delta$, a remarkable reduction of (3.16) occurs for the $\Delta = 0$ case:

$$\mathcal{E}_{0\alpha}^2 = \mathcal{E}_{0\alpha}, \quad \alpha = 1, 2, \ldots, Q - 1 \quad (3.19a)$$

$$\mathcal{E}_{0\alpha}\mathcal{E}_{0\alpha+1}\mathcal{E}_{0\alpha} \overset{(3.17)}{=} d^{-2}\mathcal{E}_{0\alpha} \quad (3.19b)$$

$$\mathcal{E}_{0\alpha}\mathcal{E}_{0\beta} = \mathcal{E}_{0\beta}\mathcal{E}_{0\alpha}, \quad |\alpha - \beta| \geq 2. \quad (3.19c)$$

This is the Temperley-Lieb algebra over a system of $Q$ qubits (TLQ). Thus, entangled world lines of commuting particles generated by $\mathcal{E}_{0\alpha}$ are isomorphic to links generated by $\mathcal{E}_{0\alpha}$. So (3.16) is a generalization of TLQ. We now consider the generalized braid that it generates: a superbraid.

\footnote{The full expressions are the following:}

\begin{align*}
X_{a,a+1} &= \Delta \left[ (e^{2i\xi}a_\alpha^\dagger a_{\alpha+2} - e^{-2i\xi}a_\alpha^\dagger a_{\alpha+2}) n_\alpha - iA^{-2} (e^{i\xi}a_\alpha^\dagger a_{\alpha+1} - e^{-i\xi}a_{\alpha+1}^\dagger a_\alpha) n_{\alpha+2} \\
& \quad - iA^2 (e^{i\xi}a_{\alpha+1}^\dagger a_{\alpha+2} - e^{-i\xi}a_{\alpha+1}^\dagger a_{\alpha+2}) n_\alpha + A^4\Delta n_{\alpha}n_{\alpha+1} + A^{-4} n_{\alpha+1}n_{\alpha+2} + n_\alpha n_{\alpha+2} \\
& \quad + (A^4 + A^{-4})(\Delta - 1)(\Delta + 1 + A^4\Delta) \right] \\
Y_{a,a+1} &= \Delta \left[ (e^{2i\xi}a_{\alpha+1}^\dagger a_{\alpha+2} - e^{-2i\xi}a_{\alpha+1}^\dagger a_{\alpha+2}) n_\alpha - iA^{-2} (e^{i\xi}a_{\alpha+1}^\dagger a_{\alpha+1} - e^{-i\xi}a_{\alpha+1}^\dagger a_\alpha) n_{\alpha+2} \\
& \quad - iA^2 (e^{i\xi}a_{\alpha+1}^\dagger a_{\alpha+2} - e^{-i\xi}a_{\alpha+1}^\dagger a_{\alpha+2}) n_\alpha + A^4\Delta n_{\alpha}n_{\alpha+1} + A^{-4} n_{\alpha+1}n_{\alpha+2} + n_\alpha n_{\alpha+2} \\
& \quad + (A^4 + A^{-4})(\Delta - 1)(\Delta + 4A^4) \right].
\end{align*}
3.5 Superbraid group

A general superbraid operator is an amalgamation of both a classical braid operator and a quantum gate

\[ b_{\Delta \alpha \beta}^s \equiv A e^{z \xi_{\Delta \alpha \beta}}, \]

where \( A \) and \( z \) are complex parameters. Equation (3.20) can be applied to any two qubits, \( \alpha \) and \( \beta \), in a system of qubits (i.e., we do not impose a restriction to the adjacency case when \( \beta = \alpha + 1 \) nor do we necessarily impose a restriction to unitary evolution). Equation (3.20) can be written in several different ways, each way useful in its own right.

Letting \( z \equiv i \zeta + \ln \tau \), the superbraid operator has the following exponential form

\[ b_{\Delta \alpha \beta}^s \equiv \tau^{-\frac{1}{4}} e^{(i\zeta + \ln \tau) \xi_{\Delta \alpha \beta}} = \tau^{-\frac{1}{4}} (e^{i\zeta})^{\xi_{\Delta \alpha \beta}}, \]

where \( A \equiv \tau^{-\frac{1}{4}} \) (and so \( \tau = A^{-4} \)). The superbraid operator can be written linearly in its generator

\[ b_{\Delta \alpha \beta}^s = A \left[ 1_Q + (A^{-4} e^{i\zeta} - 1)\xi_{\Delta \alpha \beta} \right]. \]

Thus, the superbraid operator and its inverse can be expressed in knot theory form

\[ b_{\Delta \alpha \beta}^s = A 1_Q + A^{-1} \left( \frac{1 - e^{i\zeta \tau}}{1 + \tau} \right) d \xi_{\Delta \alpha \beta} \] \hspace{1cm} (3.23a)

\[ (b_{\Delta \alpha \beta}^s)^{-1} = A^{-1} 1_Q + A \left( \frac{-e^{-i\zeta} + \tau}{1 + \tau} \right) d \xi_{\Delta \alpha \beta}. \] \hspace{1cm} (3.23b)

A nontrivial classical limit of quantum logic gates represented as (3.9) occurs at \( \zeta = \pi \) (SWAP operator). Consequently, the superbraid operator in product form is

\[ b_{\Delta \alpha \beta}^s \equiv \tau^{-\frac{1}{4}} e^{(\ln \tau + i\pi) \xi_{\Delta \alpha \beta}} e^{(i\zeta - i\pi) \xi_{\Delta \alpha \beta}} \]

\[ = b_{\Delta \alpha \beta} e^{i(\zeta - \pi) \xi_{\Delta \alpha \beta}}, \]

\( (3.24a) \hspace{1cm} (3.24b) \)
where \( b_{\Delta \alpha \beta} = r^{-\frac{1}{2}} e^{(\ln{r} + i\pi)} E_{\Delta \alpha \beta} \) is the conventional braid operator. Equation (3.24b) is useful for comprehending the physical behavior of the superbraid operator. It classically braids world lines \( \alpha \) and \( \beta \) and quantum mechanically entangles these world lines according to the deficit angle \( \zeta - \pi \).

The superbraid group is defined by

\[
\begin{align*}
    b^s_{\alpha} b^s_{\beta} &= b^s_{\beta} b^s_{\alpha}, & \text{for } |\alpha - \beta| > 1 \tag{3.25a} \\
    b^s_{\alpha} b^s_{\alpha+1} b^s_{\alpha} + \gamma b^s_{\alpha} &= b^s_{\alpha+1} b^s_{\alpha+1} b^s_{\alpha+1} + \gamma b^s_{\alpha+1}, \tag{3.25b} \\
    \quad &\text{for } 1 \leq \alpha < Q,
\end{align*}
\]

where \( \gamma \) is a constant that depends on the representation. For (3.8), we have \( \gamma = \left( A^4 + A^{-4} e^{i\zeta} \right) \left( 1 + e^{i\zeta} \right) A^{-2} d^{-2} \).

In the classical limit \( \zeta = \pi \), the superbraid operator reduces to the classical braid operator, \( b_\alpha \equiv b^s_\alpha (\pi, \tau) \), and (3.25) reduces to the Artin braid group,

\[
\begin{align*}
    b_\alpha b_\beta &= b_\beta b_\alpha, & \text{for } |\alpha - \beta| > 1 \tag{3.26a} \\
    b_\alpha b_{\alpha+1} b_\alpha &= b_{\alpha+1} b_\alpha b_{\alpha+1}, & \text{for } 1 \leq \alpha < Q. \tag{3.26b}
\end{align*}
\]

Equation (3.26) follows from Eq. (3.25) because \( \gamma = 0 \) for \( \zeta = \pi \). Also, in this classical limit, Eq. (3.22) reduces to the braid operator

\[
\begin{align*}
    b_\alpha &= A 1_\alpha + A^{-1} d E_{\Delta \alpha \beta}, \tag{3.27}
\end{align*}
\]

for \( \alpha = 1, 2, \ldots, Q-1 \) (and technically the standard braid operator when \( \beta = \alpha+1 \)).

After some ladder operator manipulations using (3.8), one finds that

\[
\begin{align*}
    b_\alpha b_{\alpha+1} b_\alpha - b_{\alpha+1} b_\alpha b_{\alpha+1} &\stackrel{(3.27)}{=} A^{-1}(A^4 - A^{-4}) d^{-2} \Delta(\Delta - 1) (1 - n_\alpha) n_{\alpha+1} n_{\alpha+2}, \tag{3.28}
\end{align*}
\]

where \( n_\alpha \equiv a_\alpha^\dagger a_\alpha \). Since \( \Delta \) is Boolean, the right-hand side vanishes, and this is just (3.26b).
3.6 Quantum skein relations

The skein relations (3.3) for directed strands are

\[ \begin{align*}
\begin{array}{rcl}
\begin{array}{c}
\text{X} \\
\text{X}
\end{array}
& = &
\begin{array}{r}
\begin{array}{c}
A
\end{array}
\end{array}
\begin{array}{c}
\text{X}
\end{array}
+ A^{-1}
\begin{array}{c}
\text{X}
\end{array}
\end{array}
\end{align*} \tag{3.29a}
\begin{align*}
\begin{array}{rcl}
\begin{array}{c}
\text{X}
\end{array}
& = &
\begin{array}{r}
\begin{array}{c}
A
\end{array}
\end{array}
\begin{array}{c}
\text{X}
\end{array}
+ A
\begin{array}{c}
\text{X}
\end{array}
\end{array}
\end{align*} \tag{3.29b}
\]

The writhe of a braid, +1 for (3.29a) and −1 for (3.29b), is determined by applying the right-hand rule at the crossing point (viz., considering the strands as vectors), rotating the strand above toward the one below with the axis of rotation either out of the plane (+1) or into the plane (−1). By inserting (3.29) into (3.14), one arrives at a remarkably simple form of the quantum skein relations:

\[ \begin{align*}
\begin{array}{rcl}
\begin{array}{c}
\text{X}
\end{array}
& = &
\begin{array}{c}
\text{X}
\end{array}
\end{array}
\end{align*} \tag{3.30a}
\begin{align*}
\begin{array}{rcl}
\begin{array}{c}
\text{X}
\end{array}
& = &
\begin{array}{c}
\text{X}
\end{array}
+ \frac{e^{i\zeta} - 1}{d} \begin{array}{c}
\text{X}
\end{array}
\end{array}
\end{align*} \tag{3.30b}
\begin{align*}
\begin{array}{rcl}
\begin{array}{c}
\text{X}
\end{array}
& = &
\begin{array}{c}
\text{X}
\end{array}
+ \frac{e^{i\zeta} - 1}{d} \begin{array}{c}
\text{X}
\end{array}
\end{array}
\end{align*} \tag{3.30c}
\begin{align*}
\begin{array}{rcl}
\begin{array}{c}
\text{X}
\end{array}
& = &
\begin{array}{c}
\text{X}
\end{array}
+ \frac{e^{i\zeta} - 1}{d} \begin{array}{c}
\text{X}
\end{array}
\end{array}
\end{align*} \tag{3.30d}
\]

Equation (3.30) is most useful for reducing a closed quantum circuit into a superposition of oriented links. The relations in the one-body sector can be written as

\[ \begin{align*}
\begin{array}{rcl}
\begin{array}{c}
\text{X}
\end{array}
& = &
\begin{array}{c}
\text{X}
\end{array}
\end{array}
\end{align*} \tag{3.31a}
\begin{align*}
\begin{array}{rcl}
\begin{array}{c}
\text{X}
\end{array}
& = &
\begin{array}{c}
\text{X}
\end{array}
+ A^{-1} \left[ \frac{A^2 (e^{i\zeta} - 1)}{d} \right] \begin{array}{c}
\text{X}
\end{array}
\end{array}
\end{align*} \tag{3.31b}
\]

for the case of a complex rotation angle (i.e., \( i\zeta \rightarrow z \)) and where we have multiplied through by \( A \) and \( A^{-1} \), respectively, and taking the adjoint of the latter relation. Now with \( e^z = A^{-4} e^{i\zeta} \) and \( A^{-4} = \tau \), we arrive at

\[ \begin{align*}
\begin{array}{rcl}
\begin{array}{c}
\text{X}
\end{array}
& = &
\begin{array}{c}
\text{X}
\end{array}
\end{array}
\end{align*} \tag{3.32a}
\begin{align*}
\begin{array}{rcl}
\begin{array}{c}
\text{X}
\end{array}
& = &
\begin{array}{c}
\text{X}
\end{array}
+ A^{-1} \left( \frac{1 - e^{i\zeta}}{1 + \tau} \right) \begin{array}{c}
\text{X}
\end{array}
\end{array}
\end{align*} \tag{3.32b}
\]
the diagrammatic representation of the superbraid operators (3.23). Thus, we have the correspondence

\[ b^a_{\Delta \alpha \beta} \leftrightarrow A \left( \begin{array}{c} \alpha \\ \beta \end{array} \right), \tag{3.33} \]

which is just (3.20) in graphical form. The superbraid operator (3.33) is unitary when \( A = \sqrt{1} \), in which case it reduces to a conservative quantum logic gate.\(^2\)

### 3.7 Superlink invariants

Let us begin by writing the conservative quantum logic gate (3.9) graphically

\[ \left( \begin{array}{c} \alpha \\ \beta \end{array} \right) = \left\langle + \frac{e^z - 1}{d} \right\rangle, \tag{3.34} \]

where we choose to use the complex time parameter \( z \). Now \( w \) number of successive superbraids is

\[ \left( \begin{array}{c} \alpha \\ \beta \end{array} \right) = \left\langle + \frac{e^{uz} - 1}{d} \right\rangle, \tag{3.35} \]

where the right-hand side follows from (3.34) by taking \( z \to wz \). Letting \( \langle b \rangle \equiv d^{-1}K_L(A) \), where \( L \) is the closure of \( b \), the Markov trace closure of (3.35), here denoted with angled brackets, is

\[ \left\langle \left( \begin{array}{c} \alpha \\ \beta \end{array} \right)^w \right\rangle = \left\langle \left( - d^{-1} \right) \right\rangle + d^{-1}e^{uwz} \left\langle \right\rangle \tag{3.36a} \]

\[ = d^{-1} \left( \right) + d^{-2}e^{uwz} \right\rangle \tag{3.36b} \]

\[ = d - d^{-1} + d^{-1}e^{uwz}. \]

\(^2\)Since flipping over a braid preserves the writhe of its crossing, we may flip over each diagram in (3.32) to have yet another way to specify operative quantum skein relations. Using this specification, if we take \( \zeta = \pi \), then the flipped-over quantum skein relations just reduce to the classical skein relations (3.29).
Multiplying through by $A^w$, we then have the trace closure of $w$-superbraids:

$$
\langle (b^w) \rangle \overset{(3.37)}{=} A^w (d - d^{-1}) + d^{-1} (A e^z)^w.
$$

In the classical limit $\zeta = \pi$ and $e^z = -A^{-4}$, then (3.37) becomes a standard $w$ braid:

$$
\langle b^w \rangle \overset{(3.38a)}{=} A^w (d - d^{-1}) + d^{-1} (-A^{-3})^w
$$

$$
= (-A^3)^{-w} d^{-1} \left[ 1 + (-A^4)^w (d^2 - 1) \right]. \quad (3.38b)
$$

The Jones polynomial is $V_L(A) \overset{(3.31)}{=} (-A^3)^{-w} \langle b^w \rangle$, so

$$
V_L(A) = (A^6)^{-w} d^{-1} \left[ 1 + (-A^4)^w (d^2 - 1) \right]. \quad (3.39)
$$

For example, considering classical links formed from the closure of two strands braided an integer number of times with $w = 0, 1, 2, 3, 4, 5 \ldots$, (3.39) gives

$$
V_{\circ \circ}(A) = -A^{-2} - A^2 \quad (3.40a)
$$

$$
V_{\circ \circ}(A) = -A^3 \quad (3.40b)
$$

$$
V_{\circ \circ \circ}(A) = -A^{-4} - A^4 \quad (3.40c)
$$

$$
V_{\circ \circ \circ \circ}(A) = A^{-7} - A^{-3} - A^5 \quad (3.40d)
$$

$$
V_{\circ \circ \circ \circ \circ}(A) = -A^{-10} + A^{-6} - A^{-2} - A^6 \quad (3.40e)
$$

$$
V_{\circ \circ \circ \circ \circ \circ}(A) = A^{13} - A^9 + A^5 - A^{-1} - A^7 \quad (3.40f)
$$

Equation (3.40b) is the Jones polynomial invariant for the unknot, (3.40c) for the Hopf link, (3.40d) for the trefoil knot, and so forth, and these Laurent polynomials are well known.

Yet the formula (3.39) follows from the quantum logic gate relation (3.36), where $w$ is a time scaling factor. Since time is a continuous variable in quantum logic, we are free to take $w$ to be a real-valued parameter whereby the formula for
the invariant Jones polynomial remains physically well defined. Thus, for example, we can evaluate (3.39) for half-integer \( w \), and calculate Jones polynomial invariants for quantum links that are “halfway” between classical links, which is to say in equal superposition of two classical links. For quantum links formed from the closure of two strands braided an half-integer number of times with \( w = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \ldots \), (3.39) then gives

\[
V_{\sqrt{\cdots}}(A) = \frac{-i - A^{-2} - A^2 - A^6}{A^{-\frac{3}{3}}(A^{-2} + A^2)} 
\]

(3.41a)

\[
V_{\sqrt{\cdots\cdots\cdots}}(A) = \frac{iA^{-3} - A^{-1} - A^3 - A^7}{A^{-\frac{3}{3}}(A^{-2} + A^2)} 
\]

(3.41b)

\[
V_{\sqrt{\cdots\cdots\cdots\cdots}}(A) = \frac{-1 - iA^{-6} - A^4 - A^8}{A^{-\frac{3}{3}}(A^{-2} + A^2)} 
\]

(3.41c)

\[
V_{\sqrt{\cdots\cdots\cdots\cdots\cdots}}(A) = \frac{iA^{-9} - A - A^5 - A^9}{A^{-\frac{3}{3}}(A^{-2} + A^2)} 
\]

(3.41d)

Equation (3.41a) is the superlink invariant for the square root of the unknot \( (\sqrt{\cdots}) \), (3.41b) for the square root of the trefoil knot \( (\sqrt{\cdots\cdots\cdots}) \), and so forth. The square root of unknot and trefoil knots are examples of quantum knots, a special class of superlinks.

3.8 Conclusion

Einstein, Podolsky and Rosen discovered nonlocal quantum entanglement over three quarters of a century ago [Einstein et al., 1935]. Although this inscrutable seminal result is the most cited one in the physics literature, quantum entanglement still remains one of the most mysterious properties of quantum physics. Here we have strived to unravel some of the mystery behind this important physical effect by rendering quantum entanglement geometrically as tangles of the most basic of strands: quantum informational spacetime trajectories (or qubit world lines). The
advantage of this approach is that it allows us to represent quantum entangled
states in terms of intuitive constructs borrowed from the mathematics developed to
understand knots.

In knot theory, the most fundamental construct is braiding (or crossing) two
adjacent strands. In quantum information theory, a fundamental construct is en-
tangling two qubits. In general, the braiding operation is nonunitary whereas an
entangling operation (2-qubit universal quantum gate) is manifestly unitary. Yet,
these two operations are not entirely unrelated—they are in fact special aspects of
a general operation, termed a superbraid. The superbraid covers both nonunitary
and unitary fundamental physical operations. It both braids qubit world lines and
entangles the qubits and in this way mathematically disambiguates these most basic
physical processes.

Analytical defining relations for a superbraid operator were presented, as was
the algebra for its generator. For \( Q \) number of qubits, the generator of a superbraid
was found to be a Hermitian operator that is a generalization of the usual generators
in knot theory satisfying the Temperley-Lieb algebra, \( \text{TL}_Q(d) \). The generalization
presented here handles both the anticommuting (\( \Delta = 1 \)) and the commuting (\( \Delta = 0 \))
cases of quantum information dynamics; the quantum particles (whose motion de-
fines the quantum informational strands) can obey either Fermi statistics or not. In
the \( \Delta = 0 \) case, the operative generators are the usual ones that satisfy \( \text{TL}_Q(d) \) and
they serve as a Hermitian representation. Our generalization of \( \text{TL}_Q(d) \) was actually
needed to handle the case of entangled fermionic world lines. These generators, and
in turn their respective superbraid operators, are analytically expressed in terms of

\[\text{3Quantum computing algorithms can be specified in terms of entangling quantum gates that act only between adjacent qubits—two-qubit entangling gate operations between nonadjacent qubits (customarily used in specifying quantum algorithms in the quantum computing literature) can each be represented as a sequence of two-qubit gates operations acting on adjacent qubit pairs. Thus, local braid and quantum gate operations are both universal operations in their respective contexts.}\]
the qubit ladder operators: qubit anticommuting creation and destruction operators and number operators.

With the technology presented, one can topologically classify closed-loop quantum circuits with various schemes for quantum wires crossed (braided) at some locations and coupled together at some locations via quantum logic gates, for example, a sequence of braid operations (particle motion) and quantum gate operations (particle-particle interactions) that specify the local dynamics of a quantum lattice gas used for a computational physics application. The closure of a sequence of superbraids is called a superlink. We have demonstrated how a superlink invariant may be computed, for example, as a generalized Jones polynomial invariant. Invariants were calculated for two-stranded superlinks, and extending this to $Q$ strands is straightforward. The approach is to reduce a superbraid with $n$ crossings to a simpler superbraid with $n - 1$ crossings by applying a quantum skein relation, a straightforward generalization of the skein relations of knot theory. The quantum skein relations are summarized as follows.

The $A$ parameter commonly used in the classical skein relation of knot theory, $\frac{1}{2} = A \uparrow \downarrow + A^{-1} \downarrow \uparrow$, a version of (3.29a) that is flipped over, may be understood in the context of quantum information processing as representing the two alternatives for the exchange of a pair of bits for configurations with one bit up (logical zero) and the other bit down (logical one). The diagrammatic convention has information flowing from top to bottom, entering in the top leads of the diagram and exiting from the bottom leads. So if the initial state is $\ldots \uparrow \downarrow \ldots$, then the final-state alternatives are: (a) no interaction (identity operation) $\ldots \uparrow \downarrow \ldots$ or (b) an exchange interaction (classical swap) $\ldots \downarrow \uparrow \ldots$. The parameter $A$ is the amplitude for the identity transition $\ldots \uparrow \downarrow \ldots \Rightarrow \ldots \uparrow \downarrow \ldots$, whereas $A^{-1}$ represents the amplitude for the exchange transition $\ldots \uparrow \downarrow \ldots \Rightarrow \ldots \downarrow \uparrow \ldots$. Since the braid operator conserves bit number and $A$ is an amplitude, we generalized the classical
skein relation by allowing the interaction alternative (b) to represent a conservative quantum mechanical exchange—one defined by a bit-conserving two-qubit entangling gate operation. This resulted in the following quantum skein relation for a superbraid operator:

\[ A \xrightarrow{\delta} = A \gamma \xi + A^{-1} \left[ (e^z - 1)/(A^{-2}d) \right] \xrightarrow{\sigma}, \]

where \( d = -A^2 - A^{-2} \). Thus, a classical point occurs for any value of \( z \) that causes the quantity in the square bracket to become unity, \( e^z - 1 = A^{-2}d \). That is, a superbraid reduces to a braid when \( e^z = -A^{-4} = A^{-4}e^{i\pi} \).

In the case when \( e^z = e^{i\xi}A^{-4} \) and \( A \) is complex unimodular, the phase of \( A \) physically acts as an internal e-bit phase angle; that is, \( A = e^{i(\xi - \frac{\pi}{2})} \) as determined by (3.11). In (3.24b) we wrote the superbraid operator as the product of a braid and conservative quantum gate. It braids two qubit world lines and entangles them according to the deficit angle \( \Delta \zeta = \zeta - \zeta_o \neq 0 \), where \( \zeta \) is the real-valued time (related to the imaginary part of \( z \)) parametrizing the operation and \( \zeta_o = \pi \) is the classical point. Entangled qubit world lines and tangled strands are related through their respective skein relations sharing a common \( A \) parameter. The approach of representing quantum information topologically in terms of tangled strands [Heydari, 2007, Zhang et al., 2005, Kauffman and Lomonaco, 2004, Asoudeh et al., 2004, Kauffman and Jr, 2002, Dye, 2003, Kauffman, 2005, Yepez, 2009, Yepez, 2010], and that we have explored here, offers insights about quantum entanglement as the quantum skein relation just mentioned, for purely imaginary \( z \), is an entangling conservative quantum gate.

The aforementioned considerations naturally lead to some relevant further outlooks, for example the observability of quantum knots such as the square root of a knot, which of course has no classical counterpart. Just how the square root of a knot may be physically realized in an experimental setup is not presently known for
certain, but according to Gell-Mann's totalitarian principle it should be experimentally compulsory as a physical phenomenon. Here is one possibility: a superbraid could exist within a Bose-Einstein condensate (BEC) superfluid as a superposition of quantum vortex loops. Furthermore, such vortex loops could represent a topologically protected qubit, and entangled states of such qubits could exist within a spinor BEC.\(^4\) In a BEC, all the vorticity in the flow is pinned to filamentary topological defects in the phase of the condensate, that is, quantum vortices with integer winding numbers [Fetter and Svidzinsky, 2001]. We explore nonlinear superfluid condensates in Chapters 5 and 6. In a spinor BEC with two or more components in the condensate, each component may have its own quantum vortices. In the dilute vortex limit for each component, these quantum vortices act like strands that may be braided and entangled as the spinor superfluid flow evolves in time.

Consider a configuration of quantum vortices in a superfluid comprising two unlinked closed loops \(\bigcirc \bigcirc\).\(^5\) Since nearby quantum vortex segments spontaneously undergo reconnection, one would expect that \(\bigcirc \Rightarrow \bigcirc \Rightarrow \bigcirc \) and so on.\(^6\) To form a qubit, one could identify the logical states with the two basic quantum vortex configurations: \(|0\rangle \equiv |\bigcirc \bigcirc \rangle\) and \(|1\rangle \equiv |\bigcirc \rangle\). So a topologically protected qubit (superbraided qubit) could be represented as a superposition of quantum vortex solitons

\[
|q\rangle = a |\bigcirc \bigcirc \rangle + b |\bigcirc \bigcirc \rangle,
\]

with amplitudes constrained by \(|a|^2 + |b|^2 = 1\).\(^7\) These amplitudes are time-dependent

\(^4\)Spinor BECs have been realized in a confined cold spinor atomic BEC with several hyperfine states [Stamper-Kurn et al., 1998, Ho, 1998].

\(^5\)The vorticity points along a quantum vortex line, so these act like directed strands. For simplicity, we omit arrow labels. Furthermore, these loops are not necessarily coplanar, for example, with the first loop in the plane of the paper, the second one could be rotated about the axis along its horizontal diameter, and perpendicularly oriented after a 90° rotation.

\(^6\)Here we tacitly assume the quantum vortices are contained in a trapping field, representing a container of genus two, so these mutually interacting quantum vortices cannot undergo a Kelvin cascade emitting phonons that escape into the bulk. That is, we assume they are constrained to interact only in the vicinity of the neighboring vortex, the reconnection region.

\(^7\)The square root of unknot \(\sqrt{\bigcirc \bigcirc}\) is realized in this qubit when \(a = b = 1/\sqrt{2}, \) or 45° polarization.
quantities, like the amplitudes of a half-integer spin precessing about a uniform magnetic field, but in this case the effective Rabi frequency is set by the inverse of two reconnection times.

In a two-component BEC, a topologically protected (perpendicular) pairwise entangled state could be formed by coupling two superbraided qubits

$$|\psi\rangle = \psi_{01} |\infty, \infty\rangle + \psi_{10} |\infty, \infty\rangle.$$  \hspace{1cm} (3.43)

Allowing for spatial overlap of the quantum vortices in each component, the two-qubit quantum vortex configuration $|\infty, \infty\rangle$ could have its two-loop configuration $\infty\infty$ simultaneously occupy the same location as its unknot quantum vortex configuration $\infty\infty$ in the spinor superfluid's second component. So, $|\infty, \infty\rangle$ might physically occur as $\infty\infty$ (overlapped). If the quantum vortex solitons can be spatially correlated in this way, then the quantum particles comprising the condensate can become physically entangled across their respective vortex cores, and in turn so too the vortex solitons themselves—a physical pathway whereby linkage may be related to entanglement.\(^8\)

Superbraid solitons such as (3.42) could store topologically protected qubits, and superlinks such as (3.43) could process topologically protected e-bits. If many superbraided qubits were coupled together to realize controllable quantum logic operations, then topological quantum computation may be directly achievable within spinor superfluids. This offers us a potential alternative to exotic non-Abelian vortices (Fibonacci anyons) recently proposed for thin-film superconductor-based topological quantum information processing.

Finally, since a superbraid is a nonunitary operation for certain values of the complex time parameter $z$, this particular feature might be akin to other behaviors of

---

\(^8\)This is allowed so long as the separation $\delta$ between the component vortices is much less than the coherence length $\xi$. This particular condition $\delta \ll \xi$ for interspinor superflow with quantum vortex solitons of unit winding number is different than the requirement $\xi \ll \delta$ in topological quantum computing with quantum logic represented in terms of braided zero-mode vortices in a $p + ip$ superconductor (as discussed in the Introduction of this chapter).
quantum systems in the real world. Quantum dynamics is effectively nonunitary because of decoherence (loss of phase coherency between previously correlated qubits) as well as the nonunitarity of projective measurement (collapse of qubit states onto a logical basis). So, the behavior of the nonunitary dynamics of superbraids may have a potential connection to measurement-based quantum computation. We establish a framework for measurement-based quantum computation in our next chapter.
CHAPTER 4

Measurement-based quantum computing

4.1 Introduction

Measurement provides a pathway for exploiting for practical purposes the non-linearities associated with wave function collapse. There are different quantum informational representations of quantum computation including the standard quantum circuit model and adiabatic quantum computing. Additionally, quantum lattice gas models that use measurement to boost the usefulness of qubit representation for physical simulation [Yepez, 1998, Yepez, 1999b, Yepez, 2001c] serve as a general representation of quantum computation. Such lattice-based qubit representations have been used to model a number of physical systems [Yepez, 2001a, Yepez, 2001b, Yepez and Boghosian, 2000, Berman et al., 2002b, Vahala et al., 2003b] [Vahala et al., 2003a, Yepez and Havel, 2004, Yepez et al., 2005b]. Measurement-based (type-II) quantum computational models were the first examples of “one-way” quantum computing relying on a parallel array of locally entangled cluster states,
an antecedent to cluster-based quantum computation [Gross and Eisert, 2007] [den Nest et al., 2006, Childs et al., 2005, Aliferis and Leung, 2004] and also to distributed quantum computing architectures and quantum multicomputers [Meter and Nemoto, 2008, Meter et al., 2009]. Type-II quantum computation has been applied to the simulation of the Ising model [Cole et al., 2004] and to the experimental implementation, for example, of Grover’s search algorithm in a one-way setup using the polarization state of photons [Walther et al., 2005].

It is useful to quantify how information, particularly joint information, is generated, transferred, and extracted from a large quantum computer during engineered quantum dynamical evolution and measurement processes, respectively. The relationships between nonlocal quantum entanglement and nonlocal quantum measurement are somewhat mysterious [Bandyopadhyay et al., 2008], so it is useful to have a toolset of operators to explore these relationships. Presented here is an analytical prescription for doing precisely this, with a focus on fundamental pairwise entanglement. Furthermore, here our focus is on analytically predicting the behavior of the entangled qubit system at the mesoscopic scale and macroscopic scale. At the mesoscopic scale, the resulting governing equation of motion is a quantum Boltzmann equation for kinetic-level (probability) variables. At the macroscopic scale, the resulting equations of motion are nonlinear and dissipative hydrodynamic equations.

4.2 Quantum measurement

4.2.1 Occupation probabilities via measurement

Our first goal is to understand quantum measurement in the context of two entangled qubits among a field of qubits. Suppose that two qubits $|q_a\rangle$ and $|q_b\rangle$ in
a many-body quantum system are initialized such that

\[ a \equiv \langle \psi | n_\alpha | \psi \rangle \quad \text{and} \quad b \equiv \langle \psi | n_\beta | \psi \rangle, \]  
\[ (4.1) \]

in the initially separable state \( |\psi\rangle \equiv |q_\alpha q_\beta\rangle \), where \( n_\alpha \) and \( n_\beta \) are the respective number operators for these qubits. Consider the following unitary evolution

\[ |\psi'\rangle = U_{\alpha\beta} |\psi\rangle, \]
\[ (4.2) \]

where \( U_{\alpha\beta} \) is an entangling quantum gate given by (2.37a) and generated by a joint number operator. Let us denote the measurement outputs as

\[ a' \equiv \langle \psi' | n_\alpha | \psi' \rangle \quad \text{and} \quad b' \equiv \langle \psi' | n_\beta | \psi' \rangle. \]
\[ (4.3) \]

Remarkably, using the joint number operators (2.39b), we can directly write the measurement outputs as matrix elements of the initial state

\[ a' = \langle \psi | n'_\alpha | \psi \rangle \quad \text{and} \quad b' = \langle \psi | n'_\beta | \psi \rangle. \]
\[ (4.4) \]

Since the \( |\psi'\rangle \) ket is entangled, a measurement that determines the value of \( a' \) (yielding one classical bit) likewise determines \( b' \). Also, the conservation of the probabilities \( a \) and \( b \) is ensured by (2.40a), the defining property of conservative quantum logic. Let us now consider a process of extracting a single bit upon measurement, which necessarily gives

\[ a' + b' = a + b. \]
\[ (4.5) \]

This is a statement about information conservation in quantum measurement that is the mesoscopic representation of (2.40a).
4.2.2 Quantum maps

A projective map, associated with quantum measurement of qubits $\alpha$ and $\beta$, going from Hilbert space to kinetic space is

$$\mathcal{P} : |\psi\rangle \rightarrow \begin{pmatrix} \langle \psi|n_\beta|\psi\rangle \\ \langle \psi|n_\alpha|\psi\rangle \end{pmatrix}.$$  \hspace{1cm} (4.6)

Oppositely, a tensor product operation is an injective map from kinetic space to Hilbert space, associated with the initial preparation of independent qubits:

$$\mathcal{I} : \begin{pmatrix} a \\ b \end{pmatrix} \rightarrow \begin{pmatrix} \sqrt{1-a} \\ \sqrt{a} \end{pmatrix} \otimes \begin{pmatrix} \sqrt{1-b} \\ \sqrt{b} \end{pmatrix}.$$ \hspace{1cm} (4.7)

The quantum evolution that entails state preparation, an entangling operation, and quantum measurement can be seen as a kinetic space transformation of probabilities [Yepez, 2001c] $\begin{pmatrix} a' \\ b' \end{pmatrix} = \mathcal{P} U_\Delta \mathcal{I} \begin{pmatrix} a \\ b \end{pmatrix}$, which can be written as the map $\hat{\mathcal{C}}$:

$$\begin{pmatrix} a \\ b \end{pmatrix} \rightarrow \begin{pmatrix} a' \\ b' \end{pmatrix} = \begin{pmatrix} \langle q_\alpha q_\beta | N_{\alpha \beta}^{1+} | q_\alpha q_\beta \rangle \\ \langle q_\alpha q_\beta | N_{\alpha \beta}^{1-} | q_\alpha q_\beta \rangle \end{pmatrix},$$ \hspace{1cm} (4.8)

where the joint entanglement operators are

$$N_{\alpha \beta}^{\Delta+} = U_\Delta^\dagger n_\beta U_\Delta \quad \text{and} \quad N_{\alpha \beta}^{\Delta-} = U_\Delta^\dagger n_\alpha U_\Delta,$$ \hspace{1cm} (4.9)

are determined by similarity transformation as usual and where we consider the special case when $U_\Delta$ acts on a pair of qubits 1 and 2 as an example of (2.37a) for half angles $\xi = \frac{\pi}{2}$ and $\vartheta = \frac{\pi}{2}$. This $U_\Delta$ is an antisymmetric square root of swap gate

$$U_\Delta \equiv e^{i\frac{\pi}{2} \epsilon_{\Delta,1,2}}|_{\xi = \frac{\pi}{2}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} + \frac{i}{2} & -\frac{1}{2} - \frac{i}{2} & 0 \\ 0 & \frac{1}{2} + \frac{i}{2} & \frac{1}{2} + \frac{i}{2} & 0 \\ 0 & 0 & 0 & (i-1)\Delta + 1 \end{pmatrix}. \hspace{1cm} (4.10)$$

We choose this special case to simplify the subsequent derivation. Entanglement drives the mesoscopic quantum dynamics, leading to a governing quantum Boltzmann equation at this scale. Can we invert this map to retrieve the incoming
probabilities \((a, b)\) only from the outgoing ones \((a', b')\)? Inverting (4.8) is not possible, because the map \(i.e.\) unitary gate (4.10) plus one measurement) induces an irreversible transition between kinetic space points. Yet, it is informative to see exactly where the inversion breaks down.

The first step towards this end is to write (4.8) explicitly in terms of the kinetic space variables [Yepez, 2006]. The map \(\tilde{C}\) is:

\[
\begin{pmatrix}
a \\
b
\end{pmatrix} \rightarrow \begin{pmatrix}
a' \\
b'
\end{pmatrix} = \begin{pmatrix}
\frac{\rho}{2} + \sqrt{(a - a^2)(b - b^2)} \\
\frac{\rho}{2} - \sqrt{(a - a^2)(b - b^2)}
\end{pmatrix},
\] (4.11)

where \(\rho \equiv a + b\) is the number density. We will define the number velocity as follows:

\[
v \equiv a' - b' = 2\sqrt{(a - a^2)(b - b^2)}.
\] (4.12)

The number density and number velocity are joint conjugate variables to the output variables. That number density and number velocity are the fundamental conserved quantities in quantum information dynamics is evidenced by the derivation leading to (2.40) that we obtained in our investigation of the basic perpendicular and parallel forms of pairwise entanglement. Squaring (4.12) gives

\[
\frac{v^2}{4} = (a - a^2)(b - b^2) = ab(1 - \rho) + (ab)^2.
\]

The quantity \(ab\) satisfies the quadratic eq. \((ab)^2 - (\rho - 1)ab - \frac{v^2}{4} = 0\), with the single physical solution

\[
ab = \frac{\rho - 1 + \sqrt{(\rho - 1)^2 + v^2}}{2}.
\] (4.13)

We had to take the positive root because \(ab \geq 0\). Finally, writing the number density as \(\rho = a + \frac{(ab)}{a}\), we can solve for the input value \(a\) in terms of the known output quantities \(\rho\) and \((ab)\). We have another quadratic equation \(a^2 - \rho a + (ab) = 0\), which has solution pairs

\[
a, b = \frac{\rho \pm \sqrt{\rho^2 - 4(ab)}}{2} \quad \text{or} \quad b, a = \frac{\rho \mp \sqrt{\rho^2 - 4(ab)}}{2}.
\] (4.14)
To disambiguate the possible orderings, we need one additional classical bit. Remarkably, we have found the bit that was lost upon measurement. It is associated with the ordering of \((a, b)\). Thus, the map (4.11) is irreversible, as we had anticipated.

\[
\begin{align*}
C^{-1}[S^2] &
\end{align*}
\]

\[
C[S^2]
\]

**FIG. 4.1:** Information preserving map \(C\) and \(C^{-1}\), both acting on a sphere \(S^2\) of configurations. (Left) The incoming preimage \(C^{-1}[(a', b')] = \{a, b\}\) and \(c = c'\), with \(\{a', b', c'\} \in S^2\), is topologically a torus with four cusps. (Right) The outgoing image \(\{a', b'\} = C[(a, b)]\) and \(c' = c\), with \(\{a, b, c\} \in S^2\), is topologically a doubly pinched sphere.

It is possible to generalize (4.11) so this bit of ordering is not lost. We can encode the ordering of the input \((a, b)\) in the output \((a', b')\). This is accomplished by generalizing (4.11) with the following nonlinear reversible map \(C\):

\[
\begin{pmatrix}
    a \\
    b
\end{pmatrix}
\rightarrow
\begin{pmatrix}
    a' \\
    b'
\end{pmatrix}
= \sigma_x^{\Theta(b-a)} \begin{pmatrix}
    \frac{p}{2} - \sqrt{(a-a^2)(b-b^2)} \\
    \frac{p}{2} + \sqrt{(a-a^2)(b-b^2)}
\end{pmatrix},
\] (4.15)

where the unit step function is \(\Theta(x) = 1\), for \(x \geq 0\), and \(\Theta(x) = 0\), for \(x < 0\), and where the Pauli matrix is \(\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\). Here is the inverse map \(C^{-1}\):

\[
\begin{pmatrix}
    a' \\
    b'
\end{pmatrix}
\rightarrow
\begin{pmatrix}
    a \\
    b
\end{pmatrix}
= \sigma_x^{\Theta(v'-a')} \begin{pmatrix}
    \rho + \sqrt{\rho^2 - 4(ab)} \\
    \rho - \sqrt{\rho^2 - 4(ab)}
\end{pmatrix},
\] (4.16)

which has the property \(C^{-1}C = 1\). The quantity \((ab)\) is computed from \((a', b')\) according to (4.13), since \(\rho = a' + b'\) and \(v = a' - b'\). The maps \(C\) and \(C^{-1}\) are
topologically expressed in Fig. 4.1 as a one-to-one mapping between distinct closed two-dimensional surfaces

\[
torus \text{ with cusps} \xrightarrow{c^{-1}} \text{ sphere} \xrightarrow{c} \text{ doubly pinched sphere.}
\]

The unit step $\Theta(b-a) = 0, 1$ encodes a single bit. (4.15) is a measurement-based (type II) quantum map [Yepez, 2001c] that conserves and localizes information but is otherwise indistinguishable from coherent evolution followed by state demolition. The term \textit{localize} denotes an intrinsic information-conserving class of wave function collapse without uncertainty in the ordering of the kinetic variables. The distinction between ordinary projective measurement and extraordinary reversible localization is quantified by the transference of one bit—a rather peculiar nonlinear quantum operation that induces state demolition while conserving all kinetic-space information in the quantum state.

4.2.3 Kinetic and hydrodynamic equations

Let us encode (4.15) with a nonlinear quantum operator, say $\Gamma$, which induces state demolition while conserving all kinetic-space information in the quantum state. (4.15) is a two-step process in Hilbert space

\[
|\psi'\rangle = U_{\alpha\beta}|q_\alpha q_\beta\rangle \quad \text{entangling operation} \tag{4.17a}
\]
\[
|q'_\alpha q'_\beta\rangle = \Gamma_{\alpha\beta}|\psi'\rangle \quad \text{disentangling operation,} \tag{4.17b}
\]

or combined into one quantum transformation

\[
|q'_\alpha q'_\beta\rangle = \Gamma_{\alpha\beta} U_{\alpha\beta}|q_\alpha q_\beta\rangle. \tag{4.18}
\]

Although reversible (i.e. $\Gamma^{-1}\Gamma = 1$ modulo the kinetic space variables), $\Gamma$ is not a unitary operator in Hilbert space (i.e. $\Gamma^{-1} \neq \Gamma^\dagger$). Analytically, we define $\Gamma$ as
a projection from Hilbert to kinetic space that is a function of $|\psi\rangle$ followed by an injection back to Hilbert space:

$$\Gamma_{\alpha\beta}[|\psi\rangle] \equiv \mathcal{I} \sigma_{x}^{1+\Theta(n_{\beta}-n_{\alpha})}\mathcal{P}. \quad (4.19)$$

Then, we can also write (4.15) in kinetic space as

$$\begin{pmatrix} a \\ b \end{pmatrix} \mapsto \begin{pmatrix} a' \\ b' \end{pmatrix} = \sigma_{x}^{1+\Theta(b-a)} \begin{pmatrix} \langle q_{\alpha}q_{\beta}|N_{1+}|q_{\alpha}q_{\beta} \rangle \\ \langle q_{\alpha}q_{\beta}|N_{1-}|q_{\alpha}q_{\beta} \rangle \end{pmatrix}. \quad (4.20)$$

**Measurement-based Q2 model**

Finally, we consider a quantum lattice gas with two qubits per point, writing (4.15) as coupled time-dependent equations

$$\begin{pmatrix} a(t + \tau) - a(t) \\ b(t + \tau) - b(t) \end{pmatrix} = \begin{pmatrix} -\Omega[a(t), b(t)] \\ \Omega[a(t), b(t)] \end{pmatrix}, \quad (4.21)$$

where $\Omega[a, b] \equiv \frac{1}{2}(b - a) + (-1)^{\Theta(b-a)}\sqrt{a(1-a)b(1-b)}$ is a collision function in kinetic space\(^1\) and $\tau$ is a relaxation time for the probabilities to equilibrate $a^{\alpha}(t + \tau) = a^{\alpha}(t)$ and $b^{\alpha}(t + \tau) = b^{\alpha}(t)$, consistent with the equilibrium condition $\Omega[a^{\alpha}, b^{\alpha}] = 0$. With $f = (f_{+}, f_{-}) \equiv (a, b)$, the operative mesoscopic Boltzmann $\mathcal{H}$-function is [Yepez, 2006]

$$\mathcal{H} = -\sum_{s=\pm} f_{s} \ln(\gamma_{s}f_{s}) + (1 - f_{s})\ln(1 - f_{s}), \quad (4.24)$$

---

\(^1\)For arbitrary gate angle $\vartheta$, the basic kinetic-level collision equations are

$$\begin{align*}
a' &= a \cos^{2} \frac{\vartheta}{2} + b \sin^{2} \frac{\vartheta}{2} + \sin(\vartheta)\sqrt{(a-a^{2})(b-b^{2})} \\
b' &= a \sin^{2} \frac{\vartheta}{2} + b \cos^{2} \frac{\vartheta}{2} - \sin(\vartheta)\sqrt{(a-a^{2})(b-b^{2})},
\end{align*} \quad (4.22a)$$

which are the expectation values of the microscopic joint number operators (2.39) with respect to the initial tensor product state $(\sqrt{a}|1+\sqrt{1-a}|0) \otimes (\sqrt{b}|1+\sqrt{1-b}|0)$ and the collision function is

$$\Omega[a, b] = (b - a) \sin^{2} \frac{\vartheta}{2} + \sin(\vartheta)\sqrt{a(1-a)b(1-b)}. \quad (4.23)$$
where $\gamma_+ = \sqrt{\alpha^2 + 1 + \alpha}$, $\gamma_- = \frac{1}{\gamma_+} = \sqrt{\alpha^2 + 1 - \alpha}$, and $\alpha = \cot \vartheta \cos \xi$. When $Q$ is large (even), partition the system into qubit pairs such that each pair is associated with a point on $\mathbb{Z}^3$. After (4.21) acts on each pair, let the particles hop to neighboring points (stream). The effective collide-localize-stream dynamics of the Q2 quantum gas is described by the linearized quantum Boltzmann equation

$$f(t + \delta t, x + c \delta t) - f(t, x) = \left( \frac{\partial f}{\partial a} \frac{\partial \Omega}{\partial b} - \frac{\partial f}{\partial b} \frac{\partial \Omega}{\partial a} \right) f_{eq} \delta f(x) + \cdots. \quad (4.25)$$

The second moment of (4.25), for $\rho \approx 1$ (near half-filling), yields the following low-energy effective field theory [Yepez, 2002c]

$$\partial_t \rho + c\alpha \partial_i \left( \frac{(1 - \rho)^2}{2} \right) - \nu \partial_{ii} \rho + \cdots = 0, \quad (4.26)$$

with viscosity $\nu = \frac{1}{2} \cot^2 \vartheta \frac{\delta x^2}{\delta t}$. With $u = c \alpha (1 - \rho)$, (4.26) is the Burgers equation. With a density (qubit pair) per direction $c \alpha (1 - \rho_i) \rightarrow u_i$, in d+1 dimensions we get

$$\partial_t \mathbf{u} + \nabla \left( \frac{\mathbf{u} \cdot \mathbf{u}}{2} \right) = \nu \nabla^2 \mathbf{u} + \cdots, \quad (4.27)$$

a realistic effective equation of motion for turbulent fluids [Yepez, 2007].

A time history of the dynamical evolution of the number density fields is plotted in Figure 4.2. The analytical solution of the Burgers equation is obtained by application of the Cole-Hopf transformation

$$\rho = \rho_0 + \frac{2\nu}{c\psi} \frac{\partial \psi}{\partial x}, \quad (4.28)$$

where

$$\psi \equiv I_0(z) + 2 \sum_{\ell=1}^{\infty} (-1)^{F_{\ell+1}/2} I_{\ell}(z) F_{\ell}(2\pi \ell x + \nu \ell t)e^{-\mu \ell t}, \quad (4.29)$$

2It is possible to add an external noise term into the right-hand side of the Burgers equation of the form $\frac{\partial \eta(x,t)}{\partial x}$. The potential field $h(x,t)$ is defined as follows: $\frac{\partial h(x,t)}{\partial x} = u(x,t)$. Then $h(x,t)$ satisfies the Kardar-Parisi-Zhang equation [Kardar et al., 1986].
FIG. 4.2: Development of a shock front in the flow field $u(x,t)$ after the system is initialized with a sinusoidal profile on a $L = 256$ site lattice for four different viscosities: (A) $\nu = 8$, (B) $\nu = 2$, (C) $\nu = \frac{1}{2}$, (D) $\nu = \frac{1}{32}$, where the viscosity is in lattice units $\frac{\delta x^2}{4\tau}$. The curves are shifted vertically one from the other by $\Delta \rho = \frac{1}{2}$ to avoid overlapping. Agreement between the numerical data (solid curves) and the analytical solution (dashed curves) is excellent. The shock fronts of the analytical solutions are slightly wider than the shock fronts of the numerical simulations which have much sharper edges. This is because these plotted analytical solutions are slightly over-damped to help stabilize the series solution (4.29), so the quantum model data is a more accurate approximation of the time-dependent solution to the Burgers equation. [For simulation details see [Yepez, 2006]].
where \( z \equiv \frac{c \rho \theta}{4 \pi \nu} \), \( \mu_\ell \equiv \nu (2 \pi \ell)^2 \), \( \nu_\ell \equiv c_s (1 - \rho_a) (2 \pi \ell) \), the \( I_\ell \)'s are modified Bessel functions, and the function \( F_\ell \) denotes the sine or cosine function when \( \ell \) is odd or even, respectively,

\[
F_\ell(x) \equiv \frac{(-1)^\ell + 1}{2} \cos(x) - \frac{(-1)^\ell - 1}{2} \sin(x).
\]  

(4.30)

To match the numerical simulations, the parameters in the analytical solution (4.29) were set to \( c = L c_s = 256 \cot \frac{\theta}{\Delta t} \) and \( \nu = \frac{1}{2} \cot^2 \frac{\theta}{\Delta t} \). Also in (4.29) the size of the system is set to unit length, that is, \( 0 \leq x \leq 1 \). The agreement between the numerical prediction and the analytical solution is excellent for all cases, as shown in Figure 4.2.

**Reverse cascade**

![Graph](image)

FIG. 4.3: Simulation of the time-reversed Burgers eq. with a shock at \( t = 0 \). (Top) \( \mathcal{H} \) function (4.24) increases under time reversal. (Bottom) Time advances right to left as the pulse evolves (amplitude of \( \rho \) grows) towards a sinusoid at \( t = 512 \) iterations of the inverse map \( C^{-1} \).

Decoherence is sufficient to explain macroscopic dissipation. Yet, in its purest form, quantum dynamics conserve information. Thus we should be able to model decoherence were the loss of microscopic phase information is retained in some other form within the qubit system. We have shown that one possibility is to have decoherence modeled as a succession of projections of the state of pairs of entangled particles whereby the lost degrees of freedom in the Hilbert space amplitudes are
precisely gained in the orderings of the degrees of freedom in the affected values of
the kinetic variables (probabilities) following the projection. Joint information is
transfered, not absolutely lost. A simple measurement archetype was offered: one
joint bit extracted from the destruction of pairwise entanglement is inserted in the
ordering of two affected kinetic variables. This has direct application to reversible
simulations of quantum processes driven by the quantum Boltzmann equation, even
when the collision hierarchy is cutoff to only handle local entanglement. The rel­
levant application is to the quantum computation of nonlinear physical dynamics,
*viz.*, mesoscopic quantum simulation that respects detailed-balance and Onsager
reciprocity relations.

To demonstrate information conservation in the quantum algorithm, the state
of the qubit system can be evolved in reverse. In Fig. 4.3, disentanglement causes
restoration of the initial profile. (4.26) evolves backward in time with negative
entropy increasing.

### 4.3 NMR experimental implementation

A measurement-based Q2 model is initialized, in the nuclear magnetic reso-
nance (NMR) case, by encoding the particles’ occupation probabilities as a spin-
magnetization profile. NMR is used as a proof-of-concept but any available quan-
tum computing technology (superconductive electronics, quantum dots, etc.) could
equally well be used as a demonstration of the quantum lattice gas model of quan-
tum computation. To handle the one-dimensional Burgers equation, it is sufficient
to use two qubits (two spin-\(\frac{1}{2}\) nuclei) per point, where each encodes a single real
valued occupation probability. A room-temperature solution of isotropically-labeled
chloroform \(^{13}CHCl_3\) was chosen for implementing the experiments, where the hy-
drogen and the labeled carbon nucleus served as qubits 1 and 2, respectively. The
### TABLE 4.1: Three different pictures at a single point

<table>
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<tr>
<th>NMR Spectroscopy</th>
<th>Quantum computing</th>
<th>Quantum Boltzmann eq.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spin-1/2 nuclei</td>
<td>Qubit</td>
<td>n_α, n_β</td>
</tr>
<tr>
<td>proton, carbon isotope C^{13}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Molecule containing above nuclei, such as chloroform, alanine dibromopropionic acid, transcrotonic acid</td>
<td>Local Hilbert space</td>
<td>Site of lattice x</td>
</tr>
<tr>
<td>Parcel of liquid ~ 10^{18} molecules</td>
<td>One-way quantum computer regular network of gates</td>
<td>Site of superlattice x at the mesoscopic scale</td>
</tr>
<tr>
<td>Relaxation</td>
<td>Memory reset</td>
<td>State demolition</td>
</tr>
<tr>
<td>ϵ_{thermal} = 1 + ε(σ^z_1 + σ^z_2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pseudo pure state</td>
<td>Ket</td>
<td></td>
</tr>
<tr>
<td>ϵ_{thermal} RF +∇ \psi</td>
<td></td>
<td></td>
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<tr>
<td>Spin-spin interaction + RF pulse sequence</td>
<td>Logic gate</td>
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<tr>
<td>Measurement of free induction decay</td>
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<td>Homogeneously Applied RF</td>
<td>Tensor Product Operator ( \hat{C} = \bigotimes_{k=1}^{V} \hat{U} )</td>
<td>parallel computation on-site collisions</td>
</tr>
</tbody>
</table>

The difference of the gyromagnetic ratio of two spins generates widely spaced resonant frequencies that allows us to address each spin independently.

A lattice of quantum information processors are related to the ensemble sample by creating a correspondence between lattice sites and spatially dependent positions in the sample. A linear magnetic field gradient is used to generate distinct spatially-dependent resonant frequencies that we can distinguish and modulate by a shaped RF pulse. In this way, the magnetic field gradient allows the entire spin ensemble to be sliced into a lattice of smaller and individually addressable subensembles. The lattice initialization starts by transforming thermal equilibrium states into pseudopure states [Pravia et al., 1999]. The equilibrium state is highly mixed and the two nuclear spins have unequal magnetizations. Thus, equalization of the magnetizations is required prior to creating the pseudopure state. The dynamical evolution is caused by a collision operator (a unitary operation), measurement (a nonunitary
operation), and streaming (an orthogonal operation) according to the quantum lattice gas algorithm. Some details of the correspondence between NMR spectroscopy, quantum computing, and the quantum lattice Boltzmann equation pictures of the method are presented in Table 4.1. This is an example of how the quantum lattice gas model can be implemented with a particular quantum information processing technology. The NMR example uses ensembles to boost the signal-to-noise ratio, but other quantum technologies that do not rely on ensembles can also be used. A promising candidate quantum information technology that is a very direct representation of the quantum lattice gas model of quantum computation are ultracold Fermi quantum gases trapped and controlled within optical lattices. These are discussed in Chapter 6.

4.3.1 Realizing a $\sqrt{\text{swap}}$ gate using carbon-13 and hydrogen nuclei

To model a $\sqrt{\text{swap}}$ gate emulating qubit state scattering, all the points locally evolve according to the Schrödinger wave equation with the unitary transformation:

$$|\psi'(n\Delta z)\rangle = e^{-i\hat{H}_{\text{NMR}}\Delta t/\hbar}|\psi(n\Delta z)\rangle. \quad (4.31)$$

The effective 2-spin Hamiltonian (averaged dipolar interaction of the spins' magnetic moments for a freely rotating molecule) is

$$\hat{H}_{\text{NMR}} = \hbar \omega_H \hat{\sigma}_z^H + \hbar \omega_C \hat{\sigma}_z^C + J \hat{\sigma}_z^H \hat{\sigma}_z^C, \quad (4.32)$$

where the resonant frequencies of the hydrogen and carbon-13 nuclei are $\omega_H = 300\text{MHz}$ and $\omega_C = 75\text{MHz}$, respectively, and where the spin-coupling resonant frequency is much smaller, $J/\hbar = 214\text{Hz}$. The interaction part of the NMR Hamiltonian, accounting for independently shaped radio frequency (RF) pulses $B_1(t)$ and
$B_2(t)$ along the transverse $\hat{x}$ and $\hat{y}$ directions, has the general form

$$\hat{H}_{\text{int}}(t) = \hbar \gamma_H B_{1x}(t) \sigma^H_x + \hbar \gamma_H B_{1y}(t) \sigma^H_y + \hbar \gamma_C B_{2x}(t) \sigma^C_x + \hbar \gamma_C B_{2y}(t) \sigma^C_y,$$

where the gyromagnetic ratio for the proton $\gamma_H$ is $2.67522212 \times 10^8 \text{ rad sec}^{-1} \text{Tesla}^{-1}$ and for the carbon-13 nucleus $\gamma_C$ is $6.728286 \times 10^7 \text{ rad sec}^{-1} \text{Tesla}^{-1}$.

In the double rotating frame, only the $J$-coupling term in (4.32) remains, and the resulting collision operator that is applied to all the lattice sites independently

$$|\psi'(n\Delta z)\rangle = \hat{G} |\psi(n\Delta z)\rangle,$$

for all $n$, has the form

$$\hat{G} = e^{-i\hat{H}_{\text{int}}(n\Delta t)/\hbar - i J_\theta H_x \sigma_x^C T_{\text{delay}}/\hbar + \cdots}.$$

This is the effective unitary evolution operator that is "programmed" by decomposing it into a sequence of external RF pulses modifying the natural spin-spin scalar coupling.

The effective components of the unitary collision gate determine the form of the macroscopic effective field theory and the value of its transport coefficients (particularly, the coefficient of the dissipative shear viscosity term in the case of the Burgers equation). The collision operator for the Burgers equation is

$$\hat{G} = e^{-i\vartheta/2 (\sigma^H_x \sigma^C_y - \sigma^H_y \sigma^C_x)},$$

where the Euler angle $\vartheta$ is determined by the physical values of the spin coupling energy, the delay time, and Planck’s constant as follows:

$$\vartheta = \frac{J T_{\text{delay}}}{\hbar}.$$

The product operators in the exponent commute with each other, resulting in

$$\hat{G} = e^{-i\vartheta/8 \sigma^H_x \sigma^C_y} e^{-i\vartheta/8 \sigma^H_y \sigma^C_x}.$$
Both terms can be expanded as natural scalar Hamiltonian couplings sandwiched with the appropriate single rotations, resulting in

\[
\hat{\mathcal{G}} = e^{-i\frac{\pi}{4}\sigma_y^C} e^{-i\frac{\pi}{4}\sigma_z^H} e^{-i\frac{\pi}{4}\sigma_z^H \sigma_y^C} e^{i\frac{\pi}{4}\sigma_y^C} \times e^{i\frac{\pi}{4}\sigma_x^C} e^{i\frac{\pi}{4}\sigma_y^H} e^{-i\frac{\pi}{4}\sigma_y^H \sigma_x^C} e^{i\frac{\pi}{4}\sigma_x^C} e^{-i\frac{\pi}{4}\sigma_x^C},
\]

which has the form of (4.35). There are many ways to encode the collision operator; the pulse sequence (4.39) is one such example.

In our test, we will set the shear viscosity to \( \nu = \frac{1}{4}, \) in lattice units where \( \Delta z = \Delta t = 1. \) We then choose \( \vartheta = \pi/3.289. \) Since the resonate spin coupling angular frequency is \( \omega_{HC} \equiv J/\hbar = 214\text{Hz} \) for our spectrometer setup, according to (4.37) we use the following delay time in the experiment, \( T_{\text{delay}} = 4.46 \text{msecs}, \) to produce the desired viscosity.

The exponential terms of single spin rotations are implemented by \( \pi/2 \) and \( \pi/4 \) pulses. The exponents of terms with \( \sigma_x^H \sigma_z^C \) represent the natural internal Hamiltonian evolutions with time period \( \hbar/2J. \) Here, the evolution of the internal Hamiltonian is ignored while the RF pulse is applied. This approximation leads to a systematic error that will accumulate during the course of the computation. In general, these errors are easy to avoid, but since one purpose of the investigation was to explore the sensitivity to accumulated errors, we did not correct it. The collision operator follows the encoding (state preparation step), and it is implemented without magnetic field gradients to ensure that all of the sites in the sample undergo the same transformation.

The experimental number densities are over-plotted in Figure 4.4 with the exact analytical solutions. Eight successive time steps of the Q2 model were implemented on 16 points. An improvement of our present experimental approach using collision operators with modulated phases is observed. The agreement of the data to the analytical solutions is encouraging.
FIG. 4.4: The experimental data are plotted together with the analytical solutions for 8 time steps on a lattice of 16 parallel two-qubit QIPs. Viscosity: $\nu = \frac{1}{2} \frac{\Delta z^2}{\Delta t}$. Experimental NMR data (dots) versus analytical solution (curves). Randomizing the error terms in the collision operator has improved the experimental results dramatically. [For simulation details see [Chen et al., 2006].]
4.4 Quantum propositions

It is possible to identify entangled states using either classical propositions or quantum propositions [Brukner and Zeilinger, 1999]. Here we consider the latter as a final point regarding the formalism of quantum measurement as represented by entangling joint number operators (2.44) for the commuting case $\Delta = 0$. These joint number operators in their analytical representation are

\[ N_{\alpha \beta}^\pm = \frac{1}{2} \left[ n_\alpha + n_\beta \pm \left( a_\alpha^\dagger a_\beta - a_\beta^\dagger a_\alpha \right) \right] - n_\alpha n_\beta \]  
\[ N_{\alpha \beta}^\pm = \frac{1}{2} \left[ n_\alpha + n_\beta \pm \left( a_\alpha^\dagger a_\beta + a_\alpha a_\beta \right) \right] - h_\alpha n_\beta, \]  

which follow from (2.44) for $\vartheta = \pi/2$ and $\xi = \pm\pi/2$. Let us consider a three qubit example. The matrix representations of (4.40) in this case are the following:

\[ N_{12}^\pm = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & \pm\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & \pm\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \pm\frac{1}{2} & 0 & \pm\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \]

\[ N_{23}^\pm = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \pm\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \pm\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & \pm\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \pm\frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \]

\[ N_{12}^\pm = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & \pm\frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & \pm\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \]

\[ N_{23}^\pm = \begin{pmatrix} \frac{1}{2} & 0 & 0 & \pm\frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \pm\frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \]

The eigenvalues of the sum of two joint operators are equivalent to the true (1) or false (0) value of a proposition. For $Q = 3$, the maximally entangled states are
the following:

\[
\Phi_0 \equiv \frac{1}{\sqrt{2}} \left( |111\rangle + |000\rangle \right) \tag{4.42a}
\]

\[
\Phi_1 \equiv \frac{1}{\sqrt{2}} \left( |110\rangle + |001\rangle \right) \tag{4.42b}
\]

\[
\Phi_2 \equiv \frac{1}{\sqrt{2}} \left( |101\rangle + |010\rangle \right) \tag{4.42c}
\]

\[
\Phi_3 \equiv \frac{1}{\sqrt{2}} \left( |100\rangle + |011\rangle \right) \tag{4.42d}
\]

\[
\Phi_4 \equiv \frac{1}{\sqrt{2}} \left( |111\rangle - |000\rangle \right) \tag{4.42e}
\]

\[
\Phi_5 \equiv \frac{1}{\sqrt{2}} \left( |110\rangle - |001\rangle \right) \tag{4.42f}
\]

\[
\Phi_6 \equiv \frac{1}{\sqrt{2}} \left( |101\rangle - |010\rangle \right) \tag{4.42g}
\]

\[
\Phi_7 \equiv \frac{1}{\sqrt{2}} \left( |100\rangle - |011\rangle \right) \tag{4.42h}
\]

This is a complete set of orthonormal states. Suppose we let \(\Psi\) denote one of the maximally entangled states in (4.42). We can determine which particular state of the set (4.42) that \(\Psi\) equals by posing three propositions. One rather simple question we may ask is whether or not the logical value of the first qubit equals the logical value of the second qubit. Such a proposition is written as \((q_1 = q_2)\), where the parenthesis around the expression denotes its logical Boolean value. A similar proposition we may employ is \((q_2 = q_3)\). Finally, a more subtle proposition is whether the state \(\Psi\) is asymmetric under complementation of bits. We write this proposition as \((q_1q_2q_3 \neq \overline{q_1}\overline{q_2}\overline{q_3})\), a proposition that is always true for classical bits but not necessarily so for qubits.\(^3\) Tracing over the last qubit, we may equivalently write this proposition as \((q_1q_2 \neq \overline{q_1}\overline{q_2})\). Altogether, our three example propositions interrogate all the qubits and consequently partition the set (4.42) as shown in Fig. 4.5. These example propositions can be represented by the following

\(^3\)The bit complement of a string of classical bits is always different than the original string.
combinations of joint number operators (4.40) as follows:

\[
\langle \Psi | N_{i2}^- + N_{i2}^- | \Psi \rangle \rightarrow (q_1 q_2 \neq \bar{q}_1 \bar{q}_2) \\
\langle \Psi | N_{i2}^+ + N_{i2}^- | \Psi \rangle \rightarrow (q_1 = q_2) \\
\langle \Psi | N_{i2}^+ + N_{i2}^+ | \Psi \rangle \rightarrow (q_2 = q_3).
\] (4.43a) (4.43b) (4.43c)

These are shown in Table 4.2 for the entangled states (4.42) and represent one choice of joint operators to disambiguate the entangled states.\(^4\) The joint operator (4.43a) is tri-idempotent while the other two operators are idempotent.

\[
\begin{array}{c|c}
(q_1 = q_2) & (q_2 = q_3) | ++ | -- | -- | -- | -- | -- | -- | (symmetric under complementation) \\
(q_2 \neq q_3) & | ++ | -- | -- | -- | -- | -- | -- | -- | (antisymmetric under complementation) \\
\end{array}
\]

\[
\begin{array}{c|c}
(q_1 \neq q_2) & (q_2 = q_3) | + + | -- | -- | -- | -- | -- | -- | (antisymmetric under complementation) \\
(q_2 \neq q_3) & | ++ | -- | -- | -- | -- | -- | -- | -- | (antisymmetric under complementation) \\
\end{array}
\]

FIG. 4.5: Logical partitioning of the \(Q = 3\) maximally entangled states using three propositions. The entangled states on the left-hand and right-hand sides are disambiguated by symmetry under the complement of qubits \(q_1 q_2\) following a partial trace of the density matrix over qubit \(q_3\), for example.

Casting a proposition such as (4.43a) with a joint number operator determines a classically multivalued property in one measurement—in this case, the asymmetry of the entangled state cannot be determined with one classical observation. In a system of size \(Q\), there are only \(Q\) classical number operators while there are \(2^Q\)

\(^4\)If one prefers to use a three qubit joint number operators, then one can directly implement the proposition \((q_1 q_2 q_3 \neq \bar{q}_1 \bar{q}_2 \bar{q}_3)\) with the joint operator \(((N_{i2}^+ + N_{i2}^-)(a_3 + a_3^\dagger))\) instead of (4.43a) to determine whether an entangled state is asymmetric under complementation of bits. In this case, one uses the \(\pm\) phase of the matrix element as the logical propositional value.
joint operators. In general, using entanglement number operators in lieu of usual number operators offers more ways to express a particular propositional value. This is the basis of the remarkable efficiency of quantum versus classical computation [Deutsch and Jozsa, 1992a]. Pathways faster than the classical pathways are the interesting ones of course.

<table>
<thead>
<tr>
<th>ENTANGLED STATE</th>
<th>PROPOSITIONS</th>
<th>VALUES</th>
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TABLE 4.2: Eight maximally entangled states in a \(Q = 3\) system. Fock state ordering is \(|q_1 q_2 q_3\rangle\), with the 1st qubit on the left and the last on the right. The propositions are cast in terms of joint operators to identify each entangled state.

4.5 Conclusion

We considered the effect of perpendicular pairwise entanglement at the mesoscopic level. Employing entanglement operators (joint number operators) made the

\[ A_0 = a_1 + a_2 + \cdots + a_{Q-1} + a_Q \]
\[ A_1 = a_1 + a_2 + \cdots + a_{Q-1} + a_Q \]
\[ A_2 = a_1 + a_2 + \cdots + a_{Q-1} + a_Q \]
\[ \vdots \]
\[ A_{2Q-2} = a_1 + a_2 + \cdots + a_{Q-1} + a_Q \]
\[ A_{2Q-1} = a_1 + a_2 + \cdots + a_{Q-1} + a_Q \]

Note that \(A_{2Q-1} = A_0^\dagger, A_{2Q-2} = A_1^\dagger\), and so forth.
analysis quite straightforward. We considered quantum measurement and tracked down where exactly information loss occurs in measurement-based quantum computing. We demonstrated that lost information can indeed be recovered even in a measurement-based quantum algorithm. Our test case was the type-II quantum algorithm for the hydrodynamic-level Burgers equation, a simple model of fluid turbulence with shocks. We also reviewed NMR-based quantum information processing and presented an experimental demonstration using this particular measurement-based quantum algorithm. Finally, as a concrete example of the utility of our joint number operators, we gave their matrix representation in the case of $Q = 3$ and demonstrated how quantum propositions can be reduced to combinations of joint number operators. Thus quantum propositions provide an efficient pathway to obtain in one observation a way to discover the value of a joint property of a system that would otherwise take many classical propositions. This is because an entangled quantum state can contain joint information in a way that represents a multifaceted classical configuration. This is a generalization of the example given in Appendix A where a two-qubit state represents a two-sided coin and entanglement offers an efficient route to solve the Deutsch problem—in one observation determining whether the coin is fair or not. This is possible when the measurement process can be reduced to a single joint number operator.
CHAPTER 5

Superfluidity in the low-temperature limit

5.1 Introduction

Feynman proposed that the superfluid turbulent state consists of a tangle of quantized vortices [Feynman, 1955]. He also correctly predicted the existence of quantized vortex lines as the source of vorticity flows in He II\(^1\), and predicted quantized vortex rings. His conjectures, which have been proven to be correct, launched an extremely active theoretical investigation of low-temperature physics that goes on until this day. This investigation has witnessed a more recent revolution driven by the experimental realization of Bose-Einstein condensates (BECs) in cold atomic vapors. Condensed matter theory of BEC superfluidity and Bardeen-Cooper-Schrieffer (BSC) superconductivity, and the interplay of their mutual crossover, is presently being sorted out, elucidating the role of quantum entanglement in the many-body dynamics underlying quantum fluids. Finally, the great mysteries underlying quan-

\(^1\)Cf. Landau conjectured superfluid vorticity derived from vortex sheets, now known to be unstable.
tum turbulence are being unraveled, presently one of the most prominent and actively pursued areas in low-temperature physics.

The isotope of Helium, $^4\text{He}$, with atomic mass of four, behaves as a quantum liquid at low temperatures. The $^4\text{He}$ atom has integer spin and is a bosonic particle. The boiling point of $^4\text{He}$ occurs at $4.2^\circ\text{K}$ and below this temperature $^4\text{He}$ is a normal viscous liquid. Yet at still lower temperatures, unlike other liquids, $^4\text{He}$ does not freeze into a spatially organized solid phase. The interatomic force between $^4\text{He}$ particles is weak enough to allow $^4\text{He}$ to remain in the liquid phase at low enough temperatures where quantum effects can dominate and give rise to an exotic state of matter. An order-disorder phase separation does occur at $2.18^\circ\text{K}$, the so-called $\lambda$-point, but remarkably, it is a second-order phase transition in momentum space. This ordered phased in momentum space is called Helium II, the superfluid phase.

The hydrodynamic properties of Helium II are fascinating, particularly the property of flow through narrow capillaries without any frictional resistance or quantum barrier tunneling manifested at macroscopic scales. Helium II behaves as a coupled two fluid system, where one fluid is a normal viscous fluid and the other is a superfluid. The underlying microscopic picture for its two fluid behavior is the following. Since Helium II is comprised of $^4\text{He}$ bosons, at zero temperature these particles can all occupy the same ground state energy level\(^2\). This state of matter is a BEC. At finite temperatures below the $\lambda$-point, thermal excitations are created, depleting the BEC, yet a macroscopic number of the $^4\text{He}$ particles remain in the condensate. In Helium II there are two types of thermal excitations: long wavelength phonons and shorter wavelength rotons. These excitations are quasiparticles, and away from the $\lambda$-point, are weakly interacting. They have an effective mass and transport

\(^2\)Even at zero temperature some virtual states at higher energies are occupied because some exclusion is created by nonlocal interactions, known as depletion of the condensate. These higher energy virtual states should not be confused with the higher energy states corresponding to thermal excitations.
momentum diffusively. As a collective system, the thermal excitations behave as a viscous fluid accounting for any convection and kinematic shear in Helium II. So the normal viscous part of Helium II is a gas of quasiparticles, while the superfluid part of Helium II is a BEC that only transports momentum coherently.

Experimentalists long ago observed that viscosity exists even below the \( \lambda \)-point for the transition to Helium II. The two-fluid model is one of the most well known attempts to understand viscous quantum fluid flow. This hydrodynamic coupled-fluid picture has Landau’s two-fluid equations modeling the nonlinear flow and interaction between the inviscid superfluid intermixed with a normal viscous fluid [Landau, 1941b]. The superfluid part of the quantum flow is comprised of the motion of quantized vortices experiencing a Magnus force [Kopnin and Salomaa, 1991]. Many nonclassical phenomena are correctly captured by this two-fluid model that incorporates mutual friction between the superfluid and normal fluid components. The most famous of these are superfluid turbulence driven by thermal counterflow, the quantum fountain effect, leaking of Helium II through a membrane (\textit{i.e.} inviscid superfluid capillary flow), and quantum tunneling through a gravitational potential (\textit{i.e.} creeping superflow up and over the walls of a shallow cup containing the quantum fluid). A review of two-fluid theory of Tisza and Landau for the Helium II phase of liquid \( ^4\text{He} \) is given in Appendix C.1.

Recently, it has been observed that at very low temperatures \(< 100 \text{ mK} \) thermal excitations are unimportant in Helium II and effectively the normal fluid component therefore vanishes in the bulk. Thus, Landau’s mutual frictional process no longer operates as a source of dissipation in the bulk region of the quantum fluid in the low-temperature limit so only the superfluid component remains. Yet, at these ultracold temperatures, dissipation has been observed [Walmsley et al., 2007]. That is, even a pure superfluid component of Helium II behaves dissipatively.

The recent discovery of BECs of atomic alkali gases provides a new way to
explore pristine superfluid behavior. The dissipation mentioned above occurs in ultracold atomic vapor BECs too, at high wave number (i.e. scales below the healing length \( \lesssim 1 \text{nm} \) in atomic BECs). We explore this phenomenon and understand it as the consequence of nonlinear Kelvin wave cascade dynamics and Kelvin mode coupling to phonon modes that escape into the bulk of the condensate.

5.1.1 Organization

This chapter is organized in two parts. We provide a comprehensive review of the superfluid dynamics, starting in Sec. 5.2 with a survey of superfluid theory and then in Sec. 5.3 a treatment of the subject of topological singularities in the condensate.

We begin the formal development in this chapter, in Sec. 5.2.1, with the many-body bosonic Hamiltonian in the grand canonical ensemble, and then derive the Gross-Pitaevskii (GP) equation in Sec. 5.2.2 using the theory of a nonrelativistic Lagrangian of a complex scalar condensate with a local self-consistent Hartree potential. Next, in Sec. 5.2.3, we consider quasiparticle excitations above the condensate and derive the Bogoliubov equations governing quasiparticle excitations in the superfluid. In Sec. 5.2.4, we generalize the ensemble representation of Bohm to handle the case of a nonlinear local interaction and then, in turn, in Sec. 5.2.5 write the average energy in a quantum fluid in terms of three components: (1) classical kinetic energy, (2) quantum kinetic energy, and (3) internal energy. This sets the stage for us to revisit the question of writing the nonlinear Schrödinger (NLS) equation in terms of a fluid equation, which we do later on in Chapter 7. The Kolomogorov power-law associated with turbulent flow follows immediately from the fact that at the hydrodynamic scale the effective governing momentum equations of a superfluid is a viscous Navier-Stokes equation, a result that depends on a straightforward
thermodynamical argument.

Then, we move on to addressing the subject of quantum vortices in a superfluid. In Sec. 5.3.1, we solve the time-independent GP equation for a single rectilinear quantum vortex. Here, we present a rigorous definition of the coherence length in a superfluid. Then, in Sec. 5.3.2, we review Fetter’s treatment of two mutually interacting quantum vortices. Like vortices orbit each other and their mutual interaction leads to the Kelvin wave instability. In Sec. 5.3.3, we present the Frenet-Serret formulation, or vortex filament model, of the dynamical motion of a quantum vortex, which is the basis of the Schwarz vortex filament model of superfluidity in the local induction approximation. Finally, in Sec. 5.4, we consider the dynamics of a Fermi condensate. In Sec. 5.4.1, we present a derivation of a model 2-spinor equation of motion for a Fermi superfluid. Then, in Sec. 5.4.2, we revisit the subject of Bogoliubov quasiparticle excitations in the context of the Fermi condensate.

5.2 Theory of superfluids

5.2.1 Grand canonical, many-body Hamiltonian

A quantum gas of Bose particles of mass \( m \) may be treated in the low-temperature limit as a many-body quantum system undergoing strictly local scattering. The interaction potential, in units of energy, is modeled as a delta function

\[
V(r - r') = g \delta^{(3)}(r - r'),
\]

where \( g \) is a real-valued coupling strength parameter with units of energy times volume. The grand canonical, many-particle Hamiltonian is [Fetter and Walecka, 1971]

\[
\hat{K} = \int d^3r \hat{\phi}^\dagger(r) (H_0 - \mu) \hat{\phi}(r)
+ \frac{g}{2} \int d^3r \hat{\phi}^\dagger(r) \hat{\phi}(r) \hat{\phi}(r) \hat{\phi}(r),
\]
where $\hat{\phi}^\dagger(r)$ and $\hat{\phi}(r)$ are the field operators that create and destroy, respectively, a particle at spatial point $r$, $H_o$ is the free particle Hamiltonian, and $\mu$ is the chemical potential. Equation (5.2) is the Hamiltonian associated with $\varphi^4$ theory in the nonrelativistic limit. The total number of particles in the grand canonical ensemble is

$$N = \int d^3r \langle \hat{\phi}^\dagger(r)\hat{\phi}(r) \rangle.$$  

(5.3)

In the low-temperature superfluid phase of the condensed matter system described by (5.2), most of the particles comprise the Bose-Einstein condensate and a few of the particles comprise the Bogoliubov quasiparticles. So, if the number of condensate particles is $N_o$ say, then the number of uncondensed particles is $N - N_o$. The Bogoliubov approximation holds when $N - N_o \ll N_o$ so the field operator may be decomposed as

$$\hat{\varphi}(r) = \varphi(r) + \hat{\phi}(r),$$  

(5.4)

where the quasiparticle field operator $\hat{\phi}(r)$ is the small fluctuation of the field operator $\varphi(r)$ about the condensate background $\varphi(r)$, which is an effective classical field with normalization $N_o = \int d^3r |\varphi(r)|^2$. In this approximation, the BEC field $\varphi(r)$ is the operative vacuum; that is, $\varphi(r)$ is the zero-quasiparticle state upon which the ladder operators $\hat{\phi}^\dagger(r)$ and $\hat{\phi}(r)$ act.

Inserting (5.4) into (5.2), we have

$$\hat{K} = \hat{K}_o + \hat{K}_{\text{int}},$$  

(5.5)

where

$$\hat{K}_o = \int d^3r \left( \varphi^*(r) + \hat{\phi}^\dagger(r) \right) \left( H_o - \mu \right) \left( \varphi(r) + \hat{\phi}(r) \right)$$  

(5.6a)

$$= \int d^3r \varphi^*(H_o - \mu)\varphi + \int d^3r \varphi^*(H_o - \mu)\hat{\phi} + \int d^3r \hat{\phi}^\dagger(H_o - \mu)\varphi + \int d^3r \hat{\phi}^\dagger(H_o - \mu)\hat{\phi}$$  

(5.6b)
and

\[
\hat{K}_\text{int} = \frac{g}{2} \int d^3r \left( \varphi^* \varphi + 2 \varphi^* \dot{\phi} + \dot{\phi}^\dagger \dot{\phi} \right) \left( \varphi^2 + 2 \varphi \dot{\phi} + \dot{\phi}^2 \right) \quad (5.6c)
\]

\[
= \frac{g}{2} \int d^3r \varphi^* |\varphi|^2 \varphi + g \int d^3r \varphi^* |\varphi|^2 \dot{\phi} + \frac{g}{2} \int d^3r \dot{\phi} \varphi^* \dot{\phi} \quad (5.6d)
\]

\[
+ \frac{g}{2} \int d^3r \dot{\phi}^\dagger |\varphi|^2 \varphi + 2g \int d^3r \dot{\phi}^\dagger |\varphi|^2 \dot{\phi} + g \int d^3r \dot{\phi}^\dagger \varphi^* \dot{\phi} \dot{\phi} \dot{\phi}^\dagger
\]

\[
+ \frac{g}{2} \int d^3r \dot{\phi}^\dagger \dot{\phi} \dot{\phi} + g \int d^3r \dot{\phi}^\dagger \dot{\phi} \dot{\phi} \dot{\phi} + \frac{g}{2} \int d^3r \dot{\phi}^\dagger \dot{\phi} \dot{\phi} \dot{\phi}^\dagger. \quad (5.6d)
\]

Then inserting (5.6) into (5.5) and collecting like terms, and arranging them in ascending order from quadratic to cubic to quartic products, the grand canonical Hamiltonian becomes

\[
\hat{K} = \int d^3r \varphi^* \left( H_0 - \mu + g |\varphi|^2 \right) \varphi
\]

\[
+ \int d^3r \varphi^* \left( H_0 - \mu + g |\varphi|^2 \right) \dot{\phi} + \int d^3r \dot{\phi}^\dagger \left( H_0 - \mu + g |\varphi|^2 \right) \varphi
\]

\[
+ \int d^3r \dot{\phi}^\dagger \left( H_0 - \mu + 2g |\varphi|^2 \right) \dot{\phi} + \frac{g}{2} \int d^3r \left( \dot{\phi}^\dagger \varphi^2 \dot{\phi} + \dot{\phi} \varphi^* \dot{\phi} \right)
\]

\[
+ g \int d^3r \dot{\phi}^\dagger \left( \varphi^* \dot{\phi} + \dot{\phi}^\dagger \varphi \right) \dot{\phi}
\]

\[
+ \frac{g}{2} \int d^3r \left( \dot{\phi}^\dagger \dot{\phi} \dot{\phi} \dot{\phi} - \varphi^* \varphi^* \varphi \varphi \right). \quad (5.7)
\]

The quasiparticle vacuum satisfies the steady-state NLS equation

\[
(H_0 + g |\varphi|^2 - \mu) \varphi = 0, \quad (5.8)
\]

so the first three terms in (5.7) vanish, and we have the Bogoliubov Hamilton for a BEC superfluid

\[
\hat{K}_\text{B} = \int d^3r \dot{\phi}^\dagger \left( H_0 - \mu + 2g |\varphi|^2 \right) \dot{\phi}
\]

\[
+ \frac{g}{2} \int d^3r \left( \dot{\phi}^\dagger \varphi^2 \dot{\phi} + \dot{\phi} \varphi^* \dot{\phi} \right) + \cdots, \quad (5.9)
\]

retaining terms only up to second order in the fluctuation of the condensate. Solutions of (5.9) has been given by Fetter, for example in the case of a spherical trapping potential [Fetter, 1996].
\subsection{Condensate dynamics}

The time-dependent theory for a nonrelativistic condensate in the zero-temperature limit in free space is

\begin{equation}
\mathcal{L}_{\text{BEC}}(t) = i\hbar \varphi^* \partial_t \varphi + \frac{\hbar^2}{2m} (\nabla \varphi^*) \cdot \nabla \varphi + \mu \varphi^* \varphi - \varphi^* V_H \varphi, \tag{5.10}
\end{equation}

where $\varphi(x)$ is a complex scalar field for the Bose-Einstein condensate, $V_H$ is a local self-consistent Hartree potential. Minimizing the action $A = \int d^4 x \mathcal{L}_{\text{NR}}(t)$ leads to the Euler-Lagrange equation

\begin{equation}
\nabla \cdot \left( \frac{\partial \mathcal{L}_{\text{BEC}}}{\partial (\nabla \varphi^*)} \right) - \frac{\partial \mathcal{L}_{\text{BEC}}}{\partial \varphi^*} = 0, \tag{5.11a}
\end{equation}

and, for $V_H = V_H(|\varphi|^2)$, this is the NLS equation

\begin{equation}
\imath \hbar \partial_t \varphi = -\frac{\hbar^2}{2m} \nabla^2 \varphi + \hbar \Omega(|\varphi|^2) \varphi, \tag{5.11b}
\end{equation}

where the "internal potential energy" is

\begin{equation}
\hbar \Omega(|\varphi|^2) \equiv V_H(|\varphi|^2) - \mu + |\varphi|^2 \frac{\partial V_H(|\varphi|^2)}{\partial |\varphi|^2}. \tag{5.12}
\end{equation}

In the case when $V_H(|\varphi|^2) = \frac{1}{2}g|\varphi|^2$, where $g$ is the real-valued coupling strength of the nonlinear interaction, (5.11b) is the GP equation [Gross, 1963, Pitaevskii, 1961]

\begin{equation}
\imath \hbar \partial_t \varphi = -\frac{\hbar^2}{2m} \nabla^2 \varphi + (g|\varphi|^2 - \mu) \varphi, \tag{5.13}
\end{equation}

and here we neglect the trapping potential. This captures a number of types of vortex physics (vortex nucleation, emission and absorption of vortex rings, vortex-line reconnection) as well as the interplay between quantum Kelvin waves (kelvon modes) riding on the vortices and sound waves (phonon modes) that escape into the bulk region of the quantum fluid.
5.2.3 Bogoliubov equations

Let us now consider quasiparticle excitations that reside on a quantum vortex in a BEC superfluid [Bogoliubov, 1947]. Let us write the nonlinear interaction with a chemical potential as $H_{\text{int}} = g|\varphi|^2 - \mu$, where the condensate wave function is normalized to $\sqrt{\mu/g}$ in the bulk (i.e. $H_{\text{int}} \sim 0$ in the bulk). The dynamical field of a quantum vortex (or collection of quantum vortices) acts like a vacuum background configuration, $\varphi_v(x)$ say, a nonuniform hydrodynamic condensate configuration on which there exists a spectrum of small fluctuations, the Bogoliubov quasiparticle excitations.

With $|u(x)|^2 + |v(x)|^2 = 1$, a constraint on the amplitudes, the bosonic scalar wave function is

$$\varphi(x, t) = \varphi_v(x, t) + \epsilon (u(x)e^{-i\omega t} - v^*(x)e^{i\omega t}) + \cdots .$$

(5.14)

Inserting (5.14) into (5.13) then gives

$$\hbar\omega \epsilon [u(x)e^{-i\omega t} + v^*(x)e^{i\omega t}] =$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + g |\varphi|^2 - \mu\right) \left[\varphi_v(x, t) + \epsilon (u(x)e^{-i\omega t} - v^*(x)e^{i\omega t})\right],$$

(5.15)

where the nonlinear interaction is

$$g|\varphi|^2 - \mu = g|\varphi_v|^2 - \mu + g\epsilon^2$$

$$+ e^{-i\omega t} g \epsilon (u\varphi^*_v - v\varphi_v) + e^{i\omega t} g \epsilon (u^*\varphi_v - v^*\varphi^*_v)$$

$$- g\epsilon^2 (e^{-2i\omega t} uv + e^{2i\omega t} u^*v^*),$$

(5.16)

where we made use of the fact that $|u|^2 + |v|^2 = 1$. Calculating all the cross-terms associated with a first-order Bogoliubov excitation $\epsilon(u(x)e^{-i\omega t} - v^*(x)e^{i\omega t})$,
the NLS equation is explicitly

\[ \hbar \omega \left[ u e^{-i\omega t} + v^* e^{i\omega t} \right] = -\frac{\hbar^2}{2m} \nabla^2 \left[ u e^{-i\omega t} - v^* e^{i\omega t} \right] \\
+ e^{-i\omega t} \left[ -g|\varphi|^2 v + (2g|\varphi|^2 - \mu + g\varepsilon^2)u \right] \\
+ e^{i\omega t} \left[ g\varphi^2 u^* - (2g|\varphi|^2 - \mu + g\varepsilon^2)v^* \right] \\
+ g \varepsilon e^{-2i\omega t} (-2\varphi, uv + \varphi^* u^2) + g \varepsilon e^{2i\omega t} (-2\varphi, u^* v^* - \varphi^* v^*^2) \\
+ 2g \varepsilon (\varphi - \varphi^* uv^*) \\
- g \varepsilon^2 e^{-3i\omega t} u^2 v + g \varepsilon^2 e^{3i\omega t} u^* v^*^2 + \cdots, \]  

(5.17)

where we have not included any other high-order nonlinear effects arising from second-order fluctuations beyond Bogoliubov quasiparticle excitations. The relevant part of the NLS equation are the zeroth order terms

\[ \hbar \omega \left[ u e^{-i\omega t} + v^* e^{i\omega t} \right] = -\frac{\hbar^2}{2m} \nabla^2 \left[ u e^{-i\omega t} - v^* e^{i\omega t} \right] \\
+ e^{-i\omega t} \left[ -g|\varphi|^2 v + (2g|\varphi|^2 - \mu + g\varepsilon^2)u \right] \\
+ e^{i\omega t} \left[ g\varphi^2 u^* - (2g|\varphi|^2 - \mu + g\varepsilon^2)v^* \right] + \cdots. \]

Finally, since the positive and negative frequency solutions are separable at zeroth order, the relevant effective field theory is basically two coupled equations

\[ \hbar \omega u = \mathcal{L} u - g\varphi^2 v + \cdots \]  

(5.18a)

\[ -\hbar \omega v = \mathcal{L} v - g\varphi^2 u^* + \cdots, \]  

(5.18b)

where \( \mathcal{L} \equiv -\frac{\hbar^2}{2m} \nabla^2 + 2g|\varphi|^2 - \mu. \) The set of coupled nonlinear equations (5.18) are known as the Bogoliubov equations, which are related to the Bogoliubov-de Gennes equations in the theory of superconductivity [de Gennes, 1966, Fetter, 2009].

The factor \( \Delta \equiv g\varphi^2 \) plays the role of the gap function in the BCS theory of superconductivity.
5.2.4 Ensemble representation

Now with the Madelung transformation $\varphi = \sqrt{\rho} e^{iS/h}$ [Madelung, 1927], the BEC Lagrangian density (5.10) can be written in terms of the conjugate fluid variables (the action $S$ and number density $\rho$) as follows

$$L_{\text{BEC}} = -\rho \partial_t S - \rho \left[ \frac{(\nabla S)^2}{2m} + \frac{\hbar^2}{2m} \left( \frac{\nabla \rho}{2\rho} \right)^2 - \mu + V_\text{in}(\rho) \right]. \quad (5.19)$$

The Madelung transformation is given in Appendix C.2. The quantity in square brackets is identified with a Hamiltonian energy functional. Bohm originally made this identification while considering quantum flow in a spatially-dependent linear external potential $V(x)$ [Bohm, 1952]. Here we consider quantum flow with a non-linear internal potential energy$^3$

$$E_{\text{in}}(\rho) \equiv V_\text{in}(\rho) - \mu. \quad (5.20)$$

So, a pseudo-classical BEC energy functional may be written as

$$H_{\text{BEC}} = \frac{(\nabla S)^2}{2m} + \frac{\hbar^2}{2m} \left( \frac{\nabla \rho}{2\rho} \right)^2 + E_{\text{in}}(\rho), \quad (5.21)$$

and the dynamics can be expressed in the form of classical Hamilton equations

$$\frac{\partial S}{\partial t} = -\frac{\delta (\rho H_{\text{BEC}})}{\delta \rho}, \quad (5.22a)$$

$$\frac{\partial \rho}{\partial t} = \frac{\delta (\rho H_{\text{BEC}})}{\delta S}. \quad (5.22b)$$

The resulting equations of motion are

$$-\frac{\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V_\text{B} + \hbar \Omega(\rho) \quad (5.23a)$$

$$\frac{\partial \rho}{\partial t} = -\frac{1}{m} \nabla \cdot (\rho \nabla S), \quad (5.23b)$$

where the quantum mechanical kinetic energy term in (5.11b) contributes the Bohm potential

$$V_\text{B} = -\frac{\hbar^2}{2m} \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}}. \quad (5.24)$$

$^3$In the BEC literature, the external potential $V(x)$ is referred to as the trapping potential, and we do not include this here since we treat superfluidity in free space.
The Hamilton equations (5.22) are just the real part (Hamilton-Jacobi equation) and imaginary part (continuity equation), respectively, of the NLS equation (5.11b).

### 5.2.5 Average energy

The average energy is calculated as a statistical volume integral

$$\overline{E} = \int d^3 x \, \rho \, H_{\text{BEC}},$$

with $\rho$ taken as the effective probability distribution

$$\overline{E} = \left. \int d^3 x \, \rho \left[ \frac{(\nabla S)^2}{2m} + \frac{\hbar^2}{2m} \left( \frac{\nabla \rho}{2\rho} \right)^2 + E_{\text{int}}(\rho) \right] \right|_{(5.21)} \tag{5.25}$$

$\overline{E}$ is a conserved quantity. Here the first two contributing time-dependent energy terms derive from the kinetic part of the BEC Lagrangian $-\frac{\hbar}{2m} |\nabla \varphi|^2$ and the last time-dependent interaction term derives from the Hartree potential $V_H = \frac{1}{2} g |\varphi|^2 \varphi$ (neglecting the constant energy shift due to the chemical potential). The result is

$$\overline{E}_{\text{TOT}} = \overline{E}_{\text{kin}}(t) + \overline{E}^{\text{qu}}_{\text{kin}}(t) + \overline{E}_{\text{int}}(t), \tag{5.26}$$

where

$$\overline{E}_{\text{kin}}(t) = \int d^3 x \, \rho(x) \left[ \frac{1}{2} m \mathbf{v}(x)^2 \right] = \frac{m}{2} \int d^3 x \, |\sqrt{\rho} \, \mathbf{v}|^2, \tag{5.27a}$$

$$\overline{E}^{\text{qu}}_{\text{kin}}(t) = \int d^3 x \, \rho(x) \left[ \frac{\hbar^2}{2m} \left( \frac{\nabla \rho(x)}{2\rho(x)} \right)^2 \right] = \frac{\hbar^2}{2m} \int d^3 x \, |\nabla \sqrt{\rho}|^2, \tag{5.27b}$$

$$\overline{E}_{\text{int}}(t) = \int d^3 x \, \rho(x) \left[ \frac{1}{2} g \rho(x) \right] = \frac{g}{2} \int d^3 x \, |\rho|^2, \tag{5.27c}$$

where in (5.27a) we made use of the de Broglie relation $m \mathbf{v} = \nabla S$.

By defining a complex vector field strength [Nore et al., 1997a]

$$\mathbf{F} = \frac{\hbar}{\sqrt{2m}} \frac{\varphi^* \nabla \varphi}{|\varphi|} = \frac{\hbar}{\sqrt{2m}} \nabla \sqrt{\rho} + i \sqrt{\frac{m}{2}} \mathbf{v}, \tag{5.28}$$

the total kinetic energy may be written as the square of the field strength, $\overline{E}_{\text{kin}} = \int d^3 x \, |\mathbf{F}|^2$, since

$$\overline{E}_{\text{kin}}^{\text{cl}} = \int d^3 x \, \Im[\mathbf{F}]^2, \quad \overline{E}_{\text{kin}}^{\text{qu}} = \int d^3 x \, \Re[\mathbf{F}]^2. \tag{5.29}$$
The Fourier transform and its inverse transform are

\[
\tilde{f}(k) = \mathcal{F}[f(x)] = \int d^3x e^{-ikx} f(x) \tag{5.30a}
\]

\[
f(x) = \mathcal{F}^{-1}[f(k)] = \int \frac{d^3k}{(2\pi)^3} e^{ikx} \tilde{f}(k). \tag{5.30b}
\]

Since \( \int d^3x e^{-ikx} = (2\pi)^3 \delta^{(3)}(k) \), Parseval’s theorem for length preservation of a function in its Fourier basis representations directly follows

\[
\int d^3x |f(x)|^2 = \int \frac{d^3k}{(2\pi)^3} |\tilde{f}(k)|^2. \tag{5.31}
\]

Using (5.31), we can rewrite (5.29) as

\[
\overline{E}_{\text{kin}}^{\text{cl}} \overset{(5.30a)}{=} \int \frac{d^3k}{(2\pi)^3} \left| \int d^3x e^{-ikx} \Im[F] \right|^2, \tag{5.32a}
\]

and

\[
\overline{E}_{\text{kin}}^{\text{qu}} \overset{(5.30a)}{=} \int \frac{d^3k}{(2\pi)^3} \left| \int d^3x e^{-ikx} \Re[F] \right|^2. \tag{5.32b}
\]

To help physically interpret the complex field strength, let us define the quantum velocity field

\[
v_{\text{qu}} = -i \sqrt{\frac{2}{m\rho}} F = (5.28) \quad v - \frac{i\hbar}{m} \nabla \sqrt{\rho}. \tag{5.33}
\]

Then, since

\[
|v_{\text{qu}}|^2 = \left( \frac{\nabla S}{m} \right)^2 + \left( \frac{\hbar}{2m} \frac{\nabla \rho}{\rho} \right)^2, \tag{5.34}
\]

we may rewrite (5.25) as

\[
\overline{E} = \int d^3x \rho \left[ \frac{1}{2} m|v_{\text{qu}}|^2 + E_{\text{int}}(\rho) \right], \tag{5.35}
\]

which corresponds to the fact that the classical and quantum average energy components in (5.29) are both kinetic energy terms. The form of (5.35) was originally obtained by Harvey [Harvey, 1966].
5.3 Quantum vortices

5.3.1 Single quantum vortex

To determine a steady-state (or background) solution of the black quantum vortex in a superfluid, with a condensate wave function denoted by \( \varphi_v \), one solves (5.8) for when \( H_0 = -\frac{\hbar^2}{2m} \nabla^2 \), which is the time-independent GP equation

\[
-\xi^2 \nabla^2 \varphi_v + \left( \frac{g}{\mu} |\varphi_v|^2 - 1 \right) \varphi_v = 0,
\]

where the healing length is \( \xi \equiv \hbar/\sqrt{2m\mu} \). A solution for the background condensate wave function of a single rectilinear quantum vortex (with vorticity along \( \hat{z} \)) is found by separation of variables in polar coordinates. Inserting \( \varphi_v(r, \theta, z) = \phi_v(r) Z_v(z)e^{i m \theta} \) into (5.36) with \( g/\mu = \xi^2 \) gives the following equations with a separation constant \( k_{||}^2 \):

\[
\begin{align*}
\frac{d^2 Z_v(z)}{dz^2} + k_{||}^2 Z_v(z) &= 0, \\
\frac{d^2 \phi_v(r)}{dr^2} + \frac{1}{r} \frac{d \phi_v(r)}{dr} - \frac{n^2}{r^2} \phi_v(r) + (a - \phi_v(r)^2) \phi_v(r) &= 0,
\end{align*}
\]

where \( a \equiv \xi^{-2} - k_{||}^2 \). Equation (5.37a) admits sinusoidal solutions and (6.76) can be solved for any integer winding number \( n \). For the simplest \( n = 1 \) case, the Padé approximant

\[
\phi_v(r) = \sqrt{a} \sqrt{\frac{11ar^2(12 + ar^2)}{384 + ar^2(128 + 11ar^2)}}
\]

solves (5.36) with errors at \( \mathcal{O}[(r \sqrt{a})^7] \) (see Sec. 6.4 and Appendix D.1). Notice that \( \phi_v(r) \to \sqrt{a} \) and \( r \to \infty \), and thus the nonlinear term in (6.76) vanishes in the bulk.

The rectilinear quantum vortex solution of (5.13) is

\[
\varphi_v(x) = \phi_v(r) \left[ Z_+^e e^{i(\omega_\parallel t + k_{||} z)} + Z_+^e e^{i(\omega_\parallel t - k_{||} z)} \right],
\]

with a parabolic dispersion relation \( h \omega_\parallel = \frac{\hbar^2 k_{||}^2}{2m} \). For a vortex line along the \( \hat{z} \)-direction in cylindrical coordinates with unit winding number, the irrotational part
of the superfluid velocity has a divergent (perpendicular) part characteristic of inviscid flow and an advective (parallel) part characteristic of rigid translation

\[ v = \frac{\hbar}{m} \nabla \left( \vartheta \pm k_\parallel z \right) \]

\[ = \frac{\hbar}{m} \left( \frac{\vartheta}{r} \frac{\partial}{\partial \vartheta} \right) \vartheta \pm \frac{\hbar k_\parallel}{m} \left( \frac{z}{\partial z} \right) z \]

\[ = \frac{\hbar}{mr} \vartheta \pm \frac{\hbar k_\parallel}{m} z. \]

This is a real velocity field, and from this we see that the circulation is quantized

\[ \kappa \equiv \oint dl \cdot v = \int_0^{2\pi} r d\vartheta \left( \frac{\hbar}{mr} \right) = \frac{h}{m}. \]

From Stokes' theorem, we have

\[ \int dS \cdot \nabla \times v = \int dS \cdot \omega = \frac{h}{m}. \]

For a rectilinear \( \hat{z} \)-directed quantum vortex, the real part of the vorticity is pinned at the vortex center

\[ \omega = \frac{\hbar}{m} \delta^{(2)}(r) \hat{z}. \]

For a vortex filament of any shape, say a curve \( C \), the velocity field in general may be written as

\[ v(r) = \frac{h}{2m} \int_C \frac{ds' \times (r - s')}{|r - s'|^3}, \]

where \( ds' \) is the differential length along the vortex filament, \( s' \) is the parametrization of \( C \), \( r \) is the field point, and \( ds' \) is the differential line element at the vortex center and parallel to the vorticity [Schwarz, 1985]. The Biot-Savart formula (5.44) reduces to \( v = \hat{\vartheta} h/(mr) \) for the case of an infinite rectilinear quantum vortex positioned along the center of a cylindrical coordinate system with \( s' = z \), \( ds' = dz \hat{z} \), and \( ds' \times (\hat{r} - \hat{s}') = \hat{\vartheta} dz |z|/|r - s'| \).
FIG. 5.1: Radial profiles for a differential length $dl$ of a linear quantum vortex (with winding number $n = 1$ and scale factor $a = 0.02$) residing in a condensate (with nonlinear coupling $g = 1$) plotted versus radial distance $r$ from the vortex center in lattice units:

**BROWN** Magnitude of radial amplitude $\phi(r)$. 
**BLUE** Angular momentum number density $\phi(r)^2 v_\theta(r)/a$. 
**THICK BLUE** Amplitude-weighted angular velocity $\phi(r) v_\theta(r)/\sqrt{a}$. 
**BLUE DASHED** Divergent angular velocity $v_\theta(r) = \hbar/(mr)$. 
**RED** $k^{-3}$ spectra occurs within one coherence length, $r \lesssim \xi$. 
**RED-GREEN** Quantum transition range is $\xi \lesssim r \lesssim \pi \xi$. 
**GREEN** $k^{-5/3}$ spectra occurs for $r \gtrsim \pi \xi$.

The average classical kinetic energy per unit length $L$ of a single linear quantum vortex is

$$\mathcal{E} \equiv \bar{E}^{cl}_{\text{kin}} / L$$

$$= \int_0^{r_b} \frac{d^3x}{L} \rho_\alpha(r) \frac{mv_\theta^2}{2}$$

$$= \int_0^{r_b} 2\pi r dr \rho_\alpha(r) \frac{mv_\theta^2}{2}$$

$$= m \rho_\alpha \int_{r_c}^{r_b} 2\pi r dr \frac{v_\theta^2}{2}$$

$$= \frac{\hbar \rho_o}{2} \int_{r_c}^{r_b} dr \ v_\theta$$

$$= \frac{\rho_o h^2}{4 \pi m} \int_{r_c}^{r_b} \frac{dr}{r}$$

$$= m \rho_o \frac{\kappa_o^2}{4 \pi} \log \frac{r_b}{r_c}$$

where $\kappa_o \equiv \hbar/m$ is the quantum of circulation and $\rho_o$ is the constant background number density of the condensate, $r_b$ is regularizing parameter associated with the
size of the vessel containing a single quantum vortex or the mean intervortex distance for a system of many quantum vortices, and \( r_c \) is an effective cutoff parameter to the divergent angular velocity field. Notice that \( r_c \) is chosen so that the integral (5.45d), with a cutoff that avoids the singularity at the origin, is equivalent to the original nonsingular integral (5.45c) with no cutoff. Therefore, \( r_c \) is technically not the usual cutoff parameter per se because the original integral is nonsingular—instead, \( r_c \) should be understood as merely a matching parameter useful for replacing a nonsingular but difficult integrand with an analytically simpler one to determine the line energy. All the expressions of the average classical kinetic energy per unit length in (5.45) are equivalent, rigorously equal in value without any approximations. That such a value of \( r_c \) exists can be seen from examining in Fig. 5.2

![Graph showing the average classical kinetic energy areal density computed in two ways in terms of the areal regions A, B, and C: (1) \( \mathcal{E} = A + B \) and (2) \( \mathcal{E} = B + C \). The latter method uses an effective cutoff parameter \( r_c \) determined by the constraint that \( A = C \). This cutoff approximately equals the coherence length, \( r_c \approx \xi \). The dashed blue curve is \( (2\pi r)\rho_0 v_0^2 / 2 \propto v_0 \) (the large radial-distance envelop) and the solid blue curve is the physical classical kinetic energy areal density, \( (2\pi r)\rho_0(r)mv_0^2 / 2 \).]

**5.3.2 Two interacting quantum vortices**

We now consider the interaction of two initially rectilinear quantum vortices in a superfluid, originally treated by Fetter [Fetter, 1967]. We take the initial (sin-
gle vortex) equilibrium states to be parallel linear filaments with an arc length parametrization given by the following vectors

\[ \mathbf{R}_1^{(0)} = (r_1, z_1) \quad \mathbf{R}_2^{(0)} = (r_2, z_2). \]  \hspace{1cm} (5.46)

The consequent deformed state to due the mutual interaction of the vortices is parametrized by

\[ \mathbf{R}_1 = (r_1 + \mathbf{u}_1(z_1), z_1) \quad \mathbf{R}_2 = (r_2 + \mathbf{u}_2(z_2), z_2), \]  \hspace{1cm} (5.47)

where \( \mathbf{u}_1 \) and \( \mathbf{u}_2 \) are treated as small amplitude perturbations in the radial directions with respect to the initial unperturbed filamentary lines. Each vortex filament is a stretched helix, approximating a nearly straight line parallel to the \( \hat{z} \)-axis.

The first step is to calculate the fluctuation in position of a vortex element at the first vortex due to the presence of the second vortex. The fluid velocity at the first vortex located at \( \mathbf{R}_1 \) caused by the second vortex at \( \mathbf{R}_2 \) is given by the Biot-Savart law (5.44)

\[ \mathbf{v}(\mathbf{R}_1) = \frac{\kappa_0}{4\pi} \oint_{\mathcal{C}_2} \frac{d\mathbf{s}_2 \times (\mathbf{R}_1 - \mathbf{R}_2)}{|\mathbf{R}_1 - \mathbf{R}_2|^3}, \]  \hspace{1cm} (5.48)

where \( \kappa_0 \equiv \hbar/m \) is the quantum of circulation. The differential arc length is

\[ ds_i = \frac{ds_i}{dz_i} dz_i = dz_i \left( \hat{z} + \frac{du_i(z_i)}{dz_i} \right), \]  \hspace{1cm} (5.49)

for \( i = 1, 2 \) denoting the vortices. Then, according to (5.48), the fluctuation of the position of the vortex element originally at \( \mathbf{R}_1^{(0)} \) is

\[ \frac{d\mathbf{u}_1}{dt} \overset{(5.49)}{=} \frac{\kappa_0}{4\pi} \int_{\mathcal{C}_2} \frac{\left( \hat{z} + \frac{du_2}{dz_2} \right) \times \left( \mathbf{R}_1^{(0)} + \mathbf{u}_1 - \mathbf{R}_2^{(0)} - \mathbf{u}_2 \right)}{|\mathbf{R}_1^{(0)} + \mathbf{u}_1 - \mathbf{R}_2^{(0)} - \mathbf{u}_2|^3} \]  \hspace{1cm} \overset{(5.50a)}{=} \frac{\kappa_0}{4\pi} \int_{\mathcal{C}_2} \frac{\left( \hat{z} + \frac{du_2}{dz_2} \right) \times (r_{12} + \hat{z} z_{12} + \mathbf{u}_{12})}{|r_{12} + \hat{z} z_{12} + \mathbf{u}_{12}|^3}, \]  \hspace{1cm} (5.50b)
where $r_{12} \equiv r_1 - r_2$, $z_{12} \equiv z_1 - z_2$, and $u_{12} \equiv u_1 - u_2$. Also, defining $R_{12}^{(0)} \equiv r_{12} + \hat{z}z_{12}$ and making use of the Taylor expansion $\frac{1}{|R_{12}^{(0)} + u_{12}|^3} = \frac{1}{|R_{12}^{(0)}|^3} - \frac{3u_{12} R_{12}^{(0)}}{|R_{12}^{(0)}|^5} + \cdots$, we can write a leading order expansion of the position fluctuation (velocity of the first vortex element at $z_1$ due to the presence of the second vortex)

$$\frac{du_1}{dt} = \frac{\kappa_0}{4\pi} \int dz_2 \left[ \frac{\hat{z} \times r_{12} + \hat{z} \times u_{12} + u_{12} \times \hat{z}z_{12}}{|R_{12}^{(0)}|^3} \right.$$

$$- \frac{3r_{12} \cdot u_{12}}{|R_{12}^{(0)}|^5} \hat{z} \times r_{12} + \cdots \left. \right]$$

$$= \frac{\kappa_0}{4\pi} \hat{z} \times \int dz_2 \left[ \frac{r_{12} + u_{12} - z_{12} \frac{du_{12}}{dz_2}}{|R_{12}^{(0)}|^3} \right.$$

$$- \frac{3r_{12} \cdot u_{12}}{|R_{12}^{(0)}|^5} r_{12} + \cdots \right].$$

Making the analogy to the mutual inductance of two line currents, the Neumann formula can be used to calculate the interaction energy of two vortices

$$E_{12} = m \rho_v \int d^3x \frac{v(x)^2}{2} (5.44) \frac{m \rho \kappa_0^2}{4\pi} \int C_1 \int C_2 \frac{ds_1 \cdot ds_2}{|R_1 - R_2|}.$$ (5.51)

The next step is to develop an expansion for the interaction energy. This is accomplished as follows

$$E_{12} = \frac{m \rho \kappa_0^2}{4\pi} \int d^3x \left[ \frac{\hat{z} \cdot \hat{u}_{12}}{|R_{12}^{(0)} + u_{12}|} \right. \left. \left( \frac{du_{12}}{dz_1} + \frac{du_{12}}{dz_2} \right) \right]$$

$$= \frac{m \rho \kappa_0^2}{4\pi} \int d^3x \left[ \frac{\hat{z} \cdot \hat{u}_{12}}{|R_{12}^{(0)} + u_{12}|} \left( 1 + \frac{du_{12}}{dz_1} \cdot \frac{du_{12}}{dz_2} + \cdots \right) \right],$$ (5.52a)

where the cross-terms vanish because, in the reference frame at the original center of the unperturbed $i$th vortex line along $\hat{z}$, the motion of the perturbed filament is in the polar direction $\frac{d\hat{u}_{12}}{dz_i} \approx \pm \hat{\theta}$. Employing Taylor’s theorem, the denominator is expanded to second order

$$\frac{1}{|R_{12}^{(0)} + u_{12}|} = \frac{1}{|R_{12}^{(0)}|} - \frac{r_{12} \cdot u_{12}}{|R_{12}^{(0)}|^3} + \frac{3(r_{12} \cdot u_{12})^2}{2|R_{12}^{(0)}|^5} - \frac{(u_{12})^2}{2|R_{12}^{(0)}|^3} + \cdots,$$
so in turn the interaction energy expansion becomes

\[
E_{12} = \frac{m\rho \kappa_0^2}{4\pi} \int \int d z_1 d z_2 \left\{ \frac{1}{|R_{12}^{(0)}|^3} \left[ \frac{1}{|R_{12}^{(0)}|^3} - \frac{r_{12} \cdot u_{12} - \frac{1}{2}(u_{12})^2}{|R_{12}^{(0)}|^3} \right] \\
+ \frac{1}{|R_{12}^{(0)}|^3} \frac{d u_1}{d z_1} \cdot \frac{d u_2}{d z_2} + \frac{3}{2} \frac{(r_{12} \cdot u_{12})^2}{|R_{12}^{(0)}|^5} + \cdots \right\} + \frac{z_{12}}{|R_{12}^{(0)}|^3} \frac{d u_2}{d z_2} \cdot u_1 + \frac{3}{2} \frac{(r_{12} \cdot u_{12})^2}{|R_{12}^{(0)}|^5} + \cdots ,
\]

(5.52d)

where in (5.52d) the term obtained by integrated by parts was rewritten as

\[
\dot{z} \frac{\dot{R}_{12}^{(0)}}{|R_{12}^{(0)}|^3} = \frac{z_{12}}{|R_{12}^{(0)}|^3}.
\]

Hence, it is straightforward to calculate the variation of the mutual interaction energy with respect to a fluctuation at \( z_1 \) of the center of the first vortex line

\[
\frac{\delta E_{12}}{\delta u_1(z_1)} = \frac{m\rho \kappa_0^2}{4\pi} \int d z_2 \left[ - \frac{r_{12} + u_{12} - z_{12} \frac{d u_2}{d z_2}}{|R_{12}^{(0)}|^3} + \frac{3}{2} \frac{r_{12} \cdot u_{12}}{|R_{12}^{(0)}|^5} r_{12} + \cdots \right].
\]

(5.53)

Comparing this result with the previous result (5.50d) yields the useful relation

\[
m\rho \kappa_0 \frac{d u_1(z_1)}{d t} = -\dot{z} \times \frac{\delta E_{12}}{\delta u_1(z_1)}.
\]

(5.54)

The mutual interaction energy part of the condensate energy arising from a perturbed quantum vortex of length \( L = \frac{\sqrt{\lambda}}{\rho} \sqrt{d z^2 + d u^2} \) is primarily due to its bending, assuming a sufficient separation distance exists between the vortices so that
vortex-vortex straining has no low-order effect. Therefore, we have

\[ \frac{\delta E_{12}}{\delta u_1(z_1)} = \frac{\delta L}{\delta u_1(z_1)} \]

Inserting this result into (5.54), yields

\[ E \frac{\delta}{\delta u_1(z_1)} \int dz \left[ 1 + \left( \frac{du_1(z)}{dz} \right)^2 \right]^{\frac{1}{2}} \]  

\[ E \frac{\delta}{\delta u_1(z_1)} \int dz \left[ 1 + \frac{1}{2} \left( \frac{du_1(z)}{dz} \right)^2 + \cdots \right] \]  

\[ E \int dz \frac{du_1(z)}{dz} \frac{d}{dz} \frac{\delta u_1(z_1)}{\delta u_1(z)} + \cdots \]  

\[ -E \int dz \frac{d^2 u_1(z)}{dz^2} \delta^{(1)}(u_1(z) - u_1(z_1)) + \cdots \]  

\[ -E \frac{d^2 u_1(z_1)}{dz_1^2} + \cdots \]

Inserting this result into (5.54), yields

\[ m \rho c_0 \frac{du_1(z_1)}{dt} = E \hat{z} \times \frac{d^2 u_1(z_1)}{dz_1^2}. \]  

We now proceed, with a geometrical perspective, to examine this relationship in more detail.

### 5.3.3 Frenet-Serret formulas

The Frenet-Serret formulas of multivariable calculus concerning the geometry of curves describe the kinematic properties of a particle at position \( \mathbf{R} \) moving along a continuous and differentiable curve \( \mathcal{C} \) (the particle's trajectory or world line) embedded in three-dimensional Euclidean space \( \mathbb{R}^3 \)

\[ \frac{d\mathbf{t}}{ds} = \kappa \mathbf{n} \]  

\[ \frac{d\mathbf{n}}{ds} = -\kappa \mathbf{t} + \tau \mathbf{b} \]  

\[ \frac{d\mathbf{b}}{ds} = -\tau \mathbf{n}, \]
where $s$ is the arc length parameter along $C$, $\hat{t}$ is the unit tangent to $C$ at the
top $R$, $\hat{n}$ is the unit normal perpendicular to $\hat{t}$ at $R$, $\hat{b}$ is the unit bi-normal
perpendicular to both $\hat{t}$ and $\hat{n}$, and $\kappa$ is the curvature and $\tau$ is the torsion of $C$ at
$R$. Remarkably, it is possible to derive the Gross-Pitaevskii equation directly from
(5.57) where the magnitude of the condensate's complex scalar field is related to the
curvature of $C$, $|\varphi| = \sqrt{\rho} \propto \kappa$, and its phase is related to the torsion integrated along
$C$, $\text{arg}(\varphi) = \int ds \tau$. This is known as the Hasimoto transformation [Hasimoto, 1972],
which is reviewed in Appendix C.3. Given a fixed curve $C$, one constructs a local
Frenet-Serret frame as follows

\[
\hat{t} \equiv \frac{R'(s)}{|R'(s)|} \quad (5.58a)
\]

\[
\hat{n} \equiv \frac{\hat{t}'(s)}{|\hat{t}'(s)|} \quad (5.58b)
\]

\[
\hat{b} \equiv \hat{t} \times \hat{n}, \quad (5.58c)
\]

where the prime indicates differentiation with respect to $s$. So $\hat{n}$ points along the
direction of the derivative of $\hat{t}$ with respect to the arc length parameter of the curve
and equating (5.57a) with (5.58b), the curvature is

\[
\kappa = |\hat{t}'(s)|. \quad (5.59)
\]

Therefore, the unit vectors $\hat{t}$, $\hat{n}$, and $\hat{b}$ serve as an orthogonal coordinate system
centered at $R$, a local reference frame that moves with the particle. For example,
specifying the points in $\mathbb{R}^3$ with the cylindrical coordinates $(r, \vartheta, z)$, if $C$ is a helix
with its axis along \( r = 0 \)

\[ \mathbf{R}(s) = \left( r \cos \frac{s}{\sqrt{r^2 + h^2}}, r \sin \frac{s}{\sqrt{r^2 + h^2}}, \frac{hs}{\sqrt{r^2 + h^2}} \right) \]  

(5.60a)

\[ = (r \cos kz, r \sin kz, 0) + (0, 0, h\, k z) \]  

(5.60b)

\[ = \mathbf{u}(kz) + \begin{cases} 
0 + \mathcal{O}\left( \frac{h}{r} \right) & h \ll r, \\
\frac{s}{r} - \mathcal{O}\left( \frac{r^2}{h^2} \right) & r \ll h 
\end{cases} \]  

(5.60c)

with \( kz = s/\sqrt{r^2 + h^2} \), then the Frenet-Serret frame is

\[ \hat{t} = \frac{r \hat{\theta} + h \hat{z}}{\sqrt{r^2 + h^2}} = \begin{cases} 
\hat{\theta} - \mathcal{O}\left( \frac{h^2}{r^2} \right) & h \ll r, \\
\hat{z} + \mathcal{O}\left( \frac{r}{h} \right) & r \ll h 
\end{cases} \]  

(5.61a)

\[ \hat{n} = -\hat{r} \]  

(5.61b)

\[ \hat{b} = \frac{-h \hat{\theta} + r \hat{z}}{\sqrt{r^2 + h^2}} = \begin{cases} 
\hat{z} + \mathcal{O}\left( \frac{h}{r} \right) & h \ll r, \\
-\hat{\theta} + \mathcal{O}\left( \frac{r^2}{h^2} \right) & r \ll h 
\end{cases} \]  

(5.61c)

and the local curvature and torsion of \( C \) are

\[ \kappa = \frac{r}{r^2 + h^2} = \begin{cases} 
\frac{1}{r} - \mathcal{O}\left( \frac{h^2}{r^2} \right) & h \ll r, \\
0 + \frac{1}{h} \mathcal{O}\left( \frac{r}{h} \right) & r \ll h 
\end{cases} \]  

(5.62a)

\[ \tau = \frac{h}{r^2 + h^2} = \begin{cases} 
0 + \frac{1}{r} \mathcal{O}\left( \frac{h}{r} \right) & h \ll r, \\
\frac{1}{h} - \mathcal{O}\left( \frac{r^2}{h^3} \right) & r \ll h. 
\end{cases} \]  

(5.62b)

In the limit \( h \ll r \), the curve is a compressed helix where each cycle approximates a circle with curvature \( 1/r \). In the opposite limit \( h \gg r \), the curve is a stretched helix where each cycle approximates a line with torsion \( 1/h \).

We may reconsider the case of a perturbation to a rectilinear quantum vortex: a quantum vortex supporting a small amplitude circularly-polarized plane Kelvin wave counterrotating in a sense opposite to the vorticity direction of the unperturbed
vortex line. The approach to tackling this problem is based on the Frenet-Serret formulas (5.57). In the limit of small curvature, the perturbed quantum vortex approximates a stretched helix. Hence, the local frame defined by (5.58), which we may choose to fix at \(z_1\) centered on the first quantum vortex, is

\[
\begin{align*}
\hat{t} &\equiv \frac{u'(z_1)}{|u'(z_1)|} = \hat{z} + \cdots \\
\hat{n} &\equiv \frac{u''(z_1)}{|u''(z_1)|} = -\hat{r} + \cdots \\
\hat{b} &\equiv \hat{t} \times \hat{n} = -\hat{\vartheta} + \cdots,
\end{align*}
\]

where the arc length is parametrized by \(s \approx z_1\).

The mutual interaction of the vortices causes them to bend into the filamentary shape of a rotating helix. This type of perturbation is known as a circularly polarized Kelvin wave. Equation (5.56) may be rewritten as

\[
\mathbf{u} (5.58a) = \frac{\mathcal{E}}{m \rho \kappa_o} \frac{u'}{|u'|} \times u''.
\]

In a parametrization whereby \(|u'| = 1\), (5.64) is known as the local induction approximation (LIA) pioneered by Schwarz as the basis of quantum turbulence simulations [Schwarz, 1985, Schwarz, 1988].

Since the second derivative of the radial perturbation of the quantum vortex center is

\[
\frac{\mathbf{u}}{5.60} = -k^2 \mathbf{u}_1,
\]

(5.56) takes the form of an undamped Bloch equation

\[
\frac{d\mathbf{u}_1(z_1)}{dt} (5.49) = \frac{\mathcal{E} k^2}{m \rho \kappa_o} \mathbf{u}_1(z_1) \times \hat{s}_2.
\]

The radial displacement \(\mathbf{u}_1\) behaves like the magnetization vector of a nuclear spin precessing about a background magnetic field along \(\hat{s}_2 \approx \hat{z}\). Thus, two segments of the mutually interacting quantum vortices behave like coupled nuclear spins. In
fact, from the Frenet-Serret formulation, we know that \( \dot{s}_2 \) is proportional to the first derivative \( u'_2 = \frac{d\theta_2}{dt} v_2 \), which is proportional to the velocity of the quantum vortex that, as mentioned in the discussion of the Biot-Savart law (5.44), is the analog of the magnetic field. Now

\[
\dot{s}_2 = \frac{u'_2}{|u'_2|} = \frac{dt}{d\theta_2} \frac{v_2}{|u'_2|} \approx \frac{1}{k \hbar \tilde{z}_2 k \tau_2} \frac{v_2}{u_2} \quad (5.67)
\]

\[
du_1(z_1) \quad (5.49) \quad \frac{dt}{dt} = \gamma u_1(z_1) \times v_2, \quad (5.68)
\]

where

\[
\gamma \equiv \frac{1}{m \rho \kappa_0 \hbar \tilde{r}_2 \tilde{z}_2} \quad (5.69)
\]

is the analog of the geomagnetic ratio.

The helix rotates in time as a sinusoidal perturbation \( u_1 \sim r_1 e^{\iota (kz - \omega t)} \), so (5.56) may be written as

\[
i \omega u_1(z_1) = \frac{\mathcal{E}(k)k^2}{m \rho \kappa_0} \tilde{z} \times u_1(z_1). \quad (5.70)
\]

Then writing \( u_1 = (x, y) \), we have

\[
i \omega (x, y) = \frac{\mathcal{E}(k)k^2}{m \rho \kappa_0} (-y, x), \quad (5.71)
\]

or in matrix form

\[
\begin{pmatrix}
i \omega & \frac{k^2}{m \rho \kappa_0} \\
-\frac{k^2}{m \rho \kappa_0} & i \omega
\end{pmatrix}
\begin{pmatrix}
x \\
y
\end{pmatrix}
= \begin{pmatrix}
0 \\
0
\end{pmatrix}. \quad (5.72)
\]

The solution follows by setting the determinant to zero, which yields the Kelvin wave dispersion relation

\[
\omega_k = \frac{\mathcal{E}(k)k^2}{m \rho \kappa_0} \quad (5.73a)
\]

\[
= \frac{\kappa_0 k^2}{4 \pi} \log \frac{1}{r_c k} \quad (5.73b)
\]

for \( r_c = 1/k \).
5.4 Fermi condensate dynamics

Superfluidity and superconductivity are closely related phenomena [Giorgini et al., 2008]. The connection between these phenomena is elucidated in the superfluid transition that occurs in chiral matter, such as in fermionic Helium-3 atoms below 2.5 mK. Fermi condensates have been recently realized in ultracold atoms in 2003, for example a condensate of molecular bosons made of \(^{40}\)K atom pairs. Remarkably, an exotic Fermi condensate, called quark a condensate, also occurs in high-energy chiral matter described by quantum chromodynamics.

5.4.1 BEC Lagrangian from an effective fermionic Lagrangian

The simplest effective fermionic Lagrangian density for a Dirac particle in a many-body system of identical quantum particles is taken to be

\[
\mathcal{L}_o = \hbar c \psi^\dagger \gamma^0 \left( i \gamma^\mu \partial_\mu - \frac{14}{\lambda} \right) \psi ,
\]

where \(\psi\) is a 4-spinor and where \(\lambda\) is the effective wavelength (i.e. over \(2\pi\)) of the particle (with broken chiral symmetry) due to a nonlinear interaction (that need not be specified at the moment) with the rest of the many-body system.\(^4\) The value

\[^4\text{As an example fermionic model consider one with a nonlinear 4-point interaction, the well known Nambu-Jona-Lasinio (NJL) model of the superfluid phase of a Fermi gas at low temperature [Nambu and Jona-Lasinio, 1961]}

\[
\mathcal{L} = i\hbar c \bar{\psi} \psi + \frac{\lambda}{4} \left[ (\bar{\psi}\psi)^2 - (\bar{\psi}\gamma^5\psi)^2 \right],
\]

where here \(\lambda\) is the nonlinear coupling constant (not the effective wavelength). The NJL interaction Lagrangian density is local, a four-point vertex

\[
\mathcal{L}_{\text{int}}^{\text{NJL}} = \frac{\lambda}{4} \left[ (\bar{\psi}\psi)^2 - (\bar{\psi}\gamma^5\psi)^2 \right]
\]

\[
= \lambda \left( \psi_R^\dagger \psi_R \right) \left( \psi_L^\dagger \psi_L \right)
\]

\[
= \lambda \left( \psi_{RL}^\dagger \psi_{RL} \psi_{L\overline{R}}^* \psi_{L\overline{R}} + \psi_{RL}^* \psi_{RL} \psi_{L\overline{R}}^* \psi_{L\overline{R}} \right)
\]

\[
= \lambda \sum_{bb'} \bar{\psi}_{b\overline{b}} \psi_{b\overline{b}'} \psi_{b\overline{b}'} \psi_{b\overline{b}'}.
\]
of $\lambda$ accounts for all particle-particle interactions and thus determines the effective mass of the quantum particle. In the chiral representation, the components of the Dirac matrices $\gamma^\mu = (\gamma^0, \bar{\gamma})$ are

$$\gamma^0 = \sigma_x \otimes 1 \quad \gamma^i = i\sigma_y \otimes \sigma_i. \quad (5.75)$$

In flat space the Minkowski metric tensor $\eta_{\mu\nu}$ is $\text{diag}(1, -1, -1, -1)$. Then with $\partial_\mu = (\frac{1}{c\partial_t}, \nabla)$, the Lagrangian density is

$$\mathcal{L}_\psi = \frac{\hbar c}{\lambda} \psi^4 \left( i\lambda \gamma^0 - \gamma^0 (1 - i\lambda \bar{\gamma} \cdot \nabla) \right) \bar{\psi}. \quad (5.76)$$

The anticommutation relations of the Dirac matrices, $\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}$, follows from the anticommutativity of the Pauli matrices

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}. \quad (5.77)$$

Consequently, we have

$$[-\gamma^0 (1 - i\lambda \bar{\gamma} \cdot \nabla)]^2 \quad (5.75)$$

$$= [-\sigma_x \otimes 1 - i\lambda \sigma_x \otimes \bar{\sigma} \cdot \nabla]^2 \quad (5.78a)$$

$$= [(\sigma_x \otimes 1)^2 + (i\lambda \sigma_x \otimes \bar{\sigma} \cdot \nabla)^2] \quad (5.78b)$$

$$= (\sigma_x \otimes 1)^2 \cdot [1 \otimes 1 + (\lambda \sigma_y \otimes \bar{\sigma} \cdot \nabla)^2] \quad (5.78c)$$

$$= (\sigma_x \otimes 1)^2 \cdot [1 \otimes 1 + \sigma_y^2 \otimes (\lambda \bar{\sigma} \cdot \nabla)^2] \quad (5.78d)$$

$$= (\sigma_x^2 \otimes 1) \cdot [1 \otimes 1 + 1 \otimes (\lambda \bar{\sigma} \cdot \nabla)^2] \quad (5.78e)$$

$$= \sigma_x^2 \otimes [1 + (\lambda \bar{\sigma} \cdot \nabla)^2] \quad (5.78f)$$

$$= \sigma_x^2 \otimes 1 \left(1 + \lambda^2 \nabla^2\right), \quad (5.78g)$$

since $(\bar{\sigma} \cdot \nabla)^2 = \nabla^2$. Taking the square root of both sides we have

$$-\gamma^0 (1 - i\lambda \bar{\gamma} \cdot \nabla) = \sigma_x \otimes 1 \sqrt{1 + \lambda^2 \nabla^2}, \quad (5.79)$$
where we select the positive root for consistency (as we will see below). In general, we would be free to take $-\gamma^0 (1_4 - i \lambda \gamma \cdot \nabla) = \pm \tau \otimes 1 \sqrt{1 + \lambda^2 \nabla^2}$, where $\tau$ must be a unimodular matrix, i.e. $\tau^2 = 1$. A unimodular matrix could be expressed as a linear combination of Pauli matrices $\tau = a \sigma_x + b \sigma_y + c \sigma_z$ provided $a^2 + b^2 + c^2 = 1$. Yet, in (5.79) we took the special case $a = 1$ and $b = c = 0$; so we choose $\tau = \sigma_x$. (In the vacuum state, if we do not distinguish between the left- and right-handed spinor components, then $\tau = \sigma_x$ is an appropriate choice. If we want to distinguish the left- and right-handed spinor components as time-reversed partners, then $\tau = \sigma_z$ is the appropriate choice.) Since the Dirac 4-spinor comprises a pair of chiral 2-spinors, $\psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}$, and each chiral 2-spinor in turn comprises a pair of spin-$\frac{1}{2}$ amplitudes, $\psi_{L,R} = \begin{pmatrix} \psi_{L,R}^1 \\ \psi_{L,R}^2 \end{pmatrix}$, the Lagrangian density (5.76) becomes

\[
\mathcal{L}_D \overset{(5.79)}{=} \frac{\hbar c}{\lambda} \psi^\dagger \left( i \lambda 1_4 \partial_t + \sigma_x \otimes 1 \sqrt{1 + \lambda^2 \nabla^2} \right) \psi \\
= \frac{\hbar c}{\lambda} \left( \begin{array}{cc} \psi_L^\dagger & \psi_R^\dagger \end{array} \right) \left[ i \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \partial_t + \begin{pmatrix} 0 & 1 \sqrt{1 + \lambda^2 \nabla^2} \\ 1 \sqrt{1 + \lambda^2 \nabla^2} & 0 \end{pmatrix} \right] \left( \begin{array}{c} \psi_L \\ \psi_R \end{array} \right) \\
= \hbar \sum_{s=L,R} \left[ i \psi_s^\dagger \partial_t \psi_s + \frac{c}{\lambda} \psi_s^\dagger \sqrt{1 + \lambda^2 \nabla^2} \psi_s \right],
\]

where $R \equiv L$ and $\overline{L} \equiv R$. We perform a small-parameter ($\epsilon$) expansion of the quantum field

\[
\psi = \psi^{(0)} + \psi^{(1)} + \psi^{(2)} + \cdots,
\]

where $\psi^{(0)}$ is the mean-field 4-spinor wave function, $\psi^{(1)} \sim \epsilon$ is the first-order fluctuation from the mean, $\psi^{(2)} \sim \epsilon^2$ is the second-order fluctuation, and so forth. Similarly, the effective wavelength of the quantum particle can be written as the deviation from equilibrium as follows

\[
\lambda = \lambda_0 + \delta \lambda,
\]
where the constant $\lambda_o \equiv \frac{\hbar}{mc}$ is the reduced Compton wavelength of the Dirac particle (i.e. $\lambda_o$ is set by the bare mass $m$ of the quantum particle) and $\delta \lambda$ is the deviation. In the nonrelativistic limit, diffusive ordering applies, so the time and space derivatives respectively scale as follows

$$\partial_t \psi^{(0)} \sim \varepsilon^2 \quad \nabla \psi^{(0)} \sim \varepsilon. \quad (5.83)$$

In turn, retaining only the lowest order terms of the geometric series we have

$$\frac{c}{\lambda} = \frac{c}{\lambda_o} \left( \frac{1}{1 + \frac{\delta \lambda}{\lambda_o}} \right) \quad (5.84a)$$

$$= \frac{c}{\lambda_o} \left( 1 - \frac{\delta \lambda}{\lambda_o} \frac{\delta \lambda^2}{\lambda_o^2} + \cdots \right) \quad (5.84b)$$

$$= \frac{c}{\lambda_o} \left[ 1 - \frac{\delta \lambda}{\lambda_o} \left( 1 - \frac{\delta \lambda}{\lambda_o} + \frac{\delta \lambda^2}{\lambda_o^2} + \cdots \right) \right] \quad (5.84c)$$

$$= \frac{c}{\lambda_o} \left[ 1 - \frac{\delta \lambda}{\lambda} \left( \frac{1}{1 + \frac{\delta \lambda}{\lambda_o}} \right) \right] \quad (5.84d)$$

$$= \frac{c}{\lambda_o} \left( 1 - \frac{\delta \lambda}{\lambda} \right) \quad (5.84e)$$

and furthermore retaining only the second-order fluctuations in the square root term we have

$$\sqrt{1 + \lambda^2 \nabla^2} = 1 + \frac{\lambda_o^2}{2} \nabla^2 + \cdots. \quad (5.85)$$

Hence, multiplying (5.84e) and (5.85) and keeping only the lowest order derivative term gives

$$\frac{c}{\lambda} \sqrt{1 + \lambda^2 \nabla^2} = \frac{c}{\lambda_o} \left( 1 + \frac{\lambda_o^2}{2} \nabla^2 - \frac{\delta \lambda}{\lambda} \right) + \cdots. \quad (5.86)$$

In the nonrelativistic limit, the Lagrangian density (5.80c) thus reduces to

$$\mathcal{L}_{NR} \overset{(5.86)}{=} \sum_{s=L,R} \left[ i \hbar \psi^\dagger_s \partial_t \psi_s + \frac{\hbar \lambda_o c}{2} \psi^\dagger_s \sigma_x \nabla^2 \psi_s + \frac{\hbar c}{\lambda_o} \psi^\dagger_s \left( 1 - \frac{\delta \lambda}{\lambda} \right) \sigma_x \psi_s \right], \quad (5.87)$$

At this point, one identifies the local Hartree potential as

$$V_H(\rho) = mc^2 \frac{\delta \lambda}{\lambda}, \quad (5.88)$$
whose explicit functional dependence on $\rho$ is not determined from the derivation leading up to (5.87). One alternative is to assume that the ordering of the fluctuations in the density

$$\rho = \rho^{(0)} + \rho^{(1)} + \rho^{(2)} + \cdots$$  \hspace{1cm} (5.89)

is exponential in the expansion parameter $\delta \lambda$. Thus, we can make an ansatz like the following

$$\rho = \rho_0 e^{\delta \lambda}. \hspace{1cm} (5.90)$$

Then the explicit $\rho$-dependence of the Hartree potential can be determined

$$V_h(\rho) = mc^2 \log \frac{\rho}{\rho_0} = mc^2 \frac{\rho}{\rho_0} - mc^2 + \cdots \hspace{1cm} (5.91)$$

In turn, the Lagrangian density becomes

$$\mathcal{L}_{NR}^{(5.90)} = \sum_{s=L,R} \psi_s \left[ i \hbar \sigma_\tau \partial_t + \frac{\hbar^2}{2m} \nabla^2 - mc^2 - V_h(\rho) \right] \psi_s. \hspace{1cm} (5.92)$$

Now the equation of motion for the 2-spinor field $\psi_s$ is governed by the Euler-Lagrange equation

$$\nabla \cdot \left( \frac{\partial \mathcal{L}_{NR}}{\partial (\nabla \psi_s^\dagger)} \right) - \frac{\partial \mathcal{L}_{NR}}{\partial \psi_s^\dagger} = 0, \hspace{1cm} (5.93)$$

which leads to the following equation of motion

$$-i\hbar \partial_t \psi_s - \frac{\hbar^2}{2m} \sigma_x \nabla^2 \psi_s + \hbar \Omega(\rho) \sigma_x \psi_s = 0, \hspace{1cm} (5.94)$$

for $s=L$ or $s=R$ and where we define the nonlinear potential as

$$\hbar \Omega(\rho) \equiv V_h(\rho) + \rho \frac{\partial V_h(\rho)}{\partial \rho} - mc^2. \hspace{1cm} (5.95)$$

Our current definition of $\hbar \Omega$ is identical to the earlier definition (5.12), just shifted by the rest energy. Equation (5.94) is the effective field theory of the quantum lattice-gas Q2 model in the nonrelativistic limit, which we treat in Chapter 6.
The 2-spinor field is \( \psi_s = \begin{pmatrix} \psi_{s1} \\ \psi_{s1} \end{pmatrix} \) and one may obtain a complex scalar bosonic field, \( \varphi_s \), by summing together the pair of chiral fermion modes

\[
\varphi_s \equiv \psi_{s1} + \psi_{s1}. \tag{5.96}
\]

Thus, adding together the component equations of (5.94), we have an effective equation of motion for the condensate

\[
-i\hbar \partial_t \varphi_s - \frac{\hbar^2}{2m} \nabla^2 \varphi_s + \hbar \Omega(\rho) \varphi_s = 0, \tag{5.97}
\]

which are two identical equations of motion of superfluid dynamics for \( \varphi_L \) and \( \varphi_n \). This is a spinor BEC. We have performed quantum simulations of (5.97) [Yepez et al., 2010], but hereafter we will consider one component of the spinor BEC. We can now write down the effective Lagrangian density for the single-component superfluid’s complex scalar quantum field—the nonrelativistic Lagrangian density is

\[
\mathcal{L}_{\text{BEC}} = \varphi^* \left[ i \hbar \partial_t + \frac{\hbar^2}{2m} \nabla^2 + mc^2 - V_n(\rho) \right] \varphi \tag{5.98a}
\]

\[
= i\hbar \varphi^* \partial_t \varphi - \frac{\hbar^2}{2m} (\nabla \varphi^*) \cdot \nabla \varphi + mc^2 \varphi^* \varphi - \varphi^* V_n(\rho) \varphi. \tag{5.98b}
\]

That is, we have just derived (5.10) with the chemical potential \( \mu = mc^2 \), the BEC Langrangian density that we used as our starting point in studying condensate dynamics of superfluids. The Euler-Lagrange equation is

\[
\nabla \cdot \left( \frac{\partial \mathcal{L}_{\text{BEC}}}{\partial (\nabla \varphi^*)} \right) = \frac{\partial \mathcal{L}_{\text{BEC}}}{\partial \varphi^*} = 0, \tag{5.99}
\]

and this yields the following NLS equation of motion

\[
i\hbar \partial_t \varphi = \hbar_{\text{BEC}} \varphi, \tag{5.100}
\]

where the BEC Hamiltonian is

\[
h_{\text{BEC}} = -\frac{\hbar^2}{2m} \nabla^2 + \hbar \Omega(\rho). \tag{5.101}
\]
Now with $\varphi = \sqrt{\rho} e^{iS/\hbar}$, we have
\[ \nabla \varphi = \left( \frac{1}{2} \nabla \rho + \frac{i}{\hbar} \nabla S \right) \varphi, \tag{5.102} \]
and in turn
\[ \frac{\hbar^2}{2m} |\nabla \varphi|^2 = \rho \left[ \frac{(\nabla S)^2}{2m} + \frac{\hbar^2}{8m} \frac{(\nabla \rho)^2}{\rho^2} \right], \tag{5.103a} \]
and
\[ i\hbar \varphi^* \partial_t \varphi = -\rho \partial_t S + \frac{i\hbar}{2} \partial_t \rho, \tag{5.103b} \]
where we can drop the second term on the right-hand side because it is a surface term that vanishes when we integrate to obtain the action, \textit{i.e.} $\int d^4x \frac{i\hbar}{2} \partial_t \rho = 0$.

Then inserting (5.103) into (5.98b) gives the nonrelativistic Lagrangian density in terms of the conjugate fluid variables
\[ \mathcal{L}_{\text{BEC}} = -\rho \partial_t S - \rho \left[ \frac{(\nabla S)^2}{2m} + \frac{\hbar^2}{2m} \left( \frac{\nabla \rho}{2\rho} \right)^2 \right] - \rho \left[ V_B(\rho) - mc^2 \right]. \tag{5.104} \]

So, we have derived (5.19). The quantity that plays the role of the potential energy density is $\rho V_B(\rho)$. The condensate action is
\[ S_{\text{BEC}} = \int d^4x \mathcal{L}_{\text{BEC}}; \tag{5.105} \]
and the equations of motion from varying the action $\frac{\delta S_{\text{BEC}}}{\delta \rho} = 0$ and $\frac{\delta S_{\text{BEC}}}{\delta S} = 0$ are, respectively
\[ \nabla \cdot \left( \frac{\partial \mathcal{L}_{\text{BEC}}}{\partial (\nabla \rho)} \right) - \frac{\partial \mathcal{L}_{\text{BEC}}}{\partial \rho} = 0 \tag{5.106a} \]
\[ \nabla \cdot \left( \frac{\partial \mathcal{L}_{\text{BEC}}}{\partial (\nabla S)} \right) - \frac{\partial \mathcal{L}_{\text{BEC}}}{\partial S} = 0. \tag{5.106b} \]

With $V_B = -\frac{\hbar^2}{2m} \frac{\nabla^2}{\sqrt{\rho}}$ and in the phase and number density conjugate variables, (5.106) are
\[ -\frac{\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V_B + \hbar \Omega(\rho), \tag{5.107a} \]
\[ \frac{\partial \rho}{\partial t} = \frac{1}{m} \nabla \cdot (\rho \nabla S). \tag{5.107b} \]
which are identical to Bohm’s form of the Hamiltonian equations [Bohm, 1952]; that is, (5.106) are equivalent to the Hamilton equations (5.22).

5.4.2 Fermi condensate excitations

In the condensed phase of an ultracold Fermi quantum gas, quasiparticles form and act like a gaseous system of “classical” particles riding above the condensate field. At the hydrodynamic scale, this quasiparticle gas behaves like a normal viscous fluid. The superfluid component, or condensate field, is strictly comprised of Cooper pairs (or momentum-anticorrelated pairs of Fermi particles) in the antisymmetric quantum state. At the hydrodynamic scale, the condensate behaves like a zero viscosity irrotational fluid. This is a well known microscopic explanation of what traditionally had been called the normal component in the two-fluid model of superfluidity due to Tisza and Landau in the 1930’s and 40’s (see Appendix C.1 for a review of the original hydrodynamic model of superfluidity) and that we previously discussed. Here we consider the Fermi condensate ground state and these excitations riding above ground state. In particular, we consider a pathway for transforming Cooper pairs into Bogoliubov quasiparticle modes. Cooper pairs are parallel pairwise entangled states whereas the Bogoliubov quasiparticles are perpendicular pairwise entangled states. With the toolset we have developed thus far, we can learn much about the interplay between these fundamental types of entangled states.

Fermi condensate ground state

The Cooper pair state has the parallel form $|\Psi_\parallel\rangle = \frac{1}{\sqrt{2}} (|11\rangle - e^{i\xi} |00\rangle)$ and the Bogoliubov quasiparticle state has the perpendicular form $|\Phi_\perp\rangle = \frac{1}{\sqrt{2}} (|01\rangle - e^{i\xi} |10\rangle)$. Let us write the completely empty vacuum as $|\text{vac}\rangle \equiv \bigotimes_{(\alpha\beta)} |00\rangle_{\alpha\beta}$, and a half-filled
classical (entanglement-free) configuration as \(|h-f\rangle \equiv \bigotimes_{(\alpha \beta)} |10\rangle_{\alpha \beta}\). The Fermi condensate ground state may then be analytically specified using the parallel joint ladder operators (2.42)

\[
|\Omega\rangle_{\parallel} \equiv \left( \prod_{(\alpha \beta)} a'_{\alpha} \right) |h-f\rangle. \tag{5.108}
\]

We began from the half-filled classical configuration because \(a'_{\alpha}\) is the sum of a destruction and a creation operator and thus preserves half-filling. That is, inserting half-filled configuration into (5.108), we have

\[
|\Omega\rangle_{\parallel} \overset{(2.42c)}{=} \bigotimes_{(\alpha \beta)} e^{i2\theta_{\alpha}} \left( \cos \frac{\theta_{\alpha}}{2} |00\rangle_{\alpha \beta} - ie^{-i\epsilon} \sin \frac{\theta_{\alpha}}{2} |11\rangle_{\alpha \beta} \right) \tag{5.109}
\]

The second-quantization technology of the joint ladder operators allowed us to write down the exact ground states of \(H_{\parallel}\) in a most expedient way. And to go further, let us define the complex coefficients \(u_{\alpha} \equiv e^{i\frac{\theta_{\alpha}}{2}} \cos \frac{\theta_{\alpha}}{2}\), and \(v_{\alpha} \equiv -ie^{i(\frac{\theta_{\alpha}}{2} - \xi)} \sin \frac{\theta_{\alpha}}{2}\).

Then, (5.109) may be expressed directly as a tensor product of qubit ladder operators

\[
|\Omega\rangle_{\parallel} \overset{(2.42c)}{=} \bigotimes_{(\alpha \beta)} \left( u_{\alpha} a_{\alpha} - v_{\alpha} a_{\alpha}^{\dagger} \right) |10\rangle_{\alpha \beta}. \tag{5.110}
\]

This intuitive result is our first application of the quantum informational representation to predict an analytical form for a pairwise entangled ground state.

Another route to obtain an analytical expression of the Fermi condensate ground state is to unitarily generating it through entangling gate rotations acting on the vacuum. The appropriate entangling gate is \(\sqrt{\text{PAIR}}\), as depicted on the bottom of Fig. 2.3. So, we may use (2.37b) to affect the needed rotation. Hence, the Fermi condensate ground state may be analytically specified as

\[
|\Omega\rangle_{\parallel} = \left[ \prod_{(\alpha \beta)} e^{i\theta_{\alpha} e_{\alpha \beta}} \right] |\text{vac}\rangle. \tag{5.111}
\]

Inserting the vacuum configuration into (5.111), and after algebraic manipulation,
one again recovers (5.109). Finally, we may insert the entanglement number operators (2.32b), which for $\Delta = 1$ is just (2.31b), into the representations (5.111) to obtain the Fermi condensate ground state

$$|\Omega\rangle_{\|} = \left[ \prod_{(\alpha)} e^{-\frac{1}{2} \vartheta_{\alpha} e^{-i \kappa_{\alpha} a_{\alpha}^\dagger a_{\beta}^\dagger}} \right] |\text{vac}\rangle. \quad (5.113)$$

This represents the quantum state of the superfluid component in the two-fluid model without a normal fluid component.

**Bogoliubov quasiparticle excitations from Cooper pairs**

A Cooper pair $|\Psi\rangle_{\|}$ can be readily transformed into a Bogoliubov quasiparticle $|\Phi\rangle_{\perp}$, and vice versa, as follows:

$$|\Phi\rangle_{\perp} = R |\Psi\rangle_{\|} \quad |\Psi\rangle_{\|} = R |\Phi\rangle_{\perp}, \quad (5.114)$$

where $R$ is an involution $R^2 = 1$ (both hermitian $R^\dagger = R$ and unitary $R^\dagger = R^{-1}$).

A qubit ladder operator representation of $R$ is

$$R_{\alpha} = a_{\alpha} + a_{\alpha}^\dagger, \quad (5.115)$$

which is manifestly hermitian and in turn unitary since $R_{\alpha} R_{\alpha}^\dagger = a_{\alpha} a_{\alpha}^\dagger + a_{\alpha}^\dagger a_{\alpha} = 1. \quad (5.116)$

Note that $R_{\alpha}$ acting on the ladder operators yields

$$R_{\alpha} a_{\alpha} R_{\alpha} = a_{\alpha}^\dagger, \quad R_{\alpha} a_{\alpha}^\dagger R_{\alpha} = a_{\alpha}, \quad (5.116a)$$

$$R_{\alpha} a_{\beta} R_{\alpha} = -a_{\beta}, \quad \text{and} \quad R_{\alpha} a_{\beta}^\dagger R_{\alpha} = -a_{\beta}^\dagger. \quad (5.116b)$$

---

5. This route leads one to alternatively express $|\Omega\rangle_{\|}$ directly using local products of qubit ladder operators

$$|\Omega\rangle_{\|} \equiv \left[ \prod_{(\alpha \beta)} (u_{\alpha} + v_{\alpha} a_{\alpha}^\dagger a_{\beta}) \right] |\text{vac}\rangle, \quad (5.112)$$

going from (5.110) to (5.112) by making use of the anticommutation relations for the qubit ladder operators: $a_{\beta}^\dagger |00\rangle_{\alpha \beta} = -a_{\alpha} a_{\beta}^\dagger |10\rangle = |01\rangle$ and $-a_{\beta}^\dagger |10\rangle_{\alpha \beta} = a_{\alpha}^\dagger a_{\beta}^\dagger |00\rangle = |11\rangle$. It is not obvious that the representation (5.112) of the ground state, which is commonly used in the literature, arises directly from a unitary transformation of the vacuum. Yet, we know that its does because the entangling gate specification (5.111). The product form (5.112) is well known in the theory of superconductivity [Schrieffer, 1988].

6. Its unitarity follows by the Euler identity, $e^{i \gamma R} = \cos \gamma + i R \sin \gamma$, that implies $R = -i e^{i \pi R/2}$ for $\gamma = \pi/2$. 

Similar relations hold for this similarity transformation of the joint ladder operators (2.42). Since \( R_\alpha |00\rangle_{\alpha\beta} = |10\rangle \), a product of \( R \)'s maps the vacuum into the half-filled configuration:

\[
\left[ \prod_{(\alpha\beta)} R_\alpha \right] |\text{vac}\rangle = |\text{h-f}\rangle. \tag{5.117}
\]

A similarity transformation from a perpendicular \( O_\perp \) to its parallel counterpart \( O_\parallel \) is

\[
O_\perp = R O_\parallel R \quad \text{or} \quad O_\parallel = R O_\perp R. \tag{5.118}
\]

Therefore, if all the Cooper pairs were to transition to Bogoliubov quasiparticles, the resulting fully excited state \( |\Omega\rangle_\perp \) can be determined directly from \( |\Omega\rangle_\parallel \):

\[
|\Omega\rangle_\perp = \left[ \prod_{(\alpha\beta)} R_\alpha \right] |\Omega\rangle_\parallel \tag{5.119a}
\]

\[
\overset{(5.112)}{=} \left[ \prod_{(\alpha\beta)} R_\alpha \left( u_\alpha + v_\alpha a_{\alpha\beta}^\dagger a_{\alpha\beta} \right) \right] |\text{vac}\rangle \tag{5.119b}
\]

\[
= \left[ \prod_{(\alpha\beta)} R_\alpha \left( u_\alpha + v_\alpha a_{\alpha\beta}^\dagger a_{\alpha\beta} \right) R_\alpha^2 \right] |\text{vac}\rangle \tag{5.119c}
\]

\[
= \left[ \prod_{(\alpha\beta)} R_\alpha \left( u_\alpha + v_\alpha a_{\alpha\beta}^\dagger a_{\alpha\beta} \right) R_\alpha \right] \left[ \prod_{(\alpha\beta)} R_\alpha \right] |\text{vac}\rangle \tag{5.119d}
\]

\[
\overset{(5.117)}{=} \left[ \prod_{(\alpha\beta)} R_\alpha \left( u_\alpha R_\alpha - v_\alpha a_{\alpha\beta}^\dagger R_\alpha a_{\alpha\beta}^\dagger \right) \right] |\text{h-f}\rangle \tag{5.119e}
\]

\[
\overset{(5.116)}{=} \left[ \prod_{(\alpha\beta)} \left( u_\alpha - v_\alpha a_{\alpha\beta}^\dagger \right) \right] |\text{h-f}\rangle. \tag{5.119f}
\]

This represents the quantum state of the normal fluid component in the two-fluid model without a superfluid component, as every Cooper pair has been converted into a Bogoliubov quasiparticle. A finite-temperature superfluid is partially excited, over a subset of the pairs in the system, and thus constitutes an intermediary state between (5.113) and (5.119f).
Two-qubit representation

The dynamical field of a quantum vortex (or collection of quantum vortices) acts like a vacuum background configuration and its 2-spinor field has the balanced form is the entangled quantum state

\[ |\psi_r(x)\rangle \overset{(5.112)}{=} u_s(x)|00\rangle + v_s(x)|11\rangle. \tag{5.120} \]

The Cooper pair (5.120) has the form it does because this is an eigenket of the \( \sqrt{\text{PAIR}} \) local quantum informational interaction, and we discuss in more detail in Sec. 6.3.2. Such an eigenket is a local equilibrium configuration with a pair at each point in the system. In the ground state, all the pairs (5.120) are identical. This is the BEC limit of a Fermi condensate where the Cooper pairs behave as a tightly bound Bose molecules.

The hydrodynamic condensate \( \varphi_r(x) \) may break down giving rise to a spectrum of small fluctuations, the Bogoliubov quasiparticle excitations. The Bogoliubov quasiparticle state is a locally entangled particle-hole pair excitation of the form

\[ |\psi_{q,p}(x)\rangle = u_n(x)e^{-i\omega t}|01\rangle - v_n^*(x)e^{i\omega t}|10\rangle, \tag{5.121} \]

where \( |u_n|^2 + |v_n|^2 = 1 \) is a constraint on the amplitudes. Notice that the Bogoliubov quasiparticle state (5.121) resides in the zero-quantum subspace (one-body sector) of the local Hilbert space of the two qubits at a point. (From the form of (5.120) and (5.121), you can see why a two qubit per point model is sufficient for representing both Cooper pairs and the spectrum of Bogoliubov quasiparticles in a Fermi condensate.) In spinor form, adding the quasiparticle (5.121) to the vacuum (5.120), we have

\[
\psi(x) = \begin{pmatrix}
\psi_0(x) \\
\psi_1(x) \\
\psi_{11}(x)
\end{pmatrix} = \begin{pmatrix}
u_s(x) \\
0 \\
0
\end{pmatrix} + \begin{pmatrix}
u_n(x)e^{-i\omega t} \\
-u_n^*(x)e^{i\omega t} \\
0
\end{pmatrix} = \psi_r(x) + \psi_{q,p}(x). \tag{5.122b}
\]
Since the bosonic wave function \( \varphi \) of the superfluid may be determined from the trace of the chiral 4-spinor field \( i.e. \varphi \equiv \text{Tr}(\mathbf{1}_4 \psi) \) the bosonic scalar wave function is

\[
\varphi(x) = \varphi_+(x) + \left( u_n(x)e^{-i\omega t} - u_n^*(x)e^{i\omega t} \right) + \cdots .
\]

This is the form we used in Sec. 5.2.3.

In summary, as the ground state formed of a fermionic condensate of entangled particle-particle zero-momentum pairs \( i.e. \) Cooper pairs, one is equally likely to find a pair of particles rotating clockwise and counterclockwise with respect to a chosen axis in position-space. The ground state has net zero angular momentum as well as net zero linear momentum. The condition of vanishing angular momentum follows from the fact that the entangled particle-particle state (localized in \( k \)-space) has both a spin configuration of \( \uparrow \downarrow \) and a flipped spin configuration of \( \downarrow \uparrow \). Thus, the quantum state of a Cooper pair, which must be an antisymmetrized Fermi state, may be written as

\[
\Psi_{\text{Cooper}}(r_1 \uparrow, r_2 \downarrow) = \sum_k v_k \left[ e^{ik(r_1 - r_2)} \uparrow \downarrow - e^{-ik(r_1 - r_2)} \downarrow \uparrow \right].
\]

This Fermi state is nonlocalized in position space (since the position-space representation is the Fourier transform of a zero-momentum pair in momentum-space). The form of (5.124) derives from a rather simple \( k \)-space number representation of a Cooper pair state, a parallel entangled state, \( |\Psi_{\text{Cooper}}\rangle = \frac{1}{\sqrt{2}} (|00\rangle - |11\rangle)_{k,-k} \). The Cooper pair, comprising two particles and two holes, has an expectation value of just a single particle: \( \langle \Psi_{\text{Cooper}}| n_1 + n_2 |\Psi_{\text{Cooper}}\rangle = 1 \). Thus, without violating number conservation, it can transition to a perpendicular state, \( |\Phi_{\text{Bogoliubov}}\rangle = \frac{1}{\sqrt{2}} (|10\rangle - |01\rangle)_{k,-k} \), that also has an expectation value of one particle: \( \langle \Psi_{\text{Bogoliubov}}| n_1 + n_2 |\Psi_{\text{Bogoliubov}}\rangle = 1 \).
Kelvin waves from gyrating Bogoliubov excitations

Consider a heuristic rendering of a quasiparticle (with net angular momentum) in position-space

\[ \text{rn}_1 \rightarrow \text{nr}_hl \rightarrow k \]

where the right-goer \( n_1 h_1 \) (red) and the left-goer \( h_1 n_1 \) (blue) of a Bogoliubov excitation rotate and counterrotate, respectively, about a common axis. The axis of rotation is the center of a quantum vortex with rotation frequency \( \Omega \) and particle gyration frequencies \(-\omega\) (red) and \(+\omega\) (blue) for \( \omega \gg \Omega \) and with the particle gyration radius greater than the vortex core size \( \xi \). If we consider the same parameters as (5.125a), but with a much slower longitudinal velocity down the axis of the quantum vortex, then an emergent Kelvin wave structure becomes evident:

\[ \text{hn}_1 \rightarrow \text{nr}_hl \rightarrow k \]
CHAPTER 6

Quantum lattice gas

representation of condensates

6.1 Introduction

The first cold atomic vapor BEC was realized by Cornell and Wieman at NIST [Anderson et al., 1995] and Ketterle at MIT [Davis et al., 1995, Mewes et al., 1996]. BEC’s are a great help in getting to the bottom of the issue regarding quantum vortex dynamics leading to quantum turbulence, and vice versa the observation of vortices in a condensate also helps the experimentalist establish the fact the BEC state was indeed created in their particular setup. The first cold atomic vapor BEC was a rubidium $^{87}$Rb gas cooled to 170 nK, and it has no normal component at all. It comprised a macroscopic number of integer spin particles in effectively a zero temperature ground state. A whole class of BECs have been realized with ultracold dilute atomic vapors (e.g. alkali-metal gases $^{87}$Rb, $^7$Li, $^{23}$Na) with low critical temperatures in the range of 0.1–1 mK.

Rarefied atom vapors (dilute alkali gas) are laser-cooled in a magneto-optical
particle traps and trapped in optical lattices (with typically $10^6$ to $10^7$ atoms of $^{87}\text{Rb}$, $^7\text{Li}$, or $^{23}\text{Na}$ atoms). These cold atomic systems are called quantum gases. Non-trapped BECs are a pure realization of an inviscid superfluid. When the cold atoms are confined to spatial nodes of an optical three-dimensional lattice as depicted in Fig. 6.1, these atomic quantum gases become quantum lattice gases. In the way of further conceptual simplification, we may consider a quantum lattice gas comprised of bits on a lattice that hop between points and that interact quantum mechanically. Atoms placed in an optical lattice, or the minimal equivalent of bits placed in a qubit lattice, may used for quantum simulation of strongly correlated condensed matter systems. This scheme constitutes a practical program of analog quantum computation for physical modeling [Yepez, 2002a].

FIG. 6.1: Optical lattices: (a) Two- and (b) three-dimensional optical lattice potentials formed by superimposing two or three orthogonal standing waves. [Taken from [Bloch et al., 2008].]

1Magnetically trapped alkali vapors are effectively confined in an external parabolic potential, for example of the asymmetric form $V(x) = k r^2$, where $r = \sqrt{\gamma_x x^2 + \gamma_y y^2 + \gamma_z z^2}$, where the gamma coefficients are not necessarily equal.
The Gross-Pitaevskii (GP) equation [Gross, 1963, Pitaevskii, 1961] is an effective model for Bose condensate dynamics in the low temperature limit and also for a Fermi condensate so long as the pairs are tightly bound as discussed in Chapter 5. So it models the low-temperature dynamics of many types of superfluids, including the Helium II phase of $^4$He below about 100 mK, dilute cold atomic vapor BECs, quark-matter condensates in neutron stars [Gusakov, 2007, Lindblom and Mendell, 2000, Andersson et al., 2002, Yoshida and Lee, 2003, Comer et al., 1999, Lin et al., 2008], ultracold Fermi gases [Regal et al., 2004, Giorgini et al., 2008], and the Q2 quantum lattice gas [Yepez et al., 2009b, Vahala et al., 2008, Yepez et al., 2009a] [Yepez et al., 2009c]. The GP equation that we derived in Sec. 5.2.2 is

$$i\hbar \partial_t \varphi = -\frac{\hbar^2}{2m} \nabla^2 \varphi + (g|\varphi|^2 - \mu) \varphi,$$

(6.1)

where $g$ is the real-valued coupling strength of the nonlinear interaction and $\mu$ is the chemical potential.

Rotating cold atom BECs form a vortex lattice analogous to that occurring in rotating $^4$He and flux-line lattices in type-II superconductors. All the rotation is pinned to topological defects in the phase of the condensate wave function. Ultracold atom BECs are useful for exploring the dynamics of mutually interacting quantum vortices, for example as shown in Fig. 6.2 for sodium condensates in a magnetic trap.

Quantum turbulence occurs in liquid Helium II and should occur in Bose-Einstein condensates (BEC) of cold atomic vapors. Remarkably, dissipation of quantum turbulence in the zero temperature limit has been recently observed in Helium II at temperatures as low as 0.08K [Walmsley et al., 2007]. It is important to compare such quantum turbulent flows to classical fluid turbulence to help us solve one of the grand challenge problems of the millennium [Barenghi, 2008]. In this regard, there is a broadly acknowledged need for high resolution quantum turbulence
FIG. 6.2: Vortex nucleation for violent stirring in an atomic BEC. The upper row shows expansion images of sodium condensates after 500 ms of stirring at the quadrupole frequency, for different laser powers of the stirring beam. The lower row shows the resulting BEC after 300 ms of equilibration time. The condensate had to be severely excited to generate many vortices. From left to right, the laser power was increased for each subsequent image by a factor of two. [Taken from [Ketterle et al., 2008].]

Fundamental to superfluid turbulence is the quantum vortex: a topological singularity with the superfluid density exactly zero at the vortex core in the simplest case [Donnelly, 1991]. Furthermore, in the simplest case, all the quantum vortices are discrete, have the same charge (i.e. quantized circulation in multiples of $\pm 2\pi$), and the flow is inviscid. This stands in sharp contrast to classical incompressible fluid turbulence where the concept of a vortex tube or eddy is imprecise and where viscosity plays an essential role. In classical turbulence there are two strongly competing effects: sweeping of small scale eddies (advection) by large scale eddies and straining of eddies (deformation) by eddies of similar scales. Building on Richardson’s local cascade of energy from large to smaller and smaller eddies till viscosity dissipates the smallest ones into heat [Richardson, 1926], Kolmogorov [Kolmogorov, 1941] assumed an inertial energy spectrum that depends only on the energy input and wave number. Assuming the energy transfer and the interacting
scales are purely local and sweeping is not important for energy transfer, he derived
the inertial energy spectrum for classical incompressible turbulence:

\[ E(k) = C_K \mathcal{E}^{3/2} k^{-5/3}, \]  

(6.2)

for some constant \( C_K \) where \( \mathcal{E} \) is the energy dissipation and \( k \) is the wave number magnitude.

As discussed in our theoretical treatment of superfluidity in Chapter 5, quantum
turbulence is envisaged to arise from dense quantum vortex tangles [Feynman, 1955]
and this is borne out by numerical simulation too. The coherence length \( \xi \) defines
the inner radius of a quantum vortex core while \( \pi \xi \) approximates its outer radius.
Since the flow outside a quantum vortex core is simple potential flow, it is thought
that for large scales \( \gg \pi \xi \) (and scales much greater than the average separation
distance between the vortex filaments) the discrete nature of the quantum vortices
is lost and the superfluid density is approximately constant while supporting phonon
radiation. Large eddies can form as aggregated quantum vortices, concomitant with
sweeping and straining (the latter important to incompressible classical turbulence),
so large scale quantum turbulence could resemble a Kolmogorov energy cascade
\( E(k) \approx k^{-5/3} \), for \( k \ll (\pi \xi)^{-1} \). The dissipation wave number \( k_{\text{diss}} = \mathcal{E}^{1/4} \nu^{-3/4} \) cuts off
the Kolmogorov energy cascade in classical turbulence—in quantum turbulence one
expects that \( k_{\text{diss}} \sim (\pi \xi)^{-1} \).

For length scales on the order of the coherence length one needs to consider the
effects of vortex reconnection—a reconnection that occurs in superfluids without
the need for viscous dissipation, unlike classical vortex tube reconnection. During
the quantum vortex-vortex reconnection/collision and vortex self-interaction, the
vortex lines are sharply distorted, supporting large amplitude Kelvin waves (large
relative to the wavelength). The Kelvin wave modes couple to generate Kelvin
waves of smaller and still smaller wavelength, emitting phonon radiation in the pro-
This Kelvin wave energy cascade continues until one reaches the shortest operable scale, *e.g.* a $k$-space cutoff on the order of half the inverse the mean-free path length in Helium II or ultracold quantum gases or the grid scale in simulations. For the $k$-dependence of the Kelvin wave cascade in quantum turbulence, one anticipates a power-law in the incompressible kinetic energy spectrum: $E(k) \approx k^{-\alpha}$, for $k \gg \xi^{-1}$ where the exponent is here determined to be $\alpha = 3.00$. There has been considerable effort to devise theories and methods [Barenghi, 2008, Kozik and Svistunov, 2004, Svistunov, 1995, Boffetta et al., 2008, L'vov et al., 2007, Kozik and Svistunov, 2008] to predict this exponent's value as well as to predict the incompressible kinetic energy spectrum in the transition region $(\pi \xi)^{-1} \lesssim k \lesssim \xi^{-1}$ between the Kolmogorov and the Kelvin wave cascade spectra. The simplest explanation that $\alpha = 3$ derives from the Fourier transform of a linear quantum vortex [Nore et al., 1997a].

Regarding the $k^{-5/3}$ part of the incompressible spectrum, GP equation starting with a Taylor-Green (TG) profile [Nore et al., 1997b] leads to (or approaches) a Richardson-Kolmogorov cascade, as does the filament-model with TG [Araki et al., 2002]. We find clean Kolmogorov-scaling in this very large grid limit ($\sim 5760^3$).\footnote{In this limit, one might that the inter-vortex spacing becomes large and most of the quantum fluid's density is constant, $|\phi|^2 \approx \rho_0$.} Thus, for sufficiently large simulations, the quantum flow in the bulk can resemble an incompressible fluid. From small to large grids, the tangles transition from dense and dilute. In the dense tangle limit, quantum turbulence is different than classical Kolmogorov turbulence. Yet, for large grids $\sim 5760^3$ (dilute tangle "classical" limit), one observes a very clean $k^{-5/3}$ line for small-$k$. Also, one finds a strong contribution in the large-$k$ compressible spectrum, due to the presence of Bogoliubov-level fluctuations within the vortex cores.
6.2 Numerical modeling approaches

Quantum turbulent studies using computational physics methods are being pursued vigorously, not only for their intrinsic importance for understanding superflows but also in the hope of shedding light on classical turbulence. There have been various attempts to begin with the NLS equation to model a BEC. For example, Leadbeater and Barenghi et al. have used a semi-implicit Crank-Nicholson algorithm to numerically predict dynamical solutions to the dimensionless GP equation to model the collision of vortex rings and the consequent emission of sound [Leadbeater et al., 2001]. Kasamatsu and Tsubota use a finite difference alternating direction implicit method [Kasamatsu et al., 2003] to numerical solve a modified GP equation

\[
(i - \gamma) \frac{\partial \varphi}{\partial t} = (-\nabla^2 + \hat{V}_{\text{ext}} + g|\varphi|^2 - \mu - \Omega\hat{L}_z)\varphi
\]  

(6.3)

where \( \hat{L}_z = -i(x\partial_y - y\partial_x) \) is the angular momentum operator and \( \Omega \) is the frequency of the frame rotating about the \( z \) axis. (6.3) has an ad hoc phenomenological dissipation term \( \gamma \) multiplying the time derivative and an orbital angular momentum term to model a turbulent BEC in a cigar shaped trap [Kasamatsu et al., 2005]. The method resolved emergent vortex lattice crystals (about 10 cores) in a rotating condensate. Yet, heretofore, the three known numerical methods that have been able to achieve (or approach) quantum turbulence are the vortex-filament method, the Fourier spectral decomposition method, and the advective real Ginzburg-Landau equation method. Numerical predictions of the incompressible spectral kinetic energy obtained by these three methods are briefly reviewed.

6.2.1 Vortex-filament method

Schwarz proposed a vortex-filament method [Schwarz, 1985, Schwarz, 1988], which is commonly used in numerical studies of superfluids and which accounts
for mutual friction. The method conserves vortex length but not energy, and it is an approximation of the Biot-Savart law for the vorticity field, with additional model reduction by the localized induction approximation (LIA) in the dilute-vortex limit given by (5.64). The velocity field of the superfluid $v(r, t)$ is

$$v(r, t) = \frac{\kappa}{4\pi} \int_C \frac{ds' \times (s' - r)}{|s' - r|^3}$$

(6.4)

where $C$ is a curve associated with the center of a quantum vortex in parametric form $s = s(\xi, t)$ and $s'$ is a point on the curve as shown in Fig. 6.3. In the vortex-filament model, one neglects the flow structure within the quantum vortex core. An example of this is the work by Barengki et al., who made an early numerical attempt to understand the Kelvin cascade with the Biot-Savart law (6.4), with large Kelvin waves coupling to smaller ones [Kivotides et al., 2001], as shown in Fig. 6.4. The numerically predicted velocity spectra from an extremely coarse grid of $64^3$ point is shown in Fig. 6.5.

Tsunehiko and Tsubota et al. used the vortex-filament method with Taylor-Green flow to capture the Kolmogorov scaling [Araki et al., 2002]. The time evolution of the Taylor-Green flow is shown in Fig. 6.6. These types of attempts to model superfluid turbulence without any quantum flow structure within the core have in
FIG. 6.4: Vortex configurations at different times. [Taken from [Kivotides et al., 2001].]

FIG. 6.5: Velocity spectra before and after the reconnections. [Taken from [Kivotides et al., 2001].]
FIG. 6.6: Time evolution of the vortex tangle at $t=0$ sec (a), $t=30.0$ sec (b), $t=50.0$ sec (c), and $t=70.0$ sec (d). [Taken from [Araki et al., 2002].]

FIG. 6.7: The energy spectra of the tangle at $t=0$ sec (dashed line), $t=30.0$ sec (dot-dashed line), $t=50.0$ sec (long-dashed line), and $t=70.0$ sec (solid line). [Taken from [Araki et al., 2002].]
the past relied on ad hoc mechanism for the filamentary reconnections. So, the main limitation of the Biot-Savart method (a Lagrangian representation of the superflow based on the motion of line vortices as opposed to an Eulerian representation based on a time-dependente condensate field governed by the GP and BdG equation set) is not that one cannot resolve the vortex core but that the vortex-vortex interactions are not correctly captured.

6.2.2 Fourier spectral decomposition method

Kobayashi and Tsubota have used a Fourier spectral decomposition method to explore the Kolmogorov spectrum of superfluid turbulence. They solve the Fourier transformed GP equation

\[ [i - \gamma(k)] \frac{\partial \tilde{\varphi}(k, t)}{\partial t} = (k^2 - \mu) \tilde{\varphi}(k, t) \]

\[ + \frac{g}{V^2} \sum_{k_1, k_2} \tilde{\varphi}(k_1, t) \tilde{\varphi}^*(k_2, t) \tilde{\varphi}(k - k_1 + k_2, t), \]

where \( V \) is the system volume and \( \tilde{\varphi}(k, t) \) is the spatial Fourier component of \( \varphi(x, t) \) with wave number \( k \), obtained with a fast Fourier transform, and where \( \gamma(k) \) is an ad hoc dissipation factor that is applied for small scales \( \leq \xi \) [Kobayashi and Tsubota, 2006]. The numerical time evolution is achieved by the Runge-Kutta-Verner method. Their energy spectrum result is shown in Fig. 6.8. They observe Kolmogorov \( k^{-5/3} \) scaling, but had to add an ad hoc dissipation term acting on scales smaller than the healing length [Kobayashi and Tsubota, 2005]. They introduced a wave number dependent dissipative term into their simulations to damp out wave numbers on the order of the vortex core. While this suppresses the Kelvin wave cascade on the quantum turbulence, it also leads to a time decay in both the total number and total energy \( E_{\text{TOT}} \). To circumvent the decay in the total number, they add a time-varying chemical potential in the GP equation although the total energy still decays. Most of
their simulations were restricted to a $512^3$ grid and did not yield a convincing incompressible kinetic energy spectrum of $k^{-\frac{5}{3}}$ for this augmented GP equation. This approach did not resolve the classical-quantum transition nor could it capture the quantum Kelvin wave cascade.

### 6.2.3 Advective real Ginzburg-Landau equation method

Nore, Abid, and Brachet used an advective real Ginzburg-Landau equation which revealed in a numerical simulation for the first time that superflow has an inertial range due to vortex reconnections [Nore et al., 1997b] as well as an NLS equation model. Time-stepping in the method is first-order accurate in ARGLE and second-order accurate in NLS equation using a Strang-type splitting. Nore uses a pseudospectral code to integrate ARGLE and NLS equation [Nore et al., 1997a], which slows down on large grids. They show how to construct a vortex array whose NLS equation dynamics mimics Taylor-Green flow with minimal emission of acoustic waves. Then they integrate to convergence the GP equation with the appropriate
adveative flow terms added

\[
\partial_t \varphi = \frac{c}{\sqrt{2\xi}} \left( \varphi - |\varphi|^2 \varphi + \xi^2 \nabla^2 \varphi \right) - i v^{\text{TG}} \cdot \nabla \varphi - \left[ \frac{(v^{\text{TG}})^2}{2\sqrt{2\xi}} \right] \varphi,
\]

and this is equivalent to minimizing the Ginzburg-Landau functional

\[
\mathcal{F} = \frac{c}{\sqrt{2\xi}} \int d^3 x \left[ - |\varphi|^2 + \frac{1}{2} |\varphi|^4 \right. \\
+ \xi^2 \left| \nabla \varphi - i \frac{v^{\text{TG}}}{\sqrt{2\xi}} \varphi \right|^2.
\]

The normalized macroscopic flow field \( \frac{v^{\text{TG}}}{\sqrt{2\xi}} \) is treated like a local gauge field that adds to the BEC momentum field. Their result for the incompressible part of the kinetic energy spectrum is shown in Fig. 6.9.

### 6.2.4 Quantum lattice gas method

We use a quantum lattice-gas model to model a superfluid. This approach represents a dynamical fermionic field on an ordered array of qubits, arranged on a cubical lattice with two qubits per lattice point. The system of quantum particles can be treated in the type-II quantum computing limit, which is appropriate to a BEC as all the pairs of quantum particles are condensed into the same state and the condensate field is factored over the points of the system. The basic quantum field that we consider is that of a chiral massive fermion, a 2-spinor. A complex scalar bose field is formed by summing together the 2-spinor fermi components. A phase rotation of the spinor components acts as a self-steering mechanism to represent the nonlinear interaction in the GP equation low-temperature approximation of a BEC. The Q2 quantum lattice gas model is a prime example of type-II quantum computation [Yepez, 2001c]. This mechanism gives rise to superfluid behavior at the large scale arising from a nonlinear \( \varphi^4 \) interaction. We observe that the Q2 quantum lattice gas is in the same universality class as a physical quantum gas superfluid.
FIG. 6.9: Plot of the incompressible kinetic energy spectrum, $E_{\text{kin}}^L(k)$. The bottom curve (a) (circles) corresponds to time $t = 0$ (Taylor-Green initial condition). The spectrum of a single axisymmetric 2D vortex multiplied by $(l/2\pi) = 175$ is shown as the bottom solid line. The top curve (b) (plusses) corresponds to time $t = 5.5$. A least-square fit over the interval $2 \geq k \geq 16$ with power law $E_{\text{kin}}^L(k) = Ak^{-n}$ gives $n = 1.70$ (top solid line). [Taken from [Nore et al., 1997b].]
With the quantum lattice gas method, previously we have predicted solutions to a number of nonlinear classical and quantum systems. These nonlinear quantum lattice gas systems have emergent nonlinear effective equations of motion governing dynamical behavior of the low energy and low momentum modes that correspond to naturally occurring quantum system. Satisfying the dual purposes of computational physics and quantum computation, these quantum lattice gas models, being strictly unitary, have proven useful for numerically predicting the time-dependent solutions of a wide class of effective nonlinear quantum wave equations that are various forms of the nonlinear Schroedinger (NLS) equation, including the Korteweg-de Vries equation [Vahala et al., 2003a], vector solitons, e.g. Manakov equations for optical solitons [Vahala et al., 2004], bright solitons [Yepez et al., 2005a], and dark solitons governed by the GP equation in 3+1 dimensions [Yepez et al., 2009b, Yepez et al., 2009a, Yepez et al., 2009c].

Quantum informational dynamics models, such as the Q2 quantum lattice gas presented here, are rather fundamental models of quantum particle dynamics. The nonlinear Q2 model can be taken as an ab initio model of a superfluid, as fundamental as the Bose-Hubbard model and the Fermi condensate superfluid limit of the BCS model for example. There are a number of advantages of the Q2 model over the standard computational physics GP solvers and Biot-Savart law models. The GP equation is merely a mean-field approximation of a quantum gas in its BEC phase, in the long-wavelength and low-temperature limits. The Q2 quantum lattice gas represents more than this as it models a quantum gas of fermions by using a qubit field to store the state information, including particle-particle correlations. Thus the Q2 quantum lattice gas captures particle entanglement, including excitations such as Bogoliubov quasiparticles, and captures the fundamental Cooper pairing not explicitly treated in the GP equation. Furthermore, the spacetime resolution of the Q2 quantum lattice gas is so high that it can capture particularly well the rich
condensed matter dynamics occurring within the three-dimensional quantum vortex core, all the high-\(k\) Kelvin wave dynamics, and consequent nonlinear vortex-vortex interactions that drive quantum turbulence.

In contrast, the Biot-Savart law vortex-filament modeling approach treats the entire vortex soliton structure as a single topological line defect. This is a rather coarse approximation since microscopically the vortex soliton is not a one-dimensional object at all. It has a very dynamically active core structure comprising a great deal of three-dimensional flow structure over the entire short wavelength range, including distances shorter than the healing length.\(^3\) In summary, actual quantum gases in the BEC phase support vortex solitons with core structure and crucial high-\(k\) dynamics and particle-particle correlations not modeled by the GP equation or Biot-Savart solvers. The unitary Q2 quantum lattice gas conserve energy exactly and faithfully captures all the high-\(k\) core dynamics and core structure, including quantum mechanical particle-particle interaction-level crossings. Its additional advantages include the following:

1. The collide operators based on two-qubit entangling gates, \(\sqrt{\text{PAIR}}\) and \(\sqrt{\text{SWAP}}\), the stream operator based on the \(\text{SWAP}\) gate, and condensate phase rotation based on one-qubit gates give rise to an algorithmically local and time-explicit representation [Yepez, 1996c, Yepez, 1996b] that approaches pseudo-spectral accuracy [Yepez and Boghosian, 2002] without the need for spectral decomposition. The quantum lattice gas representation approaches 3rd-order accuracy [Yepez, 2007].

2. Divergences typical in quantum field theories do not occur in quantum information dynamics models because the lattice provides an ultraviolet cut-off, removing high \(k\)-modes, as well as an infrared cut-off from the finite amount of information.

\(^3\)High large-\(k\) resolution is vital to capture quantum kelvons inside the vortex cores—such kelvons are known experimentally [Bretin et al., 2003]. The behavior of these quantum kelvons have been verified numerically at the Bogoliubov de Genes (BdG) level [Mizushima et al., 2003, Simula et al., 2008]. Remarkably, the cutoff \(r_c < \xi\) is inside the core and a modified Kelvin wave dispersion relation gives a corrected angular frequency [Simula et al., 2008].
(i.e. countable number of point and periodicity). The unitary quantum logic gate representation ensures the conservation of the finite information content and thus blocks divergences.

3. The low-energy effective field theory of the Q2 model, which yields the GP equation and the BdG equations, is rather easy to derive analytically. The GP equation is a rather good bench mark representation at lowest order.

4. Numerical performance of quantum lattice gas codes scales linearly with the number of processor elements, so such codes are ideally suited to massive parallelism and outperform Fourier decomposition methods on large supercomputers.

5. Quantum information dynamics models are expressed with a local and regular pattern of quantum logic gates, and are thus readily available to run on future quantum computers and can fully exploit the exponential complexity class of quantum computers. Ultracold quantum gas simulations in optical lattices represent the first realization of the quantum lattice gas model of quantum computation—presently at the state-of-the-art of quantum computation by analogs.

6.3 Q2 model

Regarding early lattice-based algorithms, the first unitary algorithm known for approximating a scalar wave function on a computer is provided by the Cayley form of the evolution operator for the Schroedinger equation [Goldberg et al., 1967]. Ultimately, we shall be concerned with using unitary algorithms to model nonlinear dynamical systems, including those with dissipation, that are efficient quantum algorithms for computational physics with high-order numerical convergence (e.g. so they can be used to model turbulence). To explain the Q2 model, we will follow the historical development of the quantum algorithm and begin with the simplest quantum lattice gas algorithm in 3+1 dimensions. In Sec. 6.3.1 we present the
original formulation, which has the merit of being quite simple but the drawback of only first-order accuracy. A revised treatment of this quantum algorithm increases the numerical accuracy to second-order and also uses a qubit representation that accommodates many-body simulations [Yepez, 2007, Yepez and Boghosian, 2002]. Next, in Sec. 6.3.2, we revisit this quantum algorithm and present the version of the algorithm used in the 3+1 dimensional GP equation simulations presented herein.

6.3.1 Lattice gas representation of the Schroedinger equation

Here we review the quantum lattice gas algorithm for the free Schroedinger equation in 3+1 dimensions. Our aim is to explain the framework for deriving an effective equation of motion starting from a given unitary evolution that is separated into a product of two fundamental operations: (1) streaming that represents the kinetic motion of the quantum particle and (2) collisions that represent local scattering events (or reversal of motion) that imparts mass to the quantum particle. We begin with a spinor representation of the quantum field over a discrete spacetime. We will postpone, until Sec. 6.3.2, a discussion of the qubit representation of the quantum field. The quantum algorithm presented here has error terms in the effective equation of motion that occur at $O(\varepsilon)$—it is a first-order accurate representation. This is not too practical for quantum simulation purposes because to reduce the numerical error by a factor of two one must likewise decrease the grid size by a factor of two. On a cubical grid this increases the number of points by $2^3$, which is a large (nearly an order of magnitude) increase in computational burden. Yet, our aim is to derive the effective equation of motion in 3+1 dimensions in the simplest way possible, so we also postpone our review of a second order accurate representation until 6.3.2. This representation allows us to model the non-
linear Schroedinger equation. The following presentation in this section originally appeared in Ref. [Yepez, 1996b, Yepez, 1996c] for the 1+1 dimensional case and the streaming operator used here for the 3+1 dimensional case originally appeared in Ref. [Yepez, 2003].

Complex amplitudes denoted by $\psi_s$, for $s = L, R$ and $\zeta = \uparrow, \downarrow$, reside at each site of the lattice, where the position of the lattice site is specified by the vector $x_i$, for $i = 1, 2, 3$. At each spacetime point $x = (t, \mathbf{x})$, a 4-spinor denoted $\Psi$ has these amplitudes as its components

$$\Psi(x) = \begin{pmatrix} \psi_{L1}(x) \\ \psi_{L\uparrow}(x) \\ \psi_{R1}(x) \\ \psi_{R\downarrow}(x) \end{pmatrix}. \quad (6.8)$$

To describe the dynamics, let us begin with the streaming operators, which is related to the Lorentz group boosts, and these directly act on the chirality-spin degrees of freedom in (6.8). The generators (for boosts) are

$$\kappa_i = \sigma_3 \otimes \sigma_i, \quad (6.9)$$

where $\sigma_i$ are the Pauli matrices, again for $i = 1, 2, 3$. The stream operators expressed in unitary exponential form are

$$T_3^3(\zeta) = e^{i\kappa_3} = 1^{\otimes 2} + i \sin(\zeta) \kappa_i + (\cos(\zeta) - 1) \kappa_i^2. \quad (6.10)$$

These stream operators preserve chirality. Note that the third generator of (6.9) is diagonal

$$\kappa_3 = \sigma_3 \otimes \sigma_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad (6.11)$$

so as a matter of algorithmic practicality, we implement all the stream operators strictly using (6.11). That is, the quantum algorithm for streaming along the $\mathbf{x}$ and
\( y \) directions is specified by

\[
\begin{align*}
\Upsilon_1^y(\zeta) &= e^{-i\frac{\pi}{4}\sigma_y} \cdot \Upsilon_3^y(\zeta) \cdot e^{i\frac{\pi}{4}\sigma_y} \\
\Upsilon_2^y(\zeta) &= e^{i\frac{\pi}{4}\sigma_x} \cdot \Upsilon_3^y(\zeta) \cdot e^{-i\frac{\pi}{4}\sigma_x}.
\end{align*}
\tag{6.12, 6.13}
\]

With \( p = -i\hbar \nabla \), the basic (quantum lattice gas) stream operator acting on the 4-spinor gives

\[
\Upsilon_3^y(\delta x \cdot p/h) \Psi(x) = \begin{pmatrix}
e^{+\delta x \cdot \nabla} \psi_{L1}(x) \\
e^{-\delta x \cdot \nabla} \psi_{L1}(x) \\
e^{-\delta x \cdot \nabla} \psi_{R1}(x) \\
e^{+\delta x \cdot \nabla} \psi_{R1}(x)
\end{pmatrix},
\tag{6.14}
\]

amounting to a shift of the amplitudes for the 4-spinor components. This is equivalent to a simple permutation between the points of the space (a unitary operation) of the amplitudes

\[
\text{Eq. (6.14)} \quad \rightarrow \quad S_{\delta x} \Psi(x) = \begin{pmatrix}
\psi_{L1}(x + \delta x, t) \\
\psi_{L1}(x - \delta x, t) \\
\psi_{R1}(x - \delta x, t) \\
\psi_{R1}(x + \delta x, t)
\end{pmatrix}.
\tag{6.15}
\]

Furthermore, in any quantum computational implementation, the shift permutations (6.15) are represented in terms of an ordered sequence of qubit-qubit interchange gates [Yepez, 2001a]. Streaming of all the 4-spinor amplitudes along the \( x, y, \) and \( z \) directions on a cubical lattice is represented by the composite operator

\[
S = \bigotimes_x \left[ e^{-i\frac{\pi}{4}\sigma_y} \cdot \Upsilon_3^y(\delta x p_x/h) \cdot e^{i\frac{\pi}{4}(\sigma_y + \sigma_x)} \cdot \Upsilon_3^y(\delta y p_y/h) \cdot e^{-i\frac{\pi}{4}\sigma_x} \cdot \Upsilon_3^y(\delta z p_z/h) \right],
\tag{6.16}
\]

where the grid sizes are a fixed length, \( \delta x = \delta y = \delta z = \varepsilon \ell \). Streaming represents the high-energy chiral motion [Yepez, 2003, Yepez, 2005, Yepez, 2007] by the following map:

\[
\Psi' = S \Psi = e^{i\varepsilon \sigma_3 \cdot \sigma \cdot \nabla} \Psi \rightarrow \Psi.
\tag{6.17}
\]

Alternatively, the stream equation (6.17) can be written exactly as a grid-level difference equation

\[
\Psi(x + \varepsilon \ell \sigma_3 \otimes \sigma, t + \varepsilon \tau) = \Psi(x, t).
\tag{6.18}
\]
In the low-energy scaling limit, obtained by Taylor expanding the spinor field in space and time under convective ordering, this in turn leads to the effective dynamical equation of motion

$$\partial_t \Psi(x) = \frac{\ell}{\tau} \sigma_3 \otimes \sigma \cdot \nabla \Psi(x) + \cdots,$$  

(6.19)

which is just the relativistically covariant Weyl equation for a 4-spinor

$$i\gamma^\mu \partial_\mu \Psi = 0,$$  

(6.20)

written in the chiral representation where the Dirac matrices are $\gamma^0 = \sigma_1 \otimes 1$ and $\gamma^i = i\sigma_2 \otimes \sigma_i$, and where the unit speed of transport is $c \equiv \ell/\tau = 1$.

Next, let us consider the unitary operator

$$U = e^{-i h_{\text{gas}} \Delta t / \hbar},$$  

(6.21)

where $h_{\text{gas}} = \hbar \omega N$, and where $N$ is an idempotent hermitian operator $N^2 = N$ that is dimensionless and represented by a $2 \times 2$ hermitian matrix. Thus, we can write

$$U = \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{-i h_{\text{gas}} \Delta t}{\hbar} \right)^n = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} (-i \omega \Delta t)^n N = 1 + J,$$  

(6.22)

where $J \equiv (e^{-i \omega \Delta t} - 1) N$ and where $1$ is the $2 \times 2$ identity matrix. (In a quantum gate representation of (6.22), the gate angle is $\omega \Delta t$.) We employ a unitary collision operator $C \equiv U \otimes 1$ to locally scatter the incoming 4-spinor $\Psi(x)$ to an outgoing 4-spinor $\Psi'(x)$:

$$\Psi'(x) = C \Psi(x).$$  

(6.23)

$C$ breaks chirality and imparts mass to the Weyl particle represented by the stream operator.

The quantum algorithm we consider is the combination of (6.17) and (6.23)

$$\Psi' = S C \Psi \mapsto \Psi,$$  

(6.24)
which can be written exactly as the following grid-level transport equation:

\[
\psi(x + \tau \mathbf{\sigma} \otimes \mathbf{\sigma}, t + \tau^2 \mathbf{\nabla}) = \psi(x, t) + \mathbf{J} \otimes \mathbf{1} \psi(x, t),
\]

(6.25)

and this is an exact expression of the quantum algorithm. Equation (6.25) is referred to as a **quantum lattice gas equation of motion**. The collide and stream based evolution (6.24) constitutes the simplest quantum lattice gas algorithm to model a free massive quantum particle in position-space in the long wavelength limit.

Taylor expanding the left-hand side of (6.25) in space gives the associated local difference equation in time, to second order in \( \tau \),

\[
J \otimes \mathbf{1} \psi(x, t) = \psi(x, t) + \psi(x, t + \tau^2 \mathbf{\nabla}) - (\mathbf{\epsilon} \mathbf{\sigma} \otimes \mathbf{\sigma} \cdot \mathbf{\nabla} + \frac{1}{2} \mathbf{\epsilon} \mathbf{\sigma} \otimes \mathbf{\sigma} \cdot \mathbf{\nabla}^2) \psi(x, t) + \cdot \cdot \cdot .
\]

Let us perform a perturbative expansion of the 4-spinor in the small dimensionless parameter \( \epsilon \) as follows:

\[
\psi = \psi^{(0)} + \psi^{(1)} + \psi^{(2)} + \cdot \cdot \cdot ,
\]

(6.27)

where \( |\psi^{(1)}| \sim \epsilon \), \( |\psi^{(2)}| \sim \epsilon^2 \), and so forth. Inserting this into (6.26) and equating terms of similar order in \( \epsilon \) gives the following zeroth, first, and second order

---

4We are using diffusive ordering where \( \delta t \sim \delta x^2 \sim \epsilon^2 \).

5Equation (6.25) was written in a form akin to the lattice Boltzmann equation but with a complex-valued distribution instead of a real-valued probability distribution [Yepez, 1996c]. My original goal around 1993 was to generalize the usual kinetic transport equation to handle complex fields. This is the form of the quantum lattice-gas equation that I originally wrote down in 1993. Although (6.25) has the drawback of being only first-order accurate, it is conceptually simple. I added a nonlinear interaction potential in 1995 and first applied the method to modeling two-fluid hydrodynamics in Helium II [Yepez, 1996b]. I presented this nonlinear quantum lattice-gas model at the Sixth International Conference on Discrete Models for Fluid Mechanics, Boston University Center for Computational Science, August 1996. I originally used two-complex amplitudes per direction. In the derivation of the effective field theory of a quantum lattice-gas system, I used an analog to the lattice Boltzmann equation with a complex distribution, all the way up 1999 [Yepez, 1999b]. A year later, in 2000, I realized that just two complex amplitudes could be used for all the Cartesian directions, so the quantum lattice-gas method was more economical with computational resources then the lattice Boltzmann method. Furthermore, because the dynamics was generated by a hermitian operator, the quantum algorithm was both reversible and unconditionally stable.
fluctuations\(^6\)

\[
J \otimes 1 \psi^{(0)}(t) = 0 \quad (6.28a)
\]

\[
J \otimes 1 \psi^{(1)}(t) = \varepsilon \ell \sigma_z \otimes \sigma \cdot \nabla \psi^{(0)}(t + \varepsilon^2 \tau) \quad (6.28b)
\]

\[
\psi^{(0)}(t + \varepsilon^2 \tau) - \psi^{(0)}(t) = -\varepsilon \ell \sigma_z \otimes \sigma \cdot \nabla \psi^{(1)}(t + \varepsilon^2 \tau)
\]

\[
-\frac{\varepsilon^2}{2} (\ell \sigma_z \otimes \sigma \cdot \nabla)^2 \psi^{(0)}(t + \varepsilon^2 \tau). \quad (6.28c)
\]

Equation (6.28b) can be inverted to solve for the first order correction to the 4-spinor field, \(\psi^{(1)}\). Substituting this into (6.28c), a difference equation for \(\psi^{(0)}\) emerges

\[
\psi^{(0)}(t + \varepsilon^2 \tau) - \psi^{(0)}(t) = -\varepsilon \ell^2 \sigma_z \otimes \sigma (J^{-1} \otimes 1) \sigma_z \otimes \sigma : \nabla \nabla \psi^{(0)}(t + 2 \varepsilon^2 \tau)
\]

\[
-\frac{\varepsilon^2 \ell^2}{2} \sigma_z^2 \otimes (\sigma \cdot \nabla)^2 \psi^{(0)}(t + \varepsilon^2 \tau),
\]

\[
(6.29a)
\]

which reduces to

\[
\tau \partial_t \psi^{(0)} = -\ell^2 \left( \sigma_z J^{-1} \sigma_z \right) \otimes (\sigma \cdot \nabla)^2 \psi^{(0)} - \frac{\ell^2}{2} \sigma_z^2 \otimes (\sigma \cdot \nabla)^2 \psi^{(0)} + \cdots, \quad (6.29b)
\]

where we have expanded both the left-hand and right-hand sides and retained only the relevant order-\(\varepsilon^2\) terms. This further simplifies since \((\sigma \cdot \nabla)^2 = \nabla^2\), an identity that follows from the anticommutativity of the Pauli matrices. So, we arrive at the effective 4-spinor equation of motion

\[
\partial_t \psi^{(0)} = -\frac{\ell^2}{\tau} \left( \sigma_z J^{-1} \sigma_z + \frac{1}{2} \right) \otimes 1 \nabla^2 \psi^{(0)}. \quad (6.30)
\]

This then separates into a pair of 2-spinor equations

\[
\partial_t \begin{pmatrix} \psi^{(0)}_{\uparrow \uparrow} \\ \psi^{(0)}_{\uparrow \downarrow} \end{pmatrix} = -\frac{\ell^2}{\tau} \left( \sigma_z J^{-1} \sigma_z + \frac{1}{2} \right) \nabla^2 \begin{pmatrix} \psi^{(0)}_{\uparrow \downarrow} \\ \psi^{(0)}_{\uparrow \downarrow} \end{pmatrix}, \quad (6.31)
\]

one equation for each of the spin-up and spin-down components, \(\zeta = \uparrow, \downarrow\).

\(^6\)At zeroth order the operator \(J\) does not affect \(\psi^{(0)}\) since this is the equilibrium state (i.e. \(J \psi^{(0)} = 0\)).
Now, we consider the equation of motion for the 2-spinor field \( \psi^{(0)} = \begin{pmatrix} \psi^{(0)}_L \\ \psi^{(0)}_R \end{pmatrix} \) (where here, for convenience, we suppress the spin index). The application of the unitary collision operator \( U = 1 + J \) may cause large changes in the 2-spinor at every time step iteration. To avoid this, it is possible to transform to a reference frame where the spinor is always near local equilibrium. Denote the spinor field in this frame by \( \eta \) and the transformation matrix by \( R \), so that \( \eta \equiv R \psi \). The requirement for being in the local equilibrium frame is that the unitary collision operator in that frame, \( C' = 1 + J' \), be diagonal. The grid-level quantum lattice gas equation in the local equilibrium frame becomes

\[
\eta(x + \varepsilon \sigma_z, t + \varepsilon^2 \tau) = C' \eta(x, t),
\]

where \( C' \) is diagonalized by the similarity transformation \( C' = R C R^{-1} \). Therefore, in the local equilibrium frame, (6.30) is diagonalized, becoming a parabolic partial differential equation in space and time for each of its 2-spinor components, independently

\[
\partial_t \eta^{(0)} = -\frac{\ell^2}{\tau} R \sigma_z \left( J^{-1} + \frac{1}{2} \right) \sigma_z R^{-1} \nabla^2 \eta^{(0)}(t). \tag{6.33}
\]

Consider the following choice for the similarity transformation\(^7\)

\[
R = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{6.34}
\]

The matrix on the right hand side of (6.33) must be diagonal, so \( \sigma_z (J^{-1} + \frac{1}{2}) \sigma_z \) must be off-diagonal. There are different choices for the form of \( J^{-1} \) available to

\(^7\)Note \( R = R^{-1} \) and it has the property that it transforms an off-diagonal matrix into a diagonal matrix

\[
R \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} R = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]
The original choice [Yepez, 1996c] was the following:

\[ J^{-1} = -\frac{1}{2} \begin{pmatrix} 1 & i \frac{\hbar}{m \nu} \\ i \frac{\hbar}{m \nu} & 1 \end{pmatrix}, \quad (6.35) \]

which when inverted gives \( J = -\frac{2}{1 + \frac{\hbar^2}{m^2 \nu^2}} \begin{pmatrix} 1 & -i \frac{\hbar}{m \nu} \\ -i \frac{\hbar}{m \nu} & 1 \end{pmatrix} \), and this in turn gives the unitary matrix

\[ U = 1 + J = \frac{1}{1 + \frac{\hbar^2}{m^2 \nu^2}} \begin{pmatrix} \frac{\hbar^2}{m^2 \nu^2} - 1 & i \frac{2 \hbar}{m \nu} \\ i \frac{2 \hbar}{m \nu} & \frac{\hbar^2}{m^2 \nu^2} - 1 \end{pmatrix}. \quad (6.36) \]

Note that \( \frac{\hbar}{m \nu} \) is a dimensionless real-valued number. That is, with these choices (6.34) and (6.36) for the similarity transformation matrix, \( R \), and the unitary matrix, \( U \), (6.30) reduces to

\[ i \hbar \partial_t \psi^{(0)} = -\frac{\hbar^2}{2m \tau \nu} \sigma_z \nabla^2 \psi^{(0)} + \cdots. \quad (6.37) \]

In turn, in the local equilibrium frame, (6.33) becomes

\[ i \hbar \partial_t \eta^{(0)} = -\frac{\hbar^2}{2m \tau \nu} \sigma_z \nabla^2 \eta^{(0)} + \cdots, \quad (6.38) \]

and letting \( \eta^{(0)} \equiv \begin{pmatrix} u \\ v \end{pmatrix} \), we have

\[ i \hbar \partial_t u = -\frac{\hbar^2}{2m} \nabla^2 u + \cdots \quad (6.39a) \]

\[ -i \hbar \partial_t v = -\frac{\hbar^2}{2m} \nabla^2 v + \cdots, \quad (6.39b) \]

where we have taken \( \nu = \ell^2 / \tau \). Since \( \eta = R \psi \), we have \( \eta = \frac{1}{\sqrt{2}} \begin{pmatrix} \psi_L + \psi_R \\ \psi_L - \psi_R \end{pmatrix} \). In (6.39), the bosonic amplitude field \( u = (\psi_L + \psi_R) / \sqrt{2} \) obeys the Schroedinger equation while \( v = (\psi_L - \psi_R) / \sqrt{2} \) obeys the time-reversed Schroedinger equation. Hence, a typical choice is \( U = e^{i \theta \sigma_z} \), so that

\[ J = \begin{pmatrix} \cos \theta & -i \sin \theta \\ i \sin \theta & \cos \theta \end{pmatrix}. \]

This has as its inverse \( J^{-1} = -\frac{1}{2} \begin{pmatrix} 1 & i \cot \frac{\theta}{2} \\ i \cot \frac{\theta}{2} & 1 \end{pmatrix} \). Hence, the determinative term on the right-hand side of (6.31) is

\[ \sigma_3 (J^{-1} + \frac{1}{2}) \sigma_3 = \frac{1}{2} \sigma_1 \cot \frac{\theta}{2}. \]}

So, the gate angle \( \theta \) sets the particle mass, \( m = \tan \frac{\theta}{2} \).
it is possible to recover the quantum fluid equations from a quantum lattice gas in analogy to the recovery of the Navier-Stokes equation from a classical lattice gas [Yepez, 1996a, Yepez, 1999a], which was the original motivation leading to the discovery of this algorithm.

The quantum algorithm (6.24) is a covariant representation of spinor dynamics as it leads to the relativistic wave equation for a Dirac particle [Yepez, 2003, Yepez, 2005, Yepez, 2007] under advective ordering where $\delta t \sim \delta x \sim \epsilon$. A variant of this quantum algorithm (6.24), that is not relativistically covariant under advective ordering, was applied to the many-particle Schroedinger equation [Boghosian and Taylor, 1996]. Our algorithm is naturally suited for a quantum computer and can be implemented in terms of simple local unitary operations on a lattice of qubits, and we subsequently found that only two qubits per point are needed to model the quantum wave equation in higher dimensions [Yepez et al., 2005a]. This serves as a basic framework for the Q2 quantum lattice gas model.

### 6.3.2 Second-order accurate representation

We have just dealt with a first-order accurate quantum algorithm for the linear Schroedinger wave equation in 3+1 dimensions. Now we will shift gears and deal with the nonlinear Schroedinger wave equation. Because the nonlinear interaction potential is highly sensitive to small fluctuations, we will require at least second-order accuracy in our representation to keep the dynamical condensate field in local equilibrium everywhere (i.e. with Cooper pair states $\psi_0 + \psi_{\uparrow 1}$ at each point). That is, we need consider a representation where the error terms that occur in the effective equation of motion are no larger than $O(\epsilon^2)$.

The evolution operator governing the time-dependent behavior of the wave function in 3+1 dimensions is cast as a local algorithm with three steps applied in
a time-interleaved fashion:

1. a classical stream operator for the point-to-point hopping

2. a quantum collision operator for the on-site interactions

3. a nonlinear operator for the $\phi^4$ self-interaction, reducing computational expense.\(^9\)

The following presentation originally appeared in Ref. [Yepez et al., 2009b]. The composition of the first and second steps is necessarily quantum mechanical, yet it does not necessarily cause an exponential explosion of quantum entanglement throughout the many-body system. In fact, the condensate requires only pairwise entangled states localized at each point in the system, so the computational complexity scales in proportion to the spatial volume of the system ($L^3$) times the Hilbert space size per point ($2^Q$). Furthermore, restricting the dynamics to be factored over the points of the system does not require nonunitary operations nor collapse of the wave function. The condensate dynamics, and that of the quantum lattice gas model, is strictly unitary.

**Qubit field**

Now we treat the qubit representation of the condensate dynamics. Quantum fields are discretized on a cubic lattice as we did in Sec. 6.3.1. We use a representation where at each lattice point is a local cluster state—the simplest case has just a single pair of qubits per point. The excited state, denoted by logical “1,” of a qubit $|q(x_n, t)\rangle$ encodes a particle at the lattice point $x_n$ at time $t$. The local ket in the Fock basis of the qubit pair is

$$|\psi\rangle = \sum_{q,q'}^1 \psi_{qq'}|qq'\rangle = \psi_0|00\rangle + \psi_{1}|01\rangle + \psi_{1}|10\rangle + \psi_{11}|11\rangle.$$  

\(^9\)This reduction comes about as the $\phi^4$ nonlinear term replaces the more expensive gauge field-chiral matter coupling in a Q4 model treatment.
The local Fock states $|01\rangle$ and $|10\rangle$ encode the spin states $|\uparrow\rangle$ and $|\downarrow\rangle$, and so the arrows as subscripts denote the respective amplitudes of those states. The local Fock states $|11\rangle$ and $|00\rangle$ encode the double-occupancy spin state $|\uparrow\downarrow\rangle$ and the empty state $|\text{empty}\rangle$. The convention used here is that the first qubit $|q\rangle$ encodes a spin-$\uparrow$ particle while the second qubit $|q'\rangle$ encodes a spin-$\downarrow$ particle. The ket (6.40) is encoded using the lattice gas convention where each bit represents a particle.

Given a system with $N$ qubits, there are $2^N$ basis kets in the number representation. The number of kets in what is termed the $p$-particle sector is equal to the binomial coefficient $(N\ \text{choose}\ p)$.

Suppose the quantum lattice gas is constrained to reside in the 1-bit sector. The number of states in the 1-bit sector Hilbert manifold identically equals the number of qubits since $(N\ \text{choose}\ 1) = N$. That is, in the 1-bit sector of the quantum Hilbert space, there are $N$ amplitudes, each a complex number. So the 1-bit sector of an $N$-qubit quantum computer can be represented exactly on a classical computer with $N$ complex numbers. While a classical computer can simulate the one-body problem using $N$ complex amplitudes, a quantum computer can simulate the full $N$-body problem using $N$ qubits because of the exponential resources of its Hilbert space. This is an advantage offered by a quantum computer [Boghosian and Taylor, 1998b].

The tensor product $|\Psi(t)\rangle = \bigotimes_{n=1}^{L^3} |\psi(x_n,t)\rangle$, where $L$ is the (linear) lattice size, will represent the state of our quantum fluid. Because the factored form of the quantum field, we can go beyond a one-body quantum simulation and still not saturate our available classical computer resources even for systems with very large $L$. To analytically recover the NLS equation (in our case, the GP equation for a superfluid), it is sufficient to employ the type-II quantum computational framework whereby the Hilbert space of the qubit system is a factored over the points of

---

10This is the Pascal triangle identity $\sum_{p=0}^{N} \binom{N}{p} = 2^N$. 

the system; hence, in the Q2 model, there are four amplitudes per point, those enumerated in (6.40). With a system comprising $L^3$ entangled clusters, we need only a small slice of size $L^3 2^2$ of the full Hilbert space of size $2^{2L^3}$. Using the (6.9) as the generator of the stream operator, the component $\psi_0(x)$ behaves as a left-goer and the component $\psi_{11}(x)$ behaves as a right-goer, or vice versa depending on the sign of the gate angle $\zeta$ in (6.10). So, the relevant 2-component amplitude field that represents the dynamical ground state of a quantum fluid is

$$
\psi(x) = \begin{pmatrix}
\psi_0(x) \\
\psi_{11}(x)
\end{pmatrix}.
$$

(6.41)

Finally, the condensate scalar wave function $\varphi$ is determined as the parallel entangled state

$$
\varphi \equiv \frac{1}{\sqrt{2}} \left( \psi_0 + \psi_{11} \right).
$$

(6.42)

This, of course, captures the important effect of quantum entanglement between the empty and doubly occupied configurations characteristic of Cooper pairing in Fermi condensates. A $\sqrt{\text{PAIR}}$ entangling gate is used to keep the 2-spinor (6.41) in its parallel entangled state. This parallel entangled state is our local equilibrium configuration of the spinor amplitudes.

**Effective GP Hamiltonian**

The evolution of $\psi$ is determined by 0–$\uparrow\downarrow$ qubit-qubit interactions (collide), free motion of the amplitudes along the cubic lattice (stream), and qubit phase shifts to model the well known “Mexican hat” interaction potential (phase rotation). The qubit-qubit interaction are generated by a collision Hamiltonian $H_c = \hbar \omega \sigma_x$, where $\hbar \omega$ is the 0–$\uparrow\downarrow$ coupling energy, and the collision time $\tau$ corresponds to the quantum logic gate time, chosen such that $\omega \tau = \frac{\pi}{4}$ to make the presentation in this section as simple as possible. Free streaming of qubit states on the lattice
(emulating the motion of particles in space) is generated by the stream Hamiltonian

\[ H_s \stackrel{(6.10)}{=} \hbar \sum_{\text{lattice}} \sigma_z \otimes c \cdot \nabla \]

acting on the qubits. \( c \equiv -\sigma / \tau \) is a streaming velocity along lattice directions.

Exploiting the fact that \([H_s, H_c] \neq 0\), we will use an interleaved compositional product of the 2-qubit quantum gates generated \( H_s \) and \( H_c \) whereby an effective Hamiltonian emerges in the scaling limit modeling the nonrelativistic free particle Hamiltonian \( H_0 \). Formally denoting this compositional product by the symbol \( \circ \), the Hamiltonian \( H_\circ \equiv \text{Tr}[H_s \circ H_c] \rightarrow -\frac{\hbar^2}{2m} \nabla^2 + \cdots \), where in our model \( m = \frac{1}{2} \)

(following from the choice \( \omega \tau = \frac{\pi}{4} \)) in lattice units and where the right arrow denotes a scaling limit. Thus \( H_\circ \) generates the evolution of a free scalar quantum field.

Phase rotation, inducing nonlinear particle-particle interactions, is generated by \( H_{\text{int}}(|\varphi|^2) = (\mu |\varphi|^2 - \mu) |\varphi|^2 \), where the quantum logic gate time \( \tau' \) is chosen such that \( g/\hbar \approx 1 \). In the low energy limit, the local evolution is effectively

\[
\varphi(t + \delta t, \mathbf{x}) = e^{-iH_0 \tau / \hbar} e^{-iH_{\text{int}} \tau'/\hbar} \varphi(t, \mathbf{x}) + \cdots \quad (6.43a)
\]

\[
\approx e^{-iH_{\text{GP}} \delta t / \hbar} \varphi(t, \mathbf{x}) \quad (6.43b)
\]

modeling (6.1) in the lowest order fluctuations. A derivation of \( H_{\text{GP}} \sim H_\circ + H_{\text{int}} \) follows from the typical scaling arguments used in kinetic lattice gases.
Entangling gates

Entangling two-qubit quantum gates presented in Chapter 2 have the form [Yepez, 2001a]

\[
U_{\perp} |\psi\rangle = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & A & B & 0 \\
0 & C & D & 0 \\
0 & 0 & 0 & \mathcal{E}
\end{pmatrix} \begin{pmatrix}
\psi_0 \\
\psi_1 \\
\psi_1 \\
\psi_{\perp 1}
\end{pmatrix}, \quad U_{\parallel} |\psi\rangle = \begin{pmatrix}
A & 0 & 0 & B \\
0 & 1 & 0 & 0 \\
0 & 0 & \mathcal{E} & 0 \\
\mathcal{C} & 0 & 0 & \mathcal{D}
\end{pmatrix} \begin{pmatrix}
\psi_0 \\
\psi_1 \\
\psi_1 \\
\psi_{\perp 1}
\end{pmatrix},
\]

(6.44)

where the block of components in the dotted box is a member of SU(2), viz. \(\begin{pmatrix} A & B \\ \mathcal{C} & \mathcal{D} \end{pmatrix} \in SU(2)\). Only the local 2-component field’s complex amplitudes \(\psi_0(x)\) and \(\psi_{\perp 1}(x)\) are quantum mechanically entangled by the action of \(U_{\parallel}\) in (6.44). Particle motion and particle-particle interactions are faithfully emulated strictly using quantum logic gates of the form of (6.44). Furthermore, to describe the quantum lattice gas algorithm, it is sufficient to consider only the type-II quantum computing slice of the full quantum Hilbert space, as discussed above. In this way, the algorithmic treatment becomes straightforward to describe using only \(2 \times 2\) matrices that represent the SU(2) subspace of (6.44).

An early example of this type of quantum algorithmic reduction is given in Ref. [Yepez, 2001a]. The quantum gate dynamics conserves particle number and consequently the effective \(H_{GP}\) in (6.43) commutes with the particle number operator. Thus, \(H_{GP}\) is block diagonal over the \(n\)-body sectors of the Hilbert space. One is justified to run a simulation in any one of the \(n\)-body sectors, for \(0 \leq n \leq 2L^3\), which is an exact representation of all the relevant quantum dynamics in that sector, independent of the dynamics in all the other sectors. The advantage of limiting the simulation to the type-II quantum computing sector is that the algorithmic complexity scales linearly with the number of points and this sector is sufficient to
capture the relevant physics of a condensate, including its quasiparticle excitations. It is for this reason that the type-II quantum algorithm can be implemented on a classical supercomputer while retaining its usefulness for quantum simulation of superfluidity.

We now describe the quantum algorithm by dealing with the subspace of the quantum logic gate operators (6.44). The SU(2) quantum operator

\[ U_C = e^{-i \frac{\pi}{4} \sigma_z} = \frac{1}{2} \begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix} \]  

(6.45)

that acts locally at every point \( x \) by the map

\[ \text{local collision : } \psi'(x) = U_C \psi(x) \rightarrow \psi(x). \]  

(6.46)

The complex scalar density \( \varphi = (1,1) \cdot \psi = \psi_0 + \psi_{\parallel} \) is conserved by (6.46), and consequently the probability \( |\psi|^2 \) is also conserved locally. Local equilibrium (i.e. \( \psi = U_C \psi \)) occurs when the amplitudes are equal (\( \psi_0 = \psi_{\parallel} \)), but in general such a local equilibrium is then broken if a spinor component is displaced in space by a vectorial amount \( \Delta x \).

**swap gate**

The sequence of swap gates used to connect points in a Q2 model on a quantum computer, when implemented on a classical supercomputer, is replaced by a global shift operation. This exactly preserves probability and unitarity. One admits only complementary displacements of the field components, induced by the stream operators of the form that acts on a 2-spinor

\[ S_{\Delta x,1} \equiv e^{h \Delta x \cdot \nabla} = n + e^{\Delta x \cdot \nabla} \cdot h = \begin{pmatrix} e^{\Delta x \cdot \nabla} & 0 \\ 0 & 1 \end{pmatrix} \]  

(6.47a)

\[ S_{\Delta x,-1} \equiv e^{n \Delta x \cdot \nabla} = h + e^{\Delta x \cdot \nabla} \cdot n = \begin{pmatrix} 1 & 0 \\ 0 & e^{\Delta x \cdot \nabla} \end{pmatrix} \]  

(6.47b)
where \( n = \frac{1}{2}(1 - \sigma_z) \) and \( h = \frac{1}{2}(1 + \sigma_z) \). Although the application of (6.47a) usually breaks local equilibrium induced by (6.46), with the appropriate boundary conditions, for example periodic boundary conditions, (6.47a) is guaranteed to conserve the total density \( \int d^3x \psi(x) \) and in turn the total probability \( \int d^3x (|\psi_0(x)|^2 + |\psi_1(x)|^2) \).

To construct a quantum algorithm using a combination of the operators \( U_C \) and \( S_{\Delta x,\sigma} \) and their respective adjoints \( U_C^\dagger \) and \( S_{\Delta x,\sigma}^\dagger \), for \( \sigma = 1 \) or \(-1\), we restrict our considerations to those combinations that are close to identity. We will use the bar notation to mean \( \bar{\sigma} = -\sigma \). To achieve high-order accuracy, our basic approach begins with the interleaved operator

\[
I_{\sigma} = S_{-\Delta x,\sigma} U_C S_{\Delta x,\sigma} U_C = \frac{1}{2} \begin{pmatrix}
1 + e^{-\sigma \Delta x \nabla} & -i + i e^{-\sigma \Delta x \nabla} \\
-i + i e^{\sigma \Delta x \nabla} & 1 + e^{\sigma \Delta x \nabla}
\end{pmatrix}
\]  

(6.48)

as the basic building block of the quantum algorithm. Since \( S_{-\Delta x,\sigma} S_{\Delta x,\sigma} = 1 \) and \( U_C^\dagger U_C = 1 \), clearly this interleaved operator is close to identity. Equivalently, (6.48) can be written as \( I_{\sigma} = S_{\Delta x,\bar{\sigma}} U_C S_{-\Delta x,\sigma} U_C^\dagger \), which adheres to the lattice gas form of (6.15) whereby the upper and lower components of a spinor stream in opposition direction.

We will need the following intermediate result, rewriting (6.48) in the analytically convenient form

\[
I_{\sigma} = \frac{1}{2} \left( 1 - i \sigma_z \right) + \frac{1}{2} \left( 1 + i \sigma_z \right) \cosh(\Delta x \cdot \nabla) - \frac{\sigma}{2} \left( \sigma_z + \sigma_y \right) \sinh(\Delta x \cdot \nabla).
\]  

(6.49)

Let us symmetrize this interleaved operator \( U_{\sigma} \)

\[
U_{\sigma} \equiv I_{\sigma} I_{\bar{\sigma}} \overset{(6.49)}{=} \sinh^2 \frac{\Delta x \cdot \nabla}{2} \left[ \cosh(\Delta x \cdot \nabla) - 1 + i(\cosh(\Delta x \cdot \nabla) + 1)\sigma_x + \sigma(\sigma_z - \sigma_y) \sinh(\Delta x \cdot \nabla) \right].
\]  

(6.50)

\[11\] Although it may not be obvious that \( S_{\Delta x,\sigma} U_C S_{-\Delta x,\sigma} U_C^\dagger \) should be close to identity since \( S_{\Delta x,\sigma} S_{-\Delta x} \neq 1 \), nevertheless this follows as it is identical to (6.48), which can be verified by carrying out the requisite matrix multiplications.

\[12\] The motivation to symmetrize the interleaved operator is to ensure the lattice gas form of its evolution is manifestly close to identity: \( I_{\sigma} I_{\bar{\sigma}} = S_{\Delta x,\sigma} U_C S_{-\Delta x,\sigma} U_C^\dagger S_{\Delta x,\sigma} U_C S_{-\Delta x,\sigma} U_C^\dagger \).
Then, to remove any dependence on spin component variable $\sigma$ that appears in the last (odd) term, we can symmetrize one last time and thus define our quantum lattice gas evolution operator as

$$U_x \equiv U_{x\sigma} U_{\sigma x} \text{(6.51)}$$

Notice that this induces unitary dynamics in one spatial dimension along $\Delta x$. Therefore, a suitable evolution operator to model a nonlinear quantum fluid in the three spatial dimensions can be constructed by a product of (6.51), one fully symmetrized operator for each of the orthogonal Cartesian directions

$$U_{\text{gas}}[\Omega(x)] \equiv U_x U_y U_z e^{-i\epsilon^2 \Omega(x)}, \text{(6.52)}$$

where $\epsilon \sim 1/L$, where $L$ is the grid resolution (i.e. $L$ is the number of grid points along one edge of the simulation volume). Equation (6.52) represents the three aspects of a type-II quantum algorithm: stream, collide, and (nonlinear) phase rotation. In dimensionless lattice units, note that $\epsilon^2 \sim \Delta x^2 \sim \Delta t$. This evolution operator is spatially dependent on the quantum field at a point only through local state reduction $\Omega(x)$:

$$\psi(x, t + \Delta t) = U_{\text{gas}}[\Omega(x)] \psi(x, t). \text{(6.53)}$$

Equation (6.53) specifies the nonlinear quantum lattice gas model of a quantum gas on a cubical grid.

**Effective field theory**

It is a rather straightforward matter to determine the effective evolution operator that corresponds to (6.53). To illustrate the procedure, we may Taylor expand (6.50) in $\epsilon \sim |\Delta x|$, and this leads to the following low-energy expansion:

$$U_{x\sigma}^{\text{eff}} = 1 + i\frac{\epsilon^2}{2} \sigma_x (\Delta x \cdot \nabla)^2 + \frac{\epsilon^3}{4} (\sigma_y - \sigma_z) \Delta x \cdot \nabla)^3 + O(\epsilon^4). \text{(6.54)}$$
Therefore, we know that the fully symmetrized evolution operator (6.51) is accurate to forth order in $\varepsilon$

\[ U_{\text{eff}} = 1 + i\varepsilon^2 \sigma_x (\Delta x \cdot \nabla)^2 + \mathcal{O}(\varepsilon^4), \quad (6.55) \]

as the second-order terms add and the third-order error terms now must necessarily cancel each other when we multiply $U_{\text{eff}}^{x\sigma}$ by $U_{\text{eff}}^{\sigma x}$. (This is why (6.51) was symmetrized to be independent of $\sigma$.) In turn, we know that $U_{\text{gas}}^{\text{eff}}$ obtained from the product (6.52) must have error terms no larger than $\mathcal{O}(\varepsilon^4)$, and so the quantum algorithm (6.53) has the following low-energy expansion:

\[ \psi(x, t + \Delta t) = \psi(x, t) - i\varepsilon^2 \left[-\sigma_x \nabla^2 + \Omega\right] \psi(x, t) + \mathcal{O}(\varepsilon^4). \quad (6.56) \]

Now with $\frac{1}{\varepsilon^2} [\psi(x, t + \Delta t) - \psi(x, t)] \sim \partial_t \psi(x, t)$, as we divide both sides of (6.56) by $\varepsilon^2$, we arrive at the effective equation of motion for the quantum lattice gas

\[ i\partial_t \psi = -\sigma_x \nabla^2 \psi + \Omega \psi + \mathcal{O}(\varepsilon^2), \quad (6.57) \]

which holds in the low energy and low momentum limits. Finally, since $\varphi = \frac{1}{\sqrt{2}} \left(\psi_0 + \psi_1\right)$, the condensate field obeys the effective scalar field equation

\[ i\partial_t \varphi = -\nabla^2 \varphi + \Omega \varphi + \mathcal{O}(\varepsilon^2), \quad (6.58) \]

which is the nonlinear Schroedinger wave equation with $m = \frac{1}{2}$ for $\hbar = 1$, so long as $|\Delta x|^2 = \Delta t = \varepsilon$. From the order of the error term in (6.58), the Taylor expansion predicts the quantum algorithm is second order convergent in space.

In summary, the low energy effective Hamiltonian that is the generator of the evolution, $U(\Delta t) = e^{-i\Delta t H_{\text{eff}}/\hbar} + \cdots$, is the following

\[ H_{\text{eff}} = -\frac{\hbar^2}{2m} \nabla^2 + \hbar \Omega(x) + \mathcal{O}(\Delta t, \Delta x^2), \quad (6.59) \]

for $m = 1/2$ and where we have written the quantum transport coefficient as

\[ \frac{\Delta x^2}{\Delta t} = \frac{\hbar}{m}. \quad (6.60) \]
This is the nonlinear GP Hamiltonian on choosing $h\Omega(\mathbf{x}) = g|\varphi(\mathbf{x})|^2$, where $g$ is the on-site interaction energy.

### 6.3.3 Considerations regarding physical accuracy

We have analytically demonstrated that the following quantum lattice gas algorithm

$$(\alpha'(\mathbf{x},t), \beta'(\mathbf{x},t)) = U_{z0}U_{y1}U_{z0}e^{-\frac{i\omega^2}{2}(g|\varphi(\mathbf{x},t-\tau)|^2 - \mu)}U_{z1}U_{y0}U_{x1}e^{-\frac{i\omega^2}{2}(g|\varphi(\mathbf{x},t-\tau)|^2 - \mu)}(\alpha(\mathbf{s},t-\tau), \beta(\mathbf{s},t-\tau))$$

(6.61)

for the 2-spinor $|\psi(\mathbf{x})\rangle = \alpha(\mathbf{x})|00\rangle + \beta(\mathbf{x})|11\rangle = \begin{pmatrix} \alpha(\mathbf{x}) \\ \beta(\mathbf{x}) \end{pmatrix}$ has the GP equation

$$i\partial_t\varphi(x) = -\nabla^2\varphi(x) + (g|\varphi(x)|^2 - \mu)\varphi(x)$$

(6.62)

(which we chose to consider without an external potential) as its low-energy effective equation of motion, where $\varphi(x) = \langle (1,1)|\psi(x)\rangle = \alpha(x) + \beta(x)$ and where the derivatives are resolved on a lattice of points with unit space and time cell sizes. These cell sizes, that we will denote as $\ell$ and $\tau$ in this section, serve as the natural lattice units for numerical implementations. In the quantum algorithm (6.61), the symbol $\bullet$ indicates that the new value of the 2-spinor field at coordinate $\mathbf{x}$ and time $t$ on the left-hand side of the question is evaluated over a stencil of spatial coordinates (centered on $\mathbf{x}$) at the earlier time $t - \tau$ on the right-hand side.

All the the amplitudes at the spacetime coordinates in the inverse light cone terminating with its apex at the coordinate $x = (t, \mathbf{x})$ contribute to the resulting 2-spinor at $x$ through quantum interference. One way to think of the algorithm is to have all of its stencils uniformly and simultaneously mapped over the entire lattice to update the 2-spinor field. That is, each point requires its own stencil and all the stencils are simultaneously overlapping. In this regard, quantum lattice gas algorithms are representations of path integrals [Yepez, 2005, Yepez, 2007]. It is
from the overlapping stencils that our method derives its numerical accuracy. Yet, the most practical way to understand the quantum lattice gas is via the configuration of its informational substrate—its regular and closed-loop linkage of quantum wires and quantum gates—which is a concept that we introduced in Chapter 1.\footnote{The grid-level equation (6.61) is only formally equivalent to a finite-difference equation even as the local spatial stencil is implicitly determined by the algorithmic protocol. It is impractical to directly specify the local stencil as it has too many terms to explicitly write out—it has about $\frac{2\pi r^2}{3} \approx 268$ points since $r/\ell \sim 4$ for protocol (6.61). Thus, the quantum lattice gas grid-level equation cannot be written as a finite-difference equation in the usual sense.}

This allows us to address the physical accuracy of the quantum lattice gas model of quantum computation by considering the dynamics that occurs on a loal plaquette of the informational substrate.

We have already proved that (6.61) is second-order accurate in space. Yet, there exist a number of constraints on the quantum information dynamics that we have yet to address and that must be respected in any numerical implementation. We may calculate limits for local fluctuations of the condensate’s phase by considering the local quantum information dynamics. Since the informational substrate is specified by the unitary interleaved operator $U_{\sigma \tau}$ in (6.61) and this in turn depends on the collision, stream, and phase rotation operators in a local and regular way, all we need to consider are any degrees of freedom in $C$, $S$, and $e^{-i e^{2\Omega}}$.

The collision operator

$$U_C = e^{-i \frac{\pi}{4} e^{i \frac{\pi}{4} \sigma_x}} = \frac{1}{2} \begin{pmatrix} 1 - i & 1 + i \\ 1 + i & 1 - i \end{pmatrix}$$

(6.63)

has no free parameters, and the stream operators (6.47a), which we may write as

$$S_{\pm \hat{x}, 1} = e^{\pm h \ell \hat{x} \cdot \nabla} = \begin{pmatrix} e^{\pm t \hat{x} \cdot \nabla} & 0 \\ 0 & 1 \end{pmatrix} \quad S_{\pm \hat{x}, -1} = e^{\pm i \ell \hat{x} \cdot \nabla} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i \ell \hat{x} \cdot \nabla} \end{pmatrix},$$

(6.64)

each have only a directional degree of freedom. That is, the displacement vector $\ell \hat{x}$ that appears in (6.64) has a fixed length $\ell$ (often taken to be unity), so the only remaining degree of freedom is the direction of $\hat{x}$. Yet, this directional degree of
freedom in $S$ is constrained by the requirement to recover the Laplacian operator $\nabla^2$ in (6.62), and is thus fixed by the algorithmic protocol (6.61). The phase rotation operator

$$e^{-i\varepsilon^2 \Omega} = e^{-i\varepsilon^2 (g|\varphi(x,t-r)|^2 - \mu)}, \quad (6.65)$$

has three parameters, but these are not all independent. With the chemical potential set to $\mu \overset{(5.987)}{=} mc^2$, (6.65) has only its number density $\rho_o = |\varphi_o|^2$ as a degree of freedom. $\rho_o$ is set by the bit filling fraction on the lattice, specified by the initial conditions of the dynamical qubit system. The coupling strength $g$ is not an independent degree of freedom in the model as it is constrained by the equilibrium relation

$$g|\varphi_o|^2 = \mu. \quad (6.66)$$

This relation derives from the requirement that the condensate be effectively described by the free Schroedinger equation (behaving as a single quantum particle) far away from any topological defect ($\varphi = 0$ nodal line) where the potential terms on the right-hand side of (6.62) necessarily cancel out, or equivalently (6.65) becomes the identity.

It is possible to use an arbitrary gate angle, say $\zeta$, so the relevant $\text{SU}(2)$ part of the $\sqrt{	ext{PAIR}}^\dagger$ collision operator is

$$U_c(\zeta) = e^{-i\zeta} \begin{pmatrix} \cos \zeta & i \sin \zeta \\ i \sin \zeta & \cos \zeta \end{pmatrix}. \quad (6.67)$$

This allows us to independently adjust the value of the mass that appears in the effective field theory that gives rise to the Schroedinger equation as the governing equation of motion of the qubit system in the low-energy limit. Setting $\zeta = \pi/4$ gives the collision operator (6.63), and in turn setting $m = 1/2$ in the equation of motion. Notice that (6.67) has eigenvector $(1, 1)$ with unity eigenvalue. Hence,
the local Cooper pair state \((|00⟩ + |11⟩)/\sqrt{2}\) is an eigenket of (6.67) with unity eigenvalue.\(^{14}\)

For numerical accuracy of the (6.61), we require that both the magnitude and phase of \(ϕ(x) = ϕ(x) e^{iθ(x)}\) vary slowly over the \(L^3\) points of the space. Using the Madelung transformation [Madelung, 1927] (see Appendix C.2), the velocity of the quantum fluid at a point is determined from the gradient of the phase

\[v = \frac{\hbar}{m} |\nabla θ| \sim \frac{\hbar}{m} \frac{Δθ}{Δx},\]  

(6.68)

where we approximate the magnitude of the gradient by the ratio of the phase change to the spatial cell size. Then, employing the lower bound of the Heisenberg uncertainty principle, \(Δx Δp = ħ/2\) (the bound defining maximally squeezed states), we can determine the velocity magnitude

\[v = \frac{ħ}{4mΔx},\]  

(6.69)

which follows from \(Δp = mΔv = 2mv\), since the velocity change \(Δv = 2v\) is due to the reversal of velocity \(v\) in lattice gases [Yepez, 2005, Yepez, 2007]. Equating (6.68) and (6.69), we find

\[Δθ = \frac{1}{4} \frac{Δx}{Δx}.\]  

(6.70)

Therefore, the smallest possible change in position is one cell size, \(Δx_{\text{min}} = 1\), so we have the upper bound

\[Δθ_{\text{max}} = \frac{1}{4} = 14.324°.\]  

(6.71a)

The largest possible (quantum mechanically coherent) change in position is one healing length, \(Δx_{\text{max}} = κ\), so we have the lower bound

\[Δθ_{\text{min}} = \frac{1}{4} \frac{κ}{κ} = \sqrt{\frac{2gρ_o}{mc^2}},\]  

(6.71b)

\(^{14}\)The small parameter \(ε^2\) is divided out of the right-hand side of the finite-difference equation (6.56) to produce the time derivative on the left-hand side of the equation, yet \(ε\) appears in (6.61), so we may treat it as an additional free parameter in the algorithm. We also have the freedom to choice the grid size, \(L\), and the size of the quantum vortex core as well.
which follows from
\[
\xi \equiv \frac{\hbar}{\sqrt{2m\mu}} \equiv \frac{\hbar}{m} \sqrt{\frac{m}{2g|\varphi_0|^2}} = c\ell \sqrt{\frac{m}{2g\rho_0}}. \tag{6.72}
\]

During the course of a numerical simulation, it is necessary to check that condition (6.71a) is not violated. It is not a simple task to predict ahead of time, solely from a knowledge of the initial conditions, whether or not (6.71a) will be violated at some later time at one or more points on the lattice. A violation of the upper bound may occur if the quantum vortices are under resolved. Generally, so long as \(\xi\) is sufficiently large (i.e., each quantum vortex is fully resolved on the grid), then the quantum lattice gas will remain near local equilibrium everywhere. A trial and error approach was used to find an appropriate value for \(\xi\). In a typical lattice gas simulation, a healing length (inner quantum vortex radius) of \(\xi \approx 10\) works well, so the lower bound in this case becomes \(\Delta \theta_{\min} \approx 1.4324^\circ\).

The GP equation is invariant under normalization and interaction strength rescaling
\[
\varphi \rightarrow s\varphi \quad \text{and} \quad g \rightarrow \frac{g}{s^2}, \tag{6.73}
\]
where \(s\) is a real-valued scaling parameter. A conventional starting point in the numerical treatment is to point normalize the wave function in the bulk so that \(|\varphi(\bm{x}, 0)|^2 = \rho_0 = 1\) for all \(\bm{x}\) far away from a nodal line.

6.4 Quantum vortex solution

The following presentation originally appeared in Ref. [Yepez et al., 2009b, Yepez et al., 2009a, Yepez et al., 2009c]. We seek a steady state solution of the black quantum vortex governed by the time-independent GP equation
\[
-\frac{1}{a} \nabla^2 \varphi + (g|\varphi|^2 - 1)\varphi = 0. \tag{6.74}
\]
A spatial rescaling parameter $\sqrt{a}$ is inserted so that the vortex core can be resolved on the substrate with a sufficient number of points so as to be consistent with the high-order of convergence of the quantum algorithm for which (6.74) represents a low-energy effective field theory in the steady state.

With the appropriate choice of nonlinear coupling $g$ and normalization of the wave function, physically the energy of a constant external potential can cancel the internal interaction energy in the region of bulk flow. This is the type of solution that we will explain here. A solution for the wave function of the quantum vortex is found by separation of variables in polar coordinates, as presented in Sec. 5.3.1. Inserting $\varphi(r, \theta) = \phi(r)e^{in\theta}$ into (6.74) with \[ g = \frac{1}{a} \] then gives

\[ \frac{d^2 \phi(r)}{dr^2} + \frac{1}{r} \frac{d\phi(r)}{dr} - \frac{n^2}{r^2} \phi(r) + (a - \phi(r)^2) \phi(r) = 0, \] \tag{6.76}

which can be solved for any integer winding number $n$. For the simplest $n = 1$ case, we take the Padé approximant of the spatially scalable form to be

\[ \phi(r) = \sqrt{\frac{r^2(a_1 + a b_2 r^2)}{1 + b_1 r^2 + b_2 r^4}} = \sqrt{\frac{11a^2r^2(12 + ar^2)}{384 + ar^2(128 + 11ar^2)}}, \] \tag{6.77}

where the solutions for the coefficients $a_1$, $b_1$, and $b_2$, worked out in Appendix D.1, have been inserted in the right-hand side. Notice that $\phi(r) \to \sqrt{a}$ and $r \to \infty$, and thus the nonlinear term in (6.76) vanishes in the bulk. Rescaling $\sqrt{a} r \to r$, and denoting the scaled solution as $R(r) \equiv \frac{1}{\sqrt{a}} \phi \left( \frac{r}{\sqrt{a}} \right)$, we have

\[ R(r) = \sqrt{\frac{11r^2(12 + r^2)}{384 + r^2(128 + 11r^2)}}, \] \tag{6.78}

This is equivalent to choosing $a = 1$ in (6.77). Thus, (6.78) is the $g = 1$ solution of the radial part of (6.74)

\[ R''(r) + \frac{1}{r} R'(r) - \frac{n^2}{r^2} R(r) + (1 - R(r)^2) R(r) = 0, \] \tag{6.79}
and (6.78) was originally found by Berloff [Berloff, 2004]. However, the more general Padé approximant (D.11) allows us to rescale the width of the quantum vortex to arbitrarily resolve its core on the computational grid to achieve sufficient numerical accuracy.

We define **bulk point normalization** to be the field configuration where (6.74) satisfies the free linear Schrödinger wave equation in the bulk and this occurs for \(|\varphi|^2 \to 1/g\) (far away from any quantum vortex center). That is, since

\[
\lim_{r \to \infty} \phi(r) = \sqrt{a},
\]

(6.80)

and so we indeed satisfy the free field condition by choosing the coupling strength according to (6.75). So with \(\sqrt{a} r \to r\), the equation we are numerically solving is

\[
\sqrt{a} \partial_t \varphi = -\nabla^2 \varphi + (|\varphi|^2 - 1)\varphi = 0.
\]

(6.81)

Thus far we have only considered a field configuration of a single quantum vortex over an infinite domain. Unfortunately, in a numerical simulation we are restricted to finite resources. Hence, we implement a field configuration in a box with periodic boundary conditions and with this restriction we cannot make do with just a single quantum vortex. We need at least two of them to enforce periodic boundary conditions in one space dimension and four of them to enforce periodic boundary conditions in two space dimensions in the phase of the \(\varphi\) field.

**6.4.1 Vortex-antivortex configuration (2 centers)**

We take the approximate form of the magnitude of vortex-antivortex configuration to be the following

\[
\phi(r) = \sqrt{a} \tanh \left[ \frac{2}{3} \sqrt{\lambda} \sin \left( \frac{\pi r}{\lambda} \sqrt{a} \right) \right].
\]

(6.82)

Expanding about \(r = 0\) to third order, (6.82) is

\[
\phi(r) = \frac{2a \pi r}{3\sqrt{\lambda}} - \frac{a^2 \pi^3 (9 + 8\lambda)}{81 \lambda^{5/2}} + \cdots
\]

(6.83)
Inserting the hyperbolic approximant (6.82) into the radial part of the steady-state GP equation (6.76), we have

\[
2 \left( a \left( n^2 - 1 \right) \pi \right) \frac{1}{3 \sqrt{\lambda} r} + \frac{a^2 \pi \left( 54 \lambda^2 + \left( n^2 - 9 \right) \pi^2 \left( 8 \lambda + 9 \right) \right)}{81 \lambda^{5/2}} r
+ \cdots = 0. \tag{6.84}
\]

For winding number \( n = 1 \) the \( 1/r \) term vanishes. Then for the first order term to vanish, (6.84) gives a quadratic equation for \( \lambda \) which has the positive solution

\[
\lambda = \frac{2\pi}{27} \left( 8 \pi + \sqrt{243 + 64 \pi^2} \right) = 12.731. \tag{6.85}
\]

Defining the separation distance between the two centers of the quantum vortices as \( 2\delta \), we find that this distance is fixed by the spatial rescaling parameter \( a \) as follows

\[
\delta = \frac{\lambda}{2\sqrt{a}}. \tag{6.86}
\]

The approximation (6.82) becomes ever more accurate for \( a \ll 1 \) as the grid resolution is increased and the high-order terms in (6.84) vanish faster than the low order terms. That the double quantum vortex is a remarkable stable structure is demonstrated in the numerical simulation shown in Fig. 6.11. In this case, even on a very small grid of size \( L = 64 \), the vortex-antivortex pair’s wave function initially set by (6.82) for \( a = \left( \frac{2\pi}{L} \right)^2 = 0.158 \) persists indefinitely in time with only small

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{quantum_vortex_antivortex.png}
\caption{Quantum vortex-antivortex magnitude (blue) for \( a = 0.81 \) compared with the black quantum vortex (brown). The size of the pair is \( 2\delta = 14.1455 \).}
\end{figure}
fluctuations a couple percent of the peak, but which are barely noticeable on the graph.

FIG. 6.11: Quantum vortex-antivortex density profile (blue) for $a = 0.158$ compared with the numerical solution (brown dots) for a small grid of size $L = 64$. The double quantum vortex is indefinitely stable.

### 6.4.2 Quadrupolar configuration (4 centers)

A simple initial condition that ensures periodicity is four symmetrically displaced vortex line solitons (parallel to the z-axis for the time being) in product form

\[
\varphi(x, y) = [\phi(r_{++})e^{i\theta_{++}}] \times [\phi(r_{+-})e^{-i\theta_{+-}}] \times [\phi(r_{-+})e^{-i\theta_{-+}}] \times [\phi(r_{--})e^{i\theta_{--}}]
\]

(6.87a)

\[
= \phi(r_{++})\phi(r_{+-})\phi(r_{-+})\phi(r_{--})e^{i(\theta_{++}-\theta_{+-}-\theta_{-+}+\theta_{--})},
\]

(6.87b)
FIG. 6.12: A slice at \( z = z_0 \) of the magnitude \( \sqrt{\rho(x, y, z_0)} \) (top, upside down) and phase \( \theta(x, y, z_0) \) (middle) and phase contours (bottom) of the wave function for a quantum vortex quadrupole, the product of 4 quantum vortex solutions on a grid of size \( L = 160 \). The density \( \rho(x, y) = |\varphi(x, y)|^2 \) and so \( \sqrt{\rho(x, y, z_0)} \to 1 \) away from a vortex core (in the bulk). From the phase diagram, plotted \( -\pi \leq \theta(x, y, z_0) \leq \pi \), going around any contour in the \( z = z_0 \) plane that encloses a single vortex singularity accumulates a phase of \( \pm 2\pi \) radians. With \( N = 4 \) line vortices one can accommodate periodic boundary conditions in the phase.
where the radial distance from a vortex line along the z-axis is

\[ r_{++}(x,y) = (x - x_o + \delta)^2 + (y - y_o + \delta)^2, \quad r_{+-}(x,y) = (x - x_o + \delta)^2 + (y - y_o - \delta)^2 \]
\[ r_{-+}(x,y) = (x - x_o - \delta)^2 + (y - y_o + \delta)^2, \quad r_{--}(x,y) = (x - x_o - \delta)^2 + (y - y_o - \delta)^2. \]

(6.88)

The size of the quantum vortex quadrupole is \(|2\delta|\), its overall center is \((x_o, y_o)\), and we define its \textbf{polarity} to be \(\text{sign}(\delta) = \pm 1\). The phase angles are

\[ \theta_{++}(x,y) = \arctan \frac{y - y_o + \delta}{x - x_o - \delta} \quad \theta_{+-}(x,y) = \arctan \frac{y - y_o + \delta}{x - x_o - \delta} \]
\[ \theta_{-+}(x,y) = \arctan \frac{y - y_o - \delta}{x - x_o + \delta} \quad \theta_{--}(x,y) = \arctan \frac{y - y_o - \delta}{x - x_o + \delta}. \]

(6.89)

The magnitude and phase of (6.87) are plotted in Fig. 6.12 with \(\delta = \frac{L}{4}\) and \(a = 0.1\) and \(L = 160\), demonstrating the periodicity of (6.87). We shall use such quantum vortex quadrupole configurations aligned along orthogonal principal lattice direction to represent initial conditions for numerical simulations.

**Clebsch potentials representation**

As an alternative representation of the vortex structure of the quadrupolar configuration (directed along the z-axis, say), we may use Clebsch potentials to analytically specify the condensate field in a box of size \(L \times L \times L\):

\[ \lambda(x, y, z) \equiv \sqrt{2} \cos \left( \frac{2\pi x}{L} \right) \]
\[ \mu(x, y, z) \equiv \sqrt{2} \cos \left( \frac{2\pi y}{L} \right). \]

(6.90a)

(6.90b)

The quantum wave function is

\[ \varphi(\lambda, \mu) = \frac{\lambda + i\mu}{\sqrt{\lambda^2 + \mu^2}} \tanh \left( \frac{\sqrt{\lambda^2 + \mu^2}}{\sqrt{2} \xi} \right), \]

(6.91)

with unity point normalization, \(|\varphi|^2 = 1\). This wave function is plotted in Fig. 6.13. An offset causes the linear vortex tubes in a quadrupole to curve into vortex rings.
FIG. 6.13: The magnitude \( \tanh \left( \frac{\sqrt{\lambda^2 + \mu^2}}{\sqrt{2} \xi} \right) \) (top) and for \( \xi = \frac{1}{10} \) and the phase \( \text{Arg}(\lambda + i\mu) \) (bottom), in two spatial dimensions on a grid of size \( L = 160 \), of the wave function (6.90) which has 4 vortex solitons in a quadrupolar arrangement consistent with periodic boundary conditions. This is a Clebsch potential representation of Fig. 6.12.
6.5 Quantum simulations

6.5.1 Poincaré recurrence

In Hamiltonian systems, the dynamics must be invertible, so it is possible to observe the system return arbitrarily closed to the initial conditions, and on time scales shorter than otherwise expected; vortex tubes untangle and reform by the absorption of sound waves to recover a configuration close to a configuration that occurred earlier in time in the flow. Recursion arising from the Hamiltonian system is observed in animations of the flow. This occurs in the limit of vanishing nonlinear interaction, \( g \ll 1 \), the vortex solitons completely untangle, as evidenced in Fig. 6.15 (by \( t = 21K \)), when the internal energy in (6.92) satisfies \( E_{\text{int}} \ll E_{\text{kin}}, E_{\text{qu}} \). Surprisingly in 3+1 dimensions, the Poincaré recursion time for the GP equation (6.1) can be extremely short.

To quantify this phenomenon, one can plot a time history of the kinetic, quantum and internal energy parts. In the \( N = 12 \) simulation with \( H_{\text{int}}(|\phi|^2) \sim 0 \), the reverse dynamics (absorption of sound waves) clearly repeats, cycling at \( t_p \sim 21K \), the Poincaré recursion time for grid size \( L = 512 \). This recurrence time is clearly evidenced in the time evolution of the (rescaled) kinetic \( E_{\text{kin}} \) and quantum \( E_{\text{qu}} \) energies plotted in Fig. 6.16.

The Poincaré recurrence theorem states that for Hamiltonian systems the solution trajectory passes arbitrarily close to the initial state provided the evolution is followed for a sufficiently long time. While for certain maps in two spatial dimensions, like the Arnold Cat Map, the Poincaré recurrence time can be short, for nearly all Hamiltonian systems the recurrence time is so long as to be effectively infinite. There have been some analytical hints that the NLS equation in 1+1 dimensions could have a fast Poincaré recurrence time [Tracy et al., 1984]—but this result was
FIG. 6.14: Starting with $N = 12$ vortex lines on a $512^3$ lattice. Vortex tubes at $t = 200K$ (left) show an onset of a Kelvin wave instability. Tangled vortices are observed, even when $H_{\text{int}} \sim 0$, at $t = 3.3K$ (right). Remarkably, one observes many vortex rings mediating the vortex line-line interactions.
FIG. 6.15: Continuing with the $N = 12$ simulation on a $512^3$ grid, at $t = 11K$ (left) is highly tangled but closer to a spherically symmetric configuration. This is just over halfway through the recurrence cycle. There are markedly different tangled configurations every few hundred time steps. Untangled vortices are observed at $t = 21K$ (right). The initial state recurs after a turbulent state. An ordered state at $t = 21K$ deterministically returns to the initial state untangling turbulence, cycling at intervals of $t_p = 21K$. 
FIG. 6.16: Top: The time evolution of the kinetic energy (blue), quantum energy (red), internal energy (green), and total constant energy (black line). The total energy is conserved. A recurrence of $t_p = 20.9K$ time steps is determined from the envelop of the forward energy cascade (dashed). Bottom: Power spectrum indicates all frequencies are represented as $|E(\nu)|^2 \sim [\nu(\nu_{max} - \nu)]^{-\frac{3}{4}}$ (red).
not expected to hold in three spatial dimensions. From a series of quantum simulations we see the Poincaré recursion time scales as $L^2$, where $L$ is the (linear) grid size. This arises from the inherent diffusive ordering of fluctuations, $\frac{\hbar}{m} \delta t \approx \delta x^2$.

### 6.5.2 Quantum Kelvin waves demarcated by Poincaré recursion

We examine hydrodynamic-scale breaking of the quantum-scale time-reversal symmetry of the free system. $H_{\text{int}} \sim g |\varphi|^2$ breaks the Poincaré recursion and has a prominent effect on the dynamics of the quantized line vortices. Yet, it remains useful to chart the pathway to turbulent configurations at intervals demarcated by the Poincaré recurrence time of the free system. In the interacting GP limit, the fast recursion is broken by nonlinear twisting (Kelvin waves) riding on the originally linear vortices, $H_{\text{int}}$ successively twisting the filamentary centers every recursion period; see Fig. 6.17. The linear vortex tubes become tangled but at the free recurrence period they do not return to their original linear configuration. Instead, they become twisted and this twisting increases with more and more free Poincaré cycles.

At very large times, the BEC manifests quantum turbulence, characteristic of nonlinear fluid behavior. In this numerical simulation, $L = 160$ and the smallness in the nonlinear interaction is set to $g \tau'/\hbar = 0.1$. To sufficiently resolve the vortex core, the scale factor in the Padé approximant is set to $a = 0.05$. A convention of unity normalization is used ($\int |\varphi(x)|^2 dx^3 = 1$). Poincaré recurrence in the $g \ll 1$ limit occurs at $t_P \approx 2020$, and this time period is used to sample the wave function configurations of the GP quantum system with $g \approx 5$. 
FIG. 6.17: Kelvin waves seen as twisting of \((N = 8)\) vortex filaments when \(H_{\text{int}}(|\phi|^2) = |\phi|^2(1 - |\phi|^2)\). In the \(g \sim 0\) limit (non-interacting particles), there is a fast Poincaré recurrence time of \(t_p = 2020\). For \(g \approx 5\), vortices at the first few Poincaré cycles \((t = 0, t_p, 2t_p, 3t_p)\) are plotted (top to bottom). The Kelvin wave twisting in the vortices eventually completely breaks the fast Poincaré recurrence. The highly tangled vortices, similar to that of Fig. 2, occurring between the Poincaré periods are not shown. The asymmetry in the time is due to the broken symmetry of the initial condition.
6.5.3 Quantum turbulence

Spectra for incompressible kinetic energy

A Kolmogorov spectrum is observed in incompressible and quantum energies of the BEC superfluid for \( k < 30 \), see Fig. 6.18. The emergence of fully developed quantum turbulence is plotted at time \( t = 27.7K \) for a \( 1024^3 \) lattice starting with \( N = 12 \) vortex solitons (1 quadrupole per spatial direction). The measured power law \( k^{-1.61} \) (black) may suggest that the theoretical \( k^{-5/3} \) Komolgorov power law describes the spectrum for \( k \lesssim 20 \), although the fit is not excellent at this small lattice size. A new power law \( k^{-5.87} \) (green) emerges in a quantum-classical transition region from \( 30 \lesssim k \lesssim 70 \). After \( k \gtrsim 70 \), the observed power law \( k^{-3.16} \) (red) agrees with the theoretical prediction of \( k^{-3} \) for a quantum vortex spectrum and excellently fits the data in this region. The power law fits were all computed using linear regression.

The bottom plot in Fig. 6.18 shows the three power regimes in a spatial view by overlaying the cut-off lengths on the vortex core profile. The \( k^{-3} \) power law characterizes fluid dynamics within the vortex core itself, with an upper cut-off scale measured to occur at \( r = 8.44 \) (in lattice units). The \( k^{-5.87} \) power law occurs near the boundary of the vortex core, with lower and upper spatial cut-offs, \( 8.44 \lesssim r \lesssim 19.71 \). The \( k^{-1.61} \) power law occurs on spatial scales larger than vortex core size. For very large wave numbers \( k \gtrsim 300 \) (with a cut-off of about just 2 lattice cell sizes), the spectrum all together drops off the chart, as expected.

In Sec. 5.2.5, we decomposed the conserved energy of the condensate into its average classical kinetic energy, quantum kinetic energy, and internal energy parts:

\[
\overline{E_{\text{TOT}}} = \overline{E_{\text{kin}}^{\text{cl}}}(t) + \overline{E_{\text{kin}}^{\text{qu}}}(t) + \overline{E_{\text{int}}}(t) = \text{const.}
\]

\[
\left( \overline{E_{\text{kin}}^{\text{cl}}}(t), \overline{E_{\text{kin}}^{\text{qu}}}(t), \overline{E_{\text{int}}}(t) \right) \overset{(5.27)}{=} \int d^3x \left( \left| \sqrt{\frac{m \rho}{2}} \mathbf{v} \right|^2, \left| \frac{\hbar}{\sqrt{2m}} \nabla \sqrt{\rho} \right|^2, \left| \sqrt{\frac{g}{2}} \right|^2 \right).
\]
FIG. 6.18: Power spectrum of the quantum fluid's incompressible kinetic energy (top). There are three regions characterized by differing power laws displayed on the vortex soliton spatial profile (bottom). Numerical data (dots) is from a supercomputer simulation of a quantum lattice gas on a $1024^3$ grid. Kolmogorov (black), transition (green), and core interior (red) regimes are shown.
The classical kinetic energy is separated into its compressible and incompressible parts by expressing the velocity field in terms of its rotational and irrotational parts, \( \mathbf{v} = \mathbf{v}^c + \mathbf{v}^i \). The following inverse Fourier transform decomposition separates the compressible part of \( \mathbf{v}(x) \) from its incompressible part:

\[
\mathbf{v}^c(x) = \int \frac{d^3k}{(2\pi)^3} e^{ik \cdot x} \left[ \hat{k} \cdot \hat{\mathbf{v}}(k) \right] \hat{k}
\]

\[
\mathbf{v}^i(x) = \int \frac{d^3k}{(2\pi)^3} e^{ik \cdot x} \hat{k} \times \hat{\mathbf{v}}(k) = \mathbf{v}(x) - \mathbf{v}^c(x),
\]

where \( \hat{\mathbf{v}}(k) \) is the Fourier transform of \( \mathbf{v}(x) \). As an analytical check of (6.93), it is straightforward to show that \( \mathbf{v}^c(x) \) is curl-free (irrotational) and \( \mathbf{v}^i(x) \) is divergence-free (rotational):

\[
\nabla \times \mathbf{v}^c(x) = \int \frac{d^3k}{(2\pi)^3} e^{ik \cdot x} i \hat{k} \times \hat{k} \left[ \hat{k} \cdot \hat{\mathbf{v}}(k) \right] = 0
\]

\[
\nabla \cdot \mathbf{v}^i(x) = \int \frac{d^3k}{(2\pi)^3} e^{ik \cdot x} i \hat{k} \cdot \left[ \hat{k} \times \hat{\mathbf{v}}(k) \right] = 0.
\]

Such a decomposition procedure is routinely used—for example by Nore, Abid, and Brachet [Nore et al., 1997b], Kobayashi and Tsubota [Kobayashi and Tsubota, 2005], and by us—to isolate the incompressible part of the flow when computing the kinetic energy spectrum. In the literature on classical turbulence, it is the incompressible part of the flow, in the inertial range, that contributes to the Kolmogorov \( k^{-5/3} \) power-law. The inertial range is demarcated by an outer scale associated with large anisotropic forcing and an inner scale associated with viscous dissipation. In this inertial range, isotropic turbulence is dominated by incompressible (rotational and convective) Eulerian flow.

Computationally, to determine the kinetic energy spectrum, one first computes the vector field

\[
\mathbf{F} = \frac{\hbar}{\sqrt{2m}} \frac{\varphi^* \nabla \varphi}{\sqrt{|\varphi|^2}}.
\]

Next, one separates the compressible and incompressible parts using the inverse Fourier transform decomposition, \( \mathbf{F} \overset{(6.93)}{=} \mathbf{F}^c + \mathbf{F}^i \). Then, one numerically determines
the right-hand side of the incompressible kinetic energy in (6.92) from $F^i$ as follows:

$$\left(\frac{h}{\sqrt{2m}}\nabla\sqrt{\rho}\right)^i = \text{Re}[F^i], \quad \left(\frac{m\rho}{2}\nu\right)^i = \text{Im}[F^i]$$

with $\rho^2 = |\varphi|^4$. \hfill (6.96)

Most of our simulations had as initial conditions a set of 12 straight line vortices consisting of three groups of 4 vortices, with the group axes in the $x$, $y$ and $z$ directions. Because the space is periodic, these lines are topologically loops. The groupings by 4 was to ensure periodicity, as discussed in Sec. 6.4.2.

On the top of Fig. 6.19 we present the incompressible kinetic energy spectrum spectra from our simulation of the GP equation on a $2048^3$ grid for $a = 0.02$ and $g = 3$ at evolution time $t = 8K$ and $t = 20K$ (in lattice units). The power laws are determined by linear regression. Thus, within a single simulation run, we find that the incompressible kinetic energy spectrum has three distinct power law $k^{-\alpha}$ regions that range from the classical turbulent regime of Kolmogorov for "large" scales (much greater than the individual quantized vortex cores) to the quantum vortex spectrum at the "small" scales (on the order of the individual quantized cores and smaller). There is a semi-classical region adjoining the Kolmogorov and quantum vortex spectra, with rich Kelvin wave dynamics. For these intermediate wave numbers, we observe a power-law behavior is $k^{-\alpha}$, where the exponent is $6 \lesssim \alpha \lesssim 7$.

These three power-law regions are quite robust as shown in middle and bottom of Figs. 6.19 from simulations on larger grids: $3072^3$ and $5760^3$ and different initial conditions. In particular, the initial conditions for the $5760^3$ grid simulation are chosen to have very long Poincaré recurrence time. Since the GP equation is Hamiltonian, Poincaré recurrence exists for arbitrary initial conditions. We found Poincaré recurrence to occur very rapidly for these simple 12-vortex systems (because of space limitations we shall discuss these results elsewhere). Hence to have very large Poincaré recurrence times we chose initial conditions of the form
FIG. 6.19: The incompressible kinetic energy spectra for a periodic 12-vortex set with $a = 0.02$, and an initial core inner radius is approximately $\xi = 10$ lattice units. The linear regression fits for power-law $k^{-\alpha}$ yield $\alpha's$ given in Table I. There are 3 distinct spectral regions: (a) $k^{-\frac{5}{3}}$ Kolmogorov energy cascade for small $k$, (b) steep semi-classical transition region for intermediate $k$, and (c) $k^{-3}$ quantum vortex spectrum for large $k$. The Kolmogorov cascade becomes robust for large grids, as seen by the insets.
The exponent $\alpha$ for the spectral $k^{-\alpha}$ are given in Table 6.1, together with the range of $k$ for these regions. A linear regression fit for the Kolmorogov range is shown in Fig. 6.19. A similar fit for the quantum vortex spectrum range is not shown since there is no point scatter about the regression line. The sharp drop-off in the spectrum at the end of the quantum vortex spectrum is due to the emission from very short wavelength phonons.

<table>
<thead>
<tr>
<th>GRID</th>
<th>KOLMOGOROV</th>
<th>SEMI-CLASSICAL</th>
<th>KELVIN WAVE</th>
</tr>
</thead>
<tbody>
<tr>
<td>2048$^3$</td>
<td>1.73 ($6&lt;k&lt;30$)</td>
<td>6.59 ($60&lt;k&lt;140$)</td>
<td>2.96 ($250&lt;k&lt;600$)</td>
</tr>
<tr>
<td>2048$^4$</td>
<td>1.84 ($6&lt;k&lt;30$)</td>
<td>6.34 ($60&lt;k&lt;140$)</td>
<td>2.97 ($250&lt;k&lt;600$)</td>
</tr>
<tr>
<td>3072$^4$</td>
<td>1.69 ($7&lt;k&lt;45$)</td>
<td>7.11 ($120&lt;k&lt;200$)</td>
<td>3.01 ($220&lt;k&lt;1000$)</td>
</tr>
<tr>
<td>5760$^4$</td>
<td>1.68 ($90&lt;k&lt;230$)</td>
<td>7.12 ($430&lt;k&lt;600$)</td>
<td>3.00 ($1000&lt;k&lt;1650$)</td>
</tr>
</tbody>
</table>

6.5.4 $k$-space power-law subranges

The Kolmogorov wave number $k_c$ marks the end of the $k^{-5/3}$ inertial subrange, characteristic of fully-developed isotropic turbulence. It is over the inertial subrange where a dissipation-free Richardson cascade is operative. To determine $k_c$, one first determines the spatial cutoff $r_c$ by matching the integrals as depicted in Fig. 5.2:

$$\int_{r_c}^{\infty} (2\pi r dr) \frac{1}{r^2} = \int_{0}^{\infty} (2\pi r dr) \frac{\rho(r)}{r^2},$$

(6.97)

where $r$ is the radial distance to the filament and one uses the Padé approximant

$$\rho(r) = \frac{11a^2+12+11ar^2}{384+ar^2(128+11ar^2)}.$$  

Then, one finds that $k_c \sim 1/(\pi r_c)$. In the quantum simulation one can recover hydrodynamic fluid dynamics for small wave numbers $< k_c$ because the quantum vortex core size $\sim r_c$ is smaller than the classical dissipation scale length $\sim \pi r_c$. The quantum coherence length $\xi \approx r_c$ is the physical length.
scale associated with the inner radius of a quantum vortex core. Within this
scale, one can observe high-\(k\) quantum Kelvin modes, however the predominant
wave number range for Kelvin waves is the transition region. The outer radius of
the quantum vortex is about a factor of \(\pi\) larger than the coherence length. These
two lengths correspond to the bends in the spectral plot of \(E_{\text{incomp}}(k)\).

Thus we define two wave number scales or transitional wavenumbers, \(k_{\text{inner}}\)
and \(k_{\text{outer}}\). The transitional wave numbers \(k_{\text{inner}}\) and \(k_{\text{outer}}\) correspond to the bends
in the spectral energy of the quantum fluid, demarcating the \(k\)-space boundaries
between the three important cascade regions. For an \(L^3\) grid, the transitional wave
numbers scale as follows:

\[
\begin{align*}
k_{\text{inner}} & \approx \frac{\sqrt{3} L}{2 \xi} \quad (6.98a) \\
k_{\text{outcr}} \equiv k_{\text{outer}} & \approx \frac{\sqrt{3} L}{2 \pi \xi}. \quad (6.98b)
\end{align*}
\]

The resolution limit of the calculation is set by the unit lattice size:

\[
k_{\text{grid}} = \frac{\sqrt{3} L}{2 \ 1.0}. \quad (6.99)
\]

The prefactor of \(\sqrt{3}\) above comes from \(\sqrt{k_x^2 + k_y^2 + k_z^2} = \sqrt{3} k\). The factor of \(1/2\) comes from the periodicity of the Fourier transform. \(k_{\text{grid}}\) is the phonon emission
limit (lattice cutoff). This ultraviolet cutoff moves to the right with increasing grid
divide \(L\). Expressing the critical wave numbers in terms of the grid size and the inverse
of the coherence length allows for a physical interpretation of these characteristic
scales. The fluid dynamics on scales \(\gg \pi \xi\) is effectively classical incompressible
viscous hydrodynamics, where the effective kinematic shear viscosity is \(\nu \equiv \pi \xi c_s\),
where \(c_s\) is the acoustic sound speed.
Intracore normal fluid dynamics

Within the core itself there exists a remarkable amount of self-similar fluidic activity that gives rise to a pronounced $k^{-3}$ quantum subrange $k_q > k_{\text{inner}}$. This subrange is universal to quantum fluids, i.e. independent of the initial large-scale flow structure. The $k^{-3}$ power-law is consistent with our theoretical understanding of the superflow dynamics: it is due to the filamentary quantum vortices in the superfluid. Furthermore, in turbulent conditions, these quantum vortices support a quantum Kelvin wave cascade, for $k \lesssim k_\xi$, where the mode-mode coupling mechanism is kelvon-kelvon coupling, but also includes kelvon-to-phonon and photon-to-kelvon indirect couplings. Thus incompressible energy (in kelvon modes) can be converted to compressible energy (phonon modes) and vice versa as driven, for example, by the right-hand side of (5.17).

6.6 Conclusion

An ab initio quantum lattice gas model of a superfluid was presented that captures the dynamical condensate vacuum governed by the GP equation as well as the Bogoliubov quasiparticle excitations vital to the quantum vortex dynamics. The method accurately captures the dynamical behavior the superfluid even in the difficult case of fully developed quantum turbulence. The quantum lattice gas method outperforms other competing numerical methods, including finite difference, spectral decomposition, vortex-filament, and advective real Ginzburg-Laudau methods.

Kolmogorov scaling of the incompressible kinetic energy spectrum should naturally occur at small wave number in low-temperature superfluids because the effective hydrodynamic-level equation of motion is a viscous Navier-Stokes equation. Thus, large-scale superfluid turbulence is akin to classical turbulence.\textsuperscript{15} The quant-

\textsuperscript{15}It has recently been observed in experimental observations of superfluid Helium II that the
The Navier-Stokes equation is derived in Chapter 7, where we address the quantum information theoretic underpinnings of turbulence. Interacting quantum vortices lead to fluid instabilities in the unitary quantum fluid that cause an energy cascade in the regime of small wave numbers, leading to power law behavior akin to $k^{-\frac{5}{3}}$ Kolmogorov turbulence in classical Navier-Stokes fluids. However, at larger wave numbers (approaching the scale of the vortex cores), the spectrum of incompressible kinetic energy transitions to another universal power law characteristic of quantum fluid flow, the quantum vortex $k^{-3}$ spectrum. For weakly nonlinear BEC superfluids, it is possible to observe fast Poincaré recurrence where at each recurrence time, Kelvin waves are observed to emerge with greater amplitude at each recurrence time, viz., vortex solitons that are successively twisted.

The distribution of velocity in decaying quantum turbulence has strongly non-Gaussian $1/v^3$ power-law tails [Paoletti et al., 2008].
CHAPTER 7

Turbulence

7.1 Introduction

Finding an analytical solution of a hydrodynamic field theory that represents turbulent flow remains the oldest and most prominent of classical grand challenge problems, open now for over 150 years. It has withstood theoretical attempts employing advanced statistical methods and perturbation methods, borrowed from quantum field theory and statistical mechanics [Kraichnan, 1973].\(^1\) Here we consider turbulence from the perspective of conserved information. The basic case we presented in Chapter 6, and continue to expound upon here, is that an analytically smooth momentum density field, \(m\rho \nu = \hbar |\phi|^2 \nabla \phi\), can represent classical turbulence. That is, at its small wave number scales, a state of quantum turbulence specified by the configuration of the nodal lines \((\varphi = \phi e^{i\theta} = 0)\) represents classical turbulence.\(^2\) That classical turbulence emerges from a turbulent condensate at small wave numbers was evidenced in Sec. 6.5.3 using the kinetic energy spectrum. This rather

\(^1\)Kraichnan began his study of turbulence while at Princeton when he and Einstein noticed great similarity between the classical theories of hydrodynamics and gravity.

\(^2\)Albeit, to correctly predict the configuration and interaction of the nodal lines one requires a microscopic quantum particle treatment.
remarkable situation follows from the property of a superfluid whereby its hydrodynamic equations of motion have the form of a viscous Navier-Stokes equation with shear viscosity \( \eta = \hbar \rho / 4 \). We derive the condensate Navier-Stokes hydrodynamic equations in Sec. 7.3.1 and show that the velocity field supporting viscous shear comes from a gradient of the condensate density, \( \mathbf{w} = \frac{\hbar}{m \rho} \nabla \rho \), and not from \( \mathbf{v} \) (as it does in classical turbulence theory). The tangled configuration of quantum vortices in the quantum turbulent state in three-dimensional space is ultimately reducible, through reconnections, to a rather simple link formed from a number of quantum vortex rings.

As commonly understood, the basic dilemma in turbulence is that in the macroscopic (hydrodynamic) limit on a many-body system, strong correlations and feedback mechanisms between large scale and small scale flow structures, over many decades of spatial separation, dominate the overall flow evolution, for example as shown in Fig. 7.1. The first high level model capturing the essential classical physics of this problem occurred in the 19th century, the incompressible Navier-Stokes equation (conservation of momentum) and continuity equation (conservation of particles)

\[
\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \mathbf{v}, \quad \nabla \cdot \mathbf{v} = 0, \quad (7.1)
\]

where \( \mathbf{v} \) is the flow field, \( P \) is the isotropic fluid pressure, \( \rho \) is the fluid (particle) density, \( \nu = \eta / \rho \) is the kinematic viscosity, and \( \eta \) is the viscosity quantifying shear dissipation, the renormalized transport coefficient for momentum diffusion.\(^3\) The strong correlation between disparate scales is captured by the extremely simple non-local convective derivative on the left-hand side of (7.1), a second order nonlinearity in the flow.

\(^3\)We are interested in inertial flow and topological dissipation mechanisms. The compressible flow equation (7.1) accommodates topological dissipation modulo bulk viscosity effects. Even though we consider energy-conserving flows, we leave out the heat equation and thus treat turbulence in a non-thermal limit. This limit, which is not to be confused with the incompressible limit, is appropriate to fluid flows where thermal excitations are not significant.
FIG. 7.1: During the onset of classical turbulence, strong coupling between large and small scale eddies is apparent in this fully resolved flow simulation of an incompressible Navier-Stokes fluid. Isosurfaces of vorticity are rendered. Helicity (dot product of the velocity and vorticity fields) is displayed in the red-blue color coding.
The reason a simple and meaningful solution of classical turbulence has remained beyond our reach for so long is that most early turbulence modelers attempted to use macroscopic scale information (i.e. averages and fluctuations of hydrodynamic variables) to represent macroscopic turbulent flow. Unfortunately, following this approach only leads to imprecision in defining a classical eddy. This imprecision inherently leads to ambiguity in sorting through the observed flow phenomenology. So with any high level approach one is left with dimensional arguments and simplifying conjectures. The standard conjecture in turbulent fluid dynamics is the Richardson cascade [Richardson, 1926]. This inertial cascade is characterized by self-similarity in the flow dynamics (picture large eddies breaking into smaller eddies and so on) that occurs above the dissipation scale, below which the hydrodynamic representation supposedly breaks down. A dissipationless Richardson energy cascade is identified in $k$-space by its characteristic power-law energy spectrum for homogeneous isotropic incompressible turbulence, the famous universal scaling law $k^{-5/3}$ predicted by Kolmogorov [Kolmogorov, 1941].

We proposed an entropic information-theoretic model of turbulence as a simpler alternative to (7.1) [Boghosian et al., 2001, Boghosian et al., 2003], [Boghosian et al., 2004a, Karlin and Gorban, 1998, Ansumali and Karlin, 2000], [Ansumali and Karlin, 2002, Chen et al., 2003]. In the entropic-informational approach, one models flow dynamics in a $Q$-dimensional kinetic phase space by tracking the probability distribution of particle occupations, where a particle at some point $x$ moves with velocity $c_q$, for $q = 1, 2, \ldots, Q$. In the Boltzmann representation, particle dynamics in position and momentum space space occur separately

$$f'_q(x) = f_q(x) + \Omega_q(f_1, \ldots f_Q) \quad (7.2a)$$

$$f_q(k) = e^{i\omega_0 k} f'_q(k), \quad (7.2b)$$
where \( f_q \) and \( f'_q \) are the incoming and outgoing kinetic variables, respectively, and \( f_q(k) \) is the momentum-space Fourier transform of \( f_q(x) \). The convex entropy function

\[
H(f_1, \ldots, f_Q) = \sum_q f_q \ln(\gamma_q f_q),
\]

(7.2c)

has self-consistently determined positive weights \( \gamma_q (\sum_q \gamma_q = 1) \). Information conservation determines the collision term \( \Omega_q \) in (7.2a) through the entropy constraint

\[
H(f'_1, \ldots, f'_Q) = H(f_1, \ldots, f_Q).
\]

(7.2d)

The hydrodynamic equations (7.1) are respectively replaced with moment equations

\[
\sum_q c_q f_q = 0, \quad \sum_q \dot{f}_q = 0,
\]

(7.2e)

where the number density is \( \rho = \sum_q f_q \) and the number current density is \( \rho \nu = \sum_q c_q f_q \). Equation (7.2e) are satisfied provided \( \sum_q c_q \Omega_q = 0 \) and \( \sum_q \Omega_q = 0 \).

In turbulent flow simulations, (7.2) is an accurate model—one that has outperformed other available methods based on (7.1). With (7.2) one can correctly resolve turbulent flow [Keating et al., 2007]—there is a dense tangle of vortex tubes. Turbulent flow regimes are attained by letting the kinematic viscosity approach zero, which occurs as entropy is locally conserved according to (7.2d). A brief review of our entropic method is given in Appendix E.1. From a large-scale flow perspective, classical eddies are represented by an organized complex of vortex tubes. Representing turbulent dynamics in informational terms is the right direction to go. Yet one can go further and represent turbulence directly in terms of microscopic quantum variables, whereby (7.2) can be recovered in the mesoscopic limit. And this represents an altogether new approach for modeling and understanding classical turbulence. In this regard, two alternatives have been investigated. The first alternative is an ab initio quantum informational model as a computationally efficient representation of (7.2), and this alternative was originally explored by the author.
This approach uses qubits to encode the local occupation probabilities, $|q_\alpha\rangle = \sqrt{f_\alpha}|1\rangle + \sqrt{1-f_\alpha}|0\rangle$. Here the hydrodynamic variables are $\rho = \sum_q \langle \psi|n_q|\psi\rangle$ and the number current density is $\rho \mathbf{v} = \sum_q c_q \langle \psi|n_q|\psi\rangle$. Unitary evolution of a $Q$ number of qubits per point followed by state localization (say via measurement) represents $\Omega_q$ in (7.2a). This quantum information model of classical fluid dynamics was the first measurement-based quantum computing algorithm, and it is the microscopic representation of (7.2) where $f_\alpha = \langle \psi|n_q|\psi\rangle$. The second alternative is an ab initio quantum information model of superfluids that uses the qubits in an altogether different way. An exposition of this second alternative was presented in Chapter 6—one approaches classical turbulence employing the flow dynamics of a superfluid in the small-$k$ limit. This approach uses $Q = 2$ number of qubits per point and employs unitary state localization. There are now two sets of hydrodynamic variables: the superfluid density $\rho_s = \langle \psi|h_{12} + n_1 n_2|\psi\rangle$ and the super current density $\rho_s \mathbf{v}_s = \hbar \nabla \arg \varphi_s$, where $\varphi_s = \psi_{00} + \psi_{11}$, as well as the normal fluid density $\rho_n = \langle \psi|h_{12} + n_1 h_2|\psi\rangle$ and the normal current density $\rho_n \mathbf{v}_n = \hbar \nabla \arg \varphi_n$, where $\varphi_n = \psi_{01} + \psi_{10}$. $\rho_s$ and $\rho_n$ are the number densities of tightly bound Cooper pairs and Bogoliubov quasiparticles.

Finally, in Sec. 7.3.3, we present a quantum information theoretic understanding of vortex reconnection and explain the localization of the quantum field. Then, in Sec. 7.3.4, we revisit the subject of the mutual interaction of two Kelvin waves (that we treated analytically in Sec. 5.3.2) and demonstrate through quantum simulation the phenomenon of vortex ring (roton) emission arising from the reconnection of two mutually interacting quantum vortices. Effective dissipation occurs as the Kelvin waves couple to phonons, during such reconnection events, when the phonons escape into the bulk of the quantum fluid.

---

4The computationally burdensome part of (7.2) is the evaluation of the collision function at any one point at any time. This collision function can be computed efficiently by a measurement-based quantum algorithm.
7.2 Navier-Stokes fluid

The long wavelength hydrodynamic behavior of a many-body system of neutral particles can be modeled at the macroscopic scale by an effective field theory, a set of coupled partial differential equations. The smooth fields of mass density, $\rho$, and flow velocity, $v$, obey a mass continuity equation and a viscous Navier-Stokes fluid equation of motion. There is also a parabolic heat equation for the energy density, yet we need not consider that for our present developments.

Because the mass increase within a region $\mathcal{R}$ is entirely accounted for by the flux of information into $\mathcal{R}$ through its boundary $\partial \mathcal{R}$, the hydrodynamic $\rho$ and $v$ fields (in the scaling limit) obey the continuity equation

$$\partial_t \rho + \partial_i (\rho v_i) = 0 + \cdots \tag{7.3}$$

which is a macroscopic scale restatement of conservation of information (bit density).

The field equation embodying Newton’s second law, for a region $\mathcal{R}$ expressing the change in the momentum density in terms of the stress applied at the boundary $\partial \mathcal{R}$, can be written in conservation form

$$\partial_t (\rho v_i) + \partial_j \Pi_{ij} = 0 + \cdots \tag{7.4}$$

a hydrodynamic scale restatement of conservation of bit flux density. Now following Landau and Lifshitz [Landau and Lifshitz, 1987], the momentum flux density tensor in Newtonian fluid can be written as

$$\Pi_{ij} = \rho \delta_{ij} + \rho v_i v_j - \eta \left( \partial_i v_j + \partial_j v_i - \frac{2}{D} \partial_k v_k \delta_{ij} \right) - \zeta \delta_{ij} \partial_k v_k + \cdots \tag{7.5}$$

where $\eta$ and $\zeta$ are the transport coefficients for the shear viscosity and bulk viscosity, respectively, and $D$ is the number of spatial dimensions of the system. The

\footnote{For non-divergent flow ($\partial_j v_j = 0$) in the incompressible fluid limit, (7.5) is $\Pi_{ij} = \rho \delta_{ij} + \rho v_i v_j - \eta (\partial_i v_j + \partial_j v_i)$. Furthermore, the gradient of the term $\eta \partial_i v_j$ in the momentum equation vanishes in this limit.}
momentum flux density tensor may be written as \( \Pi_{ij} = P\delta_{ij} + \rho v_i v_j - \sigma'_{ij} \), where the viscous stress tensor is

\[
\sigma'_{ij} \equiv \eta \left( \partial_i v_j + \partial_j v_i - \frac{2}{D} \partial_k v_k \delta_{ij} \right) + \zeta \delta_{ij} \partial_k v_k + \cdots .
\] (7.6)

The first two terms in (7.5) represent the ideal part of the momentum flux density tensor, which is the sum of the pressure term, \( P \), plus the convective term, \( \rho \mathbf{v} \mathbf{v} \), which is nonlinear in the velocity.

For a normal fluid the pressure \( P \) is a function of the mass density field, \( \rho = \rho(\mathbf{x}, t) \), whereas for a thermal fluid it also is a function of the temperature field, \( T = T(\mathbf{x}, t) \). The pressure tensor is diagonal because the fluid is isotropic. For a neutral fluid composed of independently moving particles, the pressure depends linearly on the mass density, \( P = c_s^2 \rho \), where \( c_s \) is the speed of sound in the fluid. In an hydrothermal system, the sound speed is temperature dependent, \( c_s = \sqrt{\frac{k_B T}{m}} \) (where \( k_B \) is the Boltzmann constant and \( m \) is the mass of a single quasi-particle). In this case the pressure obeys the ideal gas law, \( P = n k_B T \), where \( n = \rho/m \) is the particle number density. For an athermal hydrodynamic system (one where the system is at uniform homogeneous temperature, and where heat transport is neglected), \( c_s \) is a constant.

Substituting (7.5) into momentum equation (7.4), gives us the second equation of motion for a viscous isotropic fluid

\[
\rho \left( \partial_t v_i + v_j \partial_j v_i \right) = -\partial_i P + \rho \nu \partial^2 v_i + \left( \zeta + \frac{\eta}{D} \right) \partial_t \partial_j v_{ij} + \cdots .
\] (7.7)

This is the Navier-Stokes equation. In (7.7), \( \eta \) is the shear viscosity and \( \zeta \) is the bulk viscosity. The transport coefficient for momentum diffusion, \( \nu \equiv \eta/\rho \), is the kinematic viscosity. It gives a measure for the rate of decay of local shears in the fluid and determines how fast a perturbed fluid will relax from an anisotropic flow profile at the macroscopic scale to an isotropic steady state profile. Both the shear viscosity
and the bulk viscosity cause damping of compressional waves in the mass density field. The shear viscosity alone causes damping of shear waves in the momentum density field.

7.2.1 Dimensionless numbers

Let \( L \) and \( T \) denote the characteristic length and time scales, respectively, of a hydrodynamic scale fluctuation. That is, \( L \) and \( T \) are quantities characterizing the fluid's configuration at the macroscopic scale. Examples of the characteristic length scale for hydrodynamic flow are the wavelength of a compressional wave in the mass density field, the wavelength of a shear wave in the momentum density field, or the diameter of a fluid eddy in a normal fluid. The mean free path is the average distance a particle travels between collisions. Let \( \lambda \) and \( \tau \) denote the mean-free length and time, respectively, characterizing the microscopic particle collisions. Relevant hydrodynamic quantities are the

- characteristic flow speed, \( u \sim \frac{L}{T} \)
- sound speed, \( c_s \sim \frac{\lambda}{\tau} \)
- kinematic viscosity, \( \nu \equiv \frac{\eta}{\rho} \sim \frac{\lambda^2}{\tau} \)
- bulk viscosity, \( \zeta \).

The relevant dimensionless quantities are the

- Knudsen number, \( \text{Kn} \), defined as the ratio of the mean-free path to the characteristic length scale \( (\text{Kn} \equiv \frac{\lambda}{L}) \)
- Strouhal number, \( \text{Sh} \), defined as the ratio of the mean-free time to the characteristic time scale \( (\text{Sh} \equiv \frac{\tau}{T}) \)
• Mach number, $M$, defined as the ratio of the characteristic velocity to the sound speed ($M \equiv \frac{u}{c_s}$)

• fractional mass density variation, $\frac{\delta \rho}{\rho}$

• Reynolds number, $Re$, defined as the ratio of the product of the characteristic velocity times characteristic length to the kinematic viscosity (for incompressible flows $Re \equiv \frac{UL}{\nu}$ and compressible flows $Re \sim \frac{M}{Kn}$), about which we will say more about below.

### 7.2.2 Reynolds number

A measurement-based Q2 quantum lattice gas model in 1+1 dimensions has the effective field theory

$$
\partial_t u(x,t) + u\partial_x u(x,t) = \nu \partial_{xx} u(x,t) + \cdots,
$$

(7.8)

which is the Burgers equation, a rather simple model of shock formation with flow field $u(x,t)$ and kinematic viscosity $\nu$ but a very useful model (historically) for addressing some rudimentary issues in turbulence theory. We derived this equation in Chapter 4 as the effective field theory of the measurement-based Q2 model.

Multiplying (7.8) by $u$ and integrating over all space, with periodic boundaries, gives a relation for energy conservation where the time rate of change of the turbulent kinetic energy density $\partial_t \left( \frac{u^2}{2} \right)$ is balanced by the viscous dissipation $\varepsilon \equiv \nu \left( \frac{\partial u}{\partial x} \right)^2 \sim \frac{u_\sigma^2}{L_\sigma}$, where $L_\sigma$ is the characteristic scale of the largest feature in the flow field and $u_\sigma$ is the characteristic length scale associated with the turbulent kinetic energy (or eddy velocity) at the large scale.

The flow velocity, the kinematic viscosity, and the viscous dissipation quantities have the dimensions: $[u] = \frac{L}{T}$, $[\nu] = \frac{L^2}{T}$, and $[\varepsilon] = \frac{L^3}{T^2}$. The dissipation scale $\lambda \equiv \left( \frac{\nu^3}{\varepsilon} \right)^{\frac{1}{4}}$ is the smallest spatial scale where macroscopic effective field theory (7.8)
is physically applicable. So, the classical Kolmogorov wave number that marks the end of the $k^{-5/3}$ inertial subrange is the inverse of the dissipation scale length

$$k_c = \left( \frac{\varepsilon}{\nu^3} \right)^{1/4}.$$  \hfill (7.9)

At wave numbers $> k_c$, kinetic energy is ultimately dissipated for steady-state flows at a rate $\varepsilon$. In classical turbulence theory, one therefore considers the smallest flow velocity at the dissipation scale to be the dissipation-scale velocity $u_\lambda \equiv (\nu \varepsilon)^{1/4} = \frac{\xi}{\lambda}$.

The Reynolds number characterizing the fluid's nonlinearity is

$$\text{Re} \equiv \frac{L_o u_o}{\lambda u_\lambda} = \frac{L_o u_o}{\nu},$$  \hfill (7.10)

and using $\varepsilon = \frac{u_o^3}{L_o^3}$ to eliminate the characteristic large length scale $L_o$, we also have

$$\text{Re} = \frac{u_o^4}{\nu \varepsilon} = \left( \frac{u_o^2}{u_\lambda^2} \right)^2.$$  \hfill (7.11)

Note of course that consequently the Reynolds number can alternatively be expressed as a ratio of the large to small length scales: $\text{Re} = \left( \frac{L_o}{\lambda} \right)^{3/4}$. The minimum Reynold's number of a superfluid is a fundamental property of the superflow, and it is related to the uncertainty principle [Harvey, 1966].

### 7.3 Quantum turbulence

Quantum fluid dynamics is a topological reduction of classical fluid dynamics that brings to light crucial flow morphologies hidden at the classical level. Instead of vortex tubes disappearing at the viscous dissipation scale (the conventional viewpoint in turbulence theory), a remarkable classical-quantum flow transition occurs. Each vortex tube is represented by an organized complex of quantum vortices moving in concert, in the dilute quantum vortex limit [Kivotides, 2006, Alamri et al., 2008].

The quantum vortex (topological line defect in the phase of the complex scalar
quantum wave function at the microscopic scale) is the fundamental constituent of a classical eddy.

With further scale reduction, eventually a small multiple of the quantum coherence length is reached and one encounters a remarkable flow regime approaching the interior of the quantum vortex core itself. Then, within the quantum vortex core, there exists a rich flow dynamics that encapsulates all the macroscopic circulation in the fluid. At this small scale, the fluid dynamics is solenoidal (rotational) and effectively dissipative. Solenoidal flow is characterized by local shearing in the fluid and for this to occur there must be nonvanishing kinematic viscosity, or diffusive transport of momentum. Such a shear transport coefficient does indeed exist for a Hamiltonian-based quantum fluid. The operative kinematic viscosity is \( \frac{\hbar}{4m} \), fixed by the quantum particle mass and the Planck constant. It is a fundamental transport coefficient. Therefore, this leads one to conjecture that one way to mathematically specify a smooth momentum density flow field (with no singularities) for classical turbulence is to reduce the flow to a fundamental dynamical behavior of quantum vortices and quantum vortex-vortex interactions.

Provided the quantum vortices are well separated (in the dilute limit the separation distance between any two quantum vortices is much greater than the size of a quantum vortex) effective classical turbulence can occur. The physics underlying the Richardson cascade is ultimately reduced to well-defined reconnection events between filamentary quantum vortices, which leads for example to the exchange of small-scale intermediate quantum vortex loops. That is, at any one point in time, the turbulent flow manifold is reduced to a complex tangle (or a self-similar nested series of complex tangles in the case of fully developed turbulence) of closed quantum vortices. The complex of quantum vortices necessarily gives rise to a momentum density field that is smooth and continuous everywhere (in fact, while the velocity field has a divergent singularity at the center of quantum vortex core, the momentum
density field vanishes at the center and so is analytically well defined).

### 7.3.1 Condensate Navier-Stokes hydrodynamics

Here we demonstrate that the operative hydrodynamic-level momentum equation governing the superfluid's condensate field has the precise form of a viscous Navier-Stokes equation. We begin by physically interpreting the nonlinear term 
\( h\Omega(p) \) appearing in (5.23a). When this quantity was first defined in (5.11b), we referred to it as the “internal potential energy” of the condensate. The irrotational part of the flow, the momentum field (mass times the velocity field) can be written as the gradient of the scalar action \( S = \delta \theta \) as in (5.40)

\[
m\nu = \nabla S. \tag{7.12}
\]

In terms of the velocity potential \( \Phi \equiv S/m \), (5.23a) is the Bernoulli equation

\[
\partial_t \Phi + \frac{v^2}{2} + \frac{h\Omega(p)}{m} = -\frac{V_s}{m}, \tag{7.13}
\]

so we can identify \( h\Omega(p) \) as the enthalpy. We can employ thermodynamics to calculate the local pressure in the superfluid. The enthalpy equals the sum of the internal energy and the flow work

\[
h\Omega(p) = E_{int}(p) + \frac{P(p)}{\rho}, \tag{7.14}
\]

or

\[
P(p) = h\Omega(p) - V_n(p) + \mu \tag{7.15a}
\]

\[
= \rho^2 V_n'(p). \tag{7.15b}
\]
We now calculate the gradient of the enthalpy

\[ \nabla (h\Omega) \overset{(5.12)}{=} \nabla [V_h - \mu + \rho V_h'] \]  
(7.16a)

\[ = \nabla V_h + (\nabla \rho) V_h' + \rho \nabla V_h' \]  
(7.16b)

\[ = 2(\nabla \rho) V_h' + \rho \nabla V_h' \]  
(7.16c)

\[ = \frac{1}{\rho} \left[ 2(\rho \nabla \rho) V_h' + \rho^2 \nabla V_h' \right] \]  
(7.16d)

\[ = \frac{1}{\rho} \nabla \left( \rho^2 V_h' \right) \]  
(7.16e)

\[ \overset{(7.15b)}{=} \frac{\nabla \rho}{\rho}, \]  
(7.16f)

and the gradient of the Bohm potential (using overdot notation \( \nabla \rightarrow \partial_i \) and \( \nabla \rightarrow \partial_j \))

\[ \nabla V_b \overset{(c.52)}{=} -\frac{\hbar^2}{4m} \nabla \left[ \frac{\nabla^2 \rho}{\rho} - \frac{1}{2} \left( \frac{\nabla \rho}{\rho} \right)^2 \right] \]  
(7.17a)

\[ = -\frac{\hbar^2}{4m\rho} \nabla (\nabla^2 \rho) \]  
(7.17b)

\[ - \frac{(\nabla \rho) \nabla^2 \rho}{\rho} + \frac{(\nabla \rho)(\nabla \rho)^2}{\rho^2} - \frac{(\nabla \rho) \cdot \nabla \nabla \rho}{\rho} \]  
(7.17c)

\[ = -\frac{\hbar^2}{4m\rho} \nabla \left[ \frac{\nabla^2 \rho}{\rho} - \frac{(\nabla \rho) \nabla \rho}{\rho} \right] \]  
(7.17d)

\[ = -\frac{\hbar^2}{4m\rho} \nabla \nabla \rho - \frac{(\nabla \rho) \nabla \rho}{\rho} \]  
(7.17e)

\[ = -\frac{\hbar^2}{4m\rho} \nabla \left[ \rho \nabla \left( \frac{\nabla \rho}{\rho} \right) \right] \]  
(7.17f)

\[ = -\frac{\hbar^2}{4m\rho} \nabla \left[ \frac{\rho}{2} \left( \frac{\nabla \rho}{\rho} + \frac{\rho}{m} \frac{\nabla \sqrt{\rho}}{\sqrt{\rho}} \right) + \frac{\rho}{m} \frac{\nabla \sqrt{\rho}}{\sqrt{\rho}} \right] \]  
(7.17g)

The quantity in square brackets is a second rank tensor that has the form of a viscous stress tensor with shear viscosity

\[ \eta = \frac{\hbar \rho}{4} \]  
(7.18)
The viscous stress tensor may be rewritten as follows

\[ \sigma'_{ij} \overset{(7.17g)}{=} \eta (\partial_t w_j + \partial_j w_i), \quad (7.19a) \]

where the velocity field supporting shear is defined as

\[ \mathbf{w} \equiv \frac{\hbar}{m} \frac{\nabla \sqrt{\rho}}{\sqrt{\rho}} \overset{(5.33)}{=} -3 [\mathbf{v}_{qu}]. \quad (7.19b) \]

Then (7.17) becomes

\[ \partial_t V_b = -\frac{1}{\rho} \partial_j \sigma'_{ij}. \quad (7.20) \]

Taking the gradient of (5.23a), we can use this result for the gradient of the Bohm potential and the previous result for the gradient of the enthalpy to put the equations of motion into the form of viscous hydrodynamic fluid equations

\[ \partial_t (m v_i) + \partial_i \left( \frac{1}{2} m v^2 \right) \overset{(7.16f)}{=} \frac{\partial_i p}{\rho} + \frac{\partial_j \sigma'_{ij}}{\rho} \quad (7.21a) \]

\[ \partial_t \rho + \partial_j (\rho v_j) = 0. \quad (7.21b) \]

The set (7.21) are viscous hydrodynamic fluid equations for the form of the Navier-Stokes and continuity equations (7.1). The left-hand side of (7.21a) can be rewritten as

\[ \rho \partial_t (m \mathbf{v}) + \rho \nabla \left( \frac{1}{2} m \mathbf{v}^2 \right) = \partial_t (m \rho \mathbf{v}) - (\partial_t \rho) m \mathbf{v} \]

\[ + \ m \rho (\dot{\mathbf{v}} \cdot \nabla) \mathbf{v} + m \rho \mathbf{v} \times (\nabla \times \mathbf{v}) \overset{(7.21b)}{=} \partial_t (m \rho \mathbf{v}) + \nabla \cdot (m \rho \dot{\mathbf{v}}) \mathbf{v} \]

\[ + \ m \rho (\dot{\mathbf{v}} \cdot \nabla) \mathbf{v} + m \rho \mathbf{v} \times \mathbf{\omega} \overset{(7.21b)}{=} \partial_t (m \rho \mathbf{v}) + \nabla \cdot (m \rho \dot{\mathbf{v}} \mathbf{v}) \]

\[ + \ m \rho \mathbf{v} \times \mathbf{\omega}. \]

According to (5.43), the vorticity is maximally large at the center of a rectilinear quantum vortex but vanishes everywhere else. Since the momentum density \( m \rho \mathbf{v} \)
vanishes at the center, as shown in Fig. 7.2, the last term in (7.22c) vanishes everywhere. Thus the momentum equation (7.21a) can be written as

\[ \partial_t (m \rho v_i) + \partial_j (m \rho v_i v_j) \overset{(7.22c)}{=} -\partial_i P + \partial_j \sigma'_{ij}, \]  

(7.23a)

or

\[ \partial_t (m \rho v_i) + \partial_j \Pi_{ij} = 0, \]  

(7.23b)

where the momentum flux density tensor is

\[ \Pi_{ij} = P \delta_{ij} + \rho v_i v_j - \sigma'_{ij}. \]  

(7.24)

Equation (7.23b) is in standard fluid dynamics form of (7.4). The quantum hydrodynamic equation analog of the viscous Navier-Stokes equations have been studied as the basis of an inverse kinetic theory of the phase-space Schrödinger dynamical system [Tessarotto et al., 2007]. They have also been explored regarding a connection to the noisy Burgers equation [Ribeiro and Peixoto de Faria, 2005]. Recently, the quantum hydrodynamic equation (7.23) has been used to make a connection between Brownian motion and quantum motions with respect to Cooper pair formation in superconductivity [Isimori, 2010].

### 7.3.2 Quantum vortex as a soliton

The hallmark of a quantum vortex is that the probability at a point associated with the condensate amplitude field vanishes at the center of the vortex core and asymptotes to the background density of the bulk quantum fluid. The quantum fluid behaves like a free fluid in the bulk region satisfying the linear Schroedinger equation. Within the core, the magnitude of the condensate wave function goes to zero

\[ |\varphi(r)| = \rho(r)^{\frac{1}{2}} \approx \sqrt{a} \tanh \left( \frac{2}{3} \sqrt{\lambda \sin \frac{\pi r \sqrt{a}}{\lambda}} \right) \approx \sqrt{\frac{11 a^2 r^2 (12 + a r^2)}{384 + a^2 (128 + 11 a r^2)}}, \]  

(7.25)
where \( \lambda = \frac{2\pi}{27} (8\pi + \sqrt{243 + 64\pi^2}) \). If one follows a closed contour in the bulk region of the quantum fluid where the contour encloses a single vortex center, then the phase of the wave function must be quantized in units of \( 2\pi n \), where the quantum vortex is said to have winding number \( n = 1, 2, 3, \ldots \) \( n > 1 \) vortices separate into singly charged quantum vortices due to Kelvin wave instabilities driven by local particle dynamics within the cores.

FIG. 7.2: Quantum vortex profiles for \( g = 1 \) in lattice units with a scale factor \( a = 0.02 \):
- (BROWN) Condensate magnitude \( \rho(r)^\frac{3}{4} \).
- (BLUE) Momentum density \( u_\theta(r)/a = \rho(r)v_\theta(r)/a \).
- (BLUE DASHED) Divergent angular velocity \( v_\theta(r) = \hbar/(mr) \).
- (BLACK) Momentum density \( \Im[u_r^{\text{av}}(r)]/a = \rho(r)\Im[v_r^{\text{av}}(r)]/a \).
- (BLACK DASHED) Divergent angular velocity \( \Im[v_r^{\text{av}}(r)] \).
- (RED) Kelvin waves extend to the coherence length \( \sim \xi \).
- (GREEN) Quantum transition region extends out to \( \sim \pi \xi \).

### 7.3.3 Microscopic picture of vortex reconnection

A behavior characteristic to mutually interacting quantum vortices is vortex-vortex reconnection. Vortex reconnections contribute to the Richardson cascade [Richardson, 1926], providing a pathway whereby long vortex filaments can bend, successively, breaking ultimately into smaller vortex loops [Tsubota et al., 2000].
This reconnection process is the primary mechanism whereby a superfluid can ultimately have an inertial subrange at small $k$ with a classical Kolmogorov $k^{-5/3}$ spectrum. The bend in the particle world line is due to reconnection of the world lines of the participating quantum particles.

In Chapter 3, we have shown that perpendicular entangling gates "braid" the particle trajectory. The nonlinear interaction that is localized within the core\(^6\) decomposes the entangled state as if there had existed only one of two classical trajectories. Suppose the entangling gate operation in question occurs at $t_0$. Then the relation between the time histories are

\[
A^{-1} \left[ \frac{(e^z - 1)}{A^{-2}d} \right] \langle \tau \rangle = A \left[ \langle \tau \rangle - A \right] \langle , \right.
\]  

(7.26)

where unitary braid operator $A \langle \tau \rangle$ represents the quantum mechanical crossing (the fundamental reconnection) of both classical alternatives. This relationship connecting alternatives typifies (at the microscopic level) reconnection of two vortex solitons; it is the quantum information-theoretic representation of reconnection. An example of (7.26) at sufficiently large wave numbers to capture microscopic quantum effects cascading upward influencing the coherent flow structure of two interacting vortex cores is shown in Fig. 7.3. The vortex reconnection event occurs at time $t_0 = 48$.

Since there are only unitary processes occurring in the quantum fluid and all the time-histories of the particles are governed by a crossing relation of the form of (7.26), one might expect to see vortex solitons in superposition states, even at small wave numbers. For example, the $t = 24$ and the $t = 116$ configuration in Fig. 7.3 could exist simultaneously in quantum superposition on the large scale. Yet, in quantum simulations (run in a factored Hilbert space) we only see a progression through time from one classical alternative to the classical other. That is, we do

\(^6\)There exists a remarkable similarity between measurement and the projective nature of the nonlinear interaction that we discuss below and illustrate in Fig. 7.4.
FIG. 7.3: Time development vortex-antivortex reconnection on a $240^3$ grid. Probability isosurfaces of $|\psi|^2 = |\psi_1 + \psi_2|^2$ are plotted. At $t = 0$ (top), two independent vortex lines, oriented perpendicularly and separated in space (non-intersecting cores). By $t = 24$, the vortex-pair becomes unstable, inducing traveling Kelvin waves along the filamentary core. At $t = 48$, the two vortex cores connect, defined as $t_0$. By $t = 116$ (bottom), the cores are disconnected along the original orientations and reconnected at right angles. Induced quantum Kelvin waves are apparent.

not see a macroscopic scale superposition, the proverbial Schroedinger cat state on scales greater than the coherence (healing) length.

If we plot the condensate profile through a zero of the quantum vortex, going from one side of the center to the other including its phase that goes from plus to minus, then the profile appears as a kink (instead of a black soliton)

$$\varphi(r) \simeq \tanh \left( \frac{\pi r}{2\xi \sqrt{2}} \right), \quad -1 \leq r \leq 1,$$

(7.27)
as shown in the left side of Fig. 7.4. This profile informs us about the "one-way" informational dynamics within the core. Within the core, localization of the wave
function occurs by the nonlinear interaction, an effectively dissipative process operating within the core that self-consistently "turns-off" in the bulk. Such localization of a Q2 model in the vicinity of the core allows us to map the quantum algorithm for the Schrödinger wave dynamics onto the measurement-based quantum algorithm for Burgers dynamics. The Burgers equation admits an analytical kink solution too, derived in Appendix E.2 and shown in the bottom of Fig. 7.4. To match (7.27) where \( \varphi \to \pm 1 \) and \( r \to \pm \infty \), we can use the measurement-based quantum algorithm for the Burgers equation given in Sec. 4.2.3 for the case when the number density is bulk normalized to \( \rho = a + b = 1 \). Then, for \( b = 1 - a \), (4.23) reduces to a function of only one kinetic variable

\[
\Omega(a) = (1 - 2a) \sin^2 \frac{\vartheta}{2} + \sin(\vartheta)a(1 - a) \tag{7.28a}
\]

\[
= \sin^2 \frac{\vartheta}{2} + a(\cos \vartheta + \sin \vartheta - 1) - a^2 \sin(\vartheta). \tag{7.28b}
\]

Setting the occupation probability \( a = |\varphi|^2 \) in the measurement-based quantum algorithm, the resulting effective interaction potential is

\[
V_{\text{Burgers}}(\varphi) \approx (\cos \vartheta + \sin \vartheta - 1)|\varphi|^2 - \sin(\vartheta)|\varphi|^4, \tag{7.29a}
\]

which is diffeomorphic to

\[
V_{\text{BEC}}(\varphi) = \mu|\varphi|^2 - \frac{g}{2}|\varphi|^4 \tag{7.29b}
\]

appearing in (5.10) for the Lagrangian density of the condensate.\(^7\)

In Fig. 7.3, one expects that the alternative \( \big< \big> \) just before reconnection and \( \big\rangle \big\langle \) just after can be in quantum superposition only for a time shorter than the coherence time. This time scale corresponds to the time it takes a quasiparticle

\[^7\text{The equilibrium solution away from the kink front is found from } \Omega(a^{(0)}) = 0 \text{, which gives}
\]

\[
a^{(0)} = \frac{\csc \vartheta}{2} \left( \cos \vartheta + \sin \vartheta + \sqrt{2 - 2 \csc \vartheta - 1} \right). \tag{7.30}\n\]
to move away from the hole by a distance further than the healing length of the quantum vortex. Yet, quantum superposition (and quantum mode entanglement) between the quantum particle-hole pairs in the vicinity of the crossing point is an essential mechanism at the microscopic scale giving rise to reconnection in the scaling limit.

![Graph of a quantum vortex kink soliton](image)

**FIG. 7.4:** (LEFT) Quantum vortex is a kink soliton. The flow direction on the left of the center is the opposite from the direction on the right, viz., a phase shift of \( \pi \) radians occurs in the condensate wave function as one goes half way around a quantum vortex. (RIGHT) Time development of an analytical kink soliton solution for the velocity field \( u = 1 - \rho \) of Burgers equation (run for the case when the kinetic variables are constrained to \( \rho = a + b = 1 \)), shifted vertically for each time increment to avoid overlap. The two the kink solutions are identical. Away from the kink front, the bulk values of the respective fields are \( \pm 1 \).

### 7.3.4 Quantum Kelvin waves and intermediate vortex loop

Superfluids have two characteristic propagating excitations: acoustic sound waves (phonons) and quantum Kelvin waves (kelvons). Both are fluctuations in
the condensate density. Although phonons propagate through the bulk region (i.e., outside of the quantum vortices), kelvons exist riding on the vortex core. Kelvons arise from the gyration of particle-hole pairs as they orbit around and along the vortex axis, as shown in Fig. 7.5. These fermionic particles are Bogoliubov quasiparticles within the quantum vortex’s core [Simula et al., 2008], with a gyration frequency much slower than the orbital “cyclotron” frequency.

![Fig. 7.5](image.png)

**Fig. 7.5:** (a) Unperturbed vortex rendered over 160 cyclotron periods. (b) Four wavelengths of a kelvon riding on a larger vortex core, where $\Omega_{\text{cyc}} = \rho_c h/m_v$. (c) “Cyclotron” orbit in cross-section view, in units where the core inner radius (coherence length) is $\xi = 1.0$ (brown circle) and the gyration of a trapped quantum particle (small red circle) has a gyro-radius one quarter the core radius. The slow gyration displaces quantum vortex core (blue circle). (d) Quasiparticle trace for 20 cyclotron periods where the gyration frequency is $\Omega_{\text{cyc}}/40$, rendered as a closed world line.

A single quantum vortex can simultaneously support many kelvons. While phonons are produced as radiation emitted from the quantum vortex, kelvons are produced by vortex-vortex interactions, including reconnection, phonon exchange, and small vortex ring exchange. Regarding phonon scattering, kelvons directly couple to other kelvons, of both longer and shorter wavelengths (by phonon emission and absorption, respectively), contributing to a Kelvin wave energy cascade. They couple to themselves nonlinearly according to (5.17). There is no mechanism blocking kelvon oscillations down to scales of the vortex’s radius, and smaller.
In the case where there is a dense tangle of quantum vortices (in a turbulence superfluid), it is possible for there to be indirect kelvon-kelvon coupling between different (but adjacent) quantum vortices.\(^8\) The growth of quantum Kelvin waves due to the nonlinearity in the flow leads to rich flow morphologies, including horse-shoe shaped distortions of the quantum vortex filament. These horse-shoe distortions are large amplitude helical wave pulses and they can lead to the emission of small vortex rings as such distortions are pinched off.

\[
\text{FIG. 7.6: Simulation of vortex and anti-vortex filaments, originally linear and oriented perpendicularly on a } 1024^3 \text{ grid. Time steps } t = 1200\Delta t \text{ and } t = 4800\Delta t \text{ are plotted. Quantum Kelvin waves are seen along the vortex filaments early in the simulation. At the late stages, the filaments bend, reconnect, and exchange vortex rings.}
\]

Products of quadrupolar line solitons given in Sec. 6.4.2 may be shifted and rotated about any direction to build up more complicated initial conditions, which

\(^8\)In the low temperature physics community, it has been conjectured that quantum Kelvin waves can propagate in 3-space within a superfluid. Yet, this represents a different picture of the nature of the motion of such quantum Kelvin waves than presented here. Quantum Kelvin waves are strictly confined a filamentary core and thus propagate on some \(S^1\) embedding in 3-space. The possibility of indirect kelvon-kelvon between different filaments comprising a dense tangle should not be mistaken as Kelvin wave propagation in 3-space.
nevertheless retain periodicity. A simulation with two such orthogonal sets of vortex quadrupoles is shown in Fig. 7.6 (for a total of $N = 8$ vortex lines) on a $1024^3$ grid. In this superfluid simulation, quantum Kelvin waves occur very early on as seen in the top panel of Fig. 7.6. The filamentary cores kink into a horseshoe shape as seen in the bottom panel of Fig. 7.6, and then emit closed-loop vortex solitons that mediate the force between the larger vortex filaments. An expanded view of an emitted vortex loop is shown in Fig. 7.7.

### 7.4 Final remarks

Let us treat the filamentary quantum vortex like a directed strand (with its orientation determined by its vorticity). A single closed strand (as part of a larger link) that starts out as a simple closed loop (an unknot) can form into a complicated link through the nonlinear vortex-vortex interaction with another strand in the link as well as through a self-interaction of one segment of the strand with another segment of the same strand.\(^9\) If the global flow configuration has zero net angular momentum, then the simplest initial conditions one may consider is a quantum vortex-antivortex pair, topologically equivalent to an oriented link comprising two oppositely directed closed-loop strands. Furthermore, if periodic boundary conditions are imposed on the embedding space, then the simplest link one may consider is a quadrupole configuration of quantum vortices (a pair of quantum vortex-antivortex pairs). That is, the simplest link is a **quadrupolar flow configuration**, comprising four closed quantum vortices, that has zero net angular momentum and that may be placed in a box with periodic boundary conditions. Letting a plus sign ($\bullet +$) denote a quantum vortex oriented normal to the plane of the paper, with one unit of positive

\(^9\)In knot theory, a single closed strand is said to form a knot and multiple closed strands form a link.
FIG. 7.7: Spontaneous exchange of a vortex loop mediating a force between two orthogonally-oriented and separate vortex filaments. The exchange goes in both directions. This image is a small section of a $1024^3$ space computed with thousands of processors. Zoom-in online to see cuts in the vorticity isosurface that are inter-processor boundaries.
circulation $2\pi$ and letting a minus sign ($\bullet -$) denote one unit of negative circulation $-2\pi$, then an example quadrupolar vortex (4 quantum vortices) is

$$\bullet - \bullet + \bullet + \bullet -$$

This is a top-down view of the analytical Chebsch potentials representation of the condensate field given in Sec. 6.4.2. Three quadrupolar configurations, orthogonally oriented along the Cartesian directions, will topologically remain as a link of closed strands, but the link will become successively tangled. In the simplest case, a classical turbulent flow configuration is represented in a periodic space (obtained from a cube by gluing the opposite faces together) as a maximally tangled link comprising three quadrupoles (12 quantum vortices, each with integer winding number $n$). Therefore, turbulent viscous flow is topologically reducible to such a link (12 oriented loops, $S^1$, embedded the 3-space). The time evolution of the nodal lines, for twelve initial quantum vortex rings in a small system of size $L = 1024$, is shown in Fig. 7.8.

Reducing a snapshot of turbulent flow to a linkage of quantum vortices allows us to uniquely characterize the flow topologically at the time the snapshot is taken. Yet, in knot theory, links are basically static objects, the multiple embedding of circles ($S^1$) into three space. One considers how a link may be topologically deformed but one does not consider the dynamical process leading to the deformation of the strands in a link. In knot theory one merely imposes the restriction that the strands cannot be cut as they are deformed, nor can the deformation cause any strands to intersect one another.

There is the physically relevant question of how hydrodynamical evolution causes high-Reynolds number laminar flow configurations to ultimately fold into turbulent ones. Does there exist a simple yet comprehensive way to understand viscous flow dynamics in terms of tangles of strands? There does indeed exist another
FIG. 7.8: The evolution of quantum vortices showing the vortex bending, reconnection and formation of vortex loops on a $1024^3$ grid. Shown are ray traced surfaces of constant number density, $|\phi| = 0.08|\phi|_{\text{max}}$, that enclose the nodal lines in the condensate. (a) The initial 12 linear vortex cores (topologically equivalent to 12 vortex rings because of periodic boundaries). (b) At the early time $t = 2500$ large amplitude Kelvin waves have developed. (d) By $t = 55000$ a large number of reconnection events have occurred. (f) At $t = 60200$ the vortex tangle reduces to 12 small vortex rings topologically equivalent to the initial state. (i) The vortex cores at $t = 83500$ (green) closely resembling the initial state, but the Poincaré recurrence time occurs near $t = 167600$ (white). The “bulleys” are the intersection of the initial vortex cores with the walls at $t = 0$. 
deeper level of reduction but one must generalize knot theory to allow for the quantum mechanical interaction between strands, and this in turn leads to the notion of quantum superposition of links. In particular, this generalization allows for the quantum mechanical interaction of two strands and it is at such an “intersection point” where the fundamental physics occurs.

Up to this point in the discussion of turbulent flow expressed in terms of strands, it has been the quantum vortices themselves (or topological defect lines \( \varphi = 0 \) within the condensate wave function) that have been equated to strands. Yet, each quantum vortex is made of many quantum particles. All nonlinear vortex-vortex interactions are reducible to the level of crossing quantum particle world histories, and it is the tangle of these world histories that ultimately represents the turbulence flow topologically. The case we have pressed here is that a practical way to learn about superfluid dynamics (as well as classical fluid dynamics) is by using a quantum information theoretic model of the quantum fluid dynamics that gives rise to correlated quasiparticle pairs circulating around the quantum vortex core inherently giving rise to the quantum vortex as an emergent coherent soliton. The self-interaction of the quantum vortex soliton is due to the crossing intersection of the paths of quantum particles comprising the quantum vortex. Each crossing event is represented in an analytical way by \( \sqrt{\text{SWAP}} \) or \( \sqrt{\text{PAIR}} \) quantum logic gates. It is this quantum-gate level interaction between pairs of quantum particles in the model that is the basis for reconnection of a quantum vortex, allowing it to bend into smaller shapes. This in turn ultimately leads to the self-similarity of eddies and finally to the famous classical Richardson cascade observed at the large scales, and which is traditionally associated with classical turbulence. Therefore, a fundamental information-theoretic reason for classical turbulent flow structure is suggested, and to the best of my knowledge, for the first time. This is the first part of the turbulence puzzle.
Yet, as each quasiparticle of the quantum vortex is represented by correlated quantum particles, one can quantify how the flow configuration may be cast directly in terms of an important physical ingredient: quantum entanglement. Representation of the flow in terms of the production, transference, and destruction of quantum entanglement allows one to arrive at an even more complete physical picture. This is the second part of the puzzle. Thus, the isomorphism between links in knot theory and the quantum entanglement of many quantum particles is helpful to comprehend superflows and therefore this aspect of the research program is undergoing active investigation [Kauffman and Lomonaco, 2004, Yepez, 2009, Yepez, 2010].

As a confirmation of turbulent flow behavior, the Kolmogorov inertial subrange for small wave numbers is observed in quantum fluid simulations on sufficiently large grids that can cleanly represent large scale classical behavior: thus we have confirmed the theoretical predication that a turbulent quantum fluid behaves like a turbulent classical fluid on large scales [Yepez et al., 2009c]. These cascade effects are demonstrated with a Q2 quantum lattice gas; see Fig. 7.9 to view an example of the morphology of tangled quantum vortices comprising a state of quantum turbulence in the dense vortex limit.

In cold atomic vapor BEC experiments fully developed quantum turbulence has not been observed as it has in Helium II, yet the natural emergence of quantum vortex tangles have been recently observed in cold atom vapors. Such tangles can be observed in a freely expanding BEC after the trapping potential is turned off. Attempting to see quantum turbulence in a cold atomic vapor is presently at the forefront of BEC experimental work.
FIG. 7.9: This is a quantum lattice simulation of a BEC superfluid in 3+1 dimensions spontaneously giving rise to turbulent quantum flow. Plotted are ray-traced surfaces of constant probability density showing the cores of tangled vortex solitons (zoom-in online to view the vortex tangles). The most recent quantum lattice gas simulations are run on DoD CRAY XT-5 supercomputers that realize informational substrates with a half trillion qubits and 20 trillion gates. The amount of computational resources needed to simulate quantum turbulence is on the order of 80,000 cycle times, which comprises $10^{18}$ gate operations.
APPENDIX A

Deutsch problem and joint information

A.1 Introduction

The Deutsch problem is fundamental to understanding quantum computing as it is the simplest demonstration of computational efficiency derived from the principles of quantum mechanics [Deutsch and Jozsa, 1992b]. It is the first problem to have been solved on a quantum information processor; this was accomplished contemporaneously by Jones and Mosca [Jones and Mosca, 1998] and Chuang et al. [Chuang et al., 1998], and both experimental groups used nuclear magnetic resonance spectroscopy. It is like determining, with a single glance so to speak, if a coin is fair: balanced, heads on one side and tails on the other, or constant, heads on both sides or tails on both sides. According to classical intuition, such a determination requires two observations. Yet, a quantum circuit allows us to make the determination with a single observation. This is at the crux of quantum efficiency.

We begin by presenting a two-qubit quantum circuit for the Deutsch problem.
The circuit uses quantum superposition to gain a computational speedup and its final output comprises one qubit in a classical logical state, holding the answer to the problem, while the other qubit remains in a superposition state. This situation is typical of quantum algorithms where superposition persists to the end of the calculation on some lead while the output lead of the circuit yields the correct answer. In the original Deutsch quantum circuit design, superposition is generated by Hadamard transformations on the input qubit states, which are originally separable.

Any superposition remaining after the quantum computation decoheres by contact with the external environment, causing a loss of information. The external environment acts as an “information reservoir.” Yet, it is unnecessary to invoke the external environment as an information sink.

So next a quantum circuit is presented, the Deutsch circuit with one additional Hadamard gate acting on an output leg, that in a controlled way removes all superposition. This does not diminish quantum efficiency. This quantum circuit recasts the quantum circuit for the Deutsch problem as nearly a classical device, where the qualifier “nearly” indicates that although the device interchanges 1’s and 0’s (a classical operation), it causes an overall phase change (multiplying the input quantum state by -1) of some of the output quantum states. This quantum circuit does not transfer all accessible information that could otherwise be available for measurement. It is the kind of circuit implemented in the nuclear magnetic resonance experiments mentioned above.

The source of the quantum efficiency is seen as the capacity to flip the phase of a quantum state as well as permute states, something accomplished through the internal use of quantum superposition. Can this be achieved in a way that conserves information entirely within the quantum circuit? The answer is yes, all accessible information about the system is measurable at the end of the quantum computation. We will see how to do this by employing a symmetric quantum circuit containing
a second oracle, a dual of the original oracle. Then, with one observation following
the action of the circuit, we can learn the value of one side of the coin or its fairness,
but now the second output lead contains a valuable bit of information, the state of
one side of the coin—the last bit of available information lost in the unsymmetrical
versions of the quantum circuit. By transferring all accessible information in a way
that is available for measurement, the state of the proverbial coin is extracted in an
efficient and complete way.

A.2 Statement of the Deutsch problem

Mathematically, the Deutsch problem is equivalent to a “fair-coin” test, and

\[ f : \{0, 1\} \rightarrow \{0, 1\}. \]

Let the domain \( \{0, 1\} \) encode the two sides of the coin. Let the functional value of
\( f \) be the result of an observation of one side of the coin, with outcome heads 1 or
tails 0.

If \( f(0) = f(1) \) the function is constant, otherwise if \( f(0) \neq f(1) \) it is balanced.

There are only four possible function maps:

- **Case 0:** \( f(0) = 0 \) \( f(1) = 0 \) constant (A.1a)
- **Case 1:** \( f(0) = 0 \) \( f(1) = 1 \) balanced (A.1b)
- **Case 2:** \( f(0) = 1 \) \( f(1) = 0 \) balanced (A.1c)
- **Case 3:** \( f(0) = 1 \) \( f(1) = 1 \) constant (A.1d)

The quantum circuit for the Deutsch problem is shown in Figure A.1. Upon
measurement, the quantum circuit’s output lead tells whether \( f \) is constant or bal-
anced. The inputs to the quantum circuit on the left hand side are fixed with the
top lead set to $|0\rangle$ and the bottom lead set to $|1\rangle$. In matrix form, these input states are

$$
|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.
$$

(A.2)

The quantum circuit has three stages, where each stage is represented by a unitary matrix:

A. Superposition ($U_A$)

B. Oracle ($U_B = U_O$)

C. Inverse superposition ($U_C$).

![Quantum Circuit Diagram](image)

FIG. A.1: Quantum circuit diagram using the Deutsch oracle $U_O$. The input lines are "hardwired." Measuring the output line deterministically yields a 1 or 0 if the function $f(x)$ is balanced or constant, respectively.

### A.2.1 Superposition stage

There are two Hadamard gates, independently acting on the two input qubits, and denoted by the operator symbol $H$ with the following matrix representation:

$$
H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.
$$

(A.3)

The 2-qubit unitary operator for stage 1 is the following tensor product:

$$
U_A = H \otimes H = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}.
$$

(A.4)
Stage 1 does not cause any quantum entanglement, since the Hadamard gates act independently on the input qubits.

### A.2.2 Oracle stage

Next, there is a two-qubit quantum gate that represents the Deutsch oracle. This is denoted $U_O$. The function $f$ is applied to the bottom lead when the value of the qubit on the top lead is $|1\rangle$. That is, the oracle is controlled by the top lead.

The symbol $\oplus$ means addition modulo 2, which is binary addition. This is the classical gate operation called exclusive or, shown in Table A.1. The input state to

<table>
<thead>
<tr>
<th>$x$</th>
<th>$y$</th>
<th>$x \oplus y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

**TABLE A.1: Classical XOR gate.**

stage 2 is the tensor product $|x\rangle|y\rangle \equiv |x\rangle \otimes |y\rangle$. We leave out the $\otimes$ symbol for brevity. Sometimes to be even more brief, we simply write such a state as $|xy\rangle$. However, in the present situation, we should emphasize that our input state is separable with no quantum entanglement, and will use the notation that distinguishes each qubit individually. Also, this notation makes it easy to algebraically specify the action of $U_O$:

$$U_O |x\rangle |y\rangle \equiv |x\rangle |y \oplus f(x)\rangle. \quad (A.5)$$

To workout the matrix representation of the unitary operator for (A.5) we simply insert the qubit logical states (A.2). The unitary matrix representations of the Deutsch oracle for the four case are the following:
Case 0:

\[ U_0 = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}. \quad (A.6a) \]

Case 1:

\[ U_0 = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}. \quad (A.6b) \]

Case 2:

\[ U_0 = \begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}. \quad (A.6c) \]

Case 3:

\[ U_0 = \begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}. \quad (A.6d) \]

A.2.3 Inverse superposition stage

As a last stage, a Hadamard gate is applied to the top lead to prepare it for measurement. The unitary operator for this last stage has the following form:

\[ U_C = H \otimes 1_2 = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 \\
1 & 0 & -1 & 0 \\
0 & 1 & 0 & -1
\end{pmatrix}. \quad (A.7) \]

A.3 Unitary evolution operator

The quantum circuit for solving the Deutsch problem can be expressed by multiplying together the unitary matrices for each respective stage

\[ U = U_C U_O U_A. \quad (A.8) \]
Inserting the unitary matrices (A.4), (A.27) and (A.7) for the respective three stages into (A.8), we find the following four different resulting transformation matrices

Case 0:

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix}$$ \hspace{1cm} (A.9a)

Case 1:

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & -1 & 1 & 0 \end{pmatrix}$$ \hspace{1cm} (A.9b)

Case 2:

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$ \hspace{1cm} (A.9c)

Case 3:

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$ \hspace{1cm} (A.9d)

Now using (A.2), we can write down the following four tensor product states:

$$|0\rangle|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |0\rangle|1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1\rangle|0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |1\rangle|1\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$ \hspace{1cm} (A.10)

The output of the Deutsch quantum circuit can now be computed

Case 0:

$$U|0\rangle|1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} (|0\rangle|0\rangle - |0\rangle|1\rangle) = |0\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \quad \text{constant}$$ \hspace{1cm} (A.11a)
Case 1:

\[
U|0\rangle|1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} (|1\rangle|0\rangle - |1\rangle|1\rangle) = |1\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \quad \text{balanced}
\]

(A.11b)

Case 2:

\[
U|0\rangle|1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ -1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} (-|1\rangle|0\rangle + |1\rangle|1\rangle) = -|1\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \quad \text{balanced}
\]

(A.11c)

Case 3:

\[
U|0\rangle|1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} (-|0\rangle|0\rangle + |0\rangle|1\rangle) = -|0\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \quad \text{constant}
\]

(A.11d)

The result for the constant cases 0 and 3 are \( \pm |0\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \), while the result for the balanced cases 1 and 2 are \( \pm |1\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \). Therefore, upon measurement of the first qubit, the outcome of 0 tells us \( f \) is constant and the outcome of 1 tells us \( f \) is balanced.

### A.4 A quantum circuit with two classical output bits

In the quantum circuit for the Deutsch problem, and like all the other commonly used three-stage quantum circuits such as for the Deutsch-Jozsa, Bernstein-Varirani, and Simon algorithms, all output qubits (or qubits as the case may be) need not be observed. Some are left in a quantum superposition state that are allowed to naturally decohere. This natural process of decoherence occurs as the qubit couple
in an uncontrolled way to an external mode (say a photon or phonon mode) that escapes off to infinity. Why not avoid such uncontrolled decoherence altogether?

It is straightforward to “upgrade” the quantum circuit for the oracle so as not to leave any quantum superposition remaining and instead to have the resulting state of the circuit be a pseudo-classical state (that is, a classical state with an overall phase of \( \pm 1 \)). Figure A.2 shows the improved quantum circuit that employs an additional Hadamard gate placed on the bottom output lead. Yet, we shall see that this circuit does not conserve information.

With this circuit, the first and third stages are identical, \( U_3 = U_1 = H \otimes H \).

Therefore, the unitary transformation for the oracle can be expressed as

\[
U = (H \otimes H)U_O(H \otimes H).
\]

This has the following matrix representations:

**Case 0:**

\[
U = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]

(A.13a)

**Case 1:**

\[
U = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 \\
0 & 0 & 1 & 0 \\
0 & -1 & 0 & 0
\end{pmatrix}
\]

(A.13b)
Case 2:

\[
U = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0
\end{pmatrix}
\]

(A.13c)

Case 3:

\[
U = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & -1
\end{pmatrix}
\]

(A.13d)

These four transformation matrices are nearly classical permutation matrices. The only remaining remnants of the quantum mechanical nature of the transformation are the negative components. The consequence of these are that the resulting state of the quantum circuit may have an overall 180 degree phase shift from a pure classical state. The phase shift is necessary to uniquely distinguish the four possible mappings of \(f(x)\).

The output of the upgraded quantum circuit can now be computed

Case 0:

\[
U|0\rangle|1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = |0\rangle|1\rangle \text{ constant} \quad (A.14a)
\]

Case 1:

\[
U|0\rangle|1\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \end{pmatrix} = -|1\rangle|1\rangle \text{ balanced} \quad (A.14b)
\]

Case 2:

\[
U|0\rangle|1\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = |1\rangle|1\rangle \text{ balanced} \quad (A.14c)
\]
Case 3:

\[
U|0\rangle|1\rangle = \begin{pmatrix}
0 \\
-1 \\
0 \\
0
\end{pmatrix} = -|0\rangle|1\rangle \quad \text{constant (A.14d)}
\]

The result for the constant cases 0 and 3 are \(\pm|0\rangle|1\rangle\), while the result for the balanced cases 1 and 2 are \(\pm|1\rangle|1\rangle\). Therefore, upon measurement of the first qubit, the outcome of 0 tells us \(f\) is constant and the outcome of 1 tells us \(f\) is balanced, just as before. However, now the second qubit is always in state \(|1\rangle\), and not in internal superposition. Yet, since the value of the second qubit is fixed, information is still lost.

A.4.1 Algebraic treatment

We can algebraically express our quantum implementation and determine the output of the new circuit. For the moment, we will allow the input state to be a variable quantity, \(|x\rangle|y\rangle\). We can express (A.3) concisely as follows:

\[
H|x\rangle = \frac{1}{\sqrt{2}} \sum_{y=0}^{1} (-1)^{xy}|y\rangle.
\]  
(A.15)

Then using (A.15), the oracle becomes

\[
U|x\rangle|y\rangle = (H \otimes H)U_O(H \otimes H)|x\rangle|y\rangle
\]
\[
= \frac{1}{2} (H \otimes H)U_O \sum_{r=0}^{1} \sum_{s=0}^{1} (-1)^{xr+ys}|r\rangle|s\rangle.
\]  
(A.16)

(A.17)

Using (A.5), we then have

\[
U|x\rangle|y\rangle = \frac{1}{2} (H \otimes H) \sum_{r=0}^{1} \sum_{s=0}^{1} (-1)^{xr+ys}|r\rangle|s \oplus f(r)\rangle
\]
\[
= \frac{1}{4} \sum_{r=0}^{1} \sum_{s=0}^{1} \sum_{u=0}^{1} \sum_{v=0}^{1} (-1)^{xr+ys+ru+suf(r)}|u\rangle|v\rangle.
\]  
(A.18)

(A.19)
Noting that addition modulo 2 is the same as regular addition when it appears in the exponent of minus one, \((-1)^{s+f(r)}v = (-1)^{s+f(r)}v\), and fixing the input values to \(x = 0\) and \(y = 1\), we have

\[
U|0\rangle|1\rangle = \frac{1}{4} \sum_{rsuv} (-1)^{sru+[s+f(r)]v} |u\rangle|v\rangle. \tag{A.20}
\]

We first expand the sum over \(s\) to obtain

\[
U|0\rangle|1\rangle = \frac{1}{4} \sum_{rsuv} \left[ (-1)^{ru+f(r)v} - (-1)^{ru+[1+f(r)]v} \right] |u\rangle|v\rangle, \tag{A.21}
\]

where binary sums are understood. Then, we expand the sums over \(v\), \(u\), and \(r\), in turn, to obtain

\[
U|0\rangle|1\rangle = \frac{1}{2} \sum_{ru} (-1)^{ru+f(r)}|u\rangle|1\rangle \tag{A.22a}
\]

\[
= \frac{1}{2} \sum_{r} \left[ (-1)^{f(r)}|0\rangle|1\rangle + (-1)^{r+f(r)}|1\rangle|1\rangle \right] \tag{A.22b}
\]

\[
= \frac{1}{2} \left[ (-1)^{f(0)} + (-1)^{f(1)} \right] |0\rangle|1\rangle \tag{A.22c}
+ \frac{1}{2} \left[ (-1)^{f(0)} - (-1)^{f(1)} \right] |1\rangle|1\rangle
\]

Therefore, we obtain the final result

\[
U|0\rangle|1\rangle = \begin{cases} 
\pm|0\rangle|1\rangle, & \text{if } f \text{ is constant: } f(0) = f(1) \\
\pm|1\rangle|1\rangle, & \text{if } f \text{ is balanced: } f(0) \neq f(1)
\end{cases} \tag{A.23}
\]

as expected.

\section*{A.5 Quantum circuit for extracting all available information}

It is possible to add a fourth stage to the upgraded quantum circuit so that the bottom output line tells us the value of remaining bit of information about the
FIG. A.3: Symmetric quantum circuit diagram whose output states contain all the available classical information (two bits), again with no quantum superposition on the output. Measuring the top output line deterministically yields $q = 1$ or $q = 0$ when the function $f(x)$ is balanced or constant, respectively. Measuring the bottom output line deterministically yields $f(1)$, which corresponds to the value of one side of the coin.

Since we already know from the top output line whether the coin is constant or balanced, this last classical bit allows us to disambiguate the possibilities. The quantum logic component we need to add in the fourth stage is the dual of the Deutsch oracle. The dual of (A.5) is

$$
\overline{U}_O|x\rangle|y\rangle \equiv |x\rangle|y \oplus \bar{f}(x)\rangle.
$$

(A.24)

This has the following property

$$
\overline{U}_O U_O |x\rangle|y\rangle = |x\rangle |y \oplus f(x) \oplus \bar{f}(x)\rangle
$$

(A.25)

$$
= |x\rangle |\bar{y}\rangle.
$$

(A.26)

So $\overline{U}_O U_O = \sqrt{1} = 1_2 \otimes \sigma_x$, a NOT operation on the second qubit, which is purely linear. To be explicit, the matrix representations are

Case 0:

$$
\overline{U}_O = \begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}
$$

(A.27a)

Case 1:

$$
\overline{U}_O = \begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
$$

(A.27b)
Case 2:

\[ U_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \] (A.27c)

Case 3:

\[ U_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \] (A.27d)

and the product of the dual oracle times the original is

\[ U_0U_0 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \] (A.28)

Following (A.20), the quantum circuit

\[ U = U_0(H \otimes H)U_0(H \otimes H) \] (A.29)

can be expressed algebraically

\[ U|0\rangle|1\rangle = \frac{1}{4} \sum_{rsuv} (-1)^{s+ru+[r+f(r)]v}|u\rangle|v\rangle \oplus f(u). \] (A.30)

The final complete output is the following:

\[ U|0\rangle|1\rangle = \begin{cases} |0\rangle|1\rangle, & f(0) = f(1), \ f(1) = 1 \\ |1\rangle|0\rangle, & f(0) \neq f(1), \ f(1) = 0 \\ -|1\rangle|1\rangle, & f(0) \neq f(1), \ f(1) = 1 \\ -|0\rangle|0\rangle, & f(0) = f(1), \ f(1) = 0. \end{cases} \] (A.31)

**A.6 Remarks on the Deutsch problem**

If one were presented with a coin and asked to determine whether it is fair or not, without flipping it over to check both sides, the natural thing to do would be to go straight to the nearest mirror. When held up to the minor, one could then see the
front and back of the coin simultaneously, without having to flip it over. Of course
the light bouncing off the front of the coin and entering the observer’s eye would be
independent of the light bouncing off the back of the coin, reflecting off the mirror,
and entering the same eye. There is no quantum mechanical entanglement nor
superposition here, only two independent “photons.” This is classical parallelism,
two observations at once. So, classically, two observations are needed to obtain a
speedup.

In contradistinction, quantum superposition offers a speedup. Superposition
in the final output state is not what is remarkable about quantum logic, although
operations causing quantum superposition play an essential role as an intermediate
building blocks in the quantum circuit—in this case, to allow us to test a coin’s
fairness in one measurement. All we need in the end is an overall phase shift and
bit-flip of the final quantum state (i.e. an overall a multiplication of the state by
±1 and a permutation of the states).

The quantum circuit that we have presented in Figure A.3 illustrates the funda-
mental principle that the ideal coin can be represented as a composite of two
elementary observables, each conveyed by a bit of information: (1) the fairness of
the coin, and (2) the value of one observed side. Quantum mechanically, we can
learn the fairness of the coin with one observation, and we are guaranteed that
no more than one execution of the circuit is needed to know everything about the
coin. Therefore, a quantum circuit is more capable than a classical circuit, and
information is conserved.
APPENDIX B

Quantum logic in matrix form

B.1 Representations of perpendicular quantum gates

A type of quantum logic gate useful for casting quantum algorithms in various computational physics applications is a conservative quantum gate. It is a 2-qubit universal quantum gate associated with perpendicular pairwise entanglement. A conservative quantum gate conserves the "bit count" in the number representation of the qubit system (i.e. the total spin magnetization of a spin-$\frac{1}{2}$ system). If conservative quantum gates are used to model basic qubit-qubit interactions in a large qubit system, then the large scale dynamics of the qubit system is ultimately constrained by a number continuity equation, as was mentioned earlier.

In the most general situation, it is sufficient to consider only a block diagonal matrix that has a $2 \times 2$ sub-block, which causes entanglement and is a member of the special unitary group SU(2). We can neglect the overall phase factor because this does not affect the quantum dynamics and therefore our sub-block need not be a member of the more general unitary group U(2). If $U$ is a member of SU(2), it
can be parameterized using three real numbers, $\xi$, $\zeta$, and $\vartheta$, as follows

$$U \equiv \begin{pmatrix}
e^{i\xi} \cos \vartheta & -e^{i\zeta} \sin \vartheta \\
-e^{-i\zeta} \sin \vartheta & -e^{-i\xi} \cos \vartheta \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}. \quad (B.1)$$

We can represent a general conservative quantum logical gate by the $4 \times 4$ unitary matrix

$$\Upsilon = \begin{pmatrix} 1 & 0 & 0 & 0 \\
0 & A & B & 0 \\
0 & C & D & 0 \\
0 & 0 & 0 & E \end{pmatrix}. \quad (B.2)$$

We choose this form for $\Upsilon$ because we want to entangle only two of the basis states, $|01\rangle$ with $|10\rangle$, so as to conserve particle number, and that is why we call $\Upsilon$ a conservative quantum gate. The component in the top-left corner is set to unity because we do not want $\Upsilon$ to alter the vacuum state $|00\rangle$ in any way. However, we must allow the component in the bottom-right corner to be arbitrary. We will see that the value of this component will depend on the particle statistics, reflecting whether quantum logic gates are used to model quantum gases with particles obeying Fermi statistics or not.

### B.1.1 Ladder operator representation

It is instructive to work out the ladder operators in the $Q = 2$ case, where it is simple to write down the matrix representation. Remarkably, all the results carry over to the arbitrary size qubit systems with $Q \geq 2$. Consider the following five quadratic operators:

$$a_1^\dagger a_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 \end{pmatrix}, \quad a_2^\dagger a_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \end{pmatrix}, \quad (B.3)$$
including the compound number operators

\[
\begin{align*}
n_1(1 - n_2) &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (1 - n_1)n_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\
n_1n_2 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.
\end{align*}
\]

(B.4)

The conservative quantum gate (B.2) can be expressed in terms of the operators (B.3) and (B.4) given above:

\[
\begin{align*}
\Upsilon &= 1 + (A - 1)(1 - n_1)n_2 + Ba_2^\dagger a_1 + Ca_1^\dagger a_2 \\
&+ (D - 1)n_1(1 - n_2) + (E - 1)n_1n_2 \quad \text{(B.5)} \\
&= 1 + (A - 1)n_2 + Ba_2^\dagger a_1 + Ca_1^\dagger a_2 \\
&+ (D - 1)n_1 - (A + D - E - 1)n_1n_2. \quad \text{(B.6)}
\end{align*}
\]

We would like to find the Hamiltonian, \( H \) say, associated with \( \Upsilon \). Letting \( z \) denote a complex parameter, we begin by parametrizing (B.6) in terms of \( z \)

\[
\Upsilon(z) = e^{zH}, \quad \text{(B.7)}
\]

and then we solve for \( H \). To do this, we series expand in the parameter \( z \):

\[
\Upsilon(z) = 1 + zH + \frac{z^2}{2}H^2 + \cdots. \quad \text{(B.8)}
\]

There are two cases of interest: first when the Hamiltonian is idempotent, \( H^2 = H \), then (B.8) reduces to

\[
\Upsilon(z) = 1 + (e^z - 1)H, \quad \text{(B.9)}
\]

and second when \( H^3 = H \) and \( H^4 = H^2 \), then (B.7) reduces to

\[
\Upsilon(z) = 1 + \sinh z H + (\cosh z - 1)H^2. \quad \text{(B.10)}
\]

These cases are worked out below.
\[ H^2 = H \text{ case} \]

From (B.2) and (B.9), we can solve for \( H \):

\[
H = \frac{1}{e^z - 1} (\gamma - 1) = \frac{I}{e^z - 1} \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & A^{-1} & B & 0 \\
0 & C & D^{-1} & 0 \\
0 & 0 & 0 & E^{-1}
\end{pmatrix}. \tag{B.11}
\]

Let us pick a new set of variables to simplify matters:

\[
\begin{align*}
A &= \frac{A - 1}{e^z - 1} & B &= \frac{B}{e^z - 1} \quad \tag{B.12a} \\
C &= \frac{C}{e^z - 1} & D &= \frac{D - 1}{e^z - 1} \quad \tag{B.12b} \\
\Delta &= \frac{E - 1}{e^z - 1}. \tag{B.12c}
\end{align*}
\]

Then inserting (B.12) into (B.11), the Hamiltonian has the simple matrix and operator representation

\[
H = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & A & B & 0 \\
0 & C & D & 0 \\
0 & 0 & 0 & \Delta
\end{pmatrix}, \tag{B.13}
\]

and from this we deduce the operator form of the idempotent Hamiltonian

\[
H = Ba_1^\dagger a_1 + Ca_1^\dagger a_2 + Dn_1(1 - n_2) + A(1 - n_1)n_2 + \Delta n_1 n_2. \tag{B.14}
\]

Next, inserting the new variables (B.12) into (B.2) and (B.6), the matrix and operator representations for the conservative quantum logic gate become

\[
\begin{align*}
\gamma(z) &= e^{zH} \\
&= \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & (e^z - 1)A + 1 & (e^z - 1)B & 0 \\
0 & (e^z - 1)B^\dagger & (e^z - 1)D + 1 & 0 \\
0 & 0 & 0 & (e^z - 1)\Delta + 1
\end{pmatrix} \tag{B.15}
\end{align*}
\]

\[
= I + (e^z - 1) \left[ Ba_2^\dagger a_1 + Ca_2^\dagger a_2 + Dn_1(1 - n_2) + A(1 - n_1)n_2 + \Delta n_1 n_2 \right]. \tag{B.16}
\]

\[
= I + (e^z - 1) \left[ Ba_2^\dagger a_1 + Ca_2^\dagger a_2 \right] + \left[ Dn_1(1 - n_2) + A(1 - n_1)n_2 + \Delta n_1 n_2 \right]. \tag{B.17}
\]
Since the Hamiltonian must be Hermitian, \( H = H^\dagger \), we know that \( C = B^\dagger \) and \( \Delta = \Delta^\dagger \), so \( \Delta \) must be a real valued number. Also, since the Hamiltonian is idempotent, \( H^2 = H \), we get the additional constraint equations on the components:

\[
\begin{align*}
A^2 - A + |B|^2 &= 0 \\
A + D &= 1 \\
D^2 - D + |B|^2 &= 0,
\end{align*}
\]

which admit the solutions:

\[
\begin{align*}
A &= \frac{1}{2} \left( 1 \pm \sqrt{1 - 4|B|^2} \right) \\
D &= \frac{1}{2} \left( 1 \mp \sqrt{1 - 4|B|^2} \right).
\end{align*}
\]

Then inserting (B.21) and (B.22) into (B.13) and (B.14), we can specify the idempotent Hamiltonian with only one free complex parameter:

\[
H = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & \frac{1}{2} \pm \frac{1}{2} \sqrt{1 - 4|B|^2} & B & 0 \\
0 & B^\dagger & \frac{1}{2} \mp \frac{1}{2} \sqrt{1 - 4|B|^2} & 0 \\
0 & 0 & 0 & \Delta
\end{pmatrix}
\]

\[
= B a_1^\dagger a_1 + B^\dagger a_1^\dagger a_2 + \frac{1}{2} \left( 1 \mp \sqrt{1 - 4|B|^2} \right) n_1 (1 - n_2) \\
+ \frac{1}{2} \left( 1 \mp \sqrt{1 - 4|B|^2} \right) (1 - n_1) n_2 + \Delta n_1 n_2
\]

\[
= B a_2^\dagger a_1 + B^\dagger a_1^\dagger a_2 + \frac{1}{2} \left( 1 \mp \sqrt{1 - 4|B|^2} \right) n_1 \\
+ \frac{1}{2} \left( 1 \mp \sqrt{1 - 4|B|^2} \right) n_2 + (\Delta - 1) n_1 n_2.
\]

The associated conservative quantum logic gate can also be rewritten by inserting
(B.21) and (B.22) into (B.15):

\[
\Upsilon(z) = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{2}(e^z + 1) \pm \frac{1}{2}(e^z - 1) \sqrt{1 - 4|\mathcal{B}|^2} & 0 & (e^z - 1)\mathcal{B} \\
0 & (e^z - 1)\mathcal{B}^\dagger & \frac{1}{2}(e^z + 1) \pm \frac{1}{2}(e^z - 1) \sqrt{1 - 4|\mathcal{B}|^2} & 0 \\
0 & 0 & 0 & (e^z - 1)\Delta + 1 \\
\end{pmatrix}
\]

\[= 1 + (e^z - 1) \left[ \mathcal{B} a_2^\dagger a_1 + \mathcal{B}^\dagger a_1^\dagger a_2 \\
+ \frac{1}{2} \left( 1 \mp \sqrt{1 - 4|\mathcal{B}|^2} \right) n_1 + \frac{1}{2} \left( 1 \pm \sqrt{1 - 4|\mathcal{B}|^2} \right) n_2 + (\Delta - 1)n_1n_2 \right]. \tag{B.27} \]

A physical and useful special case occurs if we choose \( \mathcal{B} = -\frac{1}{2} e^{-i\xi} \):

\[
H = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & \frac{1}{2} & -\frac{1}{2} e^{-i\xi} & 0 \\
0 & -\frac{1}{2} e^{i\xi} & \frac{1}{2} & 0 \\
0 & 0 & 0 & \Delta \\
\end{pmatrix}
\]

\[= -\frac{1}{2} \left( a_1^\dagger a_2 e^{i\xi} + a_2^\dagger a_1 e^{-i\xi} - n_1 - n_2 \right) + (\Delta - 1)n_1n_2. \tag{B.28} \]

Since \( n_1 = a_1^\dagger a_1 \) and \( n_2 = a_2^\dagger a_2 \), we can rewrite the idempotent Hamiltonian as follows:

\[
H = \frac{1}{2} (a_1^\dagger - e^{-i\xi} a_2^\dagger)(a_1 - e^{i\xi} a_2) + (\Delta - 1)n_1n_2. \tag{B.29} \]

Also,

\[
\Upsilon(z) = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{2}(e^z + 1) & \frac{1}{2}(e^z - 1) e^{-i\xi} & 0 \\
0 & \frac{1}{2}(e^z - 1) e^{i\xi} & \frac{1}{2}(e^z + 1) & 0 \\
0 & 0 & 0 & (e^z - 1)\Delta + 1 \\
\end{pmatrix}
\]

\[= 1 + (e^z - 1) \left[ \frac{1}{2} \left( a_1^\dagger - e^{-i\xi} a_2^\dagger \right)(a_1 - e^{i\xi} a_2) \\
+ (\Delta - 1)n_1n_2 \right]. \tag{B.30} \]

\[H^3 = H \quad \text{case} \]

There exists an alternative Hamiltonian that is not idempotent but has a similar property at third order, \( H^3 = H \) (but not necessarily an involution \( H^2 = 1 \)), which
can generate a conservative quantum logic gate of the form (B.2). In this second case, the series expansion of the quantum gate (B.7) reduces to the form (B.10), which is

\[ \Upsilon(z) = 1 + (\cosh z - 1)H^2 + \sinh zH. \]

Our approach will be to assume the Hamiltonian still has the form (B.13) and that its square has a diagonal matrix form:

\[
H^2 = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & A & B & 0 \\
0 & B^\dagger & D & 0 \\
0 & 0 & 0 & \Delta
\end{pmatrix} \cdot \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & A & B & 0 \\
0 & B^\dagger & D & 0 \\
0 & 0 & 0 & \Delta
\end{pmatrix} = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & \Delta
\end{pmatrix}
\]

(B.32)

where as in the previous case either \( \Delta = 0 \) or \( \Delta = 1 \). This imposes the following constraint equations on the components:

\[
A^2 = 1 - |B|^2 \quad (B.35)
\]

\[
A + D = 0 \quad (B.36)
\]

\[
D^2 = 1 - |B|^2; \quad (B.37)
\]

which admit the solutions:

\[
A = \pm \sqrt{1 - |B|^2} \quad (B.38)
\]

\[
D = \mp \sqrt{1 - |B|^2}. \quad (B.39)
\]
Then, the Hamiltonian has the form

$$H = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & ±\sqrt{1 - |B|^2} & B & 0 \\ 0 & B^\dagger & ±\sqrt{1 - |B|^2} & 0 \\ 0 & 0 & 0 & Δ \end{pmatrix}$$

(B.40)

$$= B a_2^\dagger a_1 + B^\dagger a_1^\dagger a_2 ± \sqrt{1 - |B|^2} n_1 (1 - n_2)$$

$$± \sqrt{1 - |B|^2} (1 - n_1) n_2 + Δ n_1 n_2$$

(B.41)

$$= B a_2^\dagger a_1 + B^\dagger a_1^\dagger a_2 ± \sqrt{1 - |B|^2} n_1$$

$$± \sqrt{1 - |B|^2} n_2 + Δ n_1 n_2,$$

(B.42)

and hence, using (B.10), the matrix representation of the conservative quantum gate becomes

$$\Upsilon(z) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cosh z ± \sqrt{1 - |B|^2} \sinh z & B \sinh z & 0 \\ 0 & B^\dagger \sinh z & \cosh z ± \sqrt{1 - |B|^2} \sinh z & 0 \\ 0 & 0 & 0 & (e^z - 1)Δ + 1 \end{pmatrix}$$

(B.43a)

$$= 1 + (\cosh z - 1) [n_1 + n_2 + (\Delta - 2)n_1 n_2]$$

$$+ \sinh z \left[ B a_2^\dagger a_1 + B^\dagger a_1^\dagger a_2 ± \sqrt{1 - |B|^2} n_1 ± \sqrt{1 - |B|^2} n_2 + Δ n_1 n_2 \right]$$

(B.43b)

$$= 1 + \sinh z B a_2^\dagger a_1 + \sinh z B^\dagger a_1^\dagger a_2$$

$$+ (\cosh z - 1 ± \sqrt{1 - |B|^2}) n_1 + (\cosh z - 1 ± \sqrt{1 - |B|^2}) n_2$$

$$+ [(e^z - 1)Δ + 2(\cosh z - 1)] n_1 n_2.$$
A useful special case occurs for $B = i e^{-i\xi}$. Then,

$$H = \begin{pmatrix} 0 & 0 & 0 & 0 \\
0 & 0 & i e^{-i\xi} & 0 \\
0 & -i e^{i\xi} & 0 & 0 \\
0 & 0 & 0 & \Delta \end{pmatrix}$$ \hspace{1cm} (B.44)

$$= i e^{-i\xi} a_2^\dagger a_1 - i e^{i\xi} a_1^\dagger a_2 + \Delta n_1 n_2. \hspace{1cm} (B.45)$$

$$= (a_1^\dagger + i e^{-i\xi} a_2^\dagger) (a_1 - i e^{i\xi} a_2) - n_1 - n_2 + \Delta n_1 n_2. \hspace{1cm} (B.46)$$

The quantum gate has the form:

$$\Upsilon(z) = \begin{pmatrix} 1 & 0 & 0 & 0 \\
0 & \cosh z & i e^{-i\xi} \sinh z & 0 \\
0 & -i e^{i\xi} \sinh z & \cosh z & 0 \\
0 & 0 & 0 & (e^z - 1)\Delta + 1 \end{pmatrix} \hspace{1cm} (B.47)$$

$$= 1 + i \sinh z \left( e^{-i\xi} a_2^\dagger a_1 - e^{i\xi} a_1^\dagger a_2 \right)$$

$$+ \left( \cosh z - 1 \right) (n_1 + n_2)$$

$$+ \left[ (e^z - 1)\Delta - 2(\cosh z - 1) \right] n_1 n_2. \hspace{1cm} (B.48)$$
APPENDIX C

Superfluidity

C.1 Tisza-Landau superfluid

A two-fluid theory of Helium II superfluid was originally proposed by Tisza [Tisza, 1938, Tisza, 1947], following London’s notion of a BEC-based superfluid component [London, 1938]. Landau developed a two-fluid theory based on phonon and roton excitations [Landau, 1941a, Landau, 1941b], which for a long time has been the accepted theory of helium II. A recent review of the history of the discovery of the two-fluid theory is given by Donnelly [Donnelly, 2009].

Let \( \varepsilon(p) \) denote the excitation energy of Helium II as a function of the momentum of the thermal excitation measured in a frame of reference moving with the superfluid. The excitation spectrum for Helium II has been verified by neutron-scattering experiments and is nonlinear, see figure C.1. The large wavelength excitations correspond to phonons and have the usual linear dispersion relation between energy and momentum

\[
\varepsilon(p) = C_1 p \quad \text{for} \quad \frac{p}{\hbar} \ll 1 \text{nm}^{-1}, \tag{C.1}
\]

where \( C_1 = 239 \frac{m}{\text{sec}} \) is the sound speed of density waves that propagate at con-
FIG. C.1: Dispersion relation for He II. The initial slope at small $k^{-1}$ is linear in the phonon part of the excitation spectrum and the parabolic part of the spectrum is due to roton excitations. The dashed line indicates a solution of $\varepsilon/p = d\varepsilon/dp$ which occurs near the local minimum of the curve, the band gap energy characteristic of superfluids.

At smaller wavelengths there is a local minimum in the excitation spectrum corresponding to rotons. Locally its dispersion relation is parabolic with the form

$$
\varepsilon(p) = \Delta + \frac{(p - P_o)^2}{2\mu_r} \quad \text{for} \quad \frac{P}{\hbar} \sim 2\AA^{-1},
$$

where

$$
\frac{\Delta}{k_B} = 8.65^\circ K \quad \frac{P_o}{\hbar} = 19.1\text{nm}^{-1} \quad \mu_r = 0.16\text{m}_4.
$$

Figure C.1 is an interpolation going from the linear behavior for phonons at long wavelengths to the parabolic behavior for rotons at shorter wavelengths. Quantum liquids can receive energy in only discrete units causing a transition from the ground state to an excited state. In a fixed laboratory frame of reference, consider the following energy change

$$
\delta E = \varepsilon(p_i) + p_i v_{si}^i,
$$

where $v_{si}$ is the velocity of the superfluid and $p_i$ is the momentum of a candidate quasiparticle, either a phonon or roton. To create an excitation the situation must be energetically favorable so that the energy change is negative, $\delta E \leq 0$, which is
written as
\[ \varepsilon(p_i) + p_i v^s_i \leq 0 \quad \rightarrow \quad v_s = \frac{\varepsilon(p)}{p}. \]  \hspace{0.5cm} \text{(C.4)}

When the equality holds, this implies a critical condition for the superfluid flow speed:
\[ v^s_{cr} = \min \left( \frac{\varepsilon(p)}{p} \right) \neq 0. \]  \hspace{0.5cm} \text{(C.5)}

The creation of quasiparticles is a mechanism by which Helium II can dissipate energy. Therefore, as long as \( v^s < v_{cr} \), the creation of quasiparticles will be energetically unfavorable and Helium II will exist as a superfluid, without any friction causing energy dissipation. The minimum point of a function is found by setting its derivative to zero. In this way the excitation energy of the Helium II from (C.5) is determined
\[ \frac{d}{dp} \frac{\varepsilon(p)}{p} = 0 \quad \rightarrow \quad \varepsilon = \frac{d\varepsilon}{dp}. \]  \hspace{0.5cm} \text{(C.6)}

The solution of (C.6) is easily found by rendering the line whose slope, \( \frac{\varepsilon}{p} \), is tangent to the curve of the excitation spectrum, as shown in figure C.1. Note that the solution lies close to the local minimum of the excitation curve, where \( \varepsilon \approx \Delta \). This is the energy gap necessary for superfluidity.

In the incompressible fluid regime of Helium II, the coherent motion of the BEC is described by a wavefunction of the following form
\[ \psi(x) = \psi_0 e^{iS(x)/\hbar}. \]  \hspace{0.5cm} \text{(C.7)}

Its evolution is governed by a Schroedinger equation where the external potential is the chemical potential of the Helium II quantum fluid
\[ i\hbar \partial_t \psi = -\frac{\hbar^2}{2m_4} \partial^2 \psi + \mu \psi. \]  \hspace{0.5cm} \text{(C.8)}

It is through the chemical potential that the dynamics of the normal and superfluid parts of the Helium II are coupled. The explicit form of \( \mu \) for Helium II is given
below. The probability current is

\[ j_i^{\text{prob}}(\psi) = -\frac{i\hbar}{2m_4}(\psi^* \partial_t \psi - \psi \partial_t \psi^*). \]  

(C.9)

This implies the Helium II supercurrent density is related to the gradient of the phase of the wavefunction

\[ j_i^S \equiv m_4 j_i^{\text{prob}} = \psi_0^2 \partial_i S + j_i^{\text{prob}}, \]  

(C.10)

where \( j_i^{\text{prob}} \equiv j_i^{\text{prob}}(\psi_o) \) is the compressible part of the superfluid current density. The condition for conservation of probability

\[ \partial_t(\psi^* \psi) + \partial_i j_i^{\text{prob}} = 0 \]  

(C.11)

then becomes the continuity equation of hydrodynamics provided the mass density of the superfluid is identified as the square of the amplitude \( \rho_s \equiv m_4 \psi_0^2 \). It follows that the superfluid’s hydrodynamics flow velocity is

\[ v_i^s = \frac{1}{\rho_s} j_i^S = \frac{1}{m_4} \partial_i S + \frac{j_i^{\text{prob}}}{\psi_0^2}. \]  

(C.12)

In a singly-connected region of the quantum fluid (i.e. the bulk region), the incompressible part of the superfluid flow velocity must be curl free since it is the gradient of a scalar, the phase of the wavefunction. Inserting (C.7) into the Schroedinger’s equation for the BEC (C.8), the flow equation is expressed in terms of \( S \) and the real part takes the form of the Hamilton-Jacobi equation of motion

\[ \frac{1}{2m_4}(\nabla S)^2 + \mu = -\partial_t S + \frac{\hbar^2}{2m_4} \frac{\nabla^2 \sqrt{\rho_s}}{\sqrt{\rho_s}}. \]  

(C.13)

The last term in (C.13) vanishes in the bulk.\(^1\) Using this fact when taking the gradient of (C.13), gives the hydrodynamic flow equation, the Euler equation, for the superfluid part of Helium II in the bulk region

\[ \partial_t v_i^s + v_j^s \partial_j v_i^s = -\frac{1}{m_4} \partial_i \mu, \]  

(C.14)

\(^1\)It is not essential to assume Planck’s constant is small to be able to neglect this term since it depends only on \( \sqrt{\rho_s} \) whose gradient is negligible in the bulk region of the quantum fluid.
with a hydrostatic force due to a gradient in the chemical potential\textsuperscript{2}

What is $\nabla \mu$? Consider the thermodynamics of the fluid. Let $U_o, T, \Sigma, P, V,$ and $N$ denote the total internal energy, temperature, entropy, pressure, volume, and total particle number of the fluid. The Gibbs free energy is

\[ G = U_o - T\Sigma + PV, \quad \text{(C.15)} \]

which implies

\[ dG = dU_o - \Sigma dT - Td\Sigma + VdP + PdV. \quad \text{(C.16)} \]

Moreover, the total energy change\textsuperscript{3}

\[ dU_o = \mu dN + Td\Sigma - PdV. \quad \text{(C.17)} \]

Substituting (C.17) into (C.15) gives

\[ dG = \mu dN - \Sigma dT + VdP. \quad \text{(C.18)} \]

Therefore, the Gibbs free energy is

\[ G = N\mu \quad \text{provided} \quad Nd\mu = -\Sigma dT + VdP. \quad \text{(C.19)} \]

That is, the Gibbs free energy is the product of the number of $^4\text{He}$ particles and the chemical potential, which is expected since the chemical potential is the amount of energy it takes to add a single particle to the system\textsuperscript{4}. The total density and the

\textsuperscript{2}The identity, $\frac{1}{2} \nabla ((v^2_x)) = (v_x \cdot \nabla) v_x + v_x (\nabla \times \nabla)$, for the calculation of the gradient is used.

\textsuperscript{3}A change in the total energy can occur in three ways, $dU_o = dV + dQ + dW$, by adding a particle to the system with an “external potential” $dV = \mu dN$, by adding heat $dQ = Td\Sigma$, or by the system doing work $dW = -PdV$.

\textsuperscript{4}It is interesting to note that the phase of the condensate wave function, $S$, and the total number of particles are cannonical conjugate variables. This is directly seen by writing the Hamiltonian, $H$, as the sum of the free energy plus the bulk kinetic energy of the superfluid

\[ H = N\mu + \frac{1}{2} N m_s v_s^2. \]

The classical Hamilton’s equations are then

\[ \frac{\partial S}{\partial t} = -\frac{\partial H}{\partial N} \quad \frac{\partial N}{\partial t} = -\frac{\partial H}{\partial S}. \]
total entropy per unit mass are

\[ \rho \equiv \frac{Nm_4}{V} \quad \sigma \equiv \frac{\Sigma}{Nm_4} \]  \hspace{1cm} (C.20)

so using (C.19) the gradient of the chemical potential becomes

\[ \partial_t \mu = \frac{m_4}{\rho} \partial_t P - m_4 \sigma \partial_t T. \]  \hspace{1cm} (C.21)

The two-fluid Navier-Stokes equation for Helium II must have viscous damping arising only from the normal flow. Furthermore, the pressure must be linear in the two-fluid density and this drives first sound, \( P = c_s^2 \rho \). The two-fluid Navier-Stokes equation is then

\[ \rho_n(\partial_t v^n_i + v^n_j \partial_j v^n_i) + \rho_s(\partial_t v^s_i + v^s_j \partial_j v^s_i) = -\partial_t P + \eta \partial^2 v^n_i. \]  \hspace{1cm} (C.22)

With this equation, as well as the superfluid equation, then the hydrodynamic equation for the normal fluid can be determined. The Navier-Stokes equation for the normal fluid has a nonideal equation of state but otherwise is quite standard in form. Therefore, a model of the normal fluid equation is possible with an appropriately chosen form for an interparticle potential force.

### C.1.1 Summary of helium II hydrodynamic equations

**Mass continuity equation:**

\[ \partial_t (\rho_s + \rho_n) = -\partial_i (\rho_s v^s_i + \rho_n v^n_i). \]  \hspace{1cm} (C.23)

**Two-fluid flow equation:**

\[ \rho_n(\partial_t v^n_i + v^n_j \partial_j v^n_i) + \rho_s(\partial_t v^s_i + v^s_j \partial_j v^s_i) = -\partial_t P + \eta \partial^2 v^n_i. \]  \hspace{1cm} (C.24)

the first reducing to

\[ \partial_t S = - \left( \mu + \frac{1}{2} m_4 v^s_i \right), \]

which is exactly the Hamilton-Jacobi equation (C.13), and in this case is the integral of Euler’s equation.
Superfluid flow equation:

\[
\begin{align*}
\partial_t v_i^s + v_j^s \partial_j v_i^s &= -\frac{1}{\rho} \partial_i P + \sigma \partial_i T, \\
\mu &= -\partial_{i\mu}
\end{align*}
\]  

(C.25)

normal fluid flow equation with kinematic viscosity is \( \nu \equiv \eta/\rho_n \):

\[
\begin{align*}
\partial_t v_i^n + v_j^n \partial_j v_i^n &= -\frac{1}{\rho} \partial_i P - \frac{\rho_s}{\rho_n} \sigma \partial_i T + \nu \partial^2 v_i^n, \\
\mu &= -\partial_{i\nu}
\end{align*}
\]  

(C.26)

Entropy equation:

\[
\partial_t (\rho_s \sigma + \rho_n \sigma) = -\partial_i (\rho_s \sigma v_i^n + \rho_n \sigma v_i^n).
\]  

(C.27)

### C.1.2 Linearized helium II hydrodynamics

Consider a situation where Helium II at rest in the bulk region with constant background density, temperature, and entropy is subjected to a small perturbation so that the macroscopic dynamical variables can be \( \varepsilon \) expanded. Then considering only first order fluctuations in these variables, the linear hydrodynamics regime is obtained,

\[
\begin{align*}
v_i^s &= \varepsilon u_i^s \\
v_i^n &= \varepsilon u_i^n \\
\rho_s &= \rho_{so} + \varepsilon \theta_s \\
\rho_n &= \rho_{no} + \varepsilon \theta_n \\
\sigma &= \sigma_o + \varepsilon \zeta \\
P &= P_o + \varepsilon \tilde{P} \\
T &= T_o + \varepsilon T.
\end{align*}
\]  

(C.28)
Then neglecting damping, the linearized hydrodynamic equations for Helium II are
the following

\[
\begin{align*}
\partial_t \varrho & = -\partial_i (\rho_{so}u_i^s + \rho_{no}u_i^n) + \mathcal{O}(\varepsilon^2) \\
\partial_t u_i^s & = -\frac{1}{\rho_o} \partial_i \tilde{P} + \sigma_o \partial_i T + \mathcal{O}(\varepsilon^2) \\
\partial_t u_i^n & = -\frac{1}{\rho_o} \partial_i \tilde{P} - \frac{\rho_{so}}{\rho_{no}} \sigma_o \partial_i T + \mathcal{O}(\varepsilon^2) \\
\rho_o \partial_t \delta + \sigma_o \partial_t \varrho & = -\sigma_o \partial_i (\rho_{so}u_i^s + \rho_{no}u_i^n) + \mathcal{O}(\varepsilon^2).
\end{align*}
\]

(C.29a)  
(C.29b)  
(C.29c)  
(C.29d)

Consider a situation where Helium II is kept at a fixed temperature, so \( \nabla T = 0 \).
The fluctuating part of the two-fluid mass density is \( \varrho = \rho_o + \rho_n \) and the fluctuating
part of the two-fluid current density is \( \tilde{j}_i = \rho_{so}u_i^s + \rho_{no}u_i^n \). So the linearized two-
fluid equation, the sum of (C.29b) and (C.29c), and the linearized mass continuity
equation (C.29a) reduce to

\[
\begin{align*}
\partial_t \varrho & = -\partial_i \tilde{j}_i, \\
\partial_t \tilde{j}_i & = -\partial_i \tilde{P}.
\end{align*}
\]

(C.30a)  
(C.30b)

Eliminating \( \tilde{j}_i \) gives

\[
\partial_t^2 \varrho = \partial^2 \tilde{P}.
\]

(C.31)

Now in general the pressure is a function of density and entropy, \( P = P(\rho, \sigma) \). In
an isothermal regime we have \( \left( \frac{\partial P}{\partial \sigma} \right)_{\rho} = 0 \), so we can write

\[
\begin{align*}
\partial_t \tilde{P} & = \left( \frac{\partial P}{\partial \rho} \right)_{\sigma} \partial_t \varrho.
\end{align*}
\]

(C.32)

At constant temperature, the partial derivative of pressure with respect to density
is the square of the speed of first sound

\[
c_1 \equiv \sqrt{\left( \frac{\partial P}{\partial \rho} \right)_{\sigma}}.
\]

(C.33)

Under isothermal conditions this is constant, so we have \( \partial^2 \tilde{P} = c_1^2 \partial^2 \varrho \), and sub-
stituting this into (C.38) gives a wave equation for density fluctuations of Helium
This is the equation of motion for a phonon excitation.

Next, consider a situation where Helium Iı is kept at a fixed pressure, so \( \nabla P = 0 \). So the linearized superfluid equation (C.29b) and the linearized normal fluid equation (C.29c) reduce to

\[
\begin{align*}
\partial_t u_i^n &= \sigma \partial_i T \\
\partial_t u_i^s &= -\frac{\rho_s}{\rho_n} \sigma \partial_i T.
\end{align*}
\] (C.35a)
(C.35b)

Subtracting these gives an equation for the fluctuating velocity difference \( u_i^n - u_i^s \)

\[
\partial_t (u_i^n - u_i^s) = -\frac{\rho_s}{\rho_n} \sigma \partial_i T.
\] (C.36)

Here it is clear that a temperature gradient produces relative motion between the normal fluid and superfluid parts of Helium Iı. To obtain an equation for relative motion, insert the linearized mass continuity equation (C.29a) in the linearized entropy flow equation (C.29d), which becomes

\[
\sigma \partial_i (u_i^n - u_i^s) = -\frac{\rho_s}{\rho_n} \partial_i \zeta.
\] (C.37)

Now we have two equations from which the relative motion \( u_i^n - u_i^s \) can be eliminated to give

\[
\partial_t^2 \zeta = \frac{\rho_s}{\rho_n} \sigma^2 \partial^2 T.
\] (C.38)

In general the temperature is a function of density and entropy, \( T = T(\rho, \sigma) \). In an isobaric regime, \( \left( \frac{\partial T}{\partial \rho} \right)_\sigma = 0 \), so we can write

\[
\partial_i T = \left( \frac{\partial T}{\partial \sigma} \right)_\rho \partial_\zeta.
\] (C.39)

Under isobaric conditions \( \left( \frac{\partial T}{\partial \sigma} \right)_\rho \) is constant, so we have

\[
\partial^2 T = \left( \frac{\partial T}{\partial \sigma} \right)_\rho \partial^2 \zeta.
\] (C.40)
Denoting the speed of second sound as

\[ c_2 \equiv \sqrt{\frac{\rho_{so}}{\rho_{no}} \frac{\sigma^2}{(\partial \sigma / \partial T)_\rho}}. \]  

(C.41)

we have the equation of motion for an entropy excitation

\[ \partial_t^2 \zeta = c_2^2 \partial_x^2 \zeta, \]  

(C.42)

a second kind of hydrodynamic sound wave unique to Helium II.

C.2 Madelung transformation

It is possible to map the NLS equation (5.11b) to hydrodynamic equations. To do this, the Madelung transformation [Madelung, 1927] is employed

\[ \varphi(x) = \phi(x) e^{i \theta(x)}, \]  

(C.43)

where \( \phi(x) \) and \( \theta(x) \) are real-valued phase and magnitude fields. The first time derivative

\[ \partial_t \varphi = \left( \frac{\partial \phi}{\phi} + i \partial_t \theta \right) \varphi \]  

(C.44)

and the second space derivative is

\[ \nabla^2 \varphi = \left( \frac{\nabla \phi}{\phi} + i \nabla \theta \right)^2 \varphi + \left( \nabla \cdot \left( \frac{\nabla \phi}{\phi} \right) + i \nabla^2 \theta \right) \varphi \]  

(C.45a)

\[ = \left[ \left( \frac{\nabla \phi}{\phi} \right)^2 + \nabla \cdot \left( \frac{\nabla \phi}{\phi} \right) - (\nabla \theta)^2 \right] \varphi \]

\[ + i \left[ \frac{\nabla^2 \phi}{\phi} - (\nabla \theta)^2 \right] \varphi \]  

(C.45b)

\[ = \left[ \frac{\nabla^2 \phi}{\phi} - (\nabla \theta)^2 \right] \varphi + i \left[ 2 \left( \frac{\nabla \phi}{\phi} \right) \cdot \nabla \theta + \nabla^2 \theta \right] \varphi. \]  

(C.45c)
Then the real and imaginary parts of (5.11b) respectively are

\[-\partial_t \theta = -\frac{\hbar}{2m} \left[ \frac{\nabla^2 \phi}{\phi} - (\nabla \phi)^2 \right] + \Omega \]  
\[
\frac{\partial_t \phi}{\phi} = -\frac{\hbar}{2m} \left[ 2 \left( \frac{\nabla \phi}{\phi} \right) \cdot \nabla \theta + \nabla^2 \theta \right]. \]  

(C.46a) \hspace{1cm} (C.46b)

We apply the gradient operator $-\frac{\hbar}{m} \nabla$ to the first equation, multiply the second by $\phi^2$, and then rearrange terms

\[
\frac{\hbar}{m} \partial_t \nabla \theta + \frac{1}{2} \nabla \left( \frac{\hbar}{m} \nabla \theta \right)^2 = -\nabla \left[ \frac{\hbar \Omega}{m} - \frac{\hbar^2}{2m^2} \frac{\nabla^2 \phi}{\phi} \right] \]  

(C.47a)

\[
\phi \partial_t \phi = -\frac{\hbar}{2m} \left[ 2(\phi \nabla \phi) \cdot \nabla \theta + \phi^2 \nabla^2 \theta \right]. \]  

(C.47b)

Rearranging once again gives

\[
\partial_t \left( \frac{\hbar}{m} \nabla \theta \right) + \frac{1}{2} \nabla \left( \frac{\hbar}{m} \nabla \theta \right)^2 = -\nabla \left[ \frac{\hbar \Omega}{m} - \frac{\hbar^2}{2m^2} \frac{\nabla^2 \phi}{\phi} \right] \]  

(C.48a)

\[
\partial_t \phi^2 + \nabla \cdot \left( \phi^2 \frac{\hbar}{m} \nabla \theta \right) = 0. \]  

(C.48b)

Taking the scalar phase $S = \hbar \theta$ and number density $\rho = \phi^2$ as conjugate variables, (C.46) are Bohm’s equations [Bohm, 1952]

\[
\frac{\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V_B + \hbar \Omega(\rho) \]  

(C.49a)

\[
\frac{\partial \rho}{\partial t} = -\frac{1}{m} \nabla \cdot (\rho \nabla S), \]  

(C.49b)

where the nonlinear potential $V_B = -\frac{\hbar^2}{2m} \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}}$.

Alternatively, we may identify the conjugate variables with hydrodynamic Eulerian variables, a fluid’s density and velocity fields

\[
\rho(x) = \phi(x)^2 \]  

(C.50a)

\[
\mathbf{v}(x) = \frac{\hbar}{m} \nabla \theta(x). \]  

(C.50b)
Hence, the NLS equation is equivalent to a momentum equation (Newton’s second law) and a number continuity equation

\[\partial_t(mv) + \nabla \left( \frac{1}{2}mv^2 \right) = -\nabla \hbar \Omega - \nabla V_B \tag{C.51a}\]

\[\partial_t \rho + \nabla \cdot (\rho v) = 0, \tag{C.51b}\]

where the quantum mechanical kinetic energy term in (5.11b) contributes to the gradient of the Bohm potential

\[V_B = -\frac{\hbar^2}{2m} \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}}. \tag{C.52}\]

Carrying out the differentiation, the Bohm potential has the form

\[V_B = -\frac{\hbar^2}{4m} \left[ \frac{\nabla^2 \rho}{\rho} - \frac{1}{2} \left( \frac{\nabla \rho}{\rho} \right)^2 \right]. \tag{C.53}\]

Finally, notice that

\[\nabla \left[ -\frac{\hbar^2}{8m} \left( \frac{\nabla \rho}{\rho} \right)^2 \right] = -\frac{\hbar^2}{4m} \left[ \frac{\nabla^2 \rho}{\rho} - \frac{1}{2} \left( \frac{\nabla \rho}{\rho} \right)^2 \right] \nabla \rho, \tag{C.54}\]

so that we can write another form of the Bohm potential

\[V_B^{(C.53)} = \delta \left[ -\frac{\hbar^2}{8m} \left( \frac{\nabla \rho}{\rho} \right)^2 \right]. \tag{C.55}\]

We will consider flow with bulk density that is nearly constant \((\rho = \rho^{(0)} + \rho^{(1)} + \cdots)\). (C.50a), and in turn (C.52), is always finite and nearly constant in the bulk while supporting radiative fluctuations in \(\rho\). However, the bulk flow is driven by vortex solitons, at whose center \(\rho^{(0)}\) vanishes, so although \(V_B\) can become quite large this is regulated by the vanishing density profile. In the end, the fluid dynamics is driven by (C.52) near the core of the vortex solitons but in a stable and self-consistent way.
C.3 Hasimoto transformation

Hasimoto considered a vector quantity \( \mathbf{N} \) and a complex amplitude \( \psi \) defined along \( \mathcal{C} \) and parametrized by the arc length

\[
\mathbf{N}(s) \equiv \alpha_1 e^{i \int_0^s ds' \tau} (\mathbf{n} + i \mathbf{b}) \quad (C.56a)
\]
\[
\varphi(s) \equiv \epsilon \alpha_2 \kappa(s) e^{i \int_0^s ds' \tau}, \quad (C.56b)
\]

where \( \epsilon \) is real and \( \epsilon^2 = 1 \) and \( \varphi \) is a radial amplitude field (in two-dimensions) since the dimension of \( \varphi \) is inverse length, and \( \alpha_1 \) and \( \alpha_2 \) are a dimensionless complex numbers. Note that

\[
\epsilon \mathbf{N} = \frac{\alpha_1 \varphi}{\alpha_2 \kappa} (\mathbf{n} + i \mathbf{b}) \quad (C.57a)
\]
or

\[
\mathbf{n} + i \mathbf{b} = \frac{1}{\alpha_1} e^{-i \int_0^s ds' \tau} \mathbf{N} \quad (C.57b)
\]

and

\[
\mathbf{n} - i \mathbf{b} = \frac{1}{\alpha_1^*} \mathbf{N}^\dagger e^{i \int_0^s ds' \tau}
\]
\[
\epsilon (\mathbf{n} - i \mathbf{b}) = \frac{1}{\alpha_1^* \alpha_2 \kappa} \mathbf{N}^\dagger \varphi \quad (C.57c)
\]

Moreover, we have

\[
\varphi' = (C.56b) \left( \frac{\kappa'}{\kappa} + i \tau \right) \varphi. \quad (C.58)
\]

Using the second and third Frenet-Serret formulas, the change of \( \mathbf{N} \) with respect to the arc length is

\[
\epsilon \mathbf{N}'(s) \quad (C.56a) \equiv \alpha_1 \epsilon e^{i \int_0^s ds' \tau} (\mathbf{n}' + i \mathbf{b}')
\]
\[
+ i \alpha_1 \epsilon e^{i \int_0^s ds' \tau} (\mathbf{n} + i \mathbf{b}) \quad (C.59a)
\]
\[
= -\alpha_1 \epsilon e^{i \int_0^s ds' \tau} \mathbf{t}, \quad (C.59b)
\]
\[
= \frac{\alpha_1}{\alpha_2} \varphi \mathbf{t}. \quad (C.59c)
\]
Invoking the first Frenet-Serret formula, we have

\[ \varepsilon \dot{t}' \stackrel{(5.57)}{=} \epsilon \kappa \dot{n} \quad (C.60a) \]

\[ = \kappa \Re \left( \frac{1}{\alpha_2 \alpha_1^* \kappa} N^\dagger \varphi \right) \quad (C.60b) \]

\[ = \frac{1}{2} \left( \frac{N^\dagger \varphi + \varphi^\dagger N}{\alpha_2 \alpha_1^* + \alpha_2^* \alpha_1} \right). \quad (C.60c) \]

A fundamental geometrical property of a quantum vortex in the high-curvature limit is that its motion is directed along the bi-normal vector and with a strength proportional to the curvature

\[ \dot{R} = \beta \frac{\kappa_0}{4\pi} \kappa \dot{b}, \quad (C.61) \]

where \( \beta \) is a dimensional real-valued number. Then, choosing a parametrization with \( |R'(s)| = 1 \), for example the helix specified by \((5.60a)\), we have

\[ \dot{R} \stackrel{(5.58a)}{=} \dot{R}' \quad \text{(C.62a)} \]

\[ = \beta \frac{\kappa_0}{4\pi} \left( \kappa' \dot{b} - \tau \kappa \dot{n} \right) \quad \text{(C.62b)} \]

\[ = \beta \frac{\kappa_0}{4\pi} \kappa \Re \left[ \left( \dot{b} + i \dot{n} \right) \left( \frac{\kappa'}{\kappa} + i \tau \right) \right] \quad \text{(C.62c)} \]

\[ \dot{\Re}[\varphi] \stackrel{(C.58)}{=} \beta \frac{\kappa_0}{4\pi} \Re \left[ i e \left( \dot{n} - i \dot{b} \right) \varphi' \right] \quad \text{(C.62d)} \]

\[ \dot{N} \stackrel{(C.56)}{=} \frac{i \beta \kappa_0}{4\pi} \left( \frac{N^\dagger \varphi' \varphi}{\alpha_2^* \alpha_2} \right) \quad \text{(C.62e)} \]

where in the last line be made use of the fact that \( e^2 = 1 \). Regarding orthogonality of the Frenet-Serret basis vectors and \( N \), we have

\[ N^\dagger \cdot N \stackrel{(C.56a)}{=} 2|\alpha_1|^2, \quad N \cdot N = 0, \quad N \cdot \dot{t} = 0, \quad \cdots \quad (C.63) \]

so we can represent the time rate-of-change of \( N \) as a linear combination of \( N, N^\dagger \), and \( \dot{t} \) as follows:

\[ \dot{N} = A N + B N^\dagger + C \dot{t}, \quad (C.64) \]
where \( A, B, \) and \( C \) are unknown coefficients that we will now evaluate. First, we have

\[
\begin{align*}
\hat{N} \cdot N^\dagger &= 2|\alpha_1|^2 A \quad \text{(C.65a)} \\
N^\dagger \cdot N &= 2|\alpha_1|^2 A^* \quad \text{(C.65b)}
\end{align*}
\]

or

\[
A + A^* = \frac{1}{2|\alpha_1|^2} \left( \hat{N} \cdot N^\dagger + N^\dagger \cdot N \right) \quad \text{(C.66)}
\]

\[
= \frac{1}{2|\alpha_1|^2} \frac{\partial}{\partial t} \left( N \cdot N^\dagger \right) \quad \text{(C.67)}
\]

\[
= 0. \quad \text{(C.68)}
\]

Therefore, \( A \) must be a purely imaginary coefficient, so we will choose to write it as

\[
A = iR, \quad \text{(C.69)}
\]

where \( R \) is real. Next, we have

\[
B \overset{(C.64)}{=} \frac{1}{2|\alpha_1|^2} \hat{N} \cdot N = \frac{1}{4|\alpha_1|^2} \frac{\partial}{\partial t} (N \cdot N) \overset{(C.63)}{=} 0. \quad \text{(C.70)}
\]

Finally, from (C.62g) we have

\[
N \cdot \dot{\mathbf{i}} \overset{(C.63)}{=} i\varepsilon \beta \frac{\kappa_o}{4\pi} \frac{\alpha_1}{\alpha_2} \varphi'. \quad \text{(C.71)}
\]

and from (C.64) the last coefficient is determined

\[
\begin{align*}
C &= \mathbf{i} \cdot \mathbf{\hat{N}} \quad \text{(C.72a)} \\
&= \frac{\partial}{\partial t} \left( \mathbf{i} \cdot N \right) - N \cdot \dot{\mathbf{i}} \quad \text{(C.72b)} \\
&\overset{(C.63)}{=} -i\varepsilon \beta \frac{\kappa_o}{4\pi} \frac{\alpha_1}{\alpha_2} \varphi'. \quad \text{(C.72c)}
\end{align*}
\]

Hence, (C.64) reduces to

\[
\hat{N} \overset{(C.69),(C.70)}{=} i \left( RN - \varepsilon \beta \frac{\alpha_1}{\alpha_2} \frac{\kappa_o}{4\pi} \varphi' \mathbf{i} \right). \quad \text{(C.73)}
\]
Then, taking the derivative with respect to the arc length, we have

\[ \epsilon \mathbf{N}' = i \epsilon \left[ R' \mathbf{N} + R \mathbf{N}' - \epsilon \beta \frac{\alpha_1 \kappa_o}{\alpha_2} \frac{\varphi''}{4\pi} (\dot{\varphi} + \varphi' \dot{\varphi}') \right] \]  
(C.74a)
\[ \Rightarrow i \left[ \epsilon R' \mathbf{N} - R \frac{\alpha_1}{\alpha_2} \varphi \dot{\varphi} - \beta \frac{\alpha_1 \kappa_o}{\alpha_2} \frac{\varphi''}{4\pi} \right] \]
\[ - \epsilon \beta \frac{\alpha_1 \kappa_o}{\alpha_2} \frac{\varphi'}{4\pi} \left( \frac{\mathbf{N}^t \varphi}{\alpha_2 \alpha_1^*} + \frac{\varphi^t \mathbf{N}}{\alpha_1^*} \right). \]  
(C.74b)

Alternatively, we can calculate \( \mathbf{N}' \) directly from (C.59c)

\[ \epsilon \mathbf{N}' = - \frac{\alpha_1}{\alpha_2} \varphi \dot{\varphi} - \frac{\alpha_1}{\alpha_2} \dot{\varphi} \]  
(C.75a)
\[ \Rightarrow - \frac{\alpha_1}{\alpha_2} \varphi \dot{\varphi} - i \epsilon \frac{\alpha_1}{\alpha_2} \beta \frac{\kappa_o}{4\pi} \frac{\varphi''}{2} \left( \frac{\mathbf{N}^t \varphi'}{\alpha_2 \alpha_1^*} - \frac{\varphi^t \mathbf{N}}{\alpha_1^*} \right). \]  
(C.75b)

Thus, equating (C.74b) and (C.75b), the coefficients of \( \dot{\varphi} \) gives

\[ - \frac{\alpha_1}{\alpha_2} \varphi = - i \beta \frac{\alpha_1 \kappa_o}{\alpha_2} \frac{\varphi''}{4\pi} - i \frac{\alpha_1}{\alpha_2} R \varphi, \]
(C.76)

the coefficients of \( \mathbf{N}^t \) match, and finally the coefficients of \( \mathbf{N} \) gives

\[ R' = \frac{\beta \kappa_o}{4\pi} \frac{\alpha_1}{\alpha_2} \frac{1}{2} \left( \frac{\varphi'^t \varphi}{\alpha_2^* \alpha_1} + \frac{\varphi^t \varphi'}{\alpha_1^*} \right) \]
(C.77a)
\[ = \frac{\beta \kappa_o}{4\pi} \frac{1}{|\alpha_2|^2} \frac{\partial}{\partial s} \left( \frac{1}{2} \varphi^t \varphi \right). \]  
(C.77b)

Integrating gives

\[ R = \frac{\beta \kappa_o}{4\pi} \frac{1}{|\alpha_2|^2} \frac{\varphi^t \varphi}{2} + \frac{\mu}{\hbar} \]  
(C.77c)

where we judiciously chose the integration constant. Inserting (C.77c) into (C.76) and multiplying through by \( \hbar \) leads to the GP equation

\[ i\hbar \frac{\partial \varphi}{\partial t} = - \beta \hbar \kappa_o \frac{\partial^2 \varphi}{\partial s^2} + \left( - \frac{\beta h \kappa_o}{8\pi} \frac{1}{|\alpha_2|^2} \varphi^t \varphi - \mu \right) \varphi \]
(C.78a)
\[ = - \beta \frac{\hbar \kappa_o}{4\pi} \frac{\partial^2 \varphi}{\partial s^2} + \left( - \frac{\beta h \kappa_o}{8\pi} \frac{1}{|\alpha_2|^2} \varphi^t \varphi - \mu \right) \varphi. \]  
(C.78b)
This is the GP equation if $\beta = 1$, (in the high-torsion limit $s \approx z$)

$$\frac{\partial^2 \varphi}{\partial \beta^2} = \nabla^2 \varphi,$$  \hspace{1cm} (C.79)

and

$$g \equiv -\frac{\beta \hbar \kappa_0}{8\pi} \frac{1}{|\alpha_2|^2}.$$ \hspace{1cm} (C.80)

Thus $g < 0$ and in turn $\varphi$ is the complex scalar field of a repulsive BEC.
Vortex soliton

D.1 Padé approximant for a quantum vortex

Here we work out the values of the parameters \( a_1, b_1, b_2 \) in (6.77), the Padé approximant for a black quantum vortex. We begin by Taylor expanding \( \phi(r) \) about \( r = 0 \) to 7th order

\[
\phi(r) = \sqrt{\frac{r^2(a_1 + a_2 b_2 r^2)}{1 + b_1 r^2 + b_2 r^4}}
\]

\[
= \sqrt{a_1} r + \frac{(ab_2 - a_1 b_1) r^3}{2 \sqrt{a_1}} + \frac{(3a_1 b_1^2 - a_1^2 b_2^2 - 2a_1 (2a_1 + ab_1) b_2) r^5}{8a_1^{3/2}}
\]

\[
+ \frac{(-5a_1^2 b_1^3 + 3a_1^2 (4a_1 + ab_1) b_2 b_1 + a_1^3 b_2^3 + aa_1 (ab_1 - 4a_1) b_3^2) r^7}{16a_1^{5/2}} + \cdots
\]

Working through each term in the GP equation, and keeping terms only to 5th order, the first-order derivative term is

\[
\frac{\phi'(r)}{r} = \frac{\sqrt{a_1}}{r} + \frac{3(ab_2 - a_1 b_1)}{2 \sqrt{a_1}} + \frac{5(3a_1^2 b_1^2 - a_1^2 b_2^2 - 2a_1 (2a_1 + ab_1) b_2) r^3}{8a_1^{3/2}}
\]

\[
+ \frac{7(-5a_1^3 b_1^3 + 3a_1^2 (4a_1 + ab_1) b_2 b_1 + a_1^3 b_2^3 + aa_1 (ab_1 - 4a_1) b_3^2) r^5}{16a_1^{5/2}} + \cdots
\]
Next, the second-order derivative term is
\[
\phi''(r) = \frac{3(ab_2 - a_1 b_1)}{\sqrt{a_1}} + \frac{5(3a_1^2 b_1^2 - a_2^2 b_2^2 - 2a_1 (2a_1 + ab_1) b_2) r^3}{2a_1^{3/2}} \\
+ \frac{21 (-5a_1^3 b_1^3 + 3a_1^2 (4a_1 + ab_1) b_2 b_1 + a_2^3 b_2^3 + aa_1 (ab_1 - 4a_1) b_2^5)}{8a_1^{5/2}} + \ldots. \tag{D.2b}
\]

The orbital angular momentum terms is
\[
\frac{-n^2 \phi(r)}{r^2} = \frac{n^2 \sqrt{a_1}}{r} + \frac{n^2 (a_1 b_1 - ab_2) r}{2\sqrt{a_1}} - \frac{n^2 (3a_1^2 b_1^2 - a_2^2 b_2^2 - 2a_1 (2a_1 + ab_1) b_2) r^3}{8a_1^{3/2}} \\
+ \frac{n^2 (5a_1^3 b_1^3 - 3a_1^2 (4a_1 + ab_1) b_2 b_1 - a_2^3 b_2^3 + aa_1 (4a_1 - ab_1) b_2^5)}{16a_1^{5/2}} + \ldots. \tag{D.2c}
\]

Finally, the nonlinear term is
\[
(a - \phi(r)^2) \psi(r) = a\sqrt{a_1} r + \frac{(a^2 b_2 - a_1 (2a_1 + ab_1)) r^3}{2\sqrt{a_1}} \\
+ \frac{(-b_2^3 a^3 - 2a_1 (8a_1 + ab_1) b_2 a + 3a_1^2 b_1 (4a_1 + ab_1)) r^5}{8a_1^{3/2}} + \ldots. \tag{D.2d}
\]

The sum of the two $\frac{1}{r}$-order terms in (D.2) vanishes for winding number $n = 1$. For the sum of all the $r$-order terms to vanish
\[
\frac{a_1 (a - 4b_1) + 4ab_2}{\sqrt{a_1}} = 0 \tag{D.3}
\]
we choose
\[
b_1 = \frac{a(a_1 + 4b_2)}{4a_1}. \tag{D.4}
\]

The sum of all the $r^3$-order terms must vanish
\[
\frac{-2a_1^3 - ((a - 18b_1) b_1 + 24b_2) a_1^2 + a (a - 12b_1) b_2 a_1 - 6a^2 b_2^2}{2a_1^{3/2}} = 0 \tag{D.5}
\]
which upon inserting (D.4) reduces to
\[
\frac{(7a_1^2 - 16a_1) a_1 + 48 (a_1^2 - 4a_1) b_2}{16\sqrt{a_1}} = 0. \tag{D.6}
\]
So, we choose
\[ b_2 = \frac{a_1 (16a_1 - 7a^2)}{48 (a^2 - 4a_1)}. \]  

The sum of all the \( r^5 \)-order terms must vanish too
\[ \frac{3b_1 (4a_1 + (a - 40b_1)b_1)a_1^3 - 2(8a_1 (a - 18b_1) + a(a - 36b_1)b_1)b_2a^2_1 - a(96a_1 + a(a - 24b_1))b_2^2a_1 + 24a^3b_3^3}{8a_1^{5/2}} = 0, \]

which upon inserting (D.4) and (D.7) reduces to
\[ \frac{a (11a^2 - 32a_1) \sqrt{a_1} (a^2 + 8a_1)}{384 (a^2 - 4a_1)} = 0. \]

Finally, we choose
\[ a_1 = \frac{11a^2}{32}. \]

Next, inserting (D.10a) into (D.7), we have
\[ b_2 = \frac{11a^2}{384}. \]

In turn, inserting (D.10a) and (D.10b) into (D.4), we have
\[ b_1 = \frac{a}{3}. \]

Therefore, inserting (D.10) into (6.77), we find that the Padé approximant for winding number \( n = 1 \) yields the following radial solution for a black quantum vortex
\[ \phi(r) = \sqrt{\frac{11a^2r^2(12 + ar^2)}{384 + ar^2(128 + 11ar^2)}}. \]
APPENDIX E

Entropy conserving fluid model

E.1 Entropic lattice Boltzmann method

The basic construction of a method to simulate classical fluid hydrodynamics based on the entropic lattice Boltzmann equation starts with a suitable choice of a microscopic lattice, with finite-point group symmetry from which we can recover the desired macroscopic scale continuous symmetry of rotational invariance. We require even numbered products of the lattice vectors, within a local stencil, produce respectively ranked isotropic tensors. Therefore, we shall insist the following isotropic
lattice tensor identities hold for any acceptable model implementation:

\begin{align}
\sum_{a=1}^{n} \phi_a(\alpha) &= \Phi_0(\alpha) \quad \text{(E.1a)} \\
\sum_{a=1}^{n} \phi_a(\alpha)c_{ai} &= 0 \quad \text{(E.1b)} \\
\sum_{a=1}^{n} \phi_a(\alpha)c_{ai}c_{aj} &= \Phi_2(\alpha)\delta_{ij} \quad \text{(E.1c)} \\
\sum_{a=1}^{n} \phi_a(\alpha)c_{ai}c_{aj}c_{ak} &= 0 \quad \text{(E.1d)} \\
\sum_{a=1}^{n} \phi_a(\alpha)c_{ai}c_{aj}c_{ak}c_{ai} &= \Phi_4(\alpha)(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \quad \text{(E.1e)}
\end{align}

At each point of the lattice, a minimal representation of the single-particle phase-space distribution function is used, severely discretized over the momentum space degrees of freedom and highly resolved over the positional degrees of freedom. In the lattice model, there are \( n \) elements of the distribution, denoted \( f_a(\vec{x}, t) \) for \( a = 1, \ldots, n \). \( \vec{x} \) is the vector coordinate of a point on the lattice and \( t \) is time, measured in discrete steps of \( \Delta t = 1 \). That is, the local stencil for the numerical algorithm contains \( n \) points of the lattice; \( a \) is an index for a point in the stencil and is therefore associated with a lattice vector \( \vec{c}_a \), directed from the stencil’s center to that point.

**Equilibrium distribution**

The single-particle equilibrium occupation probabilities, \( f_a^{eq} \), are expressed in terms of a statistical distribution function, \( \phi_a \), as follows:

\[
f_a^{eq}(\vec{x}, t) = \phi_a[a(\vec{x}, t) + \vec{\beta}(\vec{x}, t) \cdot \vec{c}_a].
\]

(E.2)

Subsonic expansion of (E.2) is:

\[
f_a^{eq} = \phi_a(\alpha) + c_{ai}\beta_i\phi'_a(\alpha) + \frac{1}{2}c_{ai}c_{aj}\beta_i\beta_j\phi''_a(\alpha) + O[\beta^3].
\]

(E.3)
Zeroth, first, and second moments:

\[ \rho \equiv \sum_a f_{eq}^a \quad (E.4a) \]
\[ u_k \equiv \sum_a c_{ak} f_{eq}^a \quad (E.4b) \]
\[ \Pi_{kl} \equiv \sum_a c_{ak} c_{al} f_{eq}^a \quad (E.4c) \]

**Corrected equilibrium distribution**

Zeroth order quantities (\( \beta = 0 \)):

\[ \rho = \Phi_0(\alpha) \quad (E.5a) \]
\[ u_k = 0 \quad (E.5b) \]
\[ \Pi_{kl} = \Phi_2(\alpha) \delta_{kl} \quad (E.5c) \]

First order quantities (\( \beta \sim \epsilon \)):

\[ \rho = \Phi_0(\alpha) + \frac{\Phi''_2(\alpha)}{2} \beta^2 \quad (E.6a) \]
\[ u_k = \Phi'_2(\alpha) \beta_k \quad (E.6b) \]
\[ \Pi_{kl} = \Phi_2(\alpha) \delta_{kl} + \Phi''_4(\alpha) \left( \beta_k \beta_l + \frac{\beta^2}{2} \delta_{kl} \right) \quad (E.6c) \]

Using (E.6b) to solve for \( \beta \)

\[ \beta_k = \frac{u_k}{\Phi'_2(\alpha)} \quad (E.7) \]

and inserting this into (E.6a), one may solve for \( \Phi_0 \)

\[ \Phi_0(\alpha) = \rho - \frac{\Phi''_2(\alpha)}{2[\Phi'_2(\alpha)]^2} u^2 \quad (E.8) \]

Since \( u = \rho v \), substituting (E.5a) into the right-hand side of (E.8), we may identify the following perturbative correction (its “anti-derivative”):

\[ \phi_a(\alpha) = \phi_a(\alpha) - \phi_a(\alpha) \frac{\Phi_0(\alpha) \Phi''_2(\alpha)}{[\Phi'_2(\alpha)]^2} \frac{v^2}{2}. \quad (E.9) \]
It is because $\sum_a (E.9) = (E.8)$ that (E.9) is a consistent subsonic correction to the distribution function $\phi_a(\alpha)$, which is not unique. An alternative and more complicated way to determine a correction formula is given in our previous paper, see Eq. (23) in [Boghosian et al., 2004b]. Defining the energy density factor

$$ G = \frac{\Phi_0(\alpha)\Phi'_2(\alpha)}{[\Phi'_2(\alpha)]^2} $$

(E.10)

(E.9) is

$$ \phi_a \rightarrow \phi_a - G\frac{v^2}{2} \phi_a. $$

(E.11)

Hence, inserting (E.11) into (E.3) leads to the corrected occupation probability

$$ f_a^c = \phi_a(\alpha) + \frac{\Phi_0}{\Phi'_2} \vec{c_a} \cdot \vec{v} \phi'_a(\alpha) + \frac{G}{2} \left[ \frac{\Phi_0}{\Phi'_2} (\vec{c_a} \cdot \vec{v})^2 \phi''_a(\alpha) - v^2 \phi_a(\alpha) \right]. $$

(E.12)

As a consistency check, we can take the moments of (E.12). Second order quantities ($\beta \sim \epsilon$ and $\delta \phi_a \sim \epsilon^2$):

$$ \rho = \Phi_0(\alpha) $$

(E.13a)

$$ u_k = \Phi_0(\alpha) v_k $$

(E.13b)

$$ \Pi_{kl} = \Phi_2(\alpha) \left( 1 - G\frac{v^2}{2} \right) \delta_{kl} + g \Phi_0(\alpha) \left( v_k v_l + \frac{v^2}{2} \delta_{kl} \right), $$

(E.13c)

where the Galilean factor is

$$ g \equiv G \frac{\Phi''_4(\alpha)}{\Phi''_2(\alpha)} = \frac{\Phi_0(\alpha)\Phi''_4(\alpha)}{[\Phi'_2(\alpha)]^2}. $$

(E.14)

The pressure tensor

$$ P_{kl} \equiv \Pi_{kl} - g \Phi_0 v_k v_l $$

(E.15)

is then

$$ P_{kl} = \Phi_2(\alpha) \delta_{kl} + \left[ \Phi_0(\alpha) g - \Phi_2(\alpha) G \right] \frac{v^2}{2} \delta_{kl} $$

(E.16a)

$$ = \Phi_2(\alpha) \delta_{kl} + \left[ g - \Phi_2 \frac{G}{\Phi_0} \right] \frac{\rho v^2}{2} \delta_{kl}. $$

(E.16b)
Near equilibrium distribution

We wish to write the mesoscopic transport equation in the simplest way possible, convenient for later manipulations. We shall write all the relevant quantities as vectors in the space of the discrete momenta (irreducible Brillouin zone) denoted $\mathcal{B}$. The principle quantities are the equilibrium occupation probability $\mathbf{f} \equiv \{f_1, f_2, \ldots, f_n\}$, the collision function $\Omega[\mathbf{f}] \equiv \{\Omega_1[f_1], \Omega_2[f_2], \ldots, \Omega_n[f_n]\}$, and drift vector $\mathbf{c} \equiv \{c_1, c_2, \ldots, c_n\}$, which has as its components the constant velocity vectors. Unlabeled products of vectors are to be interpreted as multiplied component-wise, for example $\mathbf{c} \cdot \mathbf{f} \equiv \{c_1 f_1, c_2 f_2, \ldots, c_n f_n\}$. The dot product is defined as usual, for example $\mathbf{c} \cdot \mathbf{f} \equiv \sum_a c_a f_a$. It is understood that an operator acts on all the operands appearing to its right, so for example $\nabla \cdot \mathbf{c} \cdot \mathbf{f} = \mathbf{c} \cdot \nabla \mathbf{f}$, since $\mathbf{c}$ is constant and where the bullet symbol represents a slot for some operand. Consequently, $\nabla \cdot \mathbf{cf} = \{\nabla f_1, \nabla f_2, \ldots, \nabla f_n\}$ is a vector in $\mathcal{B}$ whereas $\nabla \mathbf{c} \cdot \mathbf{f} \equiv \sum_a c_a \nabla f_a$ is not. In this notation the macroscopic moments are

$$
\rho = \mathbf{1} \cdot \mathbf{f}
$$

$$
\vec{u} = \mathbf{c} \cdot \mathbf{f}
$$

$$
\vec{\Pi} = \mathbf{cc} \cdot \mathbf{f},
$$

where $\mathbf{1} \equiv (1, 1, \ldots, 1)$ and the lattice Boltzmann equation is

$$
\mathbf{f}(\mathbf{1x} + \mathbf{c} \delta t, t + \delta t) = \mathbf{f}(\mathbf{1x}, t) + \Omega[\mathbf{f}]. \tag{E.18}
$$

With the equilibrium condition $\Omega[\mathbf{fe}] = 0$, we can linearize the collision function on the right-hand side of (E.18) about the corrected equilibrium occupations. Then (E.18) may be rewritten as a matrix equation using the Jacobian matrix of the collision operator $\mathbf{J} \equiv (\partial_t \Omega)|_{\mathbf{f}=\mathbf{e}}$, where $d \equiv \Phi_0/n$. Furthermore, we introduce the space and time parabolic differential operator

$$
\mathbf{\hat{L}} \cdot \equiv (\partial_t + \nabla \cdot \mathbf{J}) \cdot, \tag{E.19}
$$
written in terms of the current operator

$$\mathcal{J} \equiv \left( c + \nabla \frac{cc}{2} \right) .$$  \hspace{1cm} (E.20)

Here $c$ act as a drift vector and $\frac{cc}{2}$ is a diffusive eigenvector, see (E.26) below. Taylor expanding the left-hand side of (E.18) about the point $(1x, t)$ yields the parabolic equation

$$\hat{L}f = J(f - f^c),$$  \hspace{1cm} (E.21)

$J$ is a $n \times n$ size matrix and the product $Jf$ is to be interpreted as the usual matrix multiplication. Then, multiplying (E.21) from the left by $c$ gives

$$\hat{L}cf = J[c(f - f^c)].$$  \hspace{1cm} (E.22)

Note that the product $cJ$ is not interpreted as a matrix multiplication operation, but instead the components of $c$ multiply the rows of $J$. Hence, we have used the identity $cJf = J[cf]$. In order to find the correction to the occupation probabilities due to collisional diffusion, we perform a perturbative approximation starting with the first order contributing term from the left-hand side of (E.22)

$$\nabla \cdot \hat{J}cf = J[c(f - f^c)]$$  \hspace{1cm} (E.23)

This implies

$$\nabla \cdot Jccf = J[c(f - f^c)] + O(\epsilon^2)$$  \hspace{1cm} (E.24)

and in turn

$$c(f - f^c) = \nabla \cdot J^{-1}ccf,$$  \hspace{1cm} (E.25)

where the generalized inverse of $J$ is taken over the kinetic subspace since the hydrodynamic subspace is the null space of eigenvectors (conserved quantities) of $J^{-1}$ with zero eigenvalue. Our lattice is chosen so the diffusive eigen-equation

$$J^{-1}cc = \frac{1}{2} \frac{cc}{\kappa_n}$$  \hspace{1cm} (E.26)
holds, whence we obtain the first order deviation of the occupation probabilities:

\[ c(f - f^c) = -\frac{1}{\kappa} \nabla \cdot ccf. \] (E.27)

This implies

\[ f = f^c - \frac{1}{\kappa} \nabla \cdot ccf + \mathcal{O}(\epsilon^3) \] (E.28)

or component-wise this reads

\[ f_a = f_a^c - \frac{1}{\kappa} c_{ai} \partial_i f_a^{(0,1)} + \mathcal{O}(\epsilon^3), \] (E.29)

where the superscript \((0, 1)\) denotes the contributing orders, perturbatively; only the zeroth and first order terms are needed since the spatial gradient of the probability field contributes an additional order \(\epsilon\). Therefore, we insert the first two (lowest order) terms of (E.12) into (E.29) to obtain a perturbation expansion of the near-equilibrium distribution, including all terms up to order \(\epsilon^2\):

\[ f_{a \text{near}} = f_a^c - \frac{1}{\kappa} c_{ai} \partial_i \left[ \phi_a(\alpha) + \frac{\Phi_0}{\Phi'_2} \phi'_a(\alpha) \right]. \] (E.30)

In vector notation, we have

\[ f_{\text{near}} = \phi + \frac{\Phi_0}{\Phi'_2} \vec{u} \cdot c \phi' + \frac{G}{2} \left[ \frac{\Phi_0}{\Phi'_2} \vec{u} \cdot c \phi'' - \vec{v} \cdot c \phi' \right] \]

\[ - \frac{1}{\kappa} \nabla \cdot c \left[ \phi + \frac{\Phi_0}{\Phi'_2} \vec{u} \cdot c \phi' \right]. \] (E.31)

Building on (E.13) we see the moments of (E.30) are the following:

\[ \rho = \Phi_0 - \frac{1}{\kappa} \partial_i \Phi_0 \bar{v}_i \] (E.32a)

\[ u_k = \Phi_0 \bar{v}_k - \frac{1}{\kappa} \partial_k \Phi_2 \] (E.32b)

\[ \Pi_{kl} = P_{kl} + \Phi_0 \bar{v}_k \bar{v}_l - \frac{g \Phi'_2}{\kappa} \left( \partial_k \bar{v}_l + \partial_l \bar{v}_k + \partial_i \bar{v}_i \delta_{kl} \right). \] (E.32c)
Navier-Stokes equation

Dotting $c$ into (E.21) (taking the first moment) yields

$$ \hat{\mathbf{L}} \mathbf{c} \cdot \mathbf{f} = 0. $$  \hspace{1cm} (E.33)

The right-hand side vanishes because $\mathbf{c} \cdot \Omega = 0$ for all distributions, whether near or far away from equilibrium. (E.33) reduces to

$$ \partial_t \mathbf{c} \cdot \mathbf{f} + \nabla \cdot \mathbf{cc} \cdot \mathbf{f} + \frac{1}{2} \nabla \nabla : \mathbf{ccc} \cdot \mathbf{f} + \mathcal{O}(\epsilon^3) = 0, $$  \hspace{1cm} (E.34)

or in component form

$$ \partial_t u_i + \partial_j \Pi_{ij} + \frac{1}{2} \partial_j \partial_k \sum_a c_{ai} c_{aj} c_{ak} f_a + \mathcal{O}(\epsilon^3) = 0. $$  \hspace{1cm} (E.35)

Inserting (E.32c) into (E.35) and retaining terms to order $\epsilon^3$ yields, in the incompressible limit when $\nabla \cdot \mathbf{v} = 0$, the following effective field theory:

$$ \partial_t (\rho v_i) + g \Phi_0 v_j \partial_j v_i = -\partial_j P_{ij} + g \Phi'_2 \left( \frac{1}{\kappa_\eta} - \frac{1}{2} \right) \partial^2 v_i + \mathcal{O}(\epsilon^4). $$  \hspace{1cm} (E.36)

Finally, dividing through by $\phi(\alpha)$ gives the incompressible Navier-Stokes equation

$$ \partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla P + \nu \nabla^2 \mathbf{v} + \mathcal{O}(\epsilon^4), $$  \hspace{1cm} (E.37)

where the pressure is

$$ P = \frac{\Phi_2}{\Phi_0} + \left[ g - \frac{\Phi_2}{\Phi_0} G \right] \frac{v^2}{2}, $$  \hspace{1cm} (E.38)

and where the kinematic viscosity is

$$ \nu = \frac{\Phi'_2}{\Phi'_0} \left( \frac{1}{\kappa_\eta} - \frac{1}{2} \right). $$  \hspace{1cm} (E.39)

For any model on a lattice that satisfies the isotropy conditions (E.1), we can choose the $\phi_a$'s so that $g = 1$ in (E.37) to impose Galilean invariance in the nonlinear convective term and also so that $g - \frac{\Phi_a}{\Phi_0} G = 0$ in (E.38) to remove any anomalous velocity dependence in the pressure term. As an example, in §E.1.2 we demonstrate this for the $n = 27$ model in 3+1 dimensions.
E.1.1 Entropic treatment

BGK collisional approximation

We take the ELBE to be the following finite-difference form of the Boltzmann kinetic transport equation:

\[ f_a(x + c_a \Delta t, t + \Delta t) = f_a(x, t) + \alpha \beta \left[ f_a^{eq}(\bar{x}, t) - f_a(\bar{x}, t) \right], \quad (E.40) \]

where the inverse relaxation time is \( \alpha \beta \sim \kappa \). This form is suitable for numerical implementation. The right-hand side is a generalization of the Bhatnager-Gross-Krook (BGK) collision function [Bhatnagar et al., 1954, Gross and Jackson, 1959] commonly used in the lattice Boltzmann equation (the Jacobian of the collision function is taken to be diagonal). The free parameter \( 0 \leq \beta \leq 1 \) allows us to tune the viscosity. For \( \alpha \sim 2 \), the inviscid limit occurs as \( \beta \to 1 \). The effective shear viscosity is

\[ \nu_{eff} = c_s^2 \Delta t \left( \frac{1}{\alpha \beta} - \frac{1}{2} \right). \quad (E.41) \]

(E.40) requires the following steps to update the distribution functions from time \( t \) to time \( t + \Delta t \):

(a) initialization of \( f_a \) using the equilibrium distribution function \( f_a^{eq}(\rho, \bar{v}, t) \);

(b) evaluation of the collision function \( \Omega_a \) (computing post-collision distribution \( f'_a \) from the pre-collision distribution \( f_a \));

(c) streaming of the distribution function information to neighboring lattice points; and

(d) calculation of the mass and velocity moments at each spatial point.

The computationally expansive step is (b), choosing the post-collision distribution \( f'_a(\bar{x}, t) \) by considering the change in the local entropy \( \mathcal{H} \) at the point \( \bar{x} \), a sum over
all $n$ entropy contributions from each of the discrete momentum directions

$$\mathcal{H}(\vec{x}) = \sum_{a=1}^{n} h_a[f_a(\vec{x})], \quad (E.42)$$

where $h_a = h_a[f_a]$ is a pre-specified function that determines the collisional dynamics, and the value of the dissipative transport coefficient, the shear viscosity $\nu$, in the macroscopic equation of motion.

FIG. E.1: Collisional inversion. The non-equilibrium part of distribution function is shown (black vectors on the left and white on the right). The curved surface is an isentrope and the diagonal plane is a constant mass surface. The incoming $f$ goes to a point at the intersection of the constant mass and entropy surfaces (black line on left and white line on right view). $f^{eq}$ is shown (middle black line on left and middle white line on right view). $f^{eq}$ contacts a lower entropy surface. The ideal $(\beta = 1)$ outgoing distribution $f' = f + \alpha \Delta$ (black line on left and white line on right view) goes to an antipodal point on the curve formed by the intersection of the constant mass and entropy surfaces. Finally for $\beta = 0.9$, the outgoing $f + \alpha \beta \Delta$ (red line on both views) illustrates $\beta < 1$ increases the entropy since $f$ does not contact the original entropy surface.

In the inviscid limit ($\nu = 0$), the change of the local entropy

$$\delta \mathcal{H} = \sum_{a=1}^{n} (h_a[f_a'(\vec{x})] - h_a[f_a(\vec{x})]) \quad (E.43)$$

vanishes at all points and at all times $\delta \mathcal{H}_{\text{min}} = 0$. In the opposite limit of maximum dissipation ($\nu = \nu_{\text{max}}$), the entropy change has its maximal value,

$$\delta \mathcal{H}_{\text{max}} = \sum_{a=1}^{n} (h_a[f^{\text{eq}}_a(\vec{x})] - h_a[f_a(\vec{x})]), \quad (E.44)$$

where the equilibrium distribution $f^{eq}_a$ is found by extremizing the entropy subject to the constraint of mass and momentum conservation and using Lagrange multipliers
for the mass density and momentum density, which are moments of the single-particle distribution: \( \sum_{a=1}^{n} f_a \{1, \vec{c}_a\} = \{\rho, \rho \vec{v}\} \), where \( m = 1 \) is the unit mass and \( \vec{c}_a \) are the lattice vectors.

\[
\frac{\partial}{\partial f_a} \left[ \mathcal{H}(f_*) - \alpha \rho - \vec{\beta} \cdot (\rho \vec{v}) \right] \bigg|_{f=f_a^*} = 0. \quad (E.45)
\]

\[
\delta \mathcal{H}_{\text{max}} = -\sum_{a=1}^{n} \delta f_a \frac{\partial}{\partial f_a} \left[ \mathcal{H}(f_*) - \alpha \rho - \vec{\beta} \cdot (\rho \vec{v}) \right], \quad (E.46)
\]

where \( \delta f = f_a' - f_a \). The entropy change is along the “uphill gradient” of the entropy hypersurface. Extremizing the entropy subject to energy conservation (second moment of the single-particle distribution) is not required in the case when we want to recover the Navier-Stokes equations in the incompressible limit.

**Isentropic dynamics**

A path along the entropy hypersurface with constant value, say \( \mathcal{H}_o \), is an isentropic path. In the \( n \)-dimensional space spanned by the occupation probabilities, the isentropic path is defined by the set of all \( f_a \)'s that satisfy the equation:

\[
\sum_{a=1}^{n} h_a[f_a] = \mathcal{H}_o. \quad (E.47)
\]

Letting the incoming distribution be denoted as \( f \) and the outgoing distribution \( f' \), the constant entropy condition is:

\[
\mathcal{H}(f) = \mathcal{H}(f'). \quad (E.48)
\]

**Collision by inversion of the distribution**

The bare collision function is \( \Delta \equiv f^{\text{eq}} - f \). The constant entropy condition is

\[
\mathcal{H}(f) = \mathcal{H}(f + \alpha \Delta), \quad (E.49)
\]

parameterized by \( 0 \leq \alpha \leq 2 \), and can be written as

\[
\mathcal{H}[f^{\text{eq}} - \Delta] = \mathcal{H}[f^{\text{eq}} + (\alpha - 1)\Delta], \quad (E.50)
\]
The trivial case occurs when $\alpha = 0$ (no collision). The other limiting case occurs when $\alpha \to 2$ (inviscid limit). We will understand the role of $\alpha$ by treating this limiting case. Here, the incoming distribution $f = f^{\text{eq}} - \Delta$ and the outgoing distribution $f' = f^{\text{eq}} + \Delta$ are exact inversions of each other in the sense that the following condition holds:

$$\mathcal{H}[f^{\text{eq}} - \Delta] = \mathcal{H}[f^{\text{eq}} + \Delta].$$

(E.51)

This represents an optimal collision mechanism to reduce momentum transport by inverting the non-equilibrium part of the incoming distribution to produce the outgoing distribution, while conserving entropy. This inversion shown in Fig. E.1 occurs by an overall sign change of the non-equilibrium part of the distribution ($-\Delta \to \Delta$), and this represents the original mechanism that led to the conception of the entropic lattice Boltzmann equation $\alpha$ parametrizes the completeness of the inversion process from $f$ to $f'$ going from $\alpha = 0$ (no inversion) up to $\alpha = 2$ (perfect inversion). The inversion of the particle distribution is used to achieve low viscosity by preserving the anisotropy of the particle distribution.

**Derivation of the equilibrium function using an entropy function approach**

Here we derive the statistical distribution function starting with a classical entropy function. The entropy of a single particle state in the mesoscopic limit is the following function:

$$h_a(f_a) = f_a \ln(\gamma_a f_a).$$

(E.52)

The equilibrium occupation probability is defined as the extrema of the entropy function:

$$\frac{\partial h_a(f_a)}{\partial f_a} \bigg|_{f=f^{\text{eq}}} = 0.$$  

(E.53)
From (E.52), we see that

\[ h'_a(f_a) = \ln(\gamma_a f_a) + 1 = \ln(e\gamma_a f_a) \quad (E.54) \]

We define the inverse function as follows

\[ \phi_a(\alpha) \equiv [h'_a(\alpha)]^{-1} \rightarrow \alpha = h'_a[\phi_a(\alpha)], \quad (E.55) \]

from which we have

\[ \alpha \overset{(E.54)}{=} \ln[e\gamma_a \phi_a(\alpha)] \rightarrow \frac{1}{e\gamma_a} e^\alpha = \phi_a(\alpha) \quad (E.56) \]

or

\[ \phi_a(\alpha) = d w_a e^\alpha, \quad (E.57) \]

where for each distribution function there is a weight \( d w_a \equiv \frac{1}{e\gamma_a} \) and where we define \( d \) to be the uniform background number density.

**Equilibrium statistical function recovered**

We extremize \( \mathcal{H} \) subject to the constraints of conserved mass and momentum. Therefore, (E.46) gives us

\[ h'_a(f_a) - \alpha - \vec{\beta} \cdot \vec{c}_a = 0. \quad (E.58) \]

Then, using the inverse function (E.55), we obtain the result for the equilibrium occupation:

\[ f^a_{eq} = \phi_a(\alpha + \vec{\beta} \cdot c_a). \quad (E.59) \]

Here we recover to our starting point (E.2). Using (E.57) we may write this as

\[ f^a_{eq} = d w_a e^{\alpha + \vec{\beta} \cdot c_a}. \quad (E.60) \]
FIG. E.2: Early stage in the development at $t = 900$ of the Kelvin-Helmholtz instability modeled with parameters $\beta = 0.9995$ and the bare viscosity is $\nu = 8.3410^{-5}$ (using $\alpha = 2$), on a $1024^2$ grid (only a horizontal strip through the middle of the grid is shown). The 2D model uses a 9-point stencil. Vortex production occurs along the fronts of the braking waves (blue is counterclockwise and red is clockwise rotation). The initial background flow speed is $u_0 = 0.51\frac{c_0}{a}$, and the Reynolds number $Re = 9.810^4$.

E.1.2 Numerical treatment

$n = 27$ model in $3+1$ dimensions

The lattice vectors are

$$c_a = \left[\left(\frac{a}{3^2}, \frac{a}{3}, a\right)\right] \mod 3 - 1,$$  \hspace{1cm} (E.61)

which is the set

$$c = \{(0, 0, 0), (0, 0, \pm 1), (0, \pm 1, 0), (\pm 1, 0, 0), (\pm 1, \pm 1, 0), (0, \pm 1, \pm 1), (\pm 1, \pm 1, \pm 1)\}.$$  \hspace{1cm} (E.62)

For each occupation probability $f_a$ is associated one element of the set, $c_a$, for $a = 1, \ldots, n$. We define a weight $w_a$ for each occupation probability as follows:

$$w_a(c_a) = \prod_{i=1}^{3} q^{1-|c_{ai}|} r^2 s^2 c_{ai} c_{ai}.$$  \hspace{1cm} (E.63)
Normalizing the weights, $\sum_a w_a = 1$, gives the following cubic equation

$$(q + r + s)^3 = 1, \quad (E.64)$$

and we take the real solution as the physical one $q = 1 - r - s$. Following (E.57), the basic approach is to write the occupation probability function in separable form

$$\phi_a(\alpha) = w_a F(\alpha). \quad (E.65)$$

Since the weights are normalized, the zeroth moment of $\phi_a$ is

$$\Phi_0(\alpha) = F(\alpha). \quad (E.66)$$

From (E.65) it follows that the second moment of $\phi_a$ is

$$\sum_a \phi_a(\alpha) \bar{c}_a \bar{c}_a = (r + s) F(\alpha) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + (r - s)^2 F(\alpha) \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad (E.67)$$

and so if we pick $r = s$ then we recover the lattice tensor identity (E.1c) where

$$\Phi_2(\alpha) = 2r F(\alpha). \quad (E.68)$$

The fourth moment of $\phi_a$ is

$$\sum_a \phi_a(\alpha) \bar{c}_a \bar{c}_a \bar{c}_a \bar{c}_a = 4r^2 F(\alpha) \begin{pmatrix} \frac{1}{2r} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (E.69)$$

To recover the lattice tensor identity (E.1e), the diagonal components must equal three, $\frac{1}{2r} = 3$, so we must have $r = \frac{1}{6}$, which gives us

$$\Phi_4(\alpha) = \frac{1}{9} F(\alpha), \quad (E.70)$$
and from (E.68) we have
\[ \Phi_2(\alpha) = \frac{1}{3} F(\alpha). \]  
(E.71)

Now using (E.71), (E.70) and (E.66), the Galilean factor (E.14) is unity,
\[ g = \frac{F'''}{F} = 1, \]  
(E.72)

and the velocity-dependent term in (E.16a) vanishes,
\[ g - \frac{\Phi_2}{\Phi_0} \Gamma = \frac{F'''}{F} - \frac{F''}{F} = 0, \]  
(E.73)

provided we have \( F(\alpha) = de^{\pm \alpha} \). This solution is consistent with (E.57). The pressure is
\[ P = \frac{1}{3}, \]  
(E.74)

and the kinematic viscosity is
\[ \nu = \frac{1}{3} \left( \frac{1}{\kappa_\eta} - \frac{1}{2} \right). \]  
(E.75)

The corrected equilibrium distribution is
\[ f^e = wde^{\alpha} \left[ 1 + 3\vec{u} \cdot \mathbf{c} + \frac{9}{2} \left( \vec{v} \cdot \mathbf{c} - \frac{\nu^2}{3} \right) \right]. \]  
(E.76)

**Simulation results**

2D interlacing Kevin-Helmholtz vorticity sheets are simulated on a 1024^2 grid at \( \text{Re} = 10^5 \), see Figure E.2. Histograms of the grid variations of the \( \alpha(x, t) \)-profiles show a significant shift from a quasi-Gaussian distribution about the equilibrium \( \alpha_{eq} = 2 \) and strongly shifted to large effective viscosities due to turbulence. At late time stages of this simulation we observed a large number of vortex pairing events. The most prominent was the paring of like-sign or co-rotating vortices, see the three stages of symmetric vortex fusion in a 2D fluid simulation shown in Figure E.3. This observed behavior agrees with experimental observations of vortex fusion by Meunier *et al.* [Meunier et al., 2002].
FIG. E.3: 3 stages of symmetric vortex fusion. 1st column \( (t < 50K) \): Vortices rotate around each other with approximately constant separation distance; the areal size of the vortices grows linearly in time because of viscous diffusion. 2nd column \( (50K < t < 70K) \): Vortices reach a critical size, about 24\% of the separation distance. Vortex centers then rapidly merge into a single core. 3rd column \( (t \geq 70K) \): Vorticity arms roll up around the central pattern, forming a spiral of vorticity, which subsequently spreads and is smoothed by diffusion.

FIG. E.4: Streamlines plot of turbulent flow arising from the initial Kida profile.
FIG. E.5: The enstrophy (integrated mean square vorticity) decay for bare viscosities ranging from $\nu = 2 \times 10^{-4}$ (for $\beta = 0.9988$) to $\nu = 8 \times 10^{-3}$ (for $\beta = 0.95$) for an initial Kida profile. In the early stages, one sees the effects of vortex stretching with exponential growth in the strength of the vortex filaments. This growth in the enstrophy is independent of viscosity. $\nu$ determines the peak in the enstrophy followed by exponential decay in the inertial range. Re $\simeq 6000$ was achieved on the $512^3$ grid.
Kida flow profile [Kida and Murakami, 1987] for the initial velocity field \( \vec{v} = (u, v, w) \) is the following:

\[
u(x, y, z, t = 0) = v(z, x, y, t = 0) = w(y, z, x, t = 0) = U_0 \sin \left( \frac{2\pi x}{N_x} \right) \left[ \cos \left( \frac{2\pi N_y y}{z} \right) \cos \left( \frac{2\pi N_z z}{y} \right) - \cos \left( \frac{2\pi N_y y}{z} \right) \cos \left( \frac{2\pi N_z z}{y} \right) \right], \tag{E.77}
\]

where the grid points \( x_i = 1, \ldots, N_x \). This is a highly symmetric periodic initial profile. We conducted many 3D simulations initialized with the Kida-Murakami velocity profile for freely decaying turbulence, see Figures E.4. The enstrophy decay is shown in Figure E.5 for the Kida profile for a range of viscosities.

### E.2 Traveling kink in the Burgers equation

#### E.2.1 Cole-Hopf Solution

The nonlinear Burgers equation

\[
\partial_t u + \partial_x \left( \frac{u^2}{2} \right) - \nu \partial_{xx} u = 0 \tag{E.78}
\]

is the effective field theory of a Q2 model with state localization. The Cole-Hopf solution method [Hopf, 1950, Cole, 1951] begins with the potential \( S \)

\[
u \equiv \partial_x S. \tag{E.79}
\]

Inserting (E.79) into (E.78) gives

\[
\partial_{xx} S + \partial_x \left[ \frac{(\partial_x S)^2}{2} \right] - \nu \partial_{xxx} S = 0. \tag{E.80}
\]

Integrating over of the space variable gives the Kardar-Parisi-Zhang equation [Kardar et al., 1986]:

\[
\partial_t S + \frac{1}{2}(\partial_x S)^2 - \nu \partial_{xx} S = 0. \tag{E.81}
\]
The exponential variable transformation is

$$\psi = e^{-\frac{S}{2\nu}} \quad \text{or} \quad S = -2\nu \ln \psi. \quad (E.82)$$

The needed partial derivatives are

$$\partial_t S = -2\nu \frac{\partial \psi}{\psi} \quad (E.83a)$$
$$\partial_x S = -2\nu \frac{\partial_x \psi}{\psi} \quad (E.83b)$$
$$\partial_{xx} S = 2\nu \frac{(\partial_x \psi)^2}{\psi^2} - 2\nu \frac{\partial_t \psi}{\psi}. \quad (E.83c)$$

The KPZ equation becomes the diffusion equation, that is inserting (E.83) into (E.81) gives

$$\partial_t \psi - \nu \partial_{xx} \psi = 0. \quad (E.84)$$

### E.2.2 Inverse solution check

Inverting the Cole-Hopf solution, inserting (E.79) into (E.82a), gives

$$\psi = \psi_0 e^{-\frac{1}{2\nu} \int dx \, u}. \quad (E.85)$$

Differentiating (E.85), we have

$$\partial_x \psi = -\frac{u}{2\nu} \psi \quad (E.86a)$$
$$\partial_{xx} \psi = -\frac{\partial_x u}{2\nu} \psi + \frac{u^2}{4\nu^2} \psi \quad (E.86b)$$
$$\partial_t \psi = -\frac{1}{2\nu} \int dx \, \partial_t u. \quad (E.86c)$$

Inserting (E.86) into (E.84) gives

$$-\frac{\int dx \, \partial_t u}{2\nu} + \frac{1}{2} \partial_x u - \frac{u^2}{4\nu} = 0. \quad (E.87)$$

Differentiating gives the Burgers equation

$$\partial_t u + \partial_x \left( \frac{u^2}{2} \right) - \nu \partial_{xx} u = 0. \quad (E.88)$$
E.2.3 Moving reference frame

Let \( k \) denote the wave number. We write an analytical solution by a kind of separation of variables in the frame moving with velocity \( \pm v \) of the shock front as follows

\[
\psi(x, t) = g(t)h[k(x \pm vt)]. \tag{E.89}
\]

Let \( z \equiv k(x \pm vt) \), then (E.89) into (E.84) gives

\[
h \partial_z g \pm kv \partial_z h - \nu k^2 g \partial_{zz} h = 0 \tag{E.90a}
\]

or

\[
\frac{\partial_z g}{g} + \frac{\partial_z (\pm kv h - \nu k^2 \partial_z h)}{h} = 0. \tag{E.90b}
\]

Now \( z \) is effectively an independent variable. Choose the separation constant to be \(-\nu k^2\):

\[
\frac{\partial_z g}{g} = -\nu k^2 \tag{E.91a}
\]

\[
\frac{\partial_z (\pm kv h - \nu k^2 \partial_z h)}{h} = \nu k^2. \tag{E.91b}
\]

The exponential damping solution of (E.91a) is

\[
g = g_0 e^{-\nu k^2 t}. \tag{E.92}
\]

Differential equation (E.91b) gives

\[
d_{zz} h \mp \frac{v}{\nu k} d_z h + h = 0. \tag{E.93}
\]

This has two solutions

\[
h(z) = h_+ e^{\frac{z}{\nu k} \left( \pm \sqrt{\frac{v^2}{\nu^2 k^2} - 4} \right)} \tag{E.94a}
\]

\[
h(z) = h_- e^{\frac{z}{\nu k} \left( \pm \sqrt{\frac{v^2}{\nu^2 k^2} - 4} \right)}. \tag{E.94b}
\]

Let \( \alpha \equiv \pm \frac{v}{2 \nu k} \), we have

\[
h(z) \overset{(E.94)}{=} h_\pm e^{z(\alpha \pm \sqrt{\alpha^2 - 1})}. \tag{E.95}
\]
Its derivatives are

\[ d_x h = (\alpha \pm \sqrt{\alpha^2 - 1})h \]  
\[ d_{xx} h = (2\alpha^2 \pm 2\alpha\sqrt{\alpha^2 - 1} - 1)h. \]  
(E.96a)  
(E.96b)

Inserting (E.96) into (E.93) gives zero. Therefore, we have the full solution of the diffusion equation in the moving reference frame, (E.92) and (E.94) → (E.89):

\[ \psi(x, t) = \psi_+ e^{-\nu k^2 t} e^{\frac{k(x \pm vt)}{2}} \left( \pm \frac{\nu}{\nu k + \sqrt{\nu^2 - \frac{k^2}{2}}} \right) + \psi_- e^{-\nu k^2 t} e^{\frac{k(x \pm vt)}{2}} \left( \pm \frac{\nu}{\nu k - \sqrt{\nu^2 - \frac{k^2}{2}}} \right). \]  
(E.97)

Inserting (E.97) into (E.84) gives zero, so (E.97) is a solution to the diffusion equation in the moving frame of reference.

Solving (E.85) for \( u \) gives

\[ u = -2\nu \frac{\partial_x \psi}{\psi}. \]  
(E.98)

Inserting (E.97) into (E.98) gives

\[ u = \mp v \]

\[ + \sqrt{\nu^2 - 4k^2 \nu^2} \left( \frac{2 \psi_-}{\psi_- + e^{(x \pm vt)\sqrt{\nu^2 - 4k^2 \nu^2}/\nu}} - 1 \right). \]  
(E.99)

Inserting (E.99) into (E.78) gives zero, so (E.99) is an analytical solution of the Burgers equation. Let us define a new wave number

\[ \kappa \equiv \frac{\sqrt{\nu^2 - 4k^2 \nu^2}}{2\nu}. \]  
(E.100)

Then (E.99) can be written in a form similar to (E.98):

\[ u(x, t) = \mp v - 2\nu \kappa \left[ \psi_+ e^{\kappa(x \pm vt)} - \psi_- e^{-\kappa(x \pm vt)} \right] \]  
\[ \psi_+ e^{\kappa(x \pm vt)} + \psi_- e^{-\kappa(x \pm vt)} \]  
(E.101)

After some algebraic manipulation, (E.101) can be written in terms of hyperbolic trigonometric functions

\[ u(x, t) = \mp v - 2\nu \kappa \tanh \kappa(x \pm vt) \]

\[ -2\nu \kappa \frac{(\psi_x - \psi_-) \sech^2 \kappa(x \pm vt)}{(\psi_x + \psi_-) + (\psi_x - \psi_-) \tanh \kappa(x \pm vt)}. \]  
(E.102)
When $\psi_+ = \psi_-$ the solution is a moving shock with a hyperbolic tangent front shape. This is called as a kink solution and is known to exist in BECs [Simula et al., 2008, Muryshev et al., 1999, Busch and Anglin, 1998].
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