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Quantum and Classical Manifestation of Hamiltonian Monodromy

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Quantum and Classical Manifestation of Hamiltonian Monodromy

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ABSTRACT

Integrable Hamiltonian systems are said to display nontrivial monodromy if fundamental action-angle loops defined on phase-space tori change their topological structure when the system is carried around a circuit. It was shown in earlier work that this topological change can be seen in families of trajectories of noninteracting particles; however, that work required use of a very abstract flow in phase space. In this dissertation, we show that the same topological change can occur as a result of application of ordinary forces. We also show how this dynamical phenomenon could be observed experimentally in cold atom systems.

Almost everything that happens in classical mechanics also shows up in quantum mechanics when we know where to look for it. In the latter half of the dissertation, we show a corresponding change in quantum wave functions: these wave functions change their topological structure in the same way that the action and angle loops change. Also the probability current associated with this wave function follows the angle loop, changing its winding number from 0 to -1.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acknowledgements</td>
<td>iv</td>
</tr>
<tr>
<td>Dedications</td>
<td>vi</td>
</tr>
<tr>
<td>List of Tables</td>
<td>vii</td>
</tr>
<tr>
<td>List of Figures</td>
<td>viii</td>
</tr>
<tr>
<td><strong>Chapter 1. Introduction</strong></td>
<td>1</td>
</tr>
<tr>
<td><strong>Chapter 2. Action and Angle Variables</strong></td>
<td>5</td>
</tr>
<tr>
<td>2.1 phase space, J-product, variable transformation</td>
<td>11</td>
</tr>
<tr>
<td>2.2 canonical transformation</td>
<td>15</td>
</tr>
<tr>
<td>2.3 canonical variables on the torus</td>
<td>24</td>
</tr>
<tr>
<td>2.3.1 integrable system, level sets, Lagrangian manifold</td>
<td>25</td>
</tr>
<tr>
<td>2.3.2 canonical transformation from ((q, p)) to ((t, f))</td>
<td>27</td>
</tr>
<tr>
<td>2.3.3 canonical transformation from ((t, f)) to ((\phi, I))</td>
<td>30</td>
</tr>
<tr>
<td><strong>Chapter 3. A Classical static manifestation of monodromy</strong></td>
<td>34</td>
</tr>
<tr>
<td>3.1 the transformation from ((t, f)) to ((\phi, I)) is not smooth</td>
<td>35</td>
</tr>
<tr>
<td>3.2 redefine action variable (I_i) to get a smooth</td>
<td></td>
</tr>
</tbody>
</table>
canonical transformation 43

3.3 topological change of the angle loop 48

Chapter 4. dynamical manifestation of monodromy 52

4.1 simulation and results 54

Chapter 5. Experimental realization 59

Chapter 6. Quantum manifestation of monodromy 74

6.1 Construct semiclassical wavefunction with topological change 83

6.1.1 Calculation of classical action-angle loops 85

6.1.2 Corresponding quantum system 87

6.1.3 Wave functions in a circular box 94

6.2 Superposition with topological change 100

6.2.1 Truncated expansion of semiclassical wavefunctions 100

6.2.2 Superposition in Mexican Hat system 108

6.2.3 The probability current under effective Hamiltonian $\mathcal{H}$ 109
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.3 Dynamical monodromy of wave functions</td>
<td>113</td>
</tr>
<tr>
<td>Chapter 7. Conclusion and outlook</td>
<td>115</td>
</tr>
<tr>
<td>Appendix A. details of the applied force</td>
<td>119</td>
</tr>
<tr>
<td>Appendix B. details of calculation of angle loop</td>
<td>122</td>
</tr>
<tr>
<td>Appendix C. details of construction of semiclassical wavefunction</td>
<td>124</td>
</tr>
<tr>
<td>Bibliography</td>
<td>129</td>
</tr>
</tbody>
</table>
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LIST OF TABLES

1. Summary of ultracold atom experiment parameters 59
LIST OF FIGURES

1. Geometric meaning of $g_i = \frac{\partial Z_i}{\partial z} = \nabla_z Z_i$ and $z_i = \frac{\partial z}{\partial Z_i}$. 24

2. Fundamental loops on the torus 31

3. Mexican Hat potential and the classical trajectory in it 37

4. Spectrum space and monodromy circuit 39

5. The angle subtended within one radial cycle in circular box 41

6. Action versus $l$ and $E$, defined in the old way 44

7. Action versus $l$ and $E$, defined in the new way 45

8. Action versus $l$ and $E$, defined in the new way (2) 46

9. The angle subtended within one radial cycle in circular box, defined in the new way 48

10. A static manifestation of Hamiltonian monodromy 51

11. Collective monodromy circuit of a family of particles 58

12. A collection of snapshots showing the evolution of the single loop and of the cold gas as the system traverses the monodromy circuit 61

13. Proposed apparatus and optical potentials for observing dynamical monodromy 65

14. Magnetic fields for producing the torque force 67

15. Torque force and central barrier modulation versus time required for completing the monodromy circuit 69

16. Time-of-flight method for measuring the total energy $E$ 71

17. Angular momentum measurement method with in situ imaging 73

18. Spectrum of eigenstates and the monodromy circuit in Mexican Hat system 77
19. Torus and its angle loops in the beginning and end of monodromy process 78

20. Monodromy of wavefunction 80

21. (a)(b) A topological change of angle variables in the circular box system 89

   (c)(d) Topological change of semiclassical wave functions in the circular box 91

   (e)(f) Topological change of superposition in the circular box 93

22. Coefficients of superposition along monodromy circuit in circular box 99

23. The sign of a radial function 103

24. Signs of radial functions on contour of smooth action 105

25. Coefficients of superposition along monodromy circuit in Mexican Hat potential 107

26. Plot of probability current 112
Chapter 1  Introduction

In recent years, there have been major advances in classical mechanics: nonlinear dynamics, chaos theory, the “butterfly effect,” new understanding of periodic orbits and their bifurcations and proliferation and their organization into families, chaotic transport and fractals, and “monodromy”. One of the motivations for studying these phenomena is that related phenomena show up in quantum systems, and we can get a new understanding of quantum systems by studying their classical counterparts.

In this dissertation we will discuss recently-discovered phenomena in classical and semiclassical mechanics that are called “nontrivial monodromy of action and angle variables”, or simply “monodromy”. Monodromy means “once around a closed path”; a system exhibits “nontrivial monodromy” if when we go around a closed path in some space, the system does not come back to its original state. The simplest example of functions that have nontrivial monodromy are $f(z) = z^2$ or $g(z) = \log(z)$ for complex $z$: on one circuit around the branch point, $z = 0$, these functions change their values. A function of two real variables $(l, E)$ with the same property is $\alpha(l, E) = l \tan^{-1}(E/l)$. If $l$ represents angular momentum and $E$ represents energy, and we multiply by constants to get the units consistent, then this function gives an approximate formula for an action variable of the system we will study: It is a multivalued function of $(l, E)$, and on one circuit around the origin of $(l, E)$ space, it changes its value.

A Hamiltonian system is said to exhibit nontrivial monodromy if the system is integrable and action and angle variables can be constructed, but they are found to be
multivalued. Angle variables are defined in such a way that they trace out fundamental loops on tori. For the systems we are considering, the angle variables change smoothly as \((l, E)\) change, but when \((l, E)\) undergo a circuit around the origin, the loops change their topological structure. Specifically, a loop that begins entirely on one side of a classically forbidden region ends by encircling that forbidden region. This is called a “static” manifestation of monodromy because it involves smooth connections among coordinates defined on “static” tori.

One reason for the research on integrable system and angle loops is that good approximations to quantum eigenvalues and eigenfunctions are obtained by examining a discrete set of tori having appropriately quantized values of action variables. These concepts, first formulated by Liouville, were carried into the old quantum theory by Einstein in 1918, and were revived starting in the 1970s by Percival \([1--3]\), Marcus and Noid \([4--13]\), and Berry \([14]\). These concepts are now a standard part of the repertoire of semiclassical physics and chemistry \([15]\). They have been used to study an immense variety of systems, such as simple nonlinear oscillators (e.g., the Henon-Heiles system) \([16--19]\), molecular vibrations and rotations \([20]\), excited states of hydrogen in electric and magnetic fields \([21,22]\), doubly excited states of helium \([23--25]\), spin-orbit coupling \([26]\), and excited states of nuclei \([27]\). (Googling the phrase “torus quantization” has given over 3000 hits.) Torus quantization also arises in problems far afield from atomic, molecular, and optical (AMO) physics: In a study of a Buffon probability problem (when a needle is dropped in random positions on a tiled floor, what is the probability that the needle intersects \(n\) of the lines between the tiles?), it was found that torus quantization gives a step on the path to the solution \([28]\).
Analysis and quantization of tori have been widely studied for so many years that it might come as a surprise that reexamination of the theory would lead to new and interesting phenomena.

Quantum implications of multivalued action variables were first described by Cushman and Duistermaat [29]: The lattice of allowed semiclassical eigenvalues \( \{ E_{m,n} \} \), defined by quantization of multivalued action variables has a defect. A motivation behind their discovery was that Cushman was looking for a “global” understanding of how tori of an integrable system fill the phase space of that system. This global perspective was brought into AMO physics primarily by Sadovskii, Zhilinskii, and their colleagues. They have used the new methods to show the presence of monodromy and related phenomena in the hydrogen atom in perpendicular fields [30–32], the CO\(_2\) molecule [33–35], HCN [36], LiCN [37], systems with coupled angular momenta [38,39], and a number of model oscillator systems [40–42]. Quasilinear molecules are discussed at length in [43–45], diatomic molecules in fields in [46], and the hydrogen atom in tilted fields in [47,48]. Experimental observations in a classical swing-spring system were made in [49].

Monodromy is not only an abstract mathematical concept, but also leads to dynamical consequences [50,51]. Initially we may start a family of particles with the same angular momentum and energy, in such a way that they form an angle loop in phase space. If we apply a time-dependent Hamiltonian to the family of particles and drive them to evolve around a closed circuit enclosing the origin in \((l,E)\) space, the family of particles will exhibit a topological change in configuration space. They will
evolve with time from a loop on one side of the origin, to a loop that encloses the origin, similar to the angle loop. This is a “dynamical manifestation of monodromy”.

This understanding of classical systems leads to understanding of their quantum counterparts. We will construct wavefunctions that show similar topological changes as the corresponding angle-loops do. When the expectation values of angular momentum \( \langle l \rangle \) and energy \( \langle E \rangle \) go along a monodromy circuit in spectrum space, originally the wave function stays on one side of the classically forbidden region, but at the end it encloses the classically forbidden region. Furthermore, we will find a continuous time-dependent unitary transformation to drive the expectation values of angular momentum and energy around a monodromy circuit, and make the wavefunction experience a topological change. Finally, we find a time-dependent Hamiltonian to implement this topological change for wavefunctions.

We will give a detailed introduction to basic concepts necessary to understand Hamiltonian monodromy in Chapter 2. We introduce symplectic geometry, a J-product of vectors, canonical transformations, Lagrangian manifolds, and the proper construction of action and angle variables. In Chapter 3, a static manifestation of monodromy is explained: we show that action and angle variables may be multivalued and have changes in their topological structure. Those results were known before I began my thesis work. New results associated with this research begin in Chapter 4, where a dynamical manifestation of monodromy is given: we show that a loop of particles driven around a monodromy circuit by ordinary forces acting in real time can have the same topological change as the action-angle loops. We also propose an experiment with ultracold atoms in optical traps to realize the dynamical monodromy in Chapter 5. In Chapter 6, we present a quantum manifestation of monodromy: a superposition of eigenfunctions has the same properties as the action and angle loops. A time-
dependent Hamiltonian is also found which causes such wavefunctions to undergo these topological changes.

Chapter 2  Action and Angle Variables

Action and angle variables are introduced in most graduate courses in classical mechanics. However, certain subtleties in their definitions are usually ignored. In certain systems, action-angle variables are not uniquely defined. The problem is the existence of branch points, which we call in this context “monodromy points”. When we make a circuit around such a branch point, the action-angle variables change their forms and their values. The resulting issues are sufficiently challenging that it is best to go back to the foundations of the theory of action-angle variables, and pay close attention to the assumptions involved in every step.

This process involves considerable effort, so let us begin by saying that the utility of action and angle variables derives from the following facts. (All of these points will be developed in detail in later sections.)

1. We examine Hamiltonian systems having \( N \) degrees of freedom, described by coordinates and momenta \((q_1, q_N, p_1, \ldots, p_N) = (q, p)\) in which there are \( N \) conserved quantities, \( \{F_i(q, p), \quad i = 1 \ldots N\} \). The Hamiltonian \( H(q, p) \) of the system must either be one of the \( F_i \)'s, or a function of some or all of them.
2. Usually each level set of the $F$'s (the set of points such that
\[ \{ F_i(q, p) = \text{constant}, \quad i = 1 \ldots N \} \) lies on an $N$-dimensional torus in the $2N$-dimensional phase space [52]. This is a theorem which holds if the gradient of $F$'s are independent, and the level set is closed and bounded (compact).

3. From those conserved quantities, it is possible to construct a set of “action variables” $\{ I_k(q, p), \quad k = 1 \ldots N \}$, which depend on phase space coordinates only through their dependence on the set of functions $F_j(q, p)$, so they are also conserved. Those action variables must be independent functions only of the $F_j$'s, and therefore the Hamiltonian can also be expressed as a function of the actions, $H(q, p) = H(I(q, p))$.

On a torus, the action variables can usually be calculated by integrals
\[ I_k = \frac{1}{2\pi} \oint \sum_j p_j dq_j \] (2.1)
where the integral goes around the $k^{th}$ fundamental loop of the torus. An important issue will be how these loops are defined, and how they change as we go from one torus to another.

4. The actions $I_k$ have a set of canonically conjugate angles $\varphi_k$, so Hamilton’s equations of motion can be written in the form
\[
\frac{dI_k}{dt} = -\frac{\partial H}{\partial \varphi_k} = 0
\]
\[
\frac{d\varphi_k}{dt} = \frac{\partial H}{\partial I_k} = \omega_k(I_1, I_N) = \text{constant}
\] (2.2)

5. When \(\varphi_k\) increases by \(2\pi\) holding the other \(\varphi\)'s fixed, the path traces out a fundamental loop on the torus.

6. There is a canonical transformation between the original variables \((q, p)\) and this set of action and angle variables \((I, \varphi)\). In this transformation, each of the original variables \((q, p)\) and any function of them must be a periodic function of the angles, with period \(2\pi\). It follows that any function of phase-space variables \(G(q, p)\) can be expressed as a Fourier series in the angles \(\varphi\) (with coefficients depending on the actions \(I\)),

\[
G(q, p) = \sum_m C_m(I(q, p) \exp(i\mathbf{m} \cdot \varphi(q, p))
\] (2.3)
with \(\mathbf{m}\) a vector of integers.

7. It therefore follows from the equations of motion (2.2) that on the physical path generated by the Hamiltonian of the system, the function varies with time according to

\[
G(q(t), p(t)) = \sum_m C_m(I(t)) \exp[i\mathbf{m} \cdot \omega(I)t]
\] (2.4)
which is called a quasiperiodic (or multiply periodic) function of time.
Further utility of action and angle variables derives from the following propositions.

A. “Action variables are adiabatic invariants.” If the system Hamiltonian is explicitly time-dependent but changes sufficiently slowly, then we can look at the tori of $H$ at each fixed time, and the trajectory of the system $(q(t), p(t))$ will move along and through these tori in such a manner that the numerical values of the action variables are, to good approximation, constant. In other words, the system point $(q(t), p(t))$ moves from one torus of the initial Hamiltonian $H(q, p; t_i)$ to a torus of the final Hamiltonian $H(q, p; t_f)$ and these tori have nearly the same numerical value of their action variables. Proposition (A) in quotation marks, is proved to the satisfaction of physicists in various textbooks of classical mechanics for systems with one degree of freedom, and it has been found in numerical calculations to be useful for systems with more degrees of freedom.

B. Quantum eigenvalues of a physical system can be found approximately by identifying “eigentori”, tori having quantized values of action variables

$$I_k = (n_k + \mu_k / 4) \hbar$$  

This formula is a corrected Bohr-Sommerfeld condition, and it gives accurate eigenvalues of quantum systems when the wavelength is short. ($n_k$ is a positive integer, and $\mu_k$ is an integer called the Maslov index, frequently 0, 2, or 4.)
In short, while action and angle variables are not necessarily easy to obtain, they give the simplest possible description of the motion, they provide adiabatic invariants, and they provide approximate quantum eigenvalues and eigenfunctions. The central problem in this chapter is how action and angle variables are computed, and how they must be defined in order to make them change continuously when we go from one torus to another.

At the risk of writing something which at this point is totally incomprehensible, we will give here the rules for defining action-angle loops, rules that sometimes lead to monodromy. Let us consider a system having two degrees of freedom, therefore a four-dimensional phase space, with two functions \((F_1(q, p), F_2(q, p))\), such that their Poisson bracket vanishes. We assume that most of the level sets of these functions, i.e. the sets of phase-space points such that \(\{ (q, p) | F_1(q, p) = f_1, F_2(q, p) = f_2 \}\), are tori, called \(\Lambda_{f_1,f_2}\). A fundamental loop on a particular torus \(\Lambda_{f_1,f_2}\) can be found by the following process.

Starting at any arbitrary point on that torus, integrate a trajectory using Hamilton's equations of motion using \(F_1(q, p)\) as the Hamiltonian for a time \(T_1\), and then continue from that point using \(F_2(q, p)\) as the Hamiltonian for a time \(T_2\). There exists a lattice of points in the \((T_1, T_2)\) plane, called \((\tilde{T}_1(f_1, f_2), \tilde{T}_2(f_1, f_2))\) such that the trajectory so computed returns to the initial point on the torus. This set of points is called the period lattice. On one torus \(\Lambda_{f_1,f_2}\), we may choose any one of these lattice points. The lattice point having the shortest (nonzero) Euclidean distance from the origin in the \((T_1, T_2)\) plane is often a good choice. The path so generated will represent one of the
fundamental loops on that torus. Now as \((f_1, f_2)\) vary, the lattice points move continuously in the \((T_1, T_2)\) plane. As we vary \((f_1, f_2)\) we are required to choose
\((\tilde{T}_1(f_1, f_2), \tilde{T}_2(f_1, f_2))\) such that they are continuous functions of \((f_1, f_2)\).

When defined in this way, for most of the familiar integrable problems in classical mechanics, \((\tilde{T}_1(f_1, f_2), \tilde{T}_2(f_1, f_2))\) will be single-valued functions of \((f_1, f_2)\). However, in systems having monodromy, there exist one or more branch points in the \((f_1, f_2)\) plane, such that on a closed circuit around that branch point, one period lattice point evolves continuously into a different one. Then \((\tilde{T}_1(f_1, f_2), \tilde{T}_2(f_1, f_2))\) are multivalued functions of \((f_1, f_2)\), and if the system is carried around such a “monodromy circuit” the fundamental loop changes its topological structure.

The purpose of this thesis is to show interesting physical phenomena that result from these topological changes. The purpose of the remainder of this chapter is to establish all the results that are stated without proof above. Everything we need is derived \textit{ab initio}, but it is done in a new way, using the methods of Symplectic Geometry. The derivation given below is based upon an unpublished article being written by John Delos and our research group.

**Hamilton’s Equations**

Hamilton’s formulation of dynamics gives equations of motion in a “canonical form”:

\[
\frac{dq}{dt} = \frac{\partial H(q, p)}{\partial p} \\
\frac{dp}{dt} = -\frac{\partial H(q, p)}{\partial q}
\]  

(2.6)
Standard courses in classical mechanics define canonical transformations to new variables \((q, p) \rightarrow (Q, P)\) : if for \((Q, P)\), Hamilton’s equation still holds, this transformation is called a canonical transformation. Equivalently, if there is a generating function \(F_2(q, P)\), such that \(p = \partial F_2 / \partial q, Q = \partial F_2 / \partial P\), the transformation is a canonical transformation. The courses also give an introduction to phase space, Liouville’s theorem and Poisson brackets.

However, as stated above, In this chapter, we will understand those basic theory in classical mechanics from a different perspective. Dynamics are described in a geometric way. Hamilton’s equation, canonical transformation, Poisson brackets and everything else in the theory are described using a “new” operation: a J-product, and a “new” type of surface in phase space called a Lagrangian manifold.

In section 2.1, we introduce the concept of phase space, and the J-product of velocity vectors on that space. In section 2.2, we define canonical transformation in a new way and prove that it is equivalent to the definitions mentioned in the previous paragraph. In section 2.3 we make canonical transformation from \((q, p)\) to action and angle variables \((\phi, I)\). During this process, the geometric meaning of variables is clearly illustrated.

### 2.1 Phase space, J-product and variable transformation

In classical mechanics, canonical coordinates \((q, p)\) are the coordinates that satisfy Hamilton’s equation. The space spanned by \((q_1, q_2, ..., q_n)\) is called configuration space. The dimension of configuration space is \(n\). The space spanned by
\((q_1, q_2 \ldots q_n, p_1, p_2 \ldots p_n)\) is called phase space, and the dimension of phase space is \(2n\).

We denote a point in the phase space as \(z = \begin{pmatrix} q \\ p \end{pmatrix}\). In phase space, the motion of a particle is described by the curve \((q_1(t), q_2(t) \ldots q_n(t), p_1(t), p_2(t) \ldots p_n(t))\). Then it is natural to define the “velocity” in phase space: \(v = \dot{z} = \begin{pmatrix} \dot{q}(t) \\ \dot{p}(t) \end{pmatrix}\).

We are familiar with the inner product for any two vectors \(u = \begin{pmatrix} u_q \\ u_p \end{pmatrix}\) and \(v = \begin{pmatrix} v_q \\ v_p \end{pmatrix}\): :

\[
\langle u | v \rangle = (u_q \ u_p)\begin{pmatrix} v_q' \\ v_p' \end{pmatrix} = u_q v_q + u_p v_p .
\]

In \(2n\) dimensional phase space, an important operation called a J-product is defined:

\[
\langle u | J | v \rangle = (u_q \ u_p) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} v_q' \\ v_p' \end{pmatrix} = u_q v_p - u_p v_q = \sum_{i=1}^{N} u_{q_i} v_{p_i} - u_{p_i} v_{q_i} .
\] (2.7)

It is also called skew product. The vectors \(u\) and \(v\) are said to be J-orthogonal if and only if \(\langle u | J | v \rangle = 0\). The J-product provides the foundation for all of our theory.

It is a common situation that we need to make coordinate transformations to simplify dynamical problems. For example, for a cylindrically symmetric problem, polar coordinates are often a better choice than Cartesian coordinates. For bound systems having a full set of conservation laws, action and angle variables are an even better choice. We will introduce these later. In order to learn how variable transformations affect operations, we introduce the famous Jacobian matrix:
\[ M(z) = \begin{bmatrix}
\frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\
\frac{\partial P}{\partial q} & \frac{\partial P}{\partial p}
\end{bmatrix} \]

(2.8)

where \( Z = (\begin{array}{c} Q \\ P \end{array}) \) are the new coordinates and \( z = (\begin{array}{c} q \\ p \end{array}) \) are the old coordinates. It is easy to notice that the Jacobian matrix from \( Z \) to \( z \) is the inverse matrix of \( M(z) \) defined above.

i.e.

\[
\begin{bmatrix}
\frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\
\frac{\partial P}{\partial q} & \frac{\partial P}{\partial p}
\end{bmatrix} \begin{bmatrix}
\frac{\partial q}{\partial Q} & \frac{\partial q}{\partial P} \\
\frac{\partial p}{\partial Q} & \frac{\partial p}{\partial P}
\end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}
\]

(2.9)

Proof: construct a function \( Q = (q(Q, P), p(Q, P)) \)

\[
\frac{\partial Q}{\partial Q} = 1 = \left( \frac{\partial Q}{\partial q} \right)_p \frac{\partial q}{\partial Q} + \left( \frac{\partial Q}{\partial p} \right)_q \frac{\partial p}{\partial Q}
\]

\[
\frac{\partial P}{\partial Q} = 1 = \left( \frac{\partial P}{\partial q} \right)_p \frac{\partial q}{\partial Q} + \left( \frac{\partial P}{\partial p} \right)_q \frac{\partial p}{\partial Q}
\]

\[
\frac{\partial Q}{\partial P} = 0 = \left( \frac{\partial Q}{\partial q} \right)_p \frac{\partial q}{\partial P} + \left( \frac{\partial Q}{\partial p} \right)_q \frac{\partial p}{\partial P}
\]

\[
\frac{\partial P}{\partial P} = 0 = \left( \frac{\partial P}{\partial q} \right)_p \frac{\partial q}{\partial P} + \left( \frac{\partial P}{\partial p} \right)_q \frac{\partial p}{\partial P}
\]
The derivative operation is affected by a variable transformation in the following way. For the gradient vector\( \left[ \begin{array}{c} u_q \\ u_p \end{array} \right] = \left[ \begin{array}{c} \frac{\partial f(z)}{\partial q} \\ \frac{\partial f(z)}{\partial p} \end{array} \right] \),

\[
\left( \begin{array}{c} \frac{\partial}{\partial Q} \\ \frac{\partial}{\partial P} \end{array} \right) = \tilde{M}^{-1}(z) \left( \begin{array}{c} \frac{\partial}{\partial q} \\ \frac{\partial}{\partial p} \end{array} \right)
\]

(Note: strictly speaking, the gradient is defined as a covector, and represented as a row vector. Above is the rule for transforming the dual, column, vector of the gradient.)

Proof:
\[
\frac{\partial}{\partial Q} = \frac{\partial q}{\partial Q} \frac{\partial}{\partial q} + \frac{\partial p}{\partial Q} \frac{\partial}{\partial p} \]
\[
\frac{\partial}{\partial P} = \frac{\partial q}{\partial P} \frac{\partial}{\partial q} + \frac{\partial p}{\partial P} \frac{\partial}{\partial p}
\]

Another quantity that is affected by variable transformation is velocity, \( \left( \begin{array}{c} \dot{q} \\ \dot{p} \end{array} \right) = \left( \begin{array}{c} \frac{dq}{dt} \\ \frac{dp}{dt} \end{array} \right) \), which follows the rule:

\[
\left( \begin{array}{c} \dot{Q} \\ \dot{P} \end{array} \right) = M(z) \left( \begin{array}{c} \dot{q} \\ \dot{p} \end{array} \right)
\]

The effect of variable transformation on the J-product of two gradient vectors is:
\[ < U | J | V > = \begin{pmatrix} U_Q & U_p \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} V_Q \\ V_p \end{pmatrix} = \begin{pmatrix} u_q & u_p \end{pmatrix} M^{-1} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tilde{M}^{-1} \begin{pmatrix} v_q \\ v_p \end{pmatrix} = < u | M^{-1} J \tilde{M}^{-1} | v > \]

note: \( \tilde{M} \) is the transposed matrix of \( M \)

### 2.2 Canonical Transformation

Now we are ready to give four equivalent definitions of canonical transformations.

**Definition 1:**
\[
J = M^{-1} J \tilde{M}^{-1} = \tilde{M}^{-1} J M^{-1} = M J M = \tilde{M} J M
\]  
(2.12)

In other words, the J-product of any two gradient vectors is invariant under a canonical transformation:
\[
< U | J | V >= < u | J | v >. \quad (2.13)
\]

**Definition 2:**
A transformation is canonical if any one of the following “generating functions” exists.

“type 1” \( S_1(q, Q) \) is defined such that
\[
dS_1 = p dq - P dQ \]
(2.14)


\[ p_i = \frac{\partial S_1}{\partial q_i}, \ \forall q_{k \neq i}, Q_k \ \text{are fixed}; \]

\[-p_i = \frac{\partial S_1}{\partial Q_i}, \ \forall Q_{k \neq i}, q_k \ \text{are fixed}; \]

A “type 2” generating function is a function \( S_2(q, P) \), such that

\[ dS_2 = pdq + QdP \tag{2.15} \]

\[ p_i = \frac{\partial S_2}{\partial q_i}, \ \forall q_{k \neq i}, P_k \ \text{are fixed}; \]

\[ Q_i = \frac{\partial S_2}{\partial P_i}, \ \forall P_{k \neq i}, q_k \ \text{are fixed}; \]

A “type 3” \( S_3(p, Q) \) is defined such that

\[ dS_3 = -qdp - PdQ \tag{2.16} \]

\[ -q_i = \frac{\partial S_3}{\partial p_i}, \ \forall q_{k \neq i}, Q_k \ \text{are fixed}; \]

\[-p_i = \frac{\partial S_3}{\partial Q_i}, \ \forall Q_{k \neq i}, p_k \ \text{are fixed}; \]

and a “type 4” generating function \( S_4(p, P) \), is such that

\[ dS_4 = -qdp + QdP \tag{2.17} \]

\[ -q_i = \frac{\partial S_4}{\partial p_i}, \ \forall p_{k \neq i}, P_k \ \text{are fixed}; \]

\[ Q_i = \frac{\partial S_4}{\partial P_i}, \ \forall P_{k \neq i}, p_k \ \text{are fixed}; \]
**Definition 3:**

Hamilton’s equations keep their form after canonical transformation: before transformation, if \( p \) are conjugate momenta of \( q \), Hamilton’s equations are

\[
\frac{dz}{dt} = J \nabla_z H(z)
\]  

(2.18)

After transformation, the equation for \( Q \) and \( P \) is still

\[
\frac{dZ}{dt} = J \nabla_Z H(z(Z))
\]

**Definition 4:**

If \((P, Q)\) are new canonical coordinates, the basic Poisson Bracket for \((P, Q)\) is:

\[
[Q_i, Q_j] = 0, \quad [P_i, P_j] = 0, \quad [Q_i, P_j] = \delta_{ij}
\]  

(2.19)

The inverse of this statement is also true.

Note: Poisson Bracket for two functions \( F_1(z) \) and \( F_2(z) \) is defined as

\[
[F_1, F_2] = \left< \nabla_z F_1 \right| \left. J \right| \nabla_z F_2 \rangle = \sum_k \frac{\partial F_1}{\partial q_k} \frac{\partial F_2}{\partial p_k} - \sum_k \frac{\partial F_1}{\partial p_k} \frac{\partial F_2}{\partial q_k}
\]  

(2.20)

In the following part, we give the proofs that all of those definitions are equivalent. They are defining the same thing from different perspective. Readers who want to skip the proofs should go to (2.21).

1) the 4 statements in definition 1 are equivalent

1a) \( J = MJ\tilde{M} \iff J = \tilde{M}JM \)

proof:
\[ J = MJM = \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial P}{\partial q} \\ \frac{\partial Q}{\partial p} & \frac{\partial P}{\partial p} \end{pmatrix} \]

\[ = \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \frac{\partial Q}{\partial q} + \frac{\partial Q}{\partial p} & \frac{\partial Q}{\partial q} \frac{\partial P}{\partial q} + \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} & \frac{\partial P}{\partial q} + \frac{\partial P}{\partial p} \end{pmatrix} \]

\[ = \begin{pmatrix} -\frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} & \frac{\partial Q}{\partial q} + \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} & \frac{\partial P}{\partial q} + \frac{\partial P}{\partial p} \end{pmatrix} \]

\[ = J \]

The proof for the opposite direction is similar.

Q.E.D

1b) \( J = M^{-1} J \tilde{M}^{-1} \iff J = \tilde{M}^{-1} J M^{-1} \)

The proof for this is similar for (1) and is omitted
1c) $J = MJ\tilde{M} \iff J = \tilde{M}^{-1}JM^{-1}$

proof:

$J = MJ\tilde{M} \Rightarrow J^{-1} = (MJ\tilde{M})^{-1} = \tilde{M}^{-1}J^{-1}M^{-1}$

$\therefore \tilde{J} = -J$

$\therefore J = \tilde{M}^{-1}JM^{-1}$

The proof for the opposite direction is similar and is omitted.

Q.E.D

1d) $J = \tilde{M}JM \iff J = M^{-1}J\tilde{M}^{-1}$

The proof for this is similar to the proof for (3) and is omitted.

2) definition 2 and definition 1 are equivalent

e.g. if $J = MJM$, there exists a generating function $S_2(q, P)$, such that

$\frac{dS_2}{dP} = pq + QdP$

Proof: the sufficient and necessary condition for the existence of $S_2(q, P)$ is that

$\frac{\partial p_i}{\partial q_j} = \frac{\partial p_j}{\partial q_i}$

$\frac{\partial Q_i}{\partial P_j} = \frac{\partial Q_j}{\partial P_i}$

$\frac{\partial Q_i}{\partial q_j} = \frac{\partial p_j}{\partial P_i}$

If written in form of matrix, these equations are:

\[
\begin{pmatrix}
\frac{dp}{dP} \\
\frac{dQ}{dP}
\end{pmatrix} =
\begin{pmatrix}
A & B \\
C & D
\end{pmatrix}
\begin{pmatrix}
\frac{dq}{dP}
\end{pmatrix}
\]
\[ A = \tilde{A} \]

\[ D = \tilde{D} \]

\[ \tilde{C} = B \]

On the other hand,

\[
\begin{pmatrix}
\frac{dQ}{dP}
\end{pmatrix} = \begin{pmatrix}
C - DB^{-1}A & DB^{-1}
\end{pmatrix}
\begin{pmatrix}
\frac{dq}{dp}
\end{pmatrix}
\]

\[
\therefore M = \begin{pmatrix}
C - DB^{-1}A & DB^{-1}
\end{pmatrix}
\begin{pmatrix}
-B^{-1}A & B^{-1}
\end{pmatrix}
\]

\[
\therefore J = \tilde{M}JM
\]

\[
\therefore \begin{pmatrix}
0 & 1 \\
-1 & 0
\end{pmatrix} = \begin{pmatrix}
\tilde{A}B^{-1}C - \tilde{C}B^{-1}A - \tilde{A}B^{-1}DB^{-1}A + \tilde{A}B^{-1}DB^{-1}A & \tilde{A}B^{-1}DB^{-1} - \tilde{A}B^{-1}DB^{-1} + \tilde{C}B^{-1} \\
-\tilde{B}^{-1}C + \tilde{B}^{-1}DB^{-1}A - \tilde{B}^{-1}DB^{-1}A & -\tilde{B}^{-1}DB^{-1} + \tilde{B}^{-1}DB^{-1}
\end{pmatrix}
\]

\[
\therefore -\tilde{B}^{-1}DB^{-1} + \tilde{B}^{-1}DB^{-1} = 0
\]

\[
\therefore D = \tilde{D}
\]

\[
\therefore 1 = \tilde{A}B^{-1}DB^{-1} - \tilde{A}B^{-1}DB^{-1} + \tilde{C}B^{-1} = \tilde{C}B^{-1}
\]

\[
\therefore B = \tilde{C}
\]

\[
\therefore 0 = \tilde{A}B^{-1}C - \tilde{C}B^{-1}A - \tilde{A}B^{-1}DB^{-1}A + \tilde{A}B^{-1}DB^{-1}A = \tilde{A}B^{-1}C - \tilde{C}B^{-1}A = \tilde{A} - A
\]

Q.E.D

Thus we have proved that
\[ \frac{\partial p_i}{\partial q_j} = \frac{\partial p_j}{\partial q_i} \]

\[ \mathbf{J} = \mathbf{M} \mathbf{J} \mathbf{M} \Rightarrow \frac{\partial Q_i}{\partial P_j} = \frac{\partial Q_j}{\partial P_i} \iff \text{there exists a generating function } S_2(q, P), \text{ such that} \]

\[ \frac{\partial Q_i}{\partial q_j} = \frac{\partial Q_j}{\partial P_i} \]

\[ dS_2 = pdq + QdP \]

The proof for the opposite direction is omitted here.

3) The four statements in definition 2 are equivalent

proof: if there exists a generating function \( S_2(q, P) \), such that \( dS_2 = pdq + QdP \)

there exists another generating function \( S_4(p, P) \), such that

\[ dS_4 = dS_2 - d(q \cdot p) = pdq + QdP - pdq - qdp = -qdp + QdP. \]

Then there exists another generating function \( S_4(p, Q) \), such that

\[ dS_3 = dS_4 - d(P \cdot Q) = -qdp + QdP - PdQ - QdP = -qdp - PdQ. \]

Then there exists another generating function \( S_3(q, Q) \), such that

\[ dS_1 = dS_3 + d(p \cdot q) = -qdp - PdQ + pdq + qdp = pdq - PdQ. \]

The proof for the opposite direction is similar and omitted.

Q.E.D

4) Definition 1 is equivalent to definition 3

Proof: before coordinate transformation, Hamilton’s equation is

\[ \frac{dz}{dt} = J \nabla_z H(z). \]

After coordinate transformation,
\[ \begin{align*}
\therefore \nabla_z H &= \left( \begin{array}{c}
\frac{\partial H}{\partial q} \\
\frac{\partial H}{\partial p}
\end{array} \right) = \tilde{M} \left( \begin{array}{c}
\frac{\partial H}{\partial q} \\
\frac{\partial H}{\partial P}
\end{array} \right) = \tilde{M} \nabla_z H
\end{align*} \]

\[ \therefore \frac{dZ}{dt} = M \frac{dz}{dt} = MJ \nabla_z H = MJ \tilde{M} \nabla_z H \]

If the coordinates transformation is canonical, \( J = MJ \tilde{M} \).

Then \( \frac{dZ}{dt} = J \nabla_z H(Z) \)

The proof for the opposite direction is obvious and is omitted.

Q.E.D

5) definition 4 is equivalent to definition 1

5a) \( J = MJ \tilde{M} \Rightarrow [Q_i, Q_j] = 0, [P_i, P_j] = 0, [Q_i, P_j] = \delta_{ij} \)

Proof:

\[ \therefore J = MJ \tilde{M} = \left( \begin{array}{cc}
\frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial P} \\
\frac{\partial P}{\partial q} & \frac{\partial P}{\partial P}
\end{array} \right) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \left( \begin{array}{cc}
\frac{\partial \tilde{Q}}{\partial q} & \frac{\partial \tilde{P}}{\partial q} \\
\frac{\partial \tilde{Q}}{\partial P} & \frac{\partial \tilde{P}}{\partial P}
\end{array} \right) \]

\[ = \left( \begin{array}{cc}
-\frac{\partial Q}{\partial P} \frac{\partial \tilde{Q}}{\partial q} + \frac{\partial Q}{\partial q} \frac{\partial \tilde{Q}}{\partial P} & -\frac{\partial Q}{\partial P} \frac{\partial \tilde{P}}{\partial q} + \frac{\partial Q}{\partial q} \frac{\partial \tilde{P}}{\partial P} \\
\frac{\partial P}{\partial q} \frac{\partial \tilde{Q}}{\partial q} - \frac{\partial P}{\partial P} \frac{\partial \tilde{Q}}{\partial q} & -\frac{\partial P}{\partial P} \frac{\partial \tilde{P}}{\partial q} + \frac{\partial P}{\partial q} \frac{\partial \tilde{P}}{\partial P}
\end{array} \right) \]
\[
\therefore -\frac{\partial Q}{\partial p} \frac{\partial \tilde{P}}{\partial q} + \frac{\partial Q}{\partial q} \frac{\partial \tilde{P}}{\partial p} = 1 \Rightarrow [Q_i, P_j] = \delta_{ij}
\]

\[
-\frac{\partial Q}{\partial p} \frac{\partial \tilde{Q}}{\partial q} + \frac{\partial Q}{\partial q} \frac{\partial \tilde{Q}}{\partial p} = 0 \Rightarrow [Q_i, Q_j] = 0
\]

\[
-\frac{\partial P}{\partial q} \frac{\partial \tilde{P}}{\partial p} + \frac{\partial P}{\partial p} \frac{\partial \tilde{P}}{\partial q} = 0 \Rightarrow [P_i, P_j] = 0
\]

Q.E.D

The proof for the opposite direction is obvious and is omitted.

Some comments about those equivalent definitions of canonical transformation: as stated in the beginning of this chapter, in most textbooks of classical mechanics, generating functions and preserved Hamilton’s equation criteria are widely used. But in this thesis, Jacobian matrix and Poisson bracket (or Lagrange bracket) are used more often.

Besides the Poisson bracket, there is another kind of bracket, called the Lagrange bracket. The definition is: for any differentiable quantities \( F_1(q, p) \), \( F_2(q, p) \), the Lagrange bracket is

\[
\{ F_i, F_j \} = \sum_j \frac{\partial q_j}{\partial F_i} \frac{\partial p_j}{\partial F_j} - \frac{\partial q_j}{\partial F_i} \frac{\partial p_j}{\partial F_j}
\]

\[ (2.21) \]

This is also a very useful concept in this dissertation. Similarly to Poisson bracket, the equivalent definition of canonical transformation can be expressed with Lagrange brackets:

\[
\{ Q_i, Q_j \} = 0, \quad \{ P_i, P_j \} = 0, \quad \{ Q_i, P_j \} = \delta_{ij}
\]

\[ (2.22) \]

Proof for this statement is similar to the proof for Poisson bracket, and is omitted.
Finally I would like to say something about the geometric meaning of two different vectors: \( \mathbf{\xi}_i = \frac{\partial Z_i}{\partial z} = \nabla_i Z_i \) and \( \mathbf{\zeta}_i = \frac{\partial z}{\partial Z_i} \) (Fig. 1)

Fig. 1. This figure shows the geometric meaning of two vectors. The curves are the new coordinate system. Each curve is a contour of a new variable. \( \mathbf{\xi}_i \), the blue arrow, points to the direction that \( Z_i \) increases but other \( Z_{k \neq i} \) are fixed:

\( \{ z | Z_k = \text{constant}, \forall k \neq i \} \).

\( \mathbf{g}_i \), the red arrow, is the gradient of \( Z_i \), pointing to the direction that \( Z_i \) increases fastest. Usually these vectors do not coincide.

2.3 canonical variables on the torus

In classical mechanics, once initial position and initial momentum are specified, the motion is fixed. However, some motions have regular pattern while some motions look like chaos. In this dissertation we focus on the motions that have very regular patterns. These systems are called integrable system. The motion of a particle in a bounded integrable system is constrained to a torus in phase space. We introduce constructions of coordinates on the tori by making a sequence of canonical transformations.
2.3.1 Integrable systems, level sets, Lagrangian manifolds

Let’s consider an n dimensional system with n independent coordinates \( q_i, i = 1,2...n \) and n conjugate momenta \( p_i, i = 1,2...n \). If there exist n independent mutually Poisson-commuting functions \( \{F_i(q,p), i = 1,2...n \} \), we say this is an integrable system. The Poisson bracket was defined in Eq. (2.20). These functions \( F_i(q,p) \) are also called conserved quantities. The surface specified by \( \{F_i(q,p) = f_i, i = 1,2,...n \} \) is called level set. Usually the surface is an n dimensional torus (Fig.3(c)). All motions under the conservation laws \( \{F_i(q,p) = f_i, i = 1,2,...n \} \) are constrained to the corresponding torus (Fig.3(c)). The space composed by the value of conserved quantities \( \{f_i, i = 1,2,...n \} \) is called spectrum space.

Let’s look at an important example. In a two-dimensional system with cylindrically symmetric potential energy, the two independent variables to describe the configuration space are \( \begin{pmatrix} x \\ y \end{pmatrix} \). Their conjugate momenta are \( \begin{pmatrix} p_x \\ p_y \end{pmatrix} \). There are two conserved quantities: \( F_1 = L = p_y x - p_x y \), \( F_2 = H = \frac{p_x^2 + p_y^2}{2m} + V(\sqrt{x^2 + y^2}) \), which are Poisson commuting:

\[
[H, L] = \frac{\partial H}{\partial x} \frac{\partial L}{\partial p_x} - \frac{\partial H}{\partial p_x} \frac{\partial L}{\partial x} + \frac{\partial H}{\partial y} \frac{\partial L}{\partial p_y} - \frac{\partial H}{\partial p_y} \frac{\partial L}{\partial y} = 0
\]  
(2.23)

The level sets are defined by fixed values of \( H \) and \( L \),

\[
H = \frac{p_x^2 + p_y^2}{2m} + V(\sqrt{x^2 + y^2}) = E, \quad L = p_y x - p_x y = l,
\]  
(2.24)
These specify a two dimensional level set in the four dimensional phase space. In most cases, it is a 2-d torus. Each level set is guaranteed to be a torus if the set is closed and bounded, and the gradients $\nabla_z F_i$ are linearly independent vectors for all points on that level set.

There can be some level sets that are not tori. Those values of $f$’s that specify a level set on which the vectors $\nabla_z F_i$ are linearly dependent at some $z$, is called a singular value in spectrum space, and the corresponding level sets $\{F_i(q,p) = f_i, i = 1,2,...n\}$ need not be a torus.

Let's look again at the example of a cylindrically symmetric potential. When $l = 0, h = 0$, $\nabla_z L(x = 0, y = 0, p_x = 0, p_y = 0) = \begin{pmatrix} p_y \\ -p_x \\ -y \\ x \end{pmatrix} = 0$, $\nabla_z H(x = 0, y = 0, p_x = 0, p_y = 0) = \begin{pmatrix} \frac{\partial V}{\partial x} \\ \frac{\partial V}{\partial y} \\ p_x/2 \\ p_y/2 \end{pmatrix} = 0$.

Therefore $l = 0, h = 0$ is a singular value in spectrum space $(l, h)$, and the level set $H = 0, L = 0$ is not a torus.

These tori have an important geometrical property, and they are examples of Lagrangian manifolds. A Lagrangian plane is a plane on which every pair of vectors
tangent to it are J-orthogonal. A manifold is a smooth surface. A manifold is a
Langrangian manifold if and only if all its tangent planes are Lagrangian planes. Now we
prove that the tori obtained as level sets of Poisson-commuting functions are Lagrangian
manifolds.

Proof:
A n dimensional torus specified by \( \{ F_i(q, p) = f_i, i = 1, 2, ... n \} \) has a tangent plane at each
point \( z \) on the torus. The tangent plane is spanned by n independent vectors:

\[ \{ v_i = J \nabla_z F_i, i = 1, 2, 3, ... n \} \]

For arbitrary pair of \( i, j \), the J-product

\[ \langle v_i | v_j \rangle = \langle J \nabla_z F_i | J \nabla_z F_j \rangle = \langle \nabla_z F_i | J \nabla_z F_j \rangle = [F_i, F_j] = 0. \]

Q.E.D

2.3.2 Canonical transformation from \((q, p)\) to \((t, f)\)

In this section we construct canonical coordinates \((t, f)\), in which \( f \) specifies a
torus and \( t \) specifies a location on that torus. We start from one torus
\( \{ F_i(q, p) = f_i, i = 1, 2, ... n \} \), and set a reference point O on it. Then

1) we follow the dynamical flow generated by \( F_i(q, p) : \nabla_z F_i(q, p) \), and record the time
on this flow \( \tau_i \). Here we prove that by following this flow, we will always stay on that
torus

\( \{ F_i(q, p) = f_i, i = 1, 2, ... n \} \).

Proof:
Under the dynamical flow generated by \( F_i(q,p) \), the equation of motion is

\[
\frac{dz}{dt} = J \nabla_x F_i(q,p)
\]

For \( \forall k = 1,2,3...n \)

\[
dF_k = \sum_i \frac{\partial F_k}{\partial z_i} dz_i = dt \sum \frac{\partial F_k}{\partial z_i} 
\frac{dz_i}{dt} = dt \langle \nabla_x F_k | J \nabla_x F_i \rangle = dt[F_k,F_i] = 0
\]

Q.E.D

Therefore all \( F_k \) are conserved under this evolution; i.e. \( F_k = f_k \) does not change during the motion.

2) Starting from the ending point in step 1), at which \( t_i = \tau_i \) on the flow \( J \nabla_x F_i(q,p) \) from reference point O, we follow the flow generated by \( F_2(q,p) : J \nabla_x F_2(q,p) \), and record the time on this flow \( \tau_2 \).

3) Repeating the procedure for other flows, \( J \nabla_x F_i(q,p) \), we use the recorded time \( t = (\tau_1, \tau_2, \tau_3, ..., \tau_n)^T \) to represent the location on the torus. There is a good quality about these time coordinates: they uniquely specify a point on the torus because the flows commute. If we exchange the sequence of flows but keep the same amount of time \( \tau_i \) on the corresponding flow \( J \nabla_x F_i(q,p) \), we will end up at the same location! As an example, we may consider again the system with cylindrically symmetric potential energy. There are two ways to get to the same point. One is to travel on the flow \( J \nabla_x L(q,p) \) for time \( \tau_i \), then travel on the flow \( J \nabla_x H(q,p) \) for time \( \tau_h \). The other way is to travel on the flow \( \nabla_x H(q,p) \) for time \( \tau_h \), then travel on the flow \( \nabla_x L(q,p) \) for time
\( \tau_i \). The two ways end up at the same point on the torus. The proof is given by Arnold [52].

Now we have constructed a coordinate system on a single torus. Let’s generalize it to the whole space:

1) We choose a reference point \( z_0 \) in phase space. This reference point also stays on a level set (torus) \( f_0 = \left( \begin{array}{c} f_1 \\ \vdots \\ f_n \end{array} \right) \). We construct \( t \) coordinates by following steps shown above.

2) We choose an \( n \) dimensional Lagrangian manifold \( \Lambda_0 \), which is transverse to a family of level sets. The intersection of \( \Lambda_0 \) and any level set \( F = f \) is a point. This point is regarded as the reference point, from which we construct \( t \) coordinates on the corresponding torus. The result is that a locally smooth coordinate system \((t, f)\) is constructed. The values of \( f \) specify which level set the points are on, while the points \( t \) identify the location on that torus.

We now assert an amazing theorem. The coordinates \((t, f)\) are canonical.

Proof:

Define \( \alpha_j = (\partial z / \partial t_j)_{t, f} \cdot t \) fixed, \( f_j \) fixed \( j \neq i \)

\( \alpha_j \) is a velocity following a dynamical flow constrained on a torus, so it is tangent to that torus.

\[ \therefore \text{torus is a Lagrangian manifold} \]

\[ \therefore < a_i | J a_j > = 0 \]
\[ \therefore < {\frac{\partial z}{\partial t_i}}_{t_i, t} \mid J \left( {\frac{\partial z}{\partial t_j}} \right)_{t_i, t} >= \{ t_i, t_j \} = 0 \]

Define \( \beta_j = \frac{\partial z}{\partial f_i} \quad t \text{ fixed}, f_j \text{ fixed } j \neq i \)

\[ \therefore \text{initial reference manifold } \Lambda_0 \text{ is Lagrangian, and Hamiltonian flow preserves Lagrangian property.} \]

\[ \therefore \text{surface } \Lambda_1 : \{ z \mid t = \text{constant} \} \text{ is also Lagrangian} \]

\[ \therefore < \beta_i \mid J \beta_j >= 0 \]

\[ \therefore < {\frac{\partial z}{\partial f_i}}_{f_i, t} \mid J \left( {\frac{\partial z}{\partial f_j}} \right)_{f_i, t} >= \{ f_i, f_j \} = 0 \]

\[ \{ t_j, f_k \} = < \alpha_i \mid J \beta_j > \]

\[ = \sum_i \frac{\partial q_i}{\partial t_j} \frac{\partial p_i}{\partial f_k} - \frac{\partial p_i}{\partial t_j} \frac{\partial q_i}{\partial f_k} \]

\[ = \sum_i \frac{\partial F_j}{\partial p_i} \frac{\partial p_i}{\partial f_k} + \frac{\partial F_j}{\partial q_i} \frac{\partial q_i}{\partial f_k} \]

\[ = \sum_i \frac{\partial F_j(q(t,f),p(t,f))}{\partial f_k} \quad t, f_i \text{ fixed, } i \neq k \]

\[ = \delta_{jk} \]

According to definition 4 of canonical transformation, it is a canonical transformation from \((q,p)\) to \((t,f)\).

Q.E.D

2.3.3 Canonical transformation from \((t,f)\) to \((\phi,I)\)

An n dimensional torus has n fundamental loops. Fundamental loops are the loops that belong to different topological classes on the tori. Each fundamental loop cannot smoothly change into other fundamental loops without breaking itself or leaving the
torus. If one loop can evolve smoothly into another loop, they are the same fundamental loop. If we cut a 2-d torus through its 2 fundamental loops $\gamma_1, \gamma_2$, we can get a rectangular surface. (Fig. 2.)

![Diagram of a torus with fundamental loops $\gamma_1$ and $\gamma_2$.](image)

(a)

![Diagram of a parallelogram representing the surface of the torus cut along its fundamental loops.](image)

(b)

**Fig. 2.** Fundamental loops on a torus. The torus (a) has two fundamental loops that are topologically different. (b) The parallelogram is the surface of the torus if it is cut along the two fundamental loops. The red edge was the fundamental loop $\gamma_1$ and the blue edge was the fundamental loop $\gamma_2$.
For fundamental loop $\chi_1$, if $z_{\text{initial}}^1$ is the starting reference point, the $t$ coordinates for the point that trace back to $z_{\text{initial}}^1$ are
\[
\left( T_1^{(1)}, T_2^{(1)} \right).
\]

For fundamental loop $\chi_2$, if $z_{\text{initial}}^2$ is the starting reference point, the $t$ coordinates for the point that trace back to $z_{\text{initial}}^2$ are
\[
\left( T_1^{(2)}, T_2^{(2)} \right). \text{ These } \left( T_1^{(2)}, T_2^{(2)} \right) \text{ do not depend on the chosen initial point. [90]}
\]

Then we define the angle coordinates as:
\[
\begin{pmatrix}
  t_1 \\
  \vdots \\
  t_n
\end{pmatrix}
= \frac{1}{2\pi}
\begin{pmatrix}
  T_1^{(1)} & \cdots & T_1^{(n)} \\
  \vdots & \ddots & \vdots \\
  T_n^{(1)} & \cdots & T_n^{(n)}
\end{pmatrix}
\begin{pmatrix}
  \theta_1 \\
  \vdots \\
  \theta_n
\end{pmatrix}
= \frac{1}{2\pi}
\begin{pmatrix}
  \theta_1 \\
  \vdots \\
  \theta_n
\end{pmatrix}
\]
\[
\Rightarrow \theta = 2\pi T^{-1} t
\]

The next step is to find a set of new conjugate momenta $I = I(t,f)$ such that the transformation from $(t,f)$ to $(\theta,I)$ is canonical. Since we already defined new "position" coordinates $Q(q,p)$, it is sensible if we ask whether there exist $P(q,p)$ conjugate to $Q(q,p)$, such that $(q,p) \rightarrow (Q,P)$ is a canonical transformation. The answer is yes.

Proof:

Starting from $Q(q,p)$, we can find an inverse function $q(Q,p)$.

If we define a function $S_1(p,Q) \equiv \int -q(Q,p')dp' - f(Q)$ and define
\[
P \equiv \sum_s \frac{\partial q(Q,p')}{\partial Q} dp' + \frac{\partial f(Q)}{\partial Q}, \quad S_1(p,Q) \text{ satisfies}
\]
\[ q = -\frac{\partial S_2}{\partial p} \text{ and } P = -\frac{\partial S_3}{\partial Q}. \]

According to definition 2 of canonical transformation, \((Q, P)\) are canonical coordinates.

\ \ Q.E.D

Knowing that the conjugate momenta exist, we want to find the analytic expression of momentum coordinates \( I(f, \phi) = i(q, p) \). There is a generating function \( S_2(q, I) \) such that \( dS_2 = p dq + \phi dI \).

\[ \therefore \phi_k = \frac{\partial S_2}{\partial I_k} = \frac{\partial}{\partial I_k} \int_{C_k} dS_2(q, I), \ C_k' \text{ is the integral path that connects a reference point for the integral to the point } (q, I). \]

\[ \phi + 2\pi = \frac{\partial S_2}{\partial I_k} = \frac{\partial}{\partial I_k} \int_{C_k'} dS_2(q, I), \ C_k'' \text{ covers } C_k' \text{ and exceed } C_k' \text{ by a fundamental loop} \]

\[ C_k: \]

on the same level set, \( \theta_{i=\phi} = \text{constant} \), starting at \( \forall \theta_k \), ending at \( \theta_k + 2\pi \).

\[ \Rightarrow 2\pi = (\phi_k + 2\pi) - \phi_k = \int_{C_k} dS_2(q, I) - \int_{C_k'} dS_2(q, I) = \int_{C_k} dS_2(q, I) \]

\[ \therefore \frac{\partial}{\partial I_k} \int_{C_k} dS_2(q, I) = 2\pi \text{ is a constant}, \]

We hope that \( I \), conjugated to position coordinates \( \phi(t) = \Phi(q, p) \), only depends on \( f \), so that along path \( C_k, dI = 0 \)
\[
I_k = \frac{1}{2\pi} \int_{C_k} dS I \cdot p = \frac{1}{2\pi} \oint_{C_k} p d q = \frac{1}{2\pi} \oint_{C_k} p d q
\]

The canonical momentum \( I_k \) is called an action variable, defined as an integral along the kth fundamental loop \( \gamma_k = C_k \) of the torus.

Chapter 3       A Classical Static Manifestation of Monodromy

After the introduction to integrable systems in Chapter 2, and the definition of action and angle variables, it is the right time to introduce Hamiltonian monodromy. In this chapter, we will show a static manifestation of Hamiltonian monodromy in classical mechanics: an unexpected topological change of angle coordinate systems on tori. Everything in this chapter leads up to the result displayed in Figure 10, which shows that
topological change. This is not my dissertation work; it had been well defined when I started my PhD research.

In the last chapter we introduced action and angle variables as new canonical variables. However, for some systems, like a circularly symmetric potential system, the canonical transformation from \((q, p)\) to \((\phi, I)\) cannot be both single-valued and smooth. If we try to make the canonical transformation from \((q, p)\) to \((\phi, I)\) smooth, at least one of the action variables and one of the angle variables must be multivalued. This fact is manifested in the topological change of the angle loop \(\gamma_1: \phi_2 = \text{constant}, \phi_1\) increases from 0 to \(2\pi\).

3.1 The transformation from \((t, f)\) to \((\phi, I)\) may not be smooth

We know that canonical coordinates satisfy Hamilton’s equation. For action and angle variables, Hamilton’s equations are

\[
\frac{d\phi}{dt} = \frac{\partial H}{\partial I}
\]

\[
\frac{dI}{dt} = -\frac{\partial H}{\partial \phi} = 0
\]

Hence the derivatives \(\frac{\partial H(I)}{\partial I}\) need to exist: \(H(I)\) needs to be differentiable.
The simplest case of failure of existence of action variables that are both smooth and single-valued is in a circularly symmetric two-dimensional system. We take the potential to be like a Mexican hat, with a central barrier and an outer well. A particle which has conserved angular momentum $l$ and conserved energy $E$ moves back and forth radially while it goes around the origin. (Fig. 3) The radial period is $T$, and the angle subtended within a radial period is $\Delta$. 
Fig. 3. Figure (a) is a cross section along the $\rho$ axis of $V(\rho)$. The potential is circularly symmetric with a central barrier and an outer soft wall. The green curve is radial momentum $p_\rho$ versus radial position $\rho$. Figure (b) is the trajectory of a single particle with fixed angular momentum and energy in the x-y plane. Figure (c) is the two-dimensional torus projected into three-dimensional space. The blue trajectory on the surface of the torus is the trajectory in figure (b) viewed in phase space. The torus can be obtained if the green loop in figure (a) is rotated around $p_\rho$ axis.

The original coordinates to describe this system are $(x, y, p_x, p_y)$ or $(\rho, \varphi, p_\rho, p_\varphi)$. The Hamiltonian of this system is

$$H = \frac{p_x^2 + p_y^2}{2m} + V(\rho).$$

As discussed in the last section, this is an integrable system with two independent Poisson-commuting
functions: \( L = p_y x - p_x y \), \( H = \frac{p_x^2 + p_y^2}{2m} + V(\rho) \). It is worth noticing that \( \nabla_z L = \begin{pmatrix} p_y \\ -p_x \\ -y \\ x \end{pmatrix} \)

and \( \nabla_z H = \begin{pmatrix} 0 \\ 0 \\ p_x / m \\ p_y / m \end{pmatrix} \) are linearly independent except at \( z = 0 \). The phase-space point \( z = 0 \) is therefore called a singular value. This point corresponds to the value \( (l = 0, \ E = 0) \) in spectrum space, which is called a singular value. The level set corresponding to \( (l = 0, \ E = 0) \) not a torus, but is usually called a “pinched torus”.

Points elsewhere in spectrum space are all regular points, for which the level sets are tori.

We consider closed circuits enclosing the singular value in spectrum space (Fig. 4) and we call them monodromy circuits.
Fig. 4. The l-E space is spectrum space. In this case, (0,0) is the singular value. The blue circuit that encloses the singular value is called a monodromy circuit.

On a monodromy circuit in spectrum space \((f_1, f_2, ..., f_n)\), each point corresponds to a level set (torus): \(\{F_i(q, p) = f_i, i = 1, 2, ..., n\}\). As we follow the monodromy circuit, the corresponding torus is changing. Since action variables are functions of the conserved values \(F, \{f_i\}\), the action variables and the associated angle variables that define a coordinate system on the torus are also varying. We would like to see a smooth evolution of action variables, so that the first order derivatives in Hamilton’s equation exist. However, unless we are careful about the definitions of the action and angle loops on the tori, this is not true when \(l = 0, E > 0\).

The explanation of this statement is the following. On a torus \(L = l, H = E\), there are two fundamental loops \(\gamma_1, \gamma_2\). \(\gamma_1\) is the loop on which angle variable \(\phi_2\) is a constant and \(\phi_1\) increases from 0 to \(2\pi\). It is also topologically equivalent to the loop

\[
\varphi = 0, p_\varphi = 0, p_\rho = \pm \sqrt{2m(h - \frac{l^2}{2m\rho^2} - V(\rho))}, \rho_{\text{min}} \leq \rho \leq \rho_{\text{max}}.
\]
\( \gamma \) is the loop on which the angle variable \( \phi \) is a constant and \( \phi \) increases from 0 to \( 2\pi \).

It is topologically equivalent to \( \rho = \rho_{\min} \), \( 0 \leq \phi \leq 2\pi \), \( p_{\phi} = l \), \( p_{\rho} = 0 \). The evaluations of action variables are

\[
I_1 = \frac{1}{2\pi} \int_{\gamma_1} dS_1(q, I) = \frac{1}{2\pi} \int_{\gamma_1} \rho d\rho + \oint_{\phi} d\phi
\]

\[
= \frac{1}{2\pi} \int_{\rho_{\min}}^{\rho_{\max}} \sqrt{2m(h - \frac{l^2}{2m\rho^2} - V(\rho))} d\rho + \frac{1}{2\pi} \int_{\rho_{\min}}^{\rho_{\max}} \sqrt{-2m(h - \frac{l^2}{2m\rho^2} - V(\rho))} d\rho
\]

\[
= \frac{1}{\pi} \int_{\rho_{\min}}^{\rho_{\max}} \sqrt{2m(h - \frac{l^2}{2m\rho^2} - V(\rho))} d\rho
\]

(3.1)

\[
I_2 = \frac{1}{2\pi} \int_{\gamma_2} dS_1(q, I) = \frac{1}{2\pi} \int_{\gamma_2} \rho d\theta + \oint_{\rho} d\rho
\]

\[
= \frac{1}{2\pi} \int_{0}^{2\pi} l d\theta = l
\]

(3.2)

Now let us evaluate \( \left( \frac{\partial H(I_1, I_2)}{\partial I_2} \right)_{I_1} \), since we hope that in Hamilton’s equation

\[
\frac{d\phi}{dt} = \frac{\partial H}{\partial I_2} \] exists. We show below that

\[
\left( \frac{\partial H(I_1, I_2)}{\partial I_2} \right)_{I_1} = -\left( \frac{\partial I_1}{\partial \ell} \right)_{E} \frac{\Delta}{T}
\]

(3.3)

i.e. the angle subtended by the trajectory in a cycle of radial motion divided by the time for that cycle. It seems everything is alright. But the tricky part is that according to the definition of \( \Delta \), it is not continuous when \( l = 0, E > 0 \).
Here I use a special system to explain why $\Delta$ is not continuous when $l = 0, E > 0$.

Consider a circular box: $V(\rho) = \begin{cases} 0, & \rho \leq \rho_{\text{max}} \\ \infty, & \rho > \rho_{\text{max}} \end{cases}$

Fig. 5. The angle subtended within one radial cycle in circular box. This figure shows how the angle subtended within a radial cycle changes as angular momentum of the particles decreases from a positive value to a negative value. The blue straight lines in the circular box are trajectories of particles with the same energy $E$, but with different angular momenta $l$. The trajectories on the right half plane are with positive angular momentum while the ones on the left half plane are with negative angular momentum. The larger the absolute value of angular momentum is, the farther the minimum of radial position.

In Fig. 5, we show how $\Delta$ changes from positive $l$ to negative $l$. While angular momentum is greater than 0, as $l$ decreases, $\Delta$ increases from 0 to $\pi$. While angular momentum is less than 0, as $l$ decreases, $\Delta$ increases from $-\pi$ to 0.

$\lim_{l \to 0^+} \Delta = \pi$

$\lim_{l \to 0^-} \Delta = -\pi$
\[ \Delta \] is not continuous at \( l = 0, E > 0 \)

\[ \begin{align*}
\left( \frac{\partial H(I_1, I_2)}{\partial I_2} \right)_{h} &= -\left( \frac{\partial I_1 / \partial \ell}{\partial E} \right)_{L} = \frac{\Delta}{T} \\
\end{align*} \]

Finally we prove here Eq. (3.3). The angle subtended within one radial cycle by a particle in this potential is

\[ \Delta = 2 \int_{0}^{\tau/2} \phi dt = 2 \int_{0}^{\tau/2} \frac{l}{m \rho^2} \frac{1}{d \rho} d \rho = 2 \int_{\rho_{\text{min}}}^{\rho_{\text{max}}} \frac{l}{m \rho^2} \frac{1}{p_{\rho}} d \rho \\
= 2 \int_{\rho_{\text{min}}}^{\rho_{\text{max}}} \frac{l}{m \rho^2} \frac{1}{p_{\rho}} d \rho = \frac{2}{m} \int \frac{1}{\sqrt{2m(E - V(\rho) - l^2 / 2m \rho^2)}} d \rho \\
= 2 \int_{\rho_{\text{min}}}^{\rho_{\text{max}}} \frac{l}{\rho^2 \sqrt{2m(E - V(\rho) - l^2 / 2m \rho^2)}} d \rho \\
\end{align*} \]

\[ \begin{align*}
\left( \frac{\partial I_1 / \partial \ell}{\partial E} \right)_{E} &= \frac{\partial}{\partial \ell} \frac{1}{\pi \rho_{\text{min}}} \int \frac{2m(E - l^2 / 2m \rho^2 - V(\rho)) d \rho}{\rho^2 \sqrt{2m(E - l^2 / 2m \rho^2 - V(\rho))}} \\
&= \frac{1}{\pi} \int_{\rho_{\text{min}}}^{\rho_{\text{max}}} \frac{-l}{\rho^2 \sqrt{2m(E - l^2 / 2m \rho^2 - V(\rho))}} d \rho \\
&= -\frac{l}{\pi} \frac{\Delta}{2} \\
\end{align*} \]

And \( \left( \frac{\partial I_1 / \partial E}{\partial E} \right)_{L} = \frac{\partial}{\partial E} \frac{1}{\pi \rho_{\text{min}}} \int \frac{2m(E - l^2 / 2m \rho^2 - V(\rho)) d \rho}{\rho^2 \sqrt{2m(E - l^2 / 2m \rho^2 - V(\rho))}} \\
= \frac{1}{\pi} \int_{\rho_{\text{min}}}^{\rho_{\text{max}}} \frac{m}{\rho^2 \sqrt{2m(E - l^2 / 2m \rho^2 - V(\rho))}} d \rho \\
\]
$$\frac{1}{\pi} \int_{\rho_{\text{min}}}^{\rho_{\text{max}}} \frac{1}{d\rho} d\rho = \frac{1}{\pi} \frac{T}{2}$$

\[ \therefore \left( \frac{\partial H(I_1, I_2)}{\partial I_2} \right)_{I_1} = -\left( \frac{\partial I_1 / \partial \ell}{\partial I_1 / \partial E} \right)_E = \frac{\Delta}{T} \]

3.2 Redefine action variable $I_1$ to get smooth variables

To fix this issue, i.e. to find a globally smooth transformation from $(q, p)$ to $(\phi, I_1)$, we must modify the definition of action and angle variables. We then find out that a smooth transformation leads to a multivalued action variable $I_1$. (It follows from arguments given in Arnold P.279 that action and angle variables are single-valued functions of phase-space variables if spectrum space is simply connected)

$I_1$ is the action variable integrated along the fundamental loop $\gamma_1$. The new definition of $I_1$ is:

$$I_1^{(\text{new})} = \begin{cases} I_1^{(\text{old})}; l \geq 0 \\ I_1^{(\text{old})} - I_2; l < 0 \end{cases} \quad (3.4)$$

To keep the coordinates canonical, the definition of angle variable $\phi_2$ needs to be modified as well:

$$\phi_2^{(\text{new})} = \begin{cases} \phi_2^{(\text{old})}; l \geq 0 \\ \phi_1^{(\text{old})} + \phi_2^{(\text{old})}; l < 0 \end{cases} \quad (3.5)$$
The following figure shows $I^{(\text{old})}_1$ (Fig.6) as function of $(l, E)$ in a Mexican Hat system:

$$V(\rho) = -\frac{3}{2} \rho^2 + \frac{1}{60} \rho^4$$

(3.6)

Fig.6 The colorful surface is the action variable $I_1(l, E)$ defined as in (3.1). We start from $(l = 0, E < 0)$ (the red dots) and follow the red trace to evaluate $I_1(l, E)$. When we pass through $(l = 0, E > 0)$ indicated by the jagged cut, the action variable $I_1(l, E)$ has a discontinuous derivative.

If we adopt the old way of defining $I_1$ (as in Eq (3.1)), starting from $(l = 0, E < 0)$ (the red dot) and following a smooth circuit, the action $I_1$ will change smoothly until $(l = 0, E > 0)$.

On that half-line there is a crease in the surface. To fix this, we redefine $I_1$. The new $I_1$ as function of $(l, E)$ is plotted together with the old $I_1$ in Fig.7. The colorful surface is for
the new $I_1$ while the grey surface is for the old $I_1$ (the same surface in Fig. 6). The new $I_1$ changes smoothly along the smooth red circuit.

Fig. 7. The grey surface is the action variable $I_1$ defined according to Eq. (3.1) while the colorful surface is $I_1$ defined according to Eq. (3.4). They coincide when $I > 0$. When we pass through $(I = 0, E > 0)$, $I_1$ changes smoothly on the new colorful surface.
If one has ambitions for a longer continuous journey to evaluate the action variable, the newer $I_1$ needs to be redefined so that it will change smoothly at $(l = 0, E < 0)$.

I show the surface in Fig.8.

Fig.8. The grey surface is the original action variable $I_1$ defined according to Eq. (3.1). The transparent light blue surface was the colorful surface in Fig.7. The colorful surface is the most newly defined action variable $I_1$ which is defined to make sure it changes smoothly when we come back and pass through $(l = 0, E < 0)$ the second time. The colorful surface coincides with the transparent light blue surface when $l < 0$.

Not only are action and angle variables redefined so that they are smooth functions of $(l, E)$, but also the angle subtended within a radial cycle $\Delta$ is redefined so that it is a smooth function of $(l, E)$.
\[ \Delta_{2}^{(\text{new})} = \begin{cases} 
\Delta_{2}^{(\text{old})}; & l \geq 0 \\
2\pi + \Delta_{1}^{(\text{old})}; & l < 0 
\end{cases} \]

(3.7)

This definition can be illustrated in Fig. 9. In Fig. 9(a), the angular momentum is positive, we do not change the definition for \( \Delta \) in this case. In Fig. 9(b), the angular momentum is negative, the new \( \Delta \) is defined as \( 2\pi \) plus the old \( \Delta \). We do this to make sure that when passing through \( l = 0 \), \( \Delta \) changes smoothly.
Fig. 9. The angle subtended within one radial cycle in circular box, defined in the new way. The dashed circle in both figures are the outer hard wall of the potential. The blue arrows are the trajectories of a particle within one radial cycle. Angles subtended within one radial cycle are labeled. In (a), the angular momentum is positive. In (b), the angular momentum is negative.

3.3 Topological change of the angle loop

Since the angle loop $\gamma_1$ is defined as angle variable $\phi_2=$constant, $\phi_1$ increases from 0 to $2\pi$, we would like to observe how the angle loop changes with $(l, E)$. This change of angle loop gives us the static manifestation of monodromy.

In Fig. 10, we show this static manifestation of monodromy. The figure in the center is a monodromy circuit in $(l, E)$ space; in this case, any counterclockwise circuit surrounding the origin gives the same result. The outer figures show seven tori
corresponding to seven different points in the \((l, E)\) spectrum space. The tori are represented in \((x, y, p_\rho)\) space [it is convenient to regard \((x, y, p_\rho)\) as orthogonal axes].

When the system is carried around such a circuit surrounding the origin in \((l, E)\) space and it returns to the original torus, the coordinate system defined by canonical angle variables on the tori changes smoothly into a different one. (The method used to calculate angle loops is given in Appendix B.)

On each torus two families of fundamental loops \([\gamma_2]\) (green curves) and \([\gamma_1]\) (blue curves) are shown, and they provide a coordinate system for each torus. Each toroidal loop \(\gamma_2\) (green) has a constant value of canonical angle variable \(\phi_1\), while \(\phi_2\) varies from zero to \(2\pi\). These loops are spaced by fixed steps of \(\phi_1\). Likewise each poloidal loop \(\gamma_1\) (blue) has a constant \(\phi_2\), while \(\phi_1\) varies from zero to \(2\pi\). Those loops are spaced by fixed steps of \(\phi_2\). One of the \(\gamma_1\) loops is stressed by a heavy curve (black).

The fundamental loops and the associated coordinate systems in the tori change smoothly as \(l\) and \(E\) change. Starting at \(l = 0\), \(E = -35\), the stressed \(\gamma_1\) (heavy black loop) is perpendicular to the toroidal (green) loops, and it is projected into the \((x, y)\) plane as a line. Moving counterclockwise in the \((l, E)\) plane, that loop is widened and tilted. For \(E > 0\), as \(l\) decreases from \((l, E) = (5, 6)\) to \((0, 5)\), the “doughnut hole” shrinks, and the innermost point of any poloidal \(\gamma_1\) loop approaches the origin in \((x, y, p_\rho)\) space. For \(l = 0\) this \((x, y, p_\rho)\) projection of the torus is singular, and the \(\gamma_1\) loops all rise vertically through the origin. When \(l\) continues to decrease for \(E > 0\), the formerly poloidal (blue) loops all go around the doughnut hole, and their projections into the \((x, y)\) plane enclose the origin. Continuing around the monodromy circuit, the loops
change smoothly; when we get back to the original torus \( l = 0, E = -35 \) the loops \( \gamma_1 \), and the associated canonical angle coordinate system, are topologically different from the original loops on that torus. The originally poloidal loop now goes around the torus in both poloidal and toroidal senses.

Also, examining the projections of the \( \gamma_1 \) loops into the \((x,y)\) plane, wherein there is a classically forbidden region surrounding the origin, the topology of the projected loop has changed. Initially it is a “trivial” loop, which in configuration space could be shrunk to a point without passing through the forbidden region, while at the end it has winding number \(-1\) about the forbidden region.

At the top of the monodromy circuit, at \((l = 0, E = 5)\) the \((x, y, p_x)\) representation of the torus is singular. However, the torus itself and its basic loops are not singular there. To display this, we show in the top line of Fig. 10 a representation of the tori in another space, \( (X = y + p_x, Y = y - p_x, P_y = x + p_y) \), where the tori and the poloidal loops (blue and black) evolve smoothly from \((l = 5, E = 6)\) to \((l = -5, E = 4)\). This change of the topological structure of the family of fundamental loops \([\gamma_1]\) is a static manifestation of monodromy.
Fig. 10. (Color) A static manifestation of Hamiltonian monodromy. Explanation is given in 3.1.3.
Chapter 4  Dynamical manifestation of monodromy

The above discussion describes the properties of angle coordinates on each \((l, E)\) torus, and how those coordinate systems change if we compare one torus with another. We call the phenomenon illustrated in Fig. 10 a static manifestation of monodromy because it is a property of static coordinate systems on static tori. A time variable \(t\) never appears in Sec. 3.3 above; there is a path variable \(s\) for the monodromy circuit \((l(s), E(s))\), but motion in real time is not considered. Therefore it may seem that monodromy is an abstract geometrical property of abstract variables, with no interesting dynamical consequences. However, we now know that monodromy has significant dynamical consequences [50,51].

What happens if in addition to the forces represented by the Hamiltonian \(H(z)\), we subject the system to an additional perturbing flow in phase space that changes the angular momentum and energy of particles in the system? Such additional forces and torques drive particles from one torus to another. Specifically, suppose we begin with a collection of noninteracting particles on an initial torus having \((l = 0, E < 0)\), and suppose that the positions and momenta of these particles correspond to the initial \(\gamma_1\) loop. Suppose then that all particles are made to change their angular momentum and their energy simultaneously, so that at every instant all particles have equal angular momentum and energy. Suppose furthermore that as they are driven from one torus to another, the change of torus leaves the value of the angle variables unchanged. (This
statement requires a definition of the origin of coordinates on each torus, which we give in 2.3.2.) Then the angle variables evolve with time as

\[
\frac{d\phi}{dt} = \alpha(l(t), E(t))
\]  

(4.1)

We may think of this evolution as occurring in incremental steps. In the first half of each step, the particles move along a static torus with \( d\phi/dt = \alpha(l, E) \), and in the second half of each step, each particle moves from a point on one torus to a point on an adjacent torus in such a way that the numerical values of the angle variables are unchanged

\[\phi(l, E) = \phi(l + dl, E + dE)\]. We call this process “ideal” evolution. It is ideal in two senses: (i) the particles all begin on a single loop on a single torus, and that loop has a constant value of the angle variable \( \phi_i \); (ii) the particles move synchronously from one loop to another. This process is one type of ideal evolution. Now suppose that the perturbing flow carries the particles in this way around a monodromy circuit in real time. In [51] a full description of such “ideal” evolution was given and it was shown that a collection of particles distributed around a \( \gamma_i \) loop remains always distributed around a \( \gamma_i \) loop. At the end of the monodromy circuit, when all particles have returned to the original torus, they occupy the final \( \gamma_i \) loop; that is, they have gone from a loop that is on one side of the potential energy barrier to a loop that surrounds the potential-energy barrier. Thus the change in the angle coordinates on the tori is manifested in the dynamical behavior in real time. The work in those references [50,51] left two important questions unanswered. (1) The ideal evolution defined therein arises from application of a perturbing flow in phase space which is (or can be) a Hamiltonian flow, but which cannot be derived from a single-valued Hamiltonian function. Can we implement a monodromy circuit by application of ordinary forces? (2) In any real system, the initial conditions
cannot be a perfect $\gamma_1$ (poloidal) loop defined on a single torus; particles will have a distribution of initial angles, initial angular momenta, and energies. Can a monodromy circuit be implemented in a real system?

4.1 Simulation and results

In this section, we show by computation that the answers to the two questions given at the end of last paragraph are “yes”: (1) a monodromy circuit can be achieved by the application of ordinary forces, and (2) it can be achieved under reasonable experimental conditions. We have carried out calculations on a variety of two-dimensional circularly symmetric potential energies having a well and a central barrier, comparable to that given in Eq.(3.6). To change the angular momenta of the particles, we apply a torque. Also, since raising and lowering the energy of the particles would not be easy to implement in an experiment, we instead lower and raise the central barrier (or equivalently, raise and lower the potential well). To answer the two questions separately, we carry out the calculations under two sets of initial conditions.

**Single loop initial conditions (case a).** We suppose that initially the particles all have the same energy and angular momentum, so their phase points lie on a single torus; we suppose that the particles are uniformly distributed on a single initial $\gamma_1$ loop on that torus, similar to the stressed (black) loop in Fig. 10. Note that whereas the particles initially all have the same angular momentum and energy, as soon as a transverse force is applied, with the same force on all particles, each particle experiences a different torque, so their angular momenta do not remain equal. Also as the potential energy changes, they gain and lose different amounts of energy. However,
the particles always occupy a single loop in phase space. That loop is close to a corresponding loop on a single torus, provided that the perturbing forces are applied slowly and gently, so that they do not change much during a radial oscillation of the particles. This is a kind of adiabatic implementation of the monodromy circuit. In our calculations, the entire monodromy circuit is implemented in approximately 30 cycles of radial oscillation.

**Cold-gas initial conditions (case b).** The Heisenberg uncertainty principle tells us that we cannot fix both the angle and the angular momentum of particles, and practical experimental limitations tell us that we cannot fix the energy exactly. We suppose that the initial conditions involve a range of initial angles and angular momenta and energies, so that the phase-space points of the particles lie on different tori, but all are reasonably close to the initial $\gamma_i$ loop of case (a). The spread of angular momenta, angles, and energies is consistent with what can be done experimentally for a cold gas described in Chapter 5, so we call this case "cold-gas initial conditions." Again the applied forces change slowly compared to the period of radial oscillation. (However, note that if the forces change too slowly, so that the time required to go around the monodromy circuit is too long, then the gas particles will spread because of their thermal motion, and the change of character of the loop will not be visible. Computational experience has shown that the topological change is visible when the entire monodromy circuit is implemented in about 30 cycles of radial oscillation.)

To drive the particles around the monodromy circuit we use the following five steps. Every step is done sufficiently slowly that there are several radial oscillations of the particles in each step. In computations, we can start a collection of particles distributed around a single loop with zero angular momentum and fixed energy, or distributed with a broader range of initial angular momenta and energy comparable to
the single-loop initial conditions. However, in an actual experiment, it is easier to start particles in a small packet near the inner turning point. Then after they have moved to the desired position, the process described below is begun.

(1) From A to B in spectrum space. Keeping the cylindrically symmetric potential unchanged, add a rotating force $F(t)$, the same force on all particles, to increase their angular momenta. The force is turned on and off gently and, in case (a), its direction is kept perpendicular to the position vector of the center of mass of the loop of particles. As a result, the force rotates counterclockwise with a frequency close to

$$f = \frac{\Delta(l, E)}{\tau(l, E)}$$

(4.2)

$\tau(l, E)$ and $\Delta(l, E)$ are, respectively, the “radial period” or time of first return, and the angle subtended in that time on the torus having angular momentum and energy respectively equal to $(l, E)$. $\bar{l}$ and $\bar{E}$ are the mean values of angular momentum and energy at the time $t$ (see Appendix A).

(2) From B to C in spectrum space. Turn off the rotating force and raise the potential well so as to increase the energies of the particles to positive values. Equivalently, we may lower the central barrier; particle energies are defined relative to the value of the potential energy at the origin $\rho = 0$.

(3) From C to E in spectrum space. Keeping the cylindrically symmetric potential fixed at the new values, apply the rotating force again the opposite way to reduce the angular momenta until they are negative. Again that force must rotate counterclockwise at a frequency close to that given in Eq. (4.2). In the “single-loop” computations of case (a) we keep the force perpendicular to the vector from the origin to the center of mass of the family of particles.
(4) From E to F in spectrum space. Turn off the rotating force and lower the well to its original depth; this decreases the energy of each particle. Equivalently, we may raise the central barrier to its original height.

(5) From F to A’ in spectrum space. Keeping the potential-energy function fixed at the new values (equal to the original values), apply the rotating force, still rotating counterclockwise with frequency (13), to increase the angular momentum of the particles, until the average angular momentum of those particles equals zero. Calculation shows that the average energy is then close to the initial energy.

Additional details about the potential energy and the perturbations are given in 4.1 and Appendix A.

Figure 11 shows the resulting monodromy circuit for “single loop initial conditions” and for “cold-gas initial conditions.” We see that the particles gain different amounts of energy and angular momentum as they traverse the monodromy circuit. However, they stay adequately close in angular momentum and energy. Figure 12 shows the configuration space and velocity space behavior for the single loop and for cold-gas initial conditions. Two important things are shown by this simulation. First, it is possible to drive a collection of particles around a monodromy circuit using ordinary forces (rather than by using the ideal flow defined in Ref. [51]). Second, while we already know that the changed structure of the loop in configuration space provides a definitive signature of monodromy, also the structure in velocity space provides another clear signature. (see Fig.12 in Chapter 5)

Thus we have shown by computation that this dynamical manifestation of monodromy can be implemented in a real system by application of ordinary forces.
Fig. 11. (Color) Spectrum-space paths, i.e., paths in angular momentum—energy space, \((l, E)\). Each line represents the path \([l, E]\) of one particle as it travels around the monodromy circuit starting at point A and proceeding through A1, B–F, and back to the final point A (called A’). Black lines represent particles with initial conditions on a single loop, and blue lines (blue) are paths of particles having cold-gas initial conditions. Particles are driven around the monodromy circuit by applying a common force acting as a torque to change the angular momentum, and by raising or lowering the potential-energy well.
Chapter 5   Experimental realization

The work described in this section was a joint project with Prof. Seth Aubin and Megan Ivory. They designed the two different proposed apparatuses, and I did the simulations. Most of the experimental details were written by Megan Ivory and Seth Aubin. This became a joint publication [53].

The experimental scheme described below uses a gas of ultracold atoms to implement dynamical monodromy. This experiment also offers the possibility of exploring the phenomenon in the presence of interparticle interactions, as well as quantum-mechanical effects such as interference and tunneling, which are beyond the scope of the theory presented in this paper. It is not an easy experiment, but it uses only standard tools of atomic physics.

A conclusive observation of dynamical monodromy should show experimentally that if one starts with a loop of initial condition points in phase space and then varies their energy and angular momentum along a closed path in spectrum space (such as in Fig. 11), then the initial and final configuration-space loops have a topologically different structure relative to the forbidden region surrounding the origin—i.e., the final, but not the initial loop encloses the energetically inaccessible region. The experimental system requires two main ingredients: (1) precision control for producing the initial phase-space loop, and for applying the torque and central potential barrier modulations to accurately implement the prescribed spectrum space path; and (2) accurate measurements of energy, angular momentum, position, and velocity to verify the phase-space and spectrum-space coordinates of the system at the start, end, and during the monodromy process.
The ultracold atoms scheme uses a ring-shaped optical trapping potential for ultracold $^{39}K$ atoms. Instead of running the full loop of initial conditions simultaneously, the atoms are placed in a short segment of the loop of initial conditions and then driven around the ring potential by the application of a uniform magnetic force, while the height of the central barrier is appropriately modulated to follow the monodromy circuit. The resulting energy and angular momentum of the atoms can then be tracked by both *in situ* and time-of-flight imaging as the system moves along the prescribed spectrum space path. The monodromy process for the full loop of initial conditions is reconstructed by combining the results of separate initial condition segments, so that the new topology of the resulting phase-space distribution can be observed.
Fig. 12. (Color) This is a collection of snapshots showing the evolution of the single loop and of the cold gas as the system traverses the monodromy circuit. The topological structure of loops of particles in configuration space changes during the monodromy circuit. Single-loop initial conditions are represented by the solid (black) curve, while gas particles are represented by dots (color). (A) and (A’) are points marked in Fig. 11. (a) Position space. Each square is a region 400 × 400 μm (±200μm about the origin). The inner and outer circles are boundaries of the classically allowed region for any single-loop particle that has \( l = \langle l \rangle \) and \( E = \langle E \rangle \). The vectors from the origin (green) represent the applied rotating force. (A) Initially all single-loop particles have the same energy and angular momentum \( (l = 0, E = E_0) \) and they form a line in configuration space \((x-y)\) plane while the “gas particles” have a spread in angle, angular momentum, and energy: \( \langle E \rangle = E_0, \Delta E > 0, \langle l \rangle = 0 \), and \( \Delta l / \Delta \varphi = \hbar / 2 \). (A1) In the second snapshot, as angular momenta increase, the line evolves into a loop always linking the inner and outer boundaries. (B
The well is lifted (equivalently, the central barrier is lowered), so the central forbidden regions reduced to a size governed by the angular momentum. With energy of the particles above the central barrier, the angular momentum is decreased from positive to negative. At some instant a single-loop particle having zero angular momentum passes over the center point \( x = y = 0 \); for that particle the central forbidden region has vanished for an instant. When it reappears, it is inside the loop. The well is lowered (equivalently, the barrier is raised) and the central forbidden region gets larger. The angular momentum is driven back up to zero. Integration is stopped when \( \langle I \rangle = 0 \), and we find that \( \langle E \rangle \) is close to the initial energy, \( E_0 \). Like the angle loop \( \gamma_1 \), the loop of particles has evolved into a topologically different loop. (b) Momentum space, \( (p_x, p_y) \). The units of momentum are \( 10^{-27} \) Kg m/s. Each square is a region 20 × 20, extending from ±10 about \( p = 0 \). From points A1–C, the loop does not enclose the origin. At D it touches the origin, and from E–A’, the winding number about the origin is 1. Initially particles are traveling equally to the left and right. At the end, they are dominantly going in a beam like a rotating searchlight.

The experimental implementation requires a number of lasers to produce a ring potential and several external magnetic fields to produce a torque that changes the angular momentum of the atoms. Figure 13 shows how lasers and magnetic coils can be combined to produce the appropriate optical potential and magnetic force for the atoms, which are then detected by a high resolution imaging system. We summarize the main suggested experimental parameters in Table I. In the following paragraphs, we describe the details of the ring trap, the atomic packet and its preparation in a segment of the ring of initial conditions, the torque force, and how to measure the total energy and angular momentum of the atomic packet.

**Ring trap.** The atoms are confined in a ring trap produced by two blue-detuned optical dipole potentials produced by two vertically directed laser beams: a focused laser that serves as the central barrier and a concentric hollow laser beam that provides the outer wall of the trap. Hollow beams can be generated with a variety of optical elements.
such as axicon lenses [54], phase plates [55], and spatial light modulators [56]. Time-averaged doughnut beams can be produced by rapid rotation of a Gaussian beam using two crossed acousto-optic modulators [57]. The Gaussian ring potential of Fig. 13(b) is well suited for ultracold atom monodromy studies and can be produced with central barrier and outer wall laser powers of 0.4 and 2.5W, respectively, at 750 nm. An additional red-detuned laser can be used to form a horizontal sheet of light that provides vertical confinement, while leaving the horizontal confinement potentials negligibly affected: For example, a 10W laser beam at 1064 nm focused to horizontal and vertical waist radii of 5 mm and 30 μm, respectively, will provide harmonic confinement of 360 Hz along the vertical axis with a trap depth of roughly 4 μK, but with a negligible 2 Hz confinement in the horizontal plane. Alternatively, vertical confinement can be provided by a one-dimensional optical lattice of horizontal “pancake traps” with the atoms spread over multiple layers. Based on simulations of atomic motion in the ring potential, the average scattering rate from all of the far off-resonant trapping light is estimated to be about 1 Hz per atom and so is negligible over the 100 ms duration of the proposed experiment.

**Atomic packets.** The atomic packets consist initially of a noninteracting Bose-Einstein condensate (BEC) of $^{39}\text{K}$ atoms designed to minimize the expansion of the atomic packet as it follows the spectrum space path. The BEC limits the expansion of the atomic packet to the Heisenberg-limited spread required of all quantum-mechanical systems, but must be carefully tailored by choosing an appropriate initial packet size: In our case, a $^{39}\text{K}$ BEC with radial and tangential half-widths of 0.3 and 2.25 μm, respectively, will expand with respective velocities of 2.7 and 0.4 μm/ms. Repulsive atom-atom interactions can also lead to relatively large expansion rates, but can be sufficiently suppressed by using the $|F = 1, mF = +1\rangle$ hyperfine ground state of $^{39}\text{K}$ at a
magnetic field of 350 G, which tunes the s-wave scattering length to zero due to a nearby Feshbach resonance \([58]\) (A slightly attractive interaction may be useful in reducing the Heisenberg-limited spreading of the packet, though simulating its precise effects on the atomic packet is beyond the scope of this paper.) Experimentally, the interactions are difficult to eliminate altogether, but even if the scattering length is reduced to \(a_s = 0.17a_0\), which for \(\frac{\partial a_s}{\partial B} = 0.55a_0\) \([58]\) corresponds to a magnetic field tuning precision of \(\Delta B = \pm 0.3G\), then interaction-induced spreading is negligible for packets with fewer than \(8 \times 10^4\) atoms. However, the atom number must also be sufficiently large to allow for high-quality imaging: Simulations of time-of-flight experiments, such as in Fig. 16, show that atom numbers of \(4 \times 10^4\) or more produce final atomic packets with optical depths of 0.5 or higher, which are suitable for absorption imaging methods \([59]\).

*Initial conditions.* The BEC is inserted into the ring trap with a multistep process. As shown in Fig. 13(c), the BEC is initially trapped by a single-beam optical dipole trap produced by an additional laser that copropagates with the 1064 nm laser sheet [not shown in Fig. 13(a)]. The BEC is located at a radius of 25 \(\mu\)m, which corresponds to a potential energy of 53 \(\mu\)K. Upon turning off this single beam confining potential, the BEC is free to oscillate in the ring potential. The specific position-velocity combination of the ring of initial conditions for the atomic packet is chosen by applying the torque force at the appropriate time of the oscillation phase. Our simulations show that a radial positioning error of \(\pm 1.25\) \(\mu\)m can be tolerated. Alternatively, if a higher precision method is needed, a multiphoton Bragg pulse \([60,61]\) can be used to impart a momentum kick (corresponding to a kinetic energy of 53 \(\mu\)K) to BEC atoms held at the minimum of the ring potential.
Fig. 13. (Color) Proposed apparatus and optical potentials for observing dynamical monodromy. (a) Sketch of apparatus for observing dynamical monodromy: The atoms are confined in a ring trap formed by the vertical downward-directed blue-detuned laser beams and the horizontal laser beam (green). The ring trap is the light (yellow) ring in the intersection of these beams. Coils (orange) generate magnetic fields for tuning the interactions to zero and producing the torque force. The camera is used for absorption imaging with an upward-directed laser probe beam (up-pointing arrow, orange). (b) Planar ring-trap potential for the ultracold $^{39}\text{K}$ atoms. The potential consists of a central Gaussian barrier with a waist radius of 73 $\mu$m and an outer Gaussian wall at a radius of 200 $\mu$m with a waist of 26 $\mu$m. (c) Trap and release method for producing the atomic packet with total energy 53 $\mu$K.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ring-trap laser power</td>
<td>2.9 W at 750 nm</td>
</tr>
<tr>
<td>Vertical trapping laser power</td>
<td>10 W at 1064 nm</td>
</tr>
<tr>
<td>Atomic state</td>
<td>(</td>
</tr>
<tr>
<td>--------------</td>
<td>--------------------------</td>
</tr>
<tr>
<td>Atomic packet population</td>
<td>(4 \times 10^4)</td>
</tr>
<tr>
<td>Energy of initial atomic packet</td>
<td>53 (\mu)K</td>
</tr>
<tr>
<td>Peak torque force</td>
<td>0.36 (m_i ) g*</td>
</tr>
<tr>
<td>Magnetic Feshbach zero</td>
<td>350 G</td>
</tr>
<tr>
<td>Duration of monodromy round trip</td>
<td>100 ms</td>
</tr>
</tbody>
</table>

*1.e. 0.36 times the weight of a potassium atom

**Torque force.** The torque force can be produced by the magnetic gradient of a horizontally oriented quadrupole coil pair with equal and opposite currents in its two coils, as shown in Fig. 13(a). As illustrated in the top three panels of Fig. 14, the central symmetry quadrupole field combines with the 350 G horizontal magnetic field required for suppressing interactions. At 350 G, the Zeeman shift of the \(|F = 1, mF = +1\rangle\) hyperfine ground state is \(-1.33 \text{ MHz/G}\). Modulation of the torque force as shown in Figs. 15(a) and 15(b) help to reduce the width of the packet in spectrum space. A maximum force of \(2.3 \times 10^{-25} \text{ N} = 0.36 \text{ mg}\) is required, which corresponds to a magnetic gradient of 2.6 G/cm. The combination of the uniform 350 G field with the weak quadrupole field results in a magnetic gradient along the direction of the 350 G field, while the gradients in the transverse horizontal and vertical directions contribute negligibly to the potential over the size of the ring trap. The orientation of the magnetic torque force can be easily rotated in the horizontal plane by changing the direction of the 350 G field, which is generated by two orthogonal Helmholtz-style coil pairs: Sinusoidal modulation of the coil
pair currents (π/2 out of phase from each other) rotates the 350 G field and the magnetic gradient in a manner similar to the magnetic field modulations in a time-orbiting potential (TOP) trap [62]. Figure 15(b) shows the orientation of the torque force and 350 G field over the course of the monodromy process: The field maintains an average angle of roughly π/2 with respect to the angular position of the atomic ensemble and is rotated at rates of up to 330 Hz, which is substantially slower than in a TOP trap [62]. Finally, the magnetic gradient produces a negligible variation of the scattering length of at most $a_s = 0.06a_0$ over the roughly 400 μm diameter of the ring trap.

Fig. 14. (Color) Magnetic fields for producing the torque force. The top three panels sketch how the quadrupole magnetic field [panel (a), thin arrows, blue] generated by the anti-Helmholtz coil pair combines with the uniform horizontal magnetic field [panel (b), thin arrows, red] produced by the two Helmholtz coil pairs to produce a magnetic gradient in the direction of the magnetic field [panel (c), thin arrows, purple], whose orientation is determined by the relative currents in the two Helmholtz coil pairs. The magnetic field line sketches in panels (a), (b), and (c) are all in the horizontal plane (view from above) and are not to scale: The thick arrows represent the current in the coil, while the thick dashed arrows indicate the current in the hidden coil underneath. The two plots (d) and (e) show the magnetic field magnitude and its associated...
effective potential. Along the field direction (d) it is nearly linear (red) while in the transverse directions (e) it is quadratic: Its horizontal variation is represented by the solid (green) curve, and its vertical variation by the dashed (blue) curve. Note the reversed right axes for the potential energy, since the $|F = 1, m_F = +1>$ state is a strong field seeker.
Fig. 15(a)(b). (Color) Torque force and central barrier modulation versus time required for completing the monodromy circuit. Top(a): Torque force magnitude (curve with arrow toward left axis, black) and central barrier amplitude (curve with arrow toward right axis, red) as a function of time. Bottom(b): Absolute torque angle with respect to starting position (arrow toward left axis, red) and torque angle relative to full atomic ensemble center of mass (arrow toward right axis, black). The letters on the top axis denote the monodromy circuit transit points of Fig. 11.
*Measuring the total energy $E$. The total energy $E$ of the atomic packet can be measured by turning off the outer laser barrier of the ring trap while the atoms are climbing the inner central barrier. The atoms convert all of their potential energy to kinetic energy as they are pushed away from the central barrier and leave the ring potential region, so that their average velocity, kinetic energy, and thus total energy can be measured by time-of-flight imaging.*

*Figure 16 shows the results of a simulation of this process. The method relies on the compactness of the atomic packet to guarantee that there are no atoms in the outer barrier region when it is turned off, and to ensure that a measurement of average velocity is representative for all the atoms in the packet. Numerical simulations show that the method functions well for all initial conditions and points along the spectrum space path: To measure the total energy $E$ at some point along the spectrum space path, the monodromy process is stopped at the desired point, and the outer barrier is turned off as the atoms are climbing the central barrier. Furthermore, the instantaneous kinetic energy of the atoms can be measured by turning off the entire ring potential and then measuring the velocity by time-of-flight imaging. In practice, the 1064 nm optical dipole laser and the torque force magnetic gradient will need to be turned off as well, since they provide very weak but sufficient horizontal confinement to affect the time-of-flight measurements.*
Fig. 16. (Color) Time-of-flight method for measuring the total energy $E$. The plot corresponds to a packet that has completed the monodromy process and returned to point A (i.e., A’) on the spectrum space path of Fig. 11.

Measuring the angular momentum $L$. The angular momentum of the atomic packet can be measured by in situ imaging of the atoms as they travel around the ring potential. The inset of Fig. 17 shows a simulated image of the atoms in the ring potential, and the radially averaged atomic population as a function of angle from which the angular center of gravity of the packet can be determined from Gaussian fits of the
distribution. A series of such images for different holding times shows the time evolution of the angular position of the packet. The main plot in Fig. 17 shows the results of a numerical simulation of this process: The average angular velocity \( \langle \dot{\theta} \rangle \) is the overall slope of the angular time evolution, but the plot also contains a periodic step feature that reflects the radial oscillations of the atoms. The angular momentum \( L \) can be extracted from the time evolution of a packet’s angular position, such as shown in Fig. 17, by determining the angle change \( \Delta \theta_r \) over the course of one radial oscillation period

\[ \Delta T_{\text{radial}} \] and then solving the following integral equation numerically for \( L \) [63]:

\[
\Delta \theta_r = 2 \int_{r_{\min}}^{r_{\max}} \frac{Ldr}{r^2 \left[ \frac{2}{m} [E - V(r)] - \frac{L^2}{m^2 r^2} \right]}
\]  

(5.1)

Where \( E \) refers to the total energy of the atoms, \( V(r) \) is the ring potential, and \( r_{\min} \) and \( r_{\max} \) are the inner and outer turning radii, respectively.

Extracting \( L \) requires knowledge of all the other quantities in Eq. (5.1). While \( \Delta \theta_r \) can be determined from the step size of the “staircase” plot of average angular position versus time, it is more reliably obtained in our simulations from the relation

\[ \Delta \theta_r = \Delta T_{\text{radial}} \langle \dot{\theta} \rangle \] : The average angular velocity \( \langle \dot{\theta} \rangle \) is the slope of a linear fit to the average angular position plot in Fig. 17, and the radial period \( \Delta T_{\text{radial}} \) of the atomic packet in the ring potential can be obtained from a Fourier transform of the average angular position time series in Fig. 17. \( V(r) \) can be determined experimentally by \textit{in situ} absorption imaging of a cold thermal gas of temperature \( T_{\text{thermal}} \) in the ring potential: The image provides the radial atomic density \( n(r) \) which can then be used to extract the potential through the relation \( n(r) \propto \exp(-V(r) / kT_{\text{thermal}}) / \Lambda^3 \), where
\[ \lambda = \frac{h}{\sqrt{2\pi mk_{thermal}}} \] is the thermal de Broglie wavelength [64]. The determination of the average total energy \( E \) of an atom in a packet was described in the previous section. The inner and outer turning radii can be determined from knowledge of the potential and the total energy or from \textit{in situ} imaging. We find through numerical simulations of the above measurement method that \( L \) can be determined with an accuracy of 5%-10% over the course of the entire spectrum space path.

Fig. 17. (Color) Angular momentum measurement method with \textit{in situ} imaging. The main plot shows the average angular position of an atomic packet versus time (wiggly curve, blue), along with a linear fit (straight line, red) that gives the average angular velocity. The simulation is for an atomic packet that has returned to point A (i.e., A') after completing the monodromy circuit of Fig. 11. Inset: Angular density of the packet (wiggly curve, blue) and Gaussian fit (smooth curve, red) versus angular position. The fit is used to determine the packet’s average angle; the inset also shows a simulated image of the atoms (dots, blue ) in the ring potential along with the maxima and minima of the radial oscillations (circles, red ).
CONCLUSION

We have shown that a dynamical monodromy circuit can be implemented by ordinary forces, and we have described two ways to realize a dynamical monodromy circuit in a physical system—an ultracold gas. All our calculations are classical, and presume no interaction between the particles, so measurements on a cold gas would raise questions about quantum behavior and about interactions between particles that are not addressed in this thesis.

Chapter 6  Quantum manifestation of monodromy

Almost everything that happens in classical mechanics also shows up in quantum mechanics when we know where to look for it. In Chapter 3-5, the phenomenon in classical mechanics involves topological changes in the loops that define action and angle variables as a result of a passage around a “monodromy circuit”. In this chapter, we show a corresponding change in quantum wave functions: these
wave functions change their topological structure in the same way that the action and angle loops change.

As in earlier chapters, we consider particles moving in two dimensions in a circularly symmetric “champagne bottle” or “Mexican hat” potential energy:

\[ H(q, p) = \frac{p_x^2 + p_y^2}{2\mu} + V(\rho) \]  \hspace{1cm} (6.1)

\[ V(\rho) = -\frac{3}{2} \rho^2 + \frac{1}{60} \rho^4 \]  \hspace{1cm} (6.2)

In quantum mechanics as well as classical mechanics, there are two conserved quantities, angular momentum \( L(q, p) = xp_y - yp_x \) with conserved value \( l \) and energy (the Hamiltonian function itself), with conserved value \( E \).

Let us briefly review the things we learned in the classical context in earlier chapters. A “level set” is the set of points \((q, p)\) in phase space corresponding to fixed values of angular momentum and energy. For the Mexican hat system, every level set except one is a torus, and the shape in phase space of these tori, and the motion on them as well, can be described by action and angle variables. The values of action variables specify the torus on which the motion occurs, and the values of angle variables specify the position on each torus.

The exceptional level set is the one having \( l = 0 \) and \( E = 0 \). That set (like all the others) is cylindrically symmetric, but forms a figure-8 rather than a torus. This seeming violation of general theorems occurs because the gradients of \( L(q, p) \) and of \( H(q, p) \) both vanish at \((q = 0, p = 0)\); accordingly the origin in phase space \((q = 0, p = 0)\) is
called a “singular point”. Connecting with quantum mechanics, we call the two-dimensional space of values of conserved quantities \((l, E)\) “spectrum space”. The origin in phase space \((q = 0, p = 0)\) corresponds to the origin in spectrum space, \((l = 0, E = 0)\), and this point is called a “singular value”.

If for each nonsingular value in spectrum space (each point other than the origin) we construct the loops that define the action and angle variables, and we insist that those loops and their associated action and angle variables must change differentiably as functions of \((l, E)\), we then find that one of the loops and its associated action and angle variables are multivalued (in Section 3.2) – on traversing a circuit around the origin (Fig. 10), one of the loops changes its topological structure. Initially, the projection of the loop into configuration space is confined to one side of a classically-forbidden region, and at the end, it surrounds that classically-forbidden region. [Fig. 19]. This topological change of classical action and angle loops is called a “static” manifestation of classical Hamiltonian monodromy.
Fig. 18  Monodromy circuits. Coordinates of spectrum space are angular momentum and energy. The grey dots represent quantized eigenvalues \( (m, E_{m,n}) \) for the Mexican Hat system defined in Eq.(6.2). The grey curves link states of the same “quantized smooth action variable”. The origin, marked by a red dot, is a singular value, also called a “monodromy center”. Any closed circuit (such as the blue curve) around this point is a monodromy circuit. The red circuit is the monodromy circuit that we often follow.
Fig. 19 In each figure is the torus in phase space specified by \((l = 0, E = E_0 < 0)\) and its projection on to the x-y plane. The two tori are the exact same two-dimensional manifold in four-dimensional phase space, but with different coordinate systems on them. The coordinate systems, marked by the blue and green loops, are defined by angle variables \((\phi_1, \phi_2)\). The bold black loop is the angle loop that we care about. It is defined by \(\phi_1 = \text{constant}, \ 0 < \phi_2 < 2\pi\). Initially, the torus with its angle loop is shown in the left figure. The black angle loop stays on one side of central forbidden region. When \((l, E)\) changes smoothly on the monodromy circuit, the torus specified by it also changes smoothly, and so does the angle loop. After traversing a monodromy circuit, when \((l, E)\) return to their initial values \((l = 0, E = E_0 < 0)\), the torus returns to the original torus but the angle loop changes into a topologically different loop, shown in the right figure.
Fig. 20. Monodromy of wave functions. Initially we make a superposition with expectation value of angular momentum $< l > = 0$, and expectation value of energy $< E > = E_{m=0, n=13}$, shown in Fig. 20a. This superposition is localized on one side of the classically forbidden region. The contour plot corresponds with the black angle loop specified by $(< l > = 0, < E > = E_{m=0, n=13})$. After carrying $(< l >, < E >)$ smoothly going along the monodromy circuit and returning to their original values $(< l > = 0, < E > = E_{m=0, n=13})$, the wave (b) smoothly changes into a topologically different wavefunction, corresponding with the topologically changed angle loop.
In Refs. [50,51] it was pointed out that this static manifestation of monodromy must have dynamical consequences: if a collection of noninteracting particles is given initial conditions corresponding to an initial angle loop on a torus, and those particles are driven continuously by an ideal Hamiltonian flow around a monodromy circuit, then the loop of particles undergoes the same topological change that is seen in the angle loop. In Ref [53], and in the previous chapter, simulations show that this phenomenon can be observed under a relatively simple time-dependent Hamilton when the appropriate torque is applied. Furthermore, the topological change also occurs under less-than-ideal conditions, with particles having a distribution of energies and angular momenta.

The question we address in this chapter is: can we construct quantum wave functions that have the same topological change that is seen in the action-angle loops? The answer is yes. In this chapter, we will show: (1) a new static quantum manifestation of monodromy -- we define a superposition of eigenfunctions of $H$ which has the appearance of an initial action-angle loop, confined to one side of a classically-forbidden region; when we carry this superposition around a monodromy circuit in spectrum space, the wave function changes its structure to a loop that surrounds the classically-forbidden region. We show also: (2) an analogous "ideal" dynamical quantum manifestation of monodromy -- a continuous time-dependent unitary transformation that drives the expectation values of angular momentum and energy around a monodromy circuit causes the wave function to make the same topological change. Finally we show: (3) a realizable manifestation -- this topological change can be implemented by a time-dependent Hamiltonian with an appropriate radiation field.

One result is shown in Figure 20. Before being carried around the monodromy circuit, the wave function is localized on one side of the origin. Afterwards it surrounds
the origin. (Spreading of a wave packet cannot produce the change shown here. In our case, spreading occurs on a longer time scale, and produces a different density.)

The topological change in classical mechanics is robust, so there are many ways to construct valid quantum analogs. In the following, we explain how we constructed these wave functions.

**Relationship to other work**

As was discussed in Chapter 1 of this thesis, this work is connected with the theory of torus quantization [65] (the modern version of the Old Quantum Theory) which has been used to study an immense variety of systems, including simple nonlinear oscillators, molecular vibrations and rotations, excited states of hydrogen in electric and magnetic fields, doubly-excited states of helium, spin-orbit coupling, and excited states of nuclei [2--4,9,10,15,27,66,67]. As discussed in earlier chapters, for the Mexican Hat system, Duistermaat, following a suggestion by Cushman, constructed action and angle variables, and showed that smoothly-defined action and angle variables cannot be single-valued. Subsequently, Cushman and Duistermaat described the quantum implications of multivalued action variables: the lattice of allowed semiclassical eigenvalues, defined by quantization of these multivalued action variables, has a defect [29,68,69].

Many classical and quantum systems display Hamiltonian monodromy and its associated spectral defects, including any cylindrically symmetric system with a quadratic barrier, the spherical pendulum, dipolar molecules in fields, the hydrogen atom in crossed fields, nearly linear molecules, elliptical billiards, and atoms in traps [30,33--
As discussed in earlier chapters, later it was shown that this seemingly abstract geometry in phase space leads to interesting dynamical consequences: in a system like the Mexican Hat, if the system is subjected to appropriate perturbations, a loop of particles can evolve smoothly in time into a topologically different loop [50,51,53].

Monodromy is the simplest and most accessible example of a class of recently uncovered phenomena (bidromy and fractional monodromy), and even attractors in field theory [40–42,75,76]. It was discovered because of new ways of thinking about classical Hamiltonian systems (the global perspective – how tori fit together in phase space) [77,78].

Finally, topological quantum states receive much attention because they are connected with the integer or fractional quantum Hall effect, because certain atom transport schemes use topological methods, and because of speculations that they can be used to implement schemes for topological quantum computing [79–91]. In Fig. 20, we have shown by computation that quantum states of very simple two-dimensional systems also can display interesting topological changes.

6.1 Construct semiclassical wavefunction with topological change

We want to carry knowledge of monodromy in classical mechanics into quantum mechanics. It is natural to think of semiclassical approximations which link classical mechanics with wavefunctions. In this section we will construct a semiclassical
wavefunction spreading along an angle loop in circular box. By expanding this semiclassical wavefunction with truncated eigenstates of circular box, we find a good way to show monodromy with superposition of eigenstates.

This is a long process, so we give a brief summary of it here.

Semiclassical approximations build approximate quantum wavefunctions from families of classical trajectories. In this section, we begin from the family of trajectories in which each trajectory in the family is an angle loop for a particle in a circular box. Those trajectories are obtained by solving Hamilton’s equations using the Hamiltonian given below in Eq. (6.7). From these trajectories, one finds a classical action, which becomes the phase of a semiclassical wavefunction, and a classical density, the square root of which becomes the amplitude of a semiclassical wavefunction. At each point in the classically allowed region there is an incoming and an outgoing trajectory. Accordingly, the full semiclassical wavefunction is a superposition of incoming and outgoing semiclassical waves.

Because we want to construct a wave packet centered on a single angle loop, we insert a weighting factor so that only the wave near that selected angle loop (the bold black one in Fig. 21(a)(b)) is emphasized. The shape of the absolute value of the semiclassical wave turns out to be like a thickened angle loop. This semiclassical construction is carried out in detail in section 6.1.

Like all semiclassical wave functions, the wave function so constructed diverges at the boundary between allowed and forbidden regions. To fix that divergence, we expand the wavefunction in a truncated set of eigenfunctions of the circular box. We find that only a small number of eigenfunctions have large coefficients; these eigenfunctions
have radial quantum number corresponding to the action integral around the angle loop,
and angular quantum number close to the angular momentum of the angle loops.

Then we return to the Mexican hat system, and construct the same type of
superposition of eigenfunctions, and show that it looks like an angle loop for the classical
Mexican hat system.

Once we have a wavefunction which is a quantum analogue of a classical angle
loop, we ask: How can we drive it around a monodromy circuit? The first step is to
define a quantum monodromy circuit. Then we implement that monodromy circuit in
three ways, which we call “static”, “ideal”, and “realistic”. In the “static” version, we
simply move the coefficients in quantum-mechanical spectrum space. We find that the
resulting wavefunction gets the same topological change that occurs in the angle loop.
This topological change is especially visible by looking at the flux density. All this is
done in section 6.2.

Now we want time dependent evolution that does the same thing. In the “ideal”
version, we fabricate a time-dependent unitary transformation that accomplishes the
same changes of coefficients. Finally, in the “realistic” version, we return to the circular
box, and solve the time-dependent Schrodinger equation using a Hamiltonian that
contains ordinary forces. Happily, the desired topological change is found.

Now let us begin.

6.1.1 Calculation of classical action-angle loops
We calculate action-angle loops on a torus using the method described in earlier chapters: we use the effective Hamiltonian \[ 53,92 \]

\[
H(q, p; l, E) = H(q, p) - \Omega(l, E)L(q, p)
\]  \hspace{1cm} (6.3)

Here \( \Omega(l, E) = \Theta(l, E) / T(l, E) \) is the angular velocity averaged over a cycle of radial motion -- \( T(l, E) \) is the radial period (time for return to the original value of \( \rho \)), and \( \Theta(l, E) \) is the azimuthal angle subtended in one radial period. Both quantities are obtained from trajectories of \( H(q, p) \), and they must be defined so that they are differentiable functions of \( (l, E) \) (See Fig. 9). Trajectories under \( H(q, p; l, E) \) are obtained by treating \( (l, E) \) as fixed parameters, and obtaining Hamiltonian equations of motion from the \( (q, p) \) dependence of \( H \). These trajectories have the form of trajectories under \( H(q, p) \) as seen in a frame of reference rotating counter-clockwise with angular velocity \( \Omega(l, E) \). Hence in one radial cycle, every orbit closes. Any trajectory of \( H(q, p; l, E) \) is an action-angle loop. The canonical angle variable associated with this loop increases linearly with time from zero to \( 2\pi \) as the trajectory goes around the loop, and the action variable is given by the integral

\[
I_{\Omega} = \int p^2 dq / 2\pi
\]  \hspace{1cm} (6.4)

around the loop. Provided that \( |\Theta(l, E)| < \pi \), these are poloidal loops.

The second family of loops can be found by calculating trajectories using \( L(q, p) = xp_y - yp_x \) as if it were a Hamiltonian. Those trajectories project to circles in
the \((x, y)\) plane. In our phase-space pictures, they are toroidal loops on each torus.

The corresponding action variable is

\[
I_\ell = \int p \, dq / 2\pi = \ell \tag{6.5}
\]

In figure 10 of Chapter 3, we showed pictures of the two families of action-angle loops for this system. These action-angle loops define a coordinate system on each torus. The relationship between those coordinates on one torus and on another constitutes a connection between coordinates on the different tori. As we change \((\ell, E)\), moving from one torus to another, these action-angle loops, and the associated coordinate systems on the tori, change gradually and smoothly, provided that we make \(\Theta(\ell, E)\) change smoothly. We define a “monodromy circuit” as any continuous closed path in spectrum space surrounding the origin. If we carry the system around such a path, when the system returns to its original \((\ell, E)\), the topological structure of the \(H\) family of loops is different. (Figure 19). The poloidal loop changes to a combination of toroidal and poloidal loops. This happens because \(\Theta(\ell, E)\) changes from zero to \(2\pi\) on traversing the monodromy circuit.

### 6.1.2 Corresponding quantum system

Now we examine stationary and nonstationary solutions of the Schrödinger equation using the quantum version of Hamiltonian (1). Every eigenfunction of

\[
H(q, -i\hbar \nabla) \quad \text{is also an eigenfunction of} \quad H(q, -i\hbar \nabla; \ell, E) , \quad \text{but the eigenvalues} \quad E_{m,n} \quad \text{of} \quad H
\]

are different from those of \(H\):

\[
E_{m,n} = E_{m,n} - \Omega(\ell = m\hbar, E_{m,n}) \hbar \tag{6.6}
\]
where $m$ is the integer angular momentum quantum number, and $n$ is the radial quantum number.
Fig. 21(a)(b) A topological change of angle variables in the circular box system. This system does not have a complete monodromy circuit, because it does not have negative energies. However, the angle loops have a topological change similar to what occurs on the upper portion of a monodromy circuit in the Mexican Hat system. Thus, we compare two tori specified by two points on the incomplete monodromy circuit respectively. 21(a) is the torus in phase space specified by $(l = 10 > 0, E = 31.5793 > 0)$ and its projection onto the x-y plane. 21(b) is the torus in phase space specified by $(l = -9 < 0, E = 14.5035 > 0)$ and its projection onto the x-y plane. Due to the outer hard wall, the “loops” and “tori” are also incomplete. The coordinate systems, marked by the blue and green loops, are defined by angle variables $(\phi_1, \phi_2)$. The bold black loop is the angle loop that we care about. It is defined by $\phi_1 = \text{constant}$, $0 < \phi_2 < 2\pi$. In figure (a), the black angle loop stays on one side of central forbidden region. When $(l, E)$ changes smoothly, the torus changes smoothly as do the angle loops. When $l < 0$, the angle loop changes into a topologically different loop, shown in figure (b).
semiclassical approximation

$m = 10$

$E = 31.5793$
Fig. 21(c)(d) Topological change of semiclassical wave functions. These two wavefunctions are localized near the emphasized angle loops on the tori shown in Fig. 21(a)(b). They were calculated from trajectories having angular momentum and energy (c) \( l = 10, E = 31.5793 \) and (d) \( l = -9, E = 14.5035 \), the same as the values in Fig. 21(a)(b). We see that these wave functions are localized close to the emphasized angle loops, so they have the desired topological change.
superposition
$m=10$
$E=31.5793$
Fig. 21(e)(f) the wave function in 21(e) is superposition with eigenstates of circular box and has expectation value of angular momentum and energy $\langle l \rangle = 10, \langle E \rangle = 31.5793$. The contour of this superposition matches the corresponding angle loop specified by $\langle l \rangle = 10, \langle E \rangle = 31.5793$ and stays on one side of the origin. The wave function in 21(f) is superposition with eigenstates of circular box and has expectation value of angular momentum.
and energy \(< l >= -9, < E >= 14.5035\). The contour of this superposition matches the corresponding angle loop specified by \(< l >= -9, < E >= 14.5035\) and encloses the origin.

### 6.1.3 Wave functions in a circular box

Now let us consider a simpler system, which does not have a complete monodromy circuit, but which nevertheless displays a comparable topological change: a circular box with

\[
V(\rho) = 0, \quad \rho \leq \rho_{\text{max}}; \quad V(\rho) = \infty, \quad \rho > \rho_{\text{max}}. \tag{6.7}
\]

We can calculate action-angle loops for this system by integrating trajectories of the effective Hamiltonian (6.3) with this circular box potential (6.7). As already stated,\( \Omega(I, E) \) must be defined such that it is differentiable when \( l \) passes through zero. We show in Fig. 21(a) trajectories under \( H \) for our selected \( l_{\text{initial}} = 10\hbar \) and \( E_{\text{initial}} = 31.5793 \).

This corresponds to a value of the poloidal action variable \( I_{\|} = 25\hbar \). We reduce \( l \) continuously until \( l_{\text{final}} = -9\hbar \). When \( l \) passes through zero, \( \Theta(l, E) \) increases smoothly through \( \pi \). The result is that the action loop defining \( I_{\|} \) changes its topological structure relative to the origin: it changes from a loop on one side of the origin to a loop that surrounds the origin. As a result,

\[
I_{\|}(-|l|, E) = I_{\|}(|l|, E) - l \tag{6.8}
\]

We follow a path similar to part of a monodromy circuit by choosing \( E \) such that \( I_{\|}(l, E) \) is held constant at \( 25\hbar \) while we reduce \( l \). As we see in Fig. 21(b), the resulting action loops have the same topological change as was obtained for the Mexican Hat potential.

The eigenfunctions of \( H \) and of \( \mathcal{H} \) are
\[ \psi_{m,n}(\rho, \varphi) = N_{m,n} J_m(k_{m,n}, \rho) \exp(im\varphi) \]  (6.9)

where \( J_m(x) \) is Bessel function, \( \{k_{m,n}\} \) are values such that \( J_m(k_{m,n}, \rho_{\text{max}}) = 0 \). The eigenvalues of \( H \) are given by

\[ E_{m,n} = (\hbar k_{m,n})^2 / 2\mu \]  (6.10)

We show in Fig. 22, the grid of eigenvalues \( (m, E_{m,n}) \). The eigenvalues of \( H \) are given by Eq. (6.6), where

\[
T(l,E) = 2\sqrt{\frac{\rho_{\text{max}}^2 - l^2}{2\mu E}}
\]

\[
\Theta(l,E) = \begin{cases}
2\arccos\left(\frac{l}{\rho_{\text{max}}\sqrt{2\mu E}}\right), & \text{if } l \geq 0 \\
2\pi - 2\arccos\left(\frac{l}{\rho_{\text{max}}\sqrt{2\mu E}}\right), & \text{if } l < 0
\end{cases}
\]  (6.11)

\[
\Omega(l,E) = \frac{\Theta(l,E)}{T(l,E)}
\]

**Semiclassical approximation to \( \psi_{m,n}(\rho, \varphi) \)**

A two-dimensional semiclassical approximation to these eigenfunctions of the circular box, \( \psi_{m,n}(\rho, \varphi) \) can be constructed by the usual rules. In this relatively simple system, analytical results can be given.

(a) Specify the quantum numbers \((m, n)\) of the target eigenfunction. The eigenvalues of angular momentum and energy \( H \) are respectively \((m\hbar, E_{m,n})\). (b) Choose an initial
curve in \((\rho, \varphi)\) space (we take \(\rho = \rho_{\text{max}}\)), and specify the value of \(\psi_{m,n}(\rho, \varphi)\) on that surface. We take it to be \(\psi_{m,n}(\rho_{\text{max}}, \varphi) = f(\varphi)\exp(i m \varphi)\). (c) Define the initial classical momentum on that curve such that
\[
p_{\varphi} = m \hbar
\]
and
\[
H(q, p; m \hbar, E_{m,n}) = E_{m,n}
\] (6.13)
which is equivalent to
\[
H(q, p) = E_{m,n}
\] (6.14)

(d) Starting at \(\rho_{\text{max}}\), for each initial \(\varphi = \varphi_0\), integrate the equations of motion under
\[
H(q, p)
\]
to obtain \(q(t, \varphi_0)\), and \(p(t, \varphi_0)\). The phase of the wavefunction is constructed by integrating one more equations to obtain the action function \(S(t, \varphi_0)\) using
\[
\frac{dS}{dt} = p(t, \varphi_0) \cdot \frac{dq(t, \varphi_0)}{dt}
\] (6.15)
with initial condition \(S(t = 0, \varphi_0) = m \varphi_0\). In the present case, the classical trajectories are given by
\[
x(\varphi_0, t) = (\rho_{\text{max}} + v_{x0} t) \cos(\Omega t - \varphi_0) + v_{y0} t \sin(\Omega t - \varphi_0)
\] (6.16)
\[
y(\varphi_0, t) = -\left(\rho_{\text{max}} + v_{x0} t\right) \sin(\Omega t - \varphi_0) + v_{y0} t \cos(\Omega t - \varphi_0)
\] (6.17)
\[
p_{x}(\varphi_0, t) = \mu v_{x0} \cos(\Omega t - \varphi_0) + \mu v_{y0} \sin(\Omega t - \varphi_0)
\] (6.18)
\[
p_{y}(\varphi_0, t) = -\mu v_{x0} \sin(\Omega t - \varphi_0) + \mu v_{y0} \cos(\Omega t - \varphi_0)
\] (6.19)
€ Invert the relationship \( q(t, \varphi_0) \) [Eqs. (6.16) and (6.17)] to obtain \( (t(q), \varphi(q)) \) and express the action as a function of \( q \). That inversion gives for each \( q \) two pairs of \( (t(q), \varphi(q)) \), corresponding to the incoming and outgoing waves. (f) The amplitude is found from

\[
A(t, \varphi_0) = f(t, \varphi_0) \left| \frac{J(t = 0, \varphi_0)}{J(t, \varphi_0)} \right|^{1/2}
\]

(6.20)

which also must be expressed as a function of \( q \). \( J(t, \varphi_0) \) is the Jacobian matrix defined as

\[
J(t, \varphi_0) \equiv \frac{\partial(x, y)}{\partial(t, \varphi_0)}.
\]

(g) The semiclassical approximation to \( \psi_{m,n}(\rho, \varphi) \) is then

\[
\psi_{m,n}^\text{sc}(\rho, \varphi) = A_{in}(\rho, \varphi) \exp \left( \frac{iS_{in}(\rho, \varphi)}{\hbar} \right) + A_{out}(\rho, \varphi) \exp \left( i \left( \frac{S_{out}(\rho, \varphi)}{\hbar} - \frac{\pi}{2} \right) \right)
\]

(6.21)

In the present case, the amplitude and the phase can be written analytically, and the result is:

for the incoming wave,

\[
S_{in}(\rho, \varphi) = -m \left[ \sqrt{\frac{\rho^2 - \rho^2_{\min}}{\rho_{\min}}} - \arccos \left( \frac{\rho_{\min}}{\rho} \right) + \sqrt{\frac{\rho^2_{\max} - \rho^2_{\min}}{\rho_{\min}}} + \arccos \left( \frac{\rho_{\min}}{\rho_{\max}} \right) \right] + m\varphi
\]

(6.22)

while for the outgoing wave,
\[ S_{\text{out}}(\rho, \varphi) = |m| \left( \sqrt{\rho^2 - \rho_{\text{min}}^2} \arccos \left( \frac{\rho_{\text{min}}}{\rho} \right) + \sqrt{\rho_{\text{max}}^2 - \rho_{\text{min}}^2} \arccos \left( \frac{\rho_{\text{min}}}{\rho_{\text{max}}} \right) \right) + m\varphi \]  

(6.23)

\[ A_{\text{in}}(\rho, \varphi) = A_{\text{out}}(\rho, \varphi) = \frac{1}{\sqrt{2|\rho_{\text{max}}^2 - \rho_{\text{min}}^2| \sqrt{\rho^2 - \rho_{\text{min}}^2}}} \]  

(6.24)

where \( \rho_{\text{min}} = |l| \sqrt{p_{\rho}^2 + p_{\varphi}^2} \).

Initial condition localized in \( \varphi \)

We now want to construct wavefunctions that are not eigenfunctions of \( H \) or of \( H \), but instead are localized near one action-angle loop. For this purpose we take \( f(\varphi_0) = \exp \left( -\varphi_0^2 / \beta^2 \right) \). This weighting factor makes only one action-angle loop and its neighboring action-angle loops play an important role in the construction of semiclassical wavefunctions. Just as above, for each \( (\rho, \varphi) \), we must find \( (\tau, \varphi_0) \), and that value of \( \varphi_0 \) is used in \( f(\varphi_0) \).

Two such wavefunctions are shown in Fig. 21(c)(d). One has initial \( m = 10 \) and initial \( n = 25 \), for which \( E_{m,n} = 31.5793 \). The other has final \( m = -9\hbar \), final \( n = 25 + (-9) \), for which \( E_{m,n} = 14.5035 \). This value of \( n \) makes the final numerical value of the continuous action variable equal to the initial value, \( 25\hbar \).
These two wavefunctions display the topological change that corresponds to the topological change in the action-angle loops.

Fig. 22 This is a three-dimensional plot in which the x-y plane is spectrum space and the z-axis is the relative magnitude of coefficients in the superposition. As described in Fig. 18, the grey dots are eigenvalues, in this case for the circular box. The red line is part of the monodromy circuit, which starts from \((l_i = 10, E_i = E_{m=10, n=25} = 31.5793\) , links states of quantized smooth action=25:

\[
\begin{aligned}
n &= 25, m \geq 0 \\
n - m &= 25, m < 0
\end{aligned}
\]

and ends at \(l_f = -9, E_f = E_{m=-9, n=16} = 14.5035\) . For a superposition with expectation value of \((<l> = l_i, <E> = E_i)\) , the coefficient before any eigenstate \(\psi_{m,n}\) is plotted as the green curve on the right: the only nonzero coefficients are those for the eigenstates of quantized smooth action=25 and with \(m\) between 4 and 16. The coefficients for that superposition has a Gaussian
distribution along the contour of smooth action=25, centered at \((l_i, E_i)\). Then we push the Gaussian distribution along monodromy circuit, until the final point \((l_f, E_f)\). The final superposition includes eigenstates of quantized smooth action variable=25. The distribution of coefficients for this distribution is Gaussian distribution along the contour of smooth action=25, centered at \((l_f, E_f)\), with \(m\) ranging between -15 and -3.

6.2 Superposition with topological change

6.2.1 Truncated expansion of semiclassical wavefunctions

Like all semiclassical approximations, these wave functions diverge at caustics (radial turning points) where \(A(\rho, \phi) \to \infty\). We can repair the divergences by expanding \(\psi_{m,n}^{sc}(\rho, \phi)\) in a small set of eigenfunctions of \(H\). Evaluation of coefficients shows that the expansion is dominated by a small number of terms. If \(m\) is substantially greater than zero, then only terms of fixed \(n = n' (= 25)\) have large coefficients, and those coefficients are distributed in \(m\) approximately as a Gaussian function (Fig. 22).

On the other hand, if \(m\) is substantially less than zero, then the only large coefficients have \(n - m = n'\), and the distribution in \(m\) is again approximately Gaussian. (Fig. 22) Two such superpositions of eigenfunctions are shown together with the corresponding semiclassical approximations in Fig. 21(c)(d) and 21(e)(f). The divergences have been repaired, and the topological change remains.
These superpositions are nonstationary states. If we incorporate the phase factors associated with $H$, $\exp \left( -iE_{m,n} t / \hbar \right)$, these wavefunctions revolve around the origin at a rate close to $\Omega \left( m\hbar, E_{m,n} \right)$.

We can use the insight gained from the circular box to obtain corresponding wave functions for the Mexican hat system. For this system, we computed eigenfunctions of $H$ with $m \geq 0$ by numerical expansion in a Bessel function basis. There is one subtle issue. For any radial eigenfunction $R^m_n (\rho)$, $R^m_n (\rho) e^{i\text{phase}}$ is also a radial eigenfunction. In order to get simple relationships between coefficients in our superpositions, the exact radial eigenfunctions $R^m_n (\rho)$ must be defined such that they have a nontrivial monodromy of their own. Specifically, we need to define what we will call a quantum-mechanical connection between $R^m_n (\rho)$ and $R^{-m}_n (\rho)$, somewhat analogous to the smooth connections of action-angle loops on tori.

We define a quantum monodromy circuit so that it connects each state $(m,n)$ to a neighboring state, $(m \pm 1, n \pm 1)$. At one point the path crosses the line $m = 0$ at a value of $n$ such that the energy $E_{m=0,n} > 0$; let’s call it the upstairs part of the circuit. At other points, the circuit crosses the $m = 0$ line at a value of $n$ such that the energy $E_{m=0,n} < 0$; let’s call it the downstairs part of the circuit.

The connection between eigenfunctions must be: upon comparing $R^m_n (\rho)$ with $R^{-m}_n (\rho)$, on any upstairs portion of the circuit,
\begin{equation}
R_n^{-m}(\rho) = (-)^m R_n^m(\rho)
\end{equation}

but on any downstairs portion,

\begin{equation}
R_n^{-m}(\rho) = R_n^m(\rho)
\end{equation}

Hence, going around a quantum monodromy circuit surrounding the origin of \((m, E)\) space,

\begin{equation}
R_n^m(\rho; \text{final}) = (-)^m R_n^m(\rho; \text{initial})
\end{equation}

Eqs. (6.26) and (6.27) correspond respectively to the symmetry relationships of Bessel functions \(J_m(\rho)\) or \(I_m(\rho)\) (the ones that are regular at the origin with \(E\) respectively greater than or less than zero).

If the description above is not clear to the reader, let us introduce the rules in another way. We define the radial eigenfunction \(R_n^m(\rho)\) as a plus-sign eigenfunction if it increases with \(\rho\) when it is close to the origin (Fig. 23).
Fig. 23. The sign of a radial eigenfunction. The blue and black curves are the eigenfunctions of opposite sign at the same eigenenergy. The blue curve which increases with $\rho$ when it is close to the origin, is defined as plus sign: +. The black curve which decreases with $\rho$ when it is close to the origin is defined as minus sign: -.

As we learned from the circular box system, we will use eigenstates on the same contour of smooth action to make the superposition. The question is: how should we define the phase of each eigenfunction? Are they going to have a plus sign, a minus sign, or a complex constant in front? I will show three examples about how we define the phase of eigenfunctions. The rule is the same as Eqs. (6.25) (6.26).
(a)

Contour:
\[
\begin{cases}
    n = 23; & \text{if } m \geq 0 \\
    n = 23 + m; & \text{if } m < 0
\end{cases}
\]
Fig. 24. Signs of radial eigenfunctions on contours of smooth action. In (a), the magenta curve $n = 10$ is a contour of smooth action for negative energies. The eigenstates on it are included in the superposition corresponding to the initial point on a monodromy circuit $m = 0, E = E_{0,10}$. Signs of each radial eigenfunction (black dots) are specified. They are all positive. In (b) the combination of the magenta curve $n = 23; m \geq 0$ and the green curve $n = 23 + m; m < 0$ is a contour of smooth action for positive energies. The eigenstates on that contour (black dots) are included in the superposition for $m = 2, E = E_{2,23}$ (the red star). Eigenfunctions with $m$ negative are $(-)^n$ times the corresponding eigenfunctions with $m$ positive. In (c) the green curve $n = 10 + m$ is the contour of smooth action after going around the monodromy circuit. Now all radial eigenfunctions have acquired the phase $(-)^n$.

If the monodromy circuit starts at $m = 0, E = E_{0,10}$ (the red star in Fig. 24(a)), the corresponding superposition includes eigenfunctions on the corresponding contour of
smooth action: \( n = 10 \) (the magenta curve in Fig.24(a)). All the eigenfunctions on the contour are set to have plus signs, as stated in (6.26) for a downstairs portion of a monodromy circuit. Suppose the monodromy circuit passes through \( m = 2, E = E_{2,23} \) (the red star in Fig. 24(b)); then the corresponding superposition includes eigenfunctions on the corresponding contour of smooth action: \( n = 23; m \geq 0 \) (the magenta curve in Fig.24(b)) and \( n = 23 + m; m < 0 \) (the green curve in Fig.24(b)). It is an upstairs portion of a monodromy circuit. All the eigenfunctions on the magenta contour are set to have plus sign, which is consistent with the sign on the magenta contour on the downstairs portion. The signs for the eigenfunctions on the green contour are set to be an alternation of plus and minus sign. The eigenstate with negative odd quantum number \( m \) have the opposite sign to that for \(|m|\). This is consistent with (6.25). When the monodromy circuit comes back down and passes through \( m = 0, E = E_{0,10} \) (the red star in Fig.24(c)), the corresponding superposition includes eigenfunctions on the corresponding contour of smooth action: \( n = 10 + m \) (the green curve in Fig.24(c)). It is a downstairs portion. The reason that the contour of smooth action in Fig.24(c) is different from the one in Fig.24(a) is that the smooth action variable is a multivalued function (Section 3.2). When \( m < 0 \), the eigenfunctions on the green contour are set to be alternation of plus and minus sign, which is consistent with the rule on the green contour of Fig. 24(b). For the continuation to the contour of \( m \geq 0 \) part, we follow the rule (6.26) to make the signs of eigenfunction are the same as what is for \(-|m|\).
Fig. 25 this is a three-dimensional plot with x-y plane is the spectrum space and z-axis is relative magnitude of coefficients in the superposition. As described in Fig. 18, the grey dots are eigenstates for Mexican Hat. The red circuit is the monodromy circuit, starting from \((l_i = 0, E_i = E_{m=0,m=13} < 0)\), moving in a counterclockwise direction, and returning to the starting point. Initially, we construct a superposition with expectation value of \(<l_i,E_i>=E_i\). All the eigenstates included in this superposition are of quantized smooth action=13 (the dashed green line). The coefficients before eigenstates are denoted with the green Gaussian curve centered at \((l_i, E_i)\). Then we take the center of Gaussian distribution along the monodromy circuit to make the superposition with expectation value and energy at the center of Gaussian distribution. Finally, when we return to the initial point \((l_i, E_i)\), the eigenstates included in the superposition are different from that in the initial superposition, because the contour of smooth action =16 is different from the initial contour.
6.2.2 Superposition in Mexican Hat system

Now we examine static superpositions of the exact eigenfunctions in Mexican Hat system

\[ \Psi(\rho, \phi) = \sum_{m,n} C_{m,n} R_{m,n}(\rho) \exp(im\phi) \]  \hspace{1cm} (6.28)

The coefficients in the superposition are defined and carried around a monodromy circuit in the following way. (i) We start with all coefficients zero except for those at one fixed \( n = n^i_{\text{downstairs}} (=13) \), and with \( m \) having a Gaussian distribution centered at \( m_{\text{center}} = 0 \), \( C_m = \exp\left(-\frac{(m - 2.5)^2}{2.5^2}\right) \). (Fig.25). The value of \( n^i_{\text{downstairs}} \) is chosen such that the energy is well below zero. (ii) Holding \( n = n^i_{\text{downstairs}} \) fixed, we increase \( m_{\text{center}} \), and keep the Gaussian distribution of coefficients, \( \exp\left(-\frac{(m - m_{\text{center}})^2}{2.5^2}\right) \). When \( m_{\text{center}} \) is sufficiently large, coefficients having \( m \leq 0 \) are negligible, and we set them to zero. (iii) Now at each \( m \), we increase \( n \) in integer steps until the energy is well above zero. We stopped at \( n = n^i_{\text{upstairs}} (=28) \). At this point the action-angle loop is plainly manifested in the quantum wavefunction, and it lies on one side of the classically forbidden region. (iv) Now we decrease \( m_{\text{center}} \), moving the Gaussian distribution to smaller \( m \). When the value of \( m \) in any term in the superposition becomes negative, we reduce the associated value of \( n \) such that \( n = n^i_{\text{upstairs}} + m = n^i_{\text{upstairs}} - |m| \). This is the quantum analogue of the classical monodromy circuit shown in red in Fig.18 and Fig.25. The quantum number \( n \) is adjusted such that the corresponding smooth action variable is
constant. Also, crossing the line \( m = 0 \) upstairs, we apply the symmetry relationship (6.25). Now the action-angle loop surrounds the origin, and the wave function does also.

(v) When \( m_{\text{center}} \) is sufficiently negative, then the coefficients for \( m \geq 0 \) are negligible, and we set them to zero. Then we reduce each value of \( n \) in steps of 1. The superposition now has a range of both \( n \) and \( m \), and in each step \( n - m = \text{constant} \). When we have reduced \( n \) such that that constant equals \( n_{\text{downstairs}}^i \), the initial \( n \), we stop reducing \( n \).

Finally we increase \( m_{\text{center}} \) (the center of the distribution) always increasing \( n \) such that \( n - m = n_{\text{downstairs}}^i \). This formula holds also for \( m > 0 \). We stop at \( m_{\text{center}} = 0 \). For the basis functions having \( m > 0 \), we have crossed the line downstairs, so we use the symmetry relationship (6.26). At this final point, we have a new superposition of eigenfunctions.

Note that the signs of the basis functions \( R_{n}^{m} \) have changed according to Eq.(6.27). This new superposition surrounds the classically forbidden region (Fig. 20).

We have obtained static monodromy of superpositions of eigenfunctions. This is a fully quantum-mechanical monodromy: only our choice of coefficients was obtained by comparison with the semiclassical approximation in the earlier section on the circular box, but at no point did we use any classical or semiclassical concept.

6.2.3 The probability current under effective Hamiltonian \( \mathcal{H} \)
In Fig. 20, we show that the superposition defined in (6.28) has the shape of the angle loop. In this section, we show that not only the shape, but also the density flux follows the corresponding angle loop.

We all know that \( \psi^* \psi \) is the probability density to find a particle at the location \((x, y)\). The probability current or flux density \( \vec{j} \) is the flow of probability density such that:

\[
\frac{d\psi^* \psi}{dt} + \nabla \cdot \vec{j} = 0
\]  

(6.29)

Under the effective Hamiltonian that generates the angle loop (6.3), we get an unusual form for the flux density:

\[
\frac{d\psi^* \psi}{dt} = \psi^* \frac{d\psi}{dt} + \frac{d\psi^*}{dt} \psi = \psi^* \frac{1}{i\hbar} H \psi + \psi \frac{1}{-i\hbar} H^\dagger \psi^* 
\]

\[
= \psi^* \frac{1}{i\hbar} \left[-\frac{\hbar^2}{2\mu} \nabla^2 \psi + V \psi - \Omega \frac{\hbar}{i} \frac{\partial \psi}{\partial y} + \Omega \frac{\hbar}{i} \frac{\partial \psi}{\partial x}\right] + \psi \frac{1}{-i\hbar} \left[-\frac{\hbar^2}{2\mu} \nabla^2 \psi^* + V \psi^* - \Omega \frac{\hbar}{i} \frac{\partial \psi^*}{\partial y} + \Omega \frac{\hbar}{i} \frac{\partial \psi^*}{\partial x}\right]
\]

\[
= \frac{\hbar}{2\mu i} \left(\psi \nabla^2 \psi^* - \psi^* \nabla^2 \psi\right) + \Omega x \frac{\partial \psi^* \psi}{\partial y} - \Omega y \frac{\partial \psi^* \psi}{\partial x}
\]

\[
= \nabla \left[\frac{\hbar}{2\mu i} \left(\psi \nabla \psi^* - \psi^* \nabla \psi\right) + \left(-\Omega \psi \psi^* \frac{\partial \psi^*}{\partial y}\right) \right]
\]

\[
= -\nabla \cdot \vec{j}
\]

It follows that the flux density is
\[
\vec{j} = \frac{\hbar}{2\mu i} \left( \psi^* \nabla \psi - \psi \nabla \psi^* \right) + \begin{pmatrix} \Omega \psi^* \psi \\
 -\Omega \psi \psi^* \end{pmatrix}
\]  

(6.30)

The term containing \( \Omega \) is unusual but important.

In Fig. 26, two superpositions along with their probability current are plotted. The one labelled (a) is before the monodromy circuit, and the one labelled (b) is after. They have the same expectation value of \( \langle l \rangle \) and \( \langle E \rangle \). But they have different topological structures and the flux densities have different winding number about the origin.
Fig. 26 The surfaces represent the absolute value of wave functions versus Cartesian coordinates $(x, y)$. Below each is the corresponding contour plot, and the probability current (black arrows). The cross markers in the center of the lower planes mark the origin of the $(x, y)$ planes. Those origins are surrounded by classically forbidden regions. The wavefunction in (a) is State 1, described in Eqs. (6.28) of the text; the one in (b) is State 2, with the same expectation value of angular momentum and energy with state 1, but it is the state after one round of following monodromy circuit starting from state 1. It is evident that these wave functions have different winding numbers around the classically forbidden regions. The flux density was computed based on the Hamiltonian $\hat{H}$; it is the same as the flux density under the
Hamiltonian $H$ as seen in a frame of reference rotating about the origin with angular velocity $\Omega$. These are nonstationary states of the Hamiltonian $H$; if we included time factors, they rotate about the origin. The bold black loops in the $(x, y)$ planes are classical action-angle loops projected into the plane. For both of these wavefunction, the angular momentum is $12\hbar$ and energy is equal to the energy of the quantum state $E_{n=23, m=12}$. The action loop and the wavefunction in (a) is a superposition of a set of eigenfunctions near $m = 12, n = 23$. The action loop and the wave function in (b) correspond to the end of one monodromy circuit, when the action loop has changed its topological structure. The wave function becomes a superposition of a different set of eigenfunctions near $m = 12, n = 23$.

6.3 Dynamical monodromy of wave functions

We may define ideal evolution leading to dynamical monodromy of superpositions of eigenfunctions by (1) making the coefficients in the superposition (6.28) time dependent, then (2) creating a unitary matrix that continuously changes the coefficients $C_{m,n}(t)$ in the superposition such that they are all given by a Gaussian function of $m$ centered at $m_{\text{center}}(t)$. On the energy-increasing step we switch the coefficients continuously between $n$ and $n+1$ as indicated in Fig. 25, and on the energy-decreasing step we similarly switch continuously between $n$ and $n-1$. This produces a kind of ideal evolution leading to wavefunction monodromy, analogous to the ideal classical evolution described in ref. [51].

Finally, let us go back to the circular box, and show that the topological change in the wavefunction that we saw in sections 6.1 and 6.2 can be produced by physical evolution under a time-dependent Hamiltonian. This is the quantum analogue of our work in Chapter 4, where we showed that classical evolution under a time-dependent Hamiltonian gives the topological change in a loop of classical particles.
Since for the circular box, the energy cannot be negative, the “downstairs” part of
the monodromy circuit does not exist, and evolution only drives the expectation values of
angular momentum and energy along the upstairs portion of the monodromy circuit, as
in Fig. 22. This time-dependent Hamiltonian is:

$$H(t) = H_0(q, -i\hbar \nabla) + P(q, t)$$

(6.31)

where $H_0(q, -i\hbar \nabla)$ is exactly the Hamiltonian in Eq.(6.7), with circular box potential.

$P(q, t)$ is a perturbation produced by a counterclockwise rotating uniform force

$|\mathbf{F}|=0.05$ with a rotation rate designed to decrease expectation value of angular
momentum $\tilde{l}$. For those who may wish to reproduce our results, the azimuthal angle
defining the direction of the force was taken to be

$$\varphi(t) = \begin{cases} 
1.937 + 0.4674t - 0.002422t^2 + 2.695e - 5t^3 - 2.183e - 7t^4 & \text{if } t \leq 43; \\
1.737 + 0.4674t - 0.002422t^2 + 2.695e - 5t^3 - 2.183e - 7t^4 & \text{if } 43 < t \leq 60.
\end{cases}$$

(6.32)

The initial superposition is as shown in the right-hand part of Fig. 22, with non-zero
coefficients only for $n=10$; the coefficient distribution is Gaussian, centered at

$$m_{\text{center}}^{\text{initial}} = 10,$$

$$|C|_{m,10} \propto \exp \left( -\left( \frac{m - m_{\text{center}}^{\text{initial}}}{2.5} \right)^2 \right)$$

(6.33)
We solve the Schrodinger equation in a basis set including $m$ from $-9$ to $15$ and $n$ from $1$ to $13$. It turns out that the dominant coefficients are always those with $n = 10$ when $m \geq 0$, or $n - m = 10$ when $m < 0$. Furthermore, the distribution in $m$ remains approximately Gaussian, with

$$|C|_{m,n} \propto \exp\left(-\frac{(m-m_{\text{center}}(t))^2}{2.5}\right).$$

As the expectation value of $m$ decreases, the expectation value of $E$ also decreases so that the path traced out by $(m \hbar, E)$ is close to the path shown in Fig. 22, which has a constant value of the continuous action variable $I_H(l, E)$. It is in effect the upstairs portion of a monodromy circuit.

It is pleasing to see that the mode of the wave function $|\psi(q, t)|$ shows the desired topological change during this process. Thus we have shown that the topological change in wave functions can be made to occur using an ordinary Hamiltonian with a rotating force.

Chapter 7 Conclusion and Outlook

This dissertation discussed a special phenomenon called “nontrivial monodromy of action and angle variables in classical mechanics”, or simply “monodromy”. We showed new consequences of this phenomenon in classical mechanics, and we showed new manifestations of monodromy in quantum mechanics.
We began by developing the theory of action–angle variables from the beginning, starting with the framework of symplectic geometry. By learning from the work done by other scholars, we understand that

- Action and angle variables are an excellent set of canonical variables to describe bounded integral system. Action variables specify which torus the point is located on, while angle variables specify the location on that torus.

- For systems with a “singular” value in its spectrum space, the old way of canonical transformation from x’s and p’s to action and angle variables is not smooth everywhere. In this situation we must modify the canonical transformation so that the transformation is smooth everywhere. The price is that at least one action variable and one angle variable become multi-valued functions.

- This multivalued property is reflected (in the systems we study) by a topological change of an angle loop after following a monodromy circuit in spectrum space. Initially the angle loop stays on one side of a classically forbidden region, but at the end of the monodromy circuit, the angle loop encloses the forbidden region.

A few years ago [51] it was recognized that this seemingly abstract property of action and angle variables has remarkable dynamical consequences. If one starts a family of noninteracting particles on an initial angle loop, and drive those particles around a monodromy circuit, then the family of particles will undergo the same topological change that occurs in the angle loop. In those references, the particles were driven around the loop by the use of a very abstract flow in phase space (for example, by using one of the angle variables as an effective Hamiltonian). No one knows how to implement such a flow in a real system.
Our new contributions to this topic are the following. (1) We showed that particles can be driven around a monodromy circuit using ordinary forces, i.e. \( \mathbf{F} = m \mathbf{a} \).

(2) Furthermore we showed that it could be done by applying the same time-dependent force to all particles in the system. (3) A first simulation had initial conditions with all particles having the same initial energy and angular momentum. (4) We showed that this phenomenon is so robust that even if the particles do not have exactly the same initial angular momentum and energy, we are still able to observe the topological change of a ring of particles. (5) Megan Ivory and Seth Aubin designed, and I simulated, an experiment using cold atoms in an optical trap to carry out a monodromy process that could display the topological change mentioned in last paragraph. All this was published in Ref 53.

All of the above was carried out using classical mechanics. We then turned to manifestations of monodromy in quantum mechanics. We built quantum mechanical wavefunctions that display the same topological change that is seen in classical action and angle loops.

We carried this out by the following process: (6) We constructed a semiclassical wave function that is localized near and travels along a classical angle loop. Like all semiclassical wave functions, this one diverges at caustics (a caustic is the multidimensional analogue of a turning point). (7) We fixed the divergences by expanding the semiclassical wavefunction in a truncated basis of eigenfunctions. (8) We found that the only important eigenfunctions in the superposition are the ones with the same “smooth action variable”. (9) We showed that when this superposition is carried around a monodromy circuit, the wavefunction has the same topological change that occurs in the action-angle loops. (10) For one case, we showed that the topological
change can be made to occur through the application of ordinary time-dependent forces
on the quantum particles.

Thus we have shown that “nontrivial monodromy of action and angle variables”
has dynamical manifestations that are interesting and robust phenomena in both
classical and quantum mechanics. Presently Perry Nerem and Dan Salmon are working
to show this phenomenon in a driven pendulum system. Corresponding experiments in
quantum systems would be a step toward dynamical control of atoms, molecules or light.
APPENDIX A: Details of the Applied Forces

The formulas for applied forces given below were obtained as a result of numerical experiments. We did not use any systematic optimization method to obtain these results, but only a modest number of trials. For single-loop initial conditions, we begin with $N$ particles, all having angular momenta equal to 0, and all having the same initial energy, uniformly distributed around a $\gamma_1$ loop on the initial torus $[I(t_0) = 0, E(t_0) = E_0]$. At each instant they have a center of mass located at $\vec{r}_0(t)$, where

$$\vec{r}_0(t) = \frac{\sum_{i=1}^{N} m_i \vec{r}_i(t)}{\sum_{i=1}^{N} m_i} = r_0(t) \cos \varphi(t)i + r_0(t) \sin \varphi(t)j$$

(A.1)

$\vec{r}_i(t)$ and $m_i$ are the instantaneous location vector and mass of the $i$th particle, and $r_0(t)$ and $\varphi(t)$ are the instantaneous length and azimuthal angle of the instantaneous center-of-mass vector $\vec{r}_0(t)$. As mentioned in the main section of this dissertation (Section 4.1), the monodromy circuit is divided into five steps, with $t_{i-1} \leq t \leq t_i$ on the $i$th step.

The driving torque that changes the angular momentum is applied as follows. The same force $\vec{F}(t)$ is applied to all particles, and this force is nearly perpendicular to the center-of-mass vector $\vec{r}_0(t)$. The direction of the force is such that the angular momentum of the center of mass increases in step 1 and in step 5, and such that it decreases in step 3. Thus, in steps 1 and 5, $\vec{F}(t)$ is $\pi/2$ “ahead of” $\vec{r}_0(t)$:
\[ \bar{F}(t) \equiv F(t) \cos[\varphi(t) + \frac{\pi}{2}] \hat{i} + F(t) \sin[\varphi(t) + \frac{\pi}{2}] \hat{j} \] (A.2)

\[ F(t) \equiv \frac{\dot{\Lambda}(t)}{\sqrt{r^2(t)}}, \quad \bar{r}^2(t) \equiv \frac{\sum_{i=1}^{N} m_i r_i^2(t)}{\sum_{i=1}^{N} m_i} \]

\( \bar{r}^2(t) \) is the mean square distance from the origin to the instantaneous location of each particle, and \( \dot{\Lambda}(t) \) is a chosen average rate of increase of angular momentum. It is made to increase and decrease smoothly, as below. In steps 2 and 4, \( \dot{\Lambda}(t) = 0 \), while in steps 1 and 3,

\[ \dot{\Lambda}(t) = c \dot{\Lambda}_0 \text{sech}\left[ \frac{(t_j - t_{j-1})}{2} \right] \left( \frac{1}{t_{j-1} - t} + \frac{1}{t_j - t} \right) \] (A.3)

\( \dot{\Lambda}_0 \) is a constant value which we take to be 0.9, and \( c_j = 1, -2, \) and 3, respectively, in steps 1, 3, and 5. The negative sign in step 3 makes the force rotate in the same sense as the center of mass, but \( \pi/2 \) “behind,” so the angular momentum is reduced in this step. Equation (A.3) makes the torque change as a \( C^\infty \) function of time.

We found that a slightly different method worked best for step 5. We took for \( t > t_4 \),

\[ \bar{F}(t) \equiv F_5 \cos[\varphi(t_4) + \omega t + \frac{\pi}{2}] \hat{i} + F_5 \sin[\varphi(t_4) + \omega t + \frac{\pi}{2}] \hat{j} \] (A.4)

where \( \varphi(t_4) \) is the azimithal angle of the center of mass at time \( t_4 \), and \( \omega \) is a constant rotation rate chosen to be

\[ \omega \equiv \frac{\Delta(l(t_4), E(t_4))}{T(l(t_4), E(t_4))}, \] (A.5)
where \((l(t_4), E(t_4))\) are the average value of angular momentum and energy when 
\(t = t_4\), and \(\Delta(l, E)\) and \(T(l, E)\) are subtended angle and time of first return as 
functions of angular momentum and energy. \(F_3\) is a constant and set to be 0.15.

During steps 2 and 4, while there is no driving torque, the parameters of the well 
are changed by changing the height of the central barrier. In our calculations this is done 
by changing the power in the strongly focused laser so that the height of the central 
barrier \(V(t)\) varies continuously between \(V_0\) and \(V_1\) as follows.

\[
V(t) = V_0 \text{ if } 0 \leq t \leq t_1
\]

\[
= V_0 + (V_1 - V_0) \left\{ \tanh \left[ \frac{t_2 - t_1}{2} \right] \left( \frac{1}{t_1 - t} + \frac{1}{t_2 - t} \right) + \frac{1}{2} \right\} \text{ if } t_1 < t \leq t_2
\]

\[
= V_1 \text{ if } t_2 < t \leq t_3
\]

\[
= V_1 + (V_0 - V_1) \left\{ \tanh \left[ \frac{t_4 - t_3}{2} \right] \left( \frac{1}{t_3 - t} + \frac{1}{t_4 - t} \right) + \frac{1}{2} \right\} \text{ if } t_3 < t \leq t_4
\]

\[
= V_0 \text{ if } t_4 < t \leq t_5
\]

\[
(A.6)
\]

Integration is stopped when the average value of the angular momentum returns to zero,
and that defines the time \(t_5\).

121
Appendix B. Details of Calculation of Angle Loop

The Hamiltonian \( H = H - \Omega(l, E)L \) generates the dynamical flow that traces out the angle loop \( \gamma \). \( H \) is the normal Hamiltonian. \( L \) is the angular momentum. \( \Omega(l, E) \) is the average angular velocity within one radial cycle under the influence of \( H \). It is a function of angular momentum and energy. In most cases, we cannot get analytic results if we want to solve Hamilton’s equation for \( H \). Only numerical results can be obtained.

But a circular box system is an exception. In a circular box potential,

\[
H = \frac{p_x^2 + p_y^2}{2m}. \quad L = p_y x - p_y y.
\]

The outer wall of the circular box is denoted as \( \rho_{\text{max}} \).

By solving Hamilton’s equations:

\[
\begin{align*}
\frac{dx}{dt} &= \frac{\partial H}{\partial p_x} = p_x - \Omega(-y) \\
\frac{dy}{dt} &= \frac{\partial H}{\partial p_y} = p_y - \Omega(x) \\
\frac{dp_x}{dt} &= -\frac{\partial H}{\partial x} = \Omega p_y \\
\frac{dp_y}{dt} &= -\frac{\partial H}{\partial y} = -\Omega p_x
\end{align*}
\]  

we derive the time-dependent solution with initial condition:

\[
\begin{align*}
x_0 &= \rho_{\text{max}} \cdot \cos \varphi_0 \\
y_0 &= \rho_{\text{max}} \cdot \sin \varphi_0 \\
p_{x0} &= mv_x \\
p_{y0} &= mv_y
\end{align*}
\]  

The solution is:
\[ x(t; \varphi_0) = (\rho_{\text{max}} + v_x t) \cos(\Omega t - \varphi_0) + v_y t \sin(\Omega t - \varphi_0) \]
\[ y(t; \varphi_0) = -(\rho_{\text{max}} + v_x t) \sin(\Omega t - \varphi_0) + v_y t \cos(\Omega t - \varphi_0) \]  

\[ p_x(t; \varphi_0) = mv_x \cos(\Omega t - \varphi_0) + mv_y \sin(\Omega t - \varphi_0) \]
\[ p_y(t; \varphi_0) = -mv_x \sin(\Omega t - \varphi_0) + mv_y \cos(\Omega t - \varphi_0) \]

(B.3)

There is another way of solving this: angle loop is the trajectory under the Hamiltonian \( H \) (in the static frame) within one radial cycle as it would be seen in a rotating frame rotating at angular velocity \( \Omega(l, E) \). In the circular box for instance, in static frame, the trajectory under the Hamiltonian \( H \) (in the static frame) within one radial cycle is:

\[ x(t, \varphi_0 = 0) = \rho_{\text{max}} + v_x t \]
\[ y(t, \varphi_0 = 0) = v_y t \]  

(B.4)

Observed in the rotating frame, the trajectory turns out to be:

\[ x(t; \varphi_0 = 0) = (\rho_{\text{max}} + v_x t) \cos \Omega t + v_y t \sin \Omega t \]
\[ y(t; \varphi_0 = 0) = -(\rho_{\text{max}} + v_x t) \sin \Omega t + v_y t \cos \Omega t \]  

(B.5)

By making a canonical transformation, it is easy to find the conjugate momenta:

\[ p_x(t; \varphi_0 = 0) = mv_x \cos \Omega t + mv_y \sin \Omega t \]
\[ p_y(t; \varphi_0 = 0) = -mv_x \sin \Omega t + mv_y \cos \Omega t \]  

(B.6)
Appendix C. Details of Construction of Semiclassical Wavefunction

We construct semiclassical wavefunctions from classical trajectories. The detailed steps are shown in Ref [93]. Here we just give analytical results of each step for the circular box.

In Appendix B, a classical angle loop is calculated. That can be regarded as a mapping from \((t, \varphi_0)\) to \((x, y)\).

Step 1: derive the inverse mapping: \((x, y)\) to \((t, \varphi_0)\):

\[
t = \left( \frac{1}{2} - \frac{\sqrt{\rho^2 - \rho_{\text{min}}^2}}{2\sqrt{\rho_{\text{max}}^2 - \rho_{\text{min}}^2}} \right) T \quad (C.1)
\]
on one part of the manifold. We call this the “incoming part of the manifold”.

\[
t = \left( \frac{1}{2} + \frac{\sqrt{\rho^2 - \rho_{\text{min}}^2}}{2\sqrt{\rho_{\text{max}}^2 - \rho_{\text{min}}^2}} \right) T \quad (C.2)
\]
on the other part of the manifold. We call this the “outgoing part of the manifold”.

\(\rho_{\text{min}}\) is the smallest radial position for the particle with conserved angular momentum \(l\) and conserved energy \(E\).

The inverse mapping to \(\varphi_0\) is more complicated.

\[
sin(\Omega t - \varphi_0) = \frac{x v_y t - y (\rho_{\text{max}} + v_x t)}{x^2 + y^2}
\]
\[
\frac{1}{\rho} \left\{ \cos \varphi \left( \frac{l}{|l|} \rho_{\min} \left( \sqrt{\rho_{\max}^2 - \rho_{\min}^2} \pm \sqrt{\rho^2 - \rho_{\min}^2} \right) \right) \\
- \sin \varphi \left[ \rho_{\max} - \sqrt{1 - \frac{\rho_{\min}^2}{\rho_{\max}^2}} \left( \sqrt{\rho_{\max}^2 - \rho_{\min}^2} \pm \sqrt{\rho^2 - \rho_{\min}^2} \right) \right] \right\} 
\]
(C.3)

\[
\cos(\Omega t - \varphi_0) = \frac{y v_y t + x (\rho_{\max} + v_x t)}{x^2 + y^2} 
\]

\[
= \frac{1}{\rho} \left\{ \sin \varphi \left( \frac{l}{|l|} \rho_{\min} \left( \sqrt{\rho_{\max}^2 - \rho_{\min}^2} \pm \sqrt{\rho^2 - \rho_{\min}^2} \right) \right) \\
+ \cos \varphi \left[ \rho_{\max} - \sqrt{1 - \frac{\rho_{\min}^2}{\rho_{\max}^2}} \left( \sqrt{\rho_{\max}^2 - \rho_{\min}^2} \pm \sqrt{\rho^2 - \rho_{\min}^2} \right) \right] \right\} 
\]
(C.4)

In \( \pm \), + is for the outgoing part of the manifold while – is for the incoming part of the manifold.

Eqs. (C.3) and (C.4) can be simplified using the notation

\[
\sin(\Omega t - \varphi_0) = f_s(\rho, \varphi) \\
\cos(\Omega t - \varphi_0) = f_c(\rho, \varphi) . 
\]

With some algebra, the final results are:

\[
\cos \varphi_0 = f_s(\rho, \varphi) \sin \Omega t + f_c(\rho, \varphi) \cos \Omega t \\
\sin \varphi_0 = f_c(\rho, \varphi) \sin \Omega t - f_s(\rho, \varphi) \cos \Omega t 
\]
(C.5)

Step 2: calculate the phase

\[ S = \int_c p \cdot dq \]

The integral path is from \((x = 0, y = 0)\) to \((x, y)\), following the red trace shown in Figure C.1.

\[
S = \int_0^{x_0} p_{\varphi} d\varphi + \int_0^{y_0} p_x(t, \varphi_0) dx(t, \varphi_0) + \int_0^{y_0} p_y(t, \varphi_0) dy(t, \varphi_0) 
\]

125
\[
= \int_0^{\phi_0} l d\varphi + \int_0^t p_x(t, \varphi_0)dx(t, \varphi_0) + \int_0^t p_y(t, \varphi_0)dy(t, \varphi_0) \\
= l\varphi_0 + 2(E - \Omega L)t \\
= l\varphi_0 + 2(E - \Omega L)(\frac{1}{2} \pm \frac{\sqrt{\rho^2 - \rho_{\min}^2}}{2\sqrt{\rho_{\max}^2 - \rho_{\min}^2}})T \tag{C.6}
\]

In \(\pm\), + is for the outgoing part of the manifold while – is for the incoming part of the manifold.
Fig. (C.1). The green circle is the outer wall of the circular box potential. Each blue loop is the trajectory of a particle with conserved angular momentum $l$ and conserved energy $E$ under $H = H - \Omega(l,E)L$, starting from different location $(\rho_{\text{max}}, \varphi_0)$. (It is also an angle loop.)

The red trace is the path for integral. It starts from $(x = 0, y = 0)$, following the outer wall until the right $\varphi_0$. Then it follows the angle loop to the target point $(x, y)$.

Step 3: calculate the Jacobian determinant

$$\left| \frac{\partial (x,y)}{\partial (t,\varphi_0)} \right| = \rho_{\text{max}} v_x + \Omega t \frac{2E}{m}$$

$$= \rho_{\text{max}} \left( -\frac{|l|}{l} \right) \sqrt{\frac{1}{\rho_{\text{min}}^2} - \frac{1}{\rho_{\text{max}}^2}} \sqrt{\frac{2m}{E}} \sqrt{\rho_{\text{max}}^2 - \rho_{\text{min}}^2}$$

$$+ \frac{2m}{E} (\rho_{\text{max}}^2 - \rho_{\text{min}}^2) \left( \frac{2E}{m} \right) \left( \frac{1}{2} \pm \frac{\sqrt{\rho_{\text{max}}^2 - \rho_{\text{min}}^2}}{2\sqrt{\rho_{\text{max}}^2 - \rho_{\text{min}}^2}} \right)$$

$$= -2 \rho_{\text{min}} \rho_{\text{max}} \sqrt{\rho_{\text{max}}^2 - \rho_{\text{min}}^2} \sqrt{\rho_{\text{max}}^2 - \rho_{\text{min}}^2}$$

$$+ 2 \left( \rho_{\text{max}}^2 - \rho_{\text{min}}^2 \right) \left( \frac{1}{2} \pm \frac{\sqrt{\rho_{\text{max}}^2 - \rho_{\text{min}}^2}}{\sqrt{\rho_{\text{max}}^2 - \rho_{\text{min}}^2}} \right)$$

with some algebra,

$$= \pm 2 \sqrt{\rho_{\text{max}}^2 - \rho_{\text{min}}^2} \sqrt{\rho^2 - \rho_{\text{min}}^2}$$

$$\therefore \left| \frac{\partial (x,y)}{\partial (t,\varphi_0)} \right| = 2 \sqrt{\rho_{\text{max}}^2 - \rho_{\text{min}}^2} \sqrt{\rho^2 - \rho_{\text{min}}^2}$$

(C.7)
Step 4: combine all the elements together

\[ \psi^{sc}_{m,n}(\rho, \varphi) = A_{in}(\rho, \varphi) \exp\left(\frac{iS_{in}(\rho, \varphi)}{\hbar}\right) + A_{out}(\rho, \varphi) \exp\left(\frac{i S_{out}(\rho, \varphi)}{\hbar} - \frac{\pi}{2}\right) \] \tag{C.8}

where \( A_{in}(\rho, \varphi) \) and \( A_{out}(\rho, \varphi) \) are given by

\[
A_{in}(\rho, \varphi) = \frac{1}{\sqrt{||\nabla(x, y)||_{in}}},
\]

\[
A_{out}(\rho, \varphi) = \frac{1}{\sqrt{||\nabla(x, y)||_{out}}},
\]
BIBLIOGRAPHY


