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## Discontinuity of maximum entropy inference and quantum phase transitions

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## PAPER

## Discontinuity of maximum entropy inference and quantum phase transitions

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and DOI.Jianxin Chen<sup>1</sup>, Zhengfeng Ji<sup>2,3</sup>, Chi-Kwong Li<sup>4</sup>, Yiu-Tung Poon<sup>5</sup>, Yi Shen<sup>6</sup>, Nengkun Yu<sup>2,7</sup>, Bei Zeng<sup>2,7,8</sup> and Duanlu Zhou<sup>9</sup><sup>1</sup> Joint Center for Quantum Information and Computer Science, University of Maryland, College Park, Maryland, USA<sup>2</sup> Institute for Quantum Computing, University of Waterloo, Waterloo, Ontario, Canada<sup>3</sup> State Key Laboratory of Computer Science, Institute of Software, Chinese Academy of Sciences, Beijing, People's Republic of China<sup>4</sup> Department of Mathematics, College of William and Mary, Williamsburg, Virginia, USA<sup>5</sup> Department of Mathematics, Iowa State University, Ames, Iowa, USA<sup>6</sup> Department of Statistics and Actuarial Science, University of Waterloo, Waterloo, Ontario, Canada<sup>7</sup> Department of Mathematics & Statistics, University of Guelph, Guelph, Ontario, Canada<sup>8</sup> Canadian Institute for Advanced Research, Toronto, Ontario, Canada<sup>9</sup> Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, People's Republic of ChinaE-mail: [zhoudl72@iphy.ac.cn](mailto:zhoudl72@iphy.ac.cn)**Keywords:** maximum entropy inference, quantum phase transition, quantum conditional mutual information, numerical range**Abstract**

In this paper, we discuss the connection between two genuinely quantum phenomena—the discontinuity of quantum maximum entropy inference and quantum phase transitions at zero temperature. It is shown that the discontinuity of the maximum entropy inference of local observable measurements signals the non-local type of transitions, where local density matrices of the ground state change smoothly at the transition point. We then propose to use the quantum conditional mutual information of the ground state as an indicator to detect the discontinuity and the non-local type of quantum phase transitions in the thermodynamic limit.

**1. Introduction**

Quantum phase transitions happen at zero temperature with no classical counterparts and are believed to be driven by quantum fluctuations [22]. The study of quantum phase transitions has been a central topic in the condensed matter physics community during the past several decades involving the study of exotic phases of matter such as superconductivity [1], fractional quantum Hall systems [12], and recently the topological insulators [2, 11, 18]. In recent years, it also becomes an intensively studied topic in quantum information science community, mainly because of its intimate connection to the study of local Hamiltonians [6].

In a usual model for quantum phase transitions, one considers a local Hamiltonian  $H(\lambda)$  which depends on some parameter vector  $\lambda$ . While  $H(\lambda)$  smoothly changes with  $\lambda$ , the change of the ground state  $|\psi_0(\lambda)\rangle$  may not be smooth when the system is undergoing a phase transition. Such kind of phenomena is naturally expected to happen at a level-crossing, or at an avoided (but near) level-crossing [22].

Intuitively, the change of ground states can then be measured by some distance between  $|\psi_0(\lambda)\rangle$  and  $|\psi_0(\lambda + \delta\lambda)\rangle$ . For a small change of the parameters  $\lambda$ , such a distance is relatively large near a transition point, while the Hamiltonian changes smoothly from  $H(\lambda)$  to  $H(\lambda + \delta\lambda)$ . The fidelity approach, using the fidelity of quantum states to measure the change of the global ground states, has demonstrated the idea successfully in many physical models for signaling quantum phase transitions [3, 5, 25, 26]. In addition, the relations between the density functional fidelity susceptibility and the Kullback–Leibler entropy or Rényi entropy have been discussed in [17, 21]. While the fidelity approach is believed to provide a signal for many kinds of quantum phase transitions, it does not distinguish between different types of the transition, for instance local or non-local (in a sense that the reduced fidelity of local density matrices may also signal the phase transition, as discussed in [5]).

Moreover, one usually needs to compute the fidelity change of a relatively large system in order to clearly signal the transition point.

In this work, we explore an information-theoretic viewpoint to quantum phase transitions. Our approach is based on the structure of the convex set given by all the possible local measurement results, and the corresponding inference of the global quantum states based on these local measurement results. By the principle of maximum entropy, the best such inference compatible with the given local measurement results is the unique quantum state  $\rho^*$  with the maximum von Neumann entropy [7].

It is known that in the classical case, the maximum entropy inference is continuous [7, 9, 24]. This means that, for any two sets of local measurement results  $\alpha$  and  $\alpha'$  close to each other, the corresponding inference  $\rho^*(\alpha)$  and  $\rho^*(\alpha')$  are also close to each other. Surprisingly, however, the quantum maximum entropy inference can be discontinuous! Namely, a small change of local measurement results may correspond to a dramatic change of the global quantum state.

The main focus of this work is to relate the discontinuity of the quantum maximum entropy inference to quantum phase transitions. We show that the discontinuity of maximum entropy inference signals level-crossings of the non-local type. That is, at the level-crossing point, a smooth change of the local Hamiltonian  $H(\lambda)$  corresponds to a smooth change of the local density matrices of the ground states, while the change of  $\rho^*$ , the maximal entropy inference of these local density matrices, is discontinuous.

We then move on to discuss the possibility of signaling quantum phase transitions by computing the discontinuity of the maximal entropy inference  $\rho^*$ . Given the observation on the relation between discontinuity of  $\rho^*$  and the non-local level-crossings, it is natural to consider signaling quantum phase transitions by directly computing where the discontinuity happens. This approach works well in finite systems, but may fail in the thermodynamic limit of infinite size systems as the places of discontinuity (i.e. where the system ‘closes gap’) may change when the system size goes to infinity. Hence, computations in finite systems may provide no information of the phase transition point. We propose to solve the problem by using the quantum conditional mutual information of two disconnected parts of the system for the ground states. This idea comes from the relationship between the three-body irreducible correlation and quantum conditional mutual information of gapped systems. As it turns out, the quantum mutual information works magically well to signature the discontinuity point, thereby also signals quantum phase transitions in the thermodynamic limit. In some sense, the quantum conditional mutual information is an analog of the Levin–Wen topological entanglement entropy [13].

We apply the concept of discontinuity of the maximum entropy inference to some well-known quantum phase transitions. In particular, we show that the non-local transition in the ground states of the transverse quantum Ising chain can be detected by the quantum mutual information of two disconnect parts of the system. The scope of the applicability of the quantum conditional mutual information was extended to many other systems, featuring different types of transitions [28, 29]. All these studies conclude that the quantum mutual information serves well as a *universal indicator* of non-trivial phase transitions.

We organize our paper as follows. In section 2, we discuss the concept of the maximum entropy inference and summarize some important relevant facts. In section 3, we analyze several examples of discontinuity of the maximum entropy inference  $\rho^*$ , ranging from simple examples in dimension 3 to more physically motivated ones. In section 4, we link the discontinuity of  $\rho^*$  to the concept of the long-range irreducible many-body correlation and propose to detect the non-local type of quantum phase transitions by the quantum conditional mutual information of two disconnect parts of the system. In section 5, further properties of discontinuity of the maximum entropy inference are discussed. We provide both a necessary condition and a sufficient condition for the discontinuity to happen. Finally, section 6 contains a summary of all the main concepts discussed and a discussion of possible future directions.

## 2. The maximum entropy inference

We start our discussion by introducing the concept of the maximum entropy inference given a set of linear constraints on the state space.

### 2.1. The general case

Let  $\mathcal{H}$  be the  $d$ -dimensional Hilbert space corresponding to the quantum system under discussion and  $\rho$  be the state of the system. Let  $\mathcal{D}$  be the set of all possible quantum states on  $\mathcal{H}$ . Any tuple  $\mathcal{F} = (F_1, F_2, \dots, F_r)$  of  $r$  observables defines a mapping

$$\rho \mapsto \boldsymbol{\alpha} = \left( \text{tr}(\rho F_1), \text{tr}(\rho F_2), \dots, \text{tr}(\rho F_r) \right), \quad (1)$$

from states  $\rho$  in  $\mathcal{D}$  to points  $\boldsymbol{\alpha}$  in the set

$$\mathcal{D}_{\mathcal{F}} = \left\{ \boldsymbol{\alpha} \mid \boldsymbol{\alpha} = \left( \text{tr}(\rho F_1), \dots, \text{tr}(\rho F_r) \right) \text{ for some } \rho \right\}.$$

The set  $\mathcal{D}_{\mathcal{F}}$  can be considered as a projection of  $\mathcal{D}$  and is a compact convex set in  $\mathbb{R}^r$ . If all the  $F_i$ 's are commuting (i.e.  $[F_i, F_j] = 0$ , corresponding to the classical case), then  $\mathcal{D}_{\mathcal{F}}$  is a polytope in  $\mathbb{R}^r$ .

The convex set  $\mathcal{D}_{\mathcal{F}}$  is mathematically related to the so-called '(joint) numerical range' of the operators  $F_i$ 's. For more mathematical aspects of these joint numerical ranges and the discontinuity of the maximum entropy inference, we refer to [20]. We remark that  $\mathcal{D}_{\mathcal{F}}$  is also known as *quantum convex support* in the literature [23].

As it will be clear in later discussions, the observables  $F_i$ 's usually come from the terms in the local Hamiltonian of interest so that the Hamiltonian is in the span of the observables  $F_i$ 's. We will call  $H = \sum_i \theta_i F_i$  the Hamiltonian related to the observables in  $\mathcal{F}$ . The energy  $\text{tr}(H\rho)$  can be written as

$$\sum_i \theta_i \text{tr}(\rho F_i),$$

the inner product of the vector  $\boldsymbol{\theta} = (\theta_i)$  and  $\boldsymbol{\alpha}$ . This means that one can think of the Hamiltonian  $H$  geometrically as the supporting hyperplanes of the convex set  $\mathcal{D}_{\mathcal{F}}$ .

Given any measurement result  $\boldsymbol{\alpha} \in \mathcal{D}_{\mathcal{F}}$ , we are interested in the set of all states in  $\mathcal{D}$  that can give  $\boldsymbol{\alpha}$  as the measurement results. We denote such a set as

$$\mathcal{L}(\boldsymbol{\alpha}) = \left\{ \rho \mid \text{tr}(\rho F_i) = \alpha_i, i = 1, \dots, r \right\}.$$

It is the preimage of  $\boldsymbol{\alpha}$  under the mapping in equation (1). In other words, it consists of the states satisfying a set of linear constraints and we call this subset of  $\mathcal{D}$  a *linear family* of quantum states.

In general, there will be many quantum states compatible with  $\boldsymbol{\alpha}$  and  $\mathcal{L}(\boldsymbol{\alpha})$  contains more than one state, unless one chooses to measure an informationally complete set of observables (for example, a basis of operators on  $\mathcal{H}$  as one often does for the case of quantum tomography). Especially, when the dimension of system  $d$  is large, it is unlikely that one can really measure an informationally complete set of observables. For instance, for an  $n$ -qubit system when  $n$  is large, we usually only have access to the expectation values of local measurements, each involving measurements only on a few number of qubits. In this case, quantum states compatible with the local observation data  $\boldsymbol{\alpha}$  are usually not unique.

The question is then what would be the best inference of the quantum states compatible with the given measurement results  $\boldsymbol{\alpha}$ . The answer to this question is well-known, and is given by the principle of maximum entropy [7, 24]. That is, for any given measurement results  $\boldsymbol{\alpha}$ , there is a unique state  $\rho^* \in \mathcal{L}(\boldsymbol{\alpha})$ , given by

$$\rho^*(\boldsymbol{\alpha}) = \underset{\rho \in \mathcal{L}(\boldsymbol{\alpha})}{\text{argmax}} S(\rho), \quad (2)$$

where  $S(\rho)$  is the von Neumann entropy of  $\rho$ . We call  $\rho^*(\boldsymbol{\alpha})$  the *maximum entropy inference* for the given measurement results  $\boldsymbol{\alpha}$ . More explicitly, it is the optimal solution of the following optimization problem

$$\begin{aligned} & \text{Maximize: } S(\rho) \\ & \text{Subject to: } \text{tr}(\rho F_i) = \alpha_i, \text{ for all } i = 1, 2, \dots, k, \\ & \rho \in \mathcal{D}. \end{aligned}$$

It may seem counter-intuitive that both the maximum entropy inference  $\rho^*$  and its entropy can be discontinuous [9] as functions of the local measurement data  $\boldsymbol{\alpha}$ . When we say  $\rho^*$  is discontinuous, we mean the state itself, not its entropy, is discontinuous. Indeed there could be examples where these two concepts are not the same (e.g. the energy gap of the system closes but the ground-state degeneracy does not change). For all examples considered in this paper, however, the entropy is also discontinuous when the state is. We note that the discontinuity of the maximum entropy inference is a genuinely quantum effect as the classical maximum entropy inference is always continuous [7, 24].

## 2.2. The case of local measurements

The discussions in the above subsection specialize to the important case of many-body physics with local measurements.

Consider an  $n$ -particle system where each particle has dimension  $d$ . The Hilbert space  $\mathcal{H}$  of the systems is  $(\mathbb{C}^d)^{\otimes n}$ , with dimension  $d^n$ . We know that, for an  $n$ -particle state  $\rho$ , we usually only have access to the measurement results of a set of local measurements  $\mathcal{F} = (F_1, \dots, F_r)$  on the system, where each  $F_i$  acts on at most

$k$  particles for  $k \leq n$ . The most interesting case is where  $n$  is large and  $k$  is small (usually a constant independent of  $n$ ). In this sense, we will just call such a measurement setting  $k$ -local.

Notice that each measurement result  $\text{tr}(\rho F_i)$  now depends only on the  $k$ -particle reduced density matrix ( $k$ -RDM) of the particles that  $F_i$  is acting non-trivially on. It is convenient to write the set of all the  $k$ -RDMs of  $\rho$  (in some fixed order) as a vector  $\boldsymbol{\rho}^{(k)} = \{\rho_1^{(k)}, \dots, \rho_m^{(k)}\}$ , where each component is a  $k$ -RDM of  $\rho$  and  $m = \binom{n}{k}$ . The  $k$ -RDMs  $\rho^{(k)}$  will play the role of expectation values  $\alpha$  as in the general case.

Along this line, the set of results of all  $k$ -local measurements can be defined in terms of  $k$ -RDMs, and we write the set  $\mathcal{D}^{(k)}$  of all such measurement results as

$$\mathcal{D}^{(k)} = \{\boldsymbol{\rho}^{(k)} \mid \boldsymbol{\rho}^{(k)} \text{ is the } k\text{-RDMs of some } \rho\}. \quad (3)$$

Similarly, the linear family can also be defined in terms of  $k$ -RDMs

$$\mathcal{L}(\boldsymbol{\rho}^{(k)}) = \{\rho \mid \rho \text{ has the } k\text{-RDMs } \boldsymbol{\rho}^{(k)}\}. \quad (4)$$

The maximum entropy inference given the  $k$ -RDMs  $\boldsymbol{\rho}^{(k)}$  is

$$\rho^*(\boldsymbol{\rho}^{(k)}) = \underset{\rho \in \mathcal{L}(\boldsymbol{\rho}^{(k)})}{\text{argmax}} S(\rho). \quad (5)$$

We remark that, in practice, one may not be interested in all the  $m = \binom{n}{k}$   $k$ -RDMs, but rather only those  $k$ -RDMs that are *geometrically* local. For instance, for a lattice spin model, one may only be interested in the two-RDMs of the nearest-neighbour spins. Our discussion can also be generalized to these cases, as in the discussion in [29] for one-dimensional spin chains. There could also be cases that the system has certain symmetry (for instance a bosonic system or fermionic system where all the  $k$ -RDMs are the same), and our theory can be naturally adapted to these cases.

The maximum entropy inference  $\rho^*$  given local density matrices has a more concrete physical meaning. For any  $n$ -particle state  $\rho$ , if  $\rho = \rho^*(\boldsymbol{\rho}^{(k)})$ , then  $\rho$  is uniquely determined by its  $k$ -RDMs using the maximum entropy principle. One can argue, in this case, that all the information (including all correlations among particles) contained in  $\rho$  are already contained in its  $k$ -RDMs. In other words,  $\rho$  does not contain any irreducible correlation [30] of order higher than  $k$ . On the other hand, if  $\rho \neq \rho^*$ , then  $\rho$  can not be determined by its  $k$ -RDMs and there are more information/correlations in  $\rho$  than those in its  $k$ -RDMs. Therefore,  $\rho$  contains non-local irreducible correlation that can not be obtained from its local RDMs.

### 3. Discontinuity of $\rho^*$

In this section, we explore the discontinuity of  $\rho^*$  based on several simple examples. The first three of them involve only two different measurement observables, but they do demonstrate almost all the key ideas in the general case.

#### 3.1. The examples of two observables

We will choose  $d = 3$  for the Hilbert space dimension as it is enough to demonstrate most of the phenomena we need to see. Fix an arbitrary orthonormal basis of  $\mathbb{C}^3$ , say,  $\{|0\rangle, |1\rangle, |2\rangle\}$ .

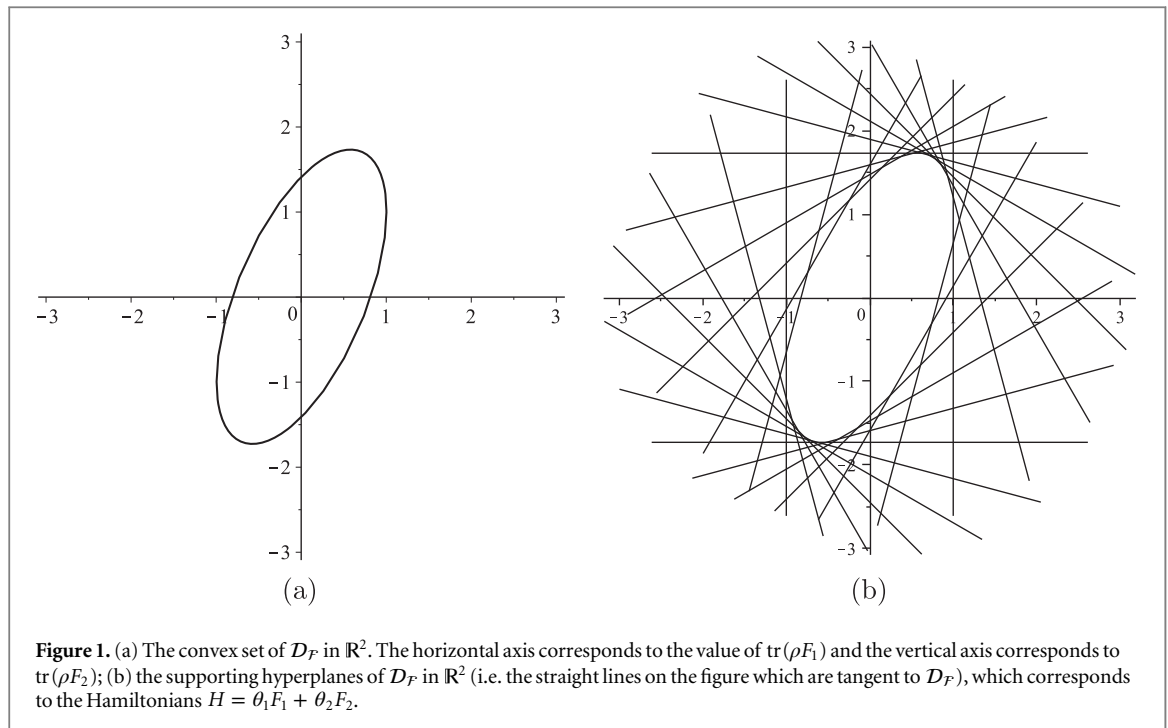
**Example 1.**  $\mathcal{F}$  consists of the following two observables

$$F_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad F_2 = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & -1 \end{pmatrix}. \quad (6)$$

First, notice that  $F_1, F_2$  do not commute. The set of all possible measurement results  $\mathcal{D}_{\mathcal{F}}$  is a convex set in  $\mathbb{R}^2$ . We plot this convex set in figure 1(a). To obtain this figure, we let  $\rho$  vary for all the density matrices on  $\mathbb{C}^3$ , and let the corresponding  $\text{tr}(\rho F_1)$  be the horizontal coordinate and  $\text{tr}(\rho F_2)$  the vertical coordinate. The resulting picture is nothing but the numerical range of the matrix  $F_1 + iF_2$ .

As discussed in section 2, the Hamiltonian  $H$  related to  $\mathcal{F}$  has the form

$$H = \theta_1 F_1 + \theta_2 F_2 \quad (7)$$



for some parameters  $\theta_1, \theta_2 \in \mathbb{R}$ . Notice that the Hamiltonian corresponds to supporting hyperplanes of  $\mathcal{D}_{\mathcal{F}}$ , as the inner product has the form  $\text{tr}(H\rho) = (\theta_1, \theta_2) \cdot (\alpha_1, \alpha_2)^T$ . We demonstrate these supporting hyperplanes of  $\mathcal{D}_{\mathcal{F}}$  in figure 1(b).

It is straightforward to see that the ground state of  $H$  is non-degenerate except for the case  $\theta_1 < 0, \theta_2 = 0$ , where the ground space is two-fold degenerate with a basis  $\{|0\rangle, |1\rangle\}$  corresponding to the measurement results  $\alpha_0 = (1, 1)$ .

We now show that the maximum entropy inference  $\rho^*(\alpha)$  is indeed discontinuous at the point  $\alpha_0 = (1, 1)$ . To see this, first notice that the corresponding  $\rho^* = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$ . While for any small  $\epsilon$ , the corresponding ground state space of  $-F_1 + \epsilon F_2$  is no longer degenerate, which means  $\rho^*(\alpha)$  is a pure state for  $\alpha \neq \alpha_0$ . Therefore, for any sequence of  $\alpha$  on the boundary of  $\mathcal{D}_{\mathcal{F}}$  approaching  $\alpha_0$ ,

$$\rho^*(\alpha) \not\rightarrow \rho^*(\alpha_0) \text{ when } \alpha \rightarrow \alpha_0, \tag{8}$$

and the discontinuity of  $\rho^*(\alpha)$  follows.

This example seems to indicate that the discontinuity simply comes from degeneracy: as in general degeneracy is rare, whenever such a point of degeneracy exists, we have a singularity on the boundary of  $\mathcal{D}_{\mathcal{F}}$  so discontinuity happens. However, it is important to point out that this is not quite true. For example, degeneracy also happens in classical systems where there can have no discontinuity of  $\rho^*$ . We further explain this point in the following example.

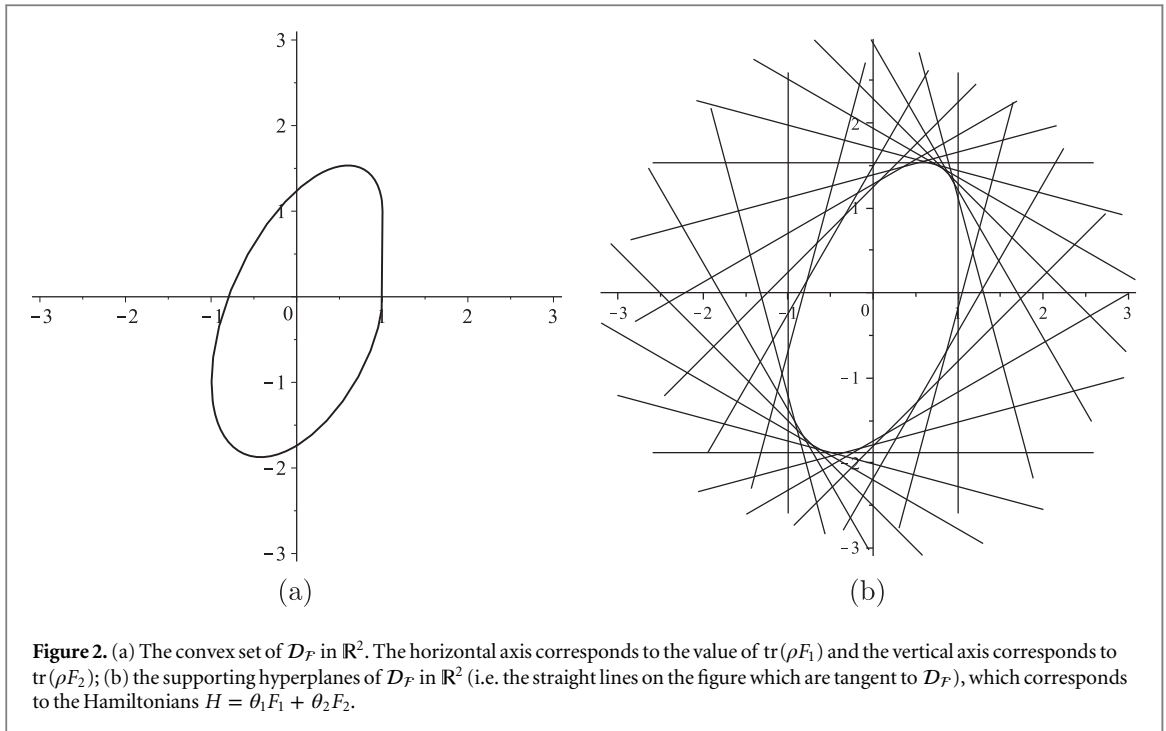
**Example 2.**  $\mathcal{F}$  consists of the following two observables

$$F_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad F_2 = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & -1 \end{pmatrix}. \tag{9}$$

Notice that again  $[F_1, F_2] \neq 0$ . And we show the convex set  $\mathcal{D}_{\mathcal{F}}$  in figure 2(a).

Consider the Hamiltonian  $H = \theta_1 F_1 + \theta_2 F_2$  for some  $\theta_1, \theta_2 \in \mathbb{R}$ , as illustrated as supporting hyperplanes in figure 2(b). Similarly, the ground state of  $H$  is two-fold degenerate for  $\theta_1 < 0, \theta_2 = 0$  (corresponding to the vertical line at  $\alpha_1 = 1$ ) with a basis  $\{|0\rangle, |1\rangle\}$ . However, different from example 1, the ground states do not correspond to a single measurement result  $\alpha_1 = (1, 1)$ . Instead, they are on the line  $[(1, 0), (1, 1)]$ .

By simple calculations, now the maximum entropy inference  $\rho^*(\alpha)$  is in fact continuous at the point  $\alpha_1 = (1, 1)$ , and on the entire line  $[(1, 0), (1, 1)]$ . In fact,  $\rho^*(\alpha_p) = p |0\rangle\langle 0| + (1 - p)|1\rangle\langle 1|$  for  $\alpha_p = (1, p)$ .



For any small perturbation  $\epsilon$ , the corresponding ground state space of  $-F_1 + \epsilon F_2$  is non-degenerate, meaning  $\rho^*(\alpha)$  is a pure state. This change of  $\rho^*(\alpha)$  from  $\epsilon < 0$  to  $\epsilon > 0$  is *sudden* with respect to the small change of  $\epsilon$ , which, however, is accompanied by a sudden change also in the measurement results (from a point near  $(1, 1)$  to  $(1, 0)$ ). As we are considering the discontinuity of  $\rho^*$  with respect to the measurement data  $\alpha$ , not the parameter  $\epsilon$  in the Hamiltonian,  $\rho^*$  is in fact continuous.

This example demonstrates that when Hamiltonian changes smoothly, ground states have sudden changes accompanied with the sudden change of measurement results. In other words, the change of ground states can be described already by the change of local measurement results. This is somewhat a classical feature, as discussed in the next example.

**Example 3.**  $\mathcal{F}$  consists of the following two observables

$$F_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad F_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (10)$$

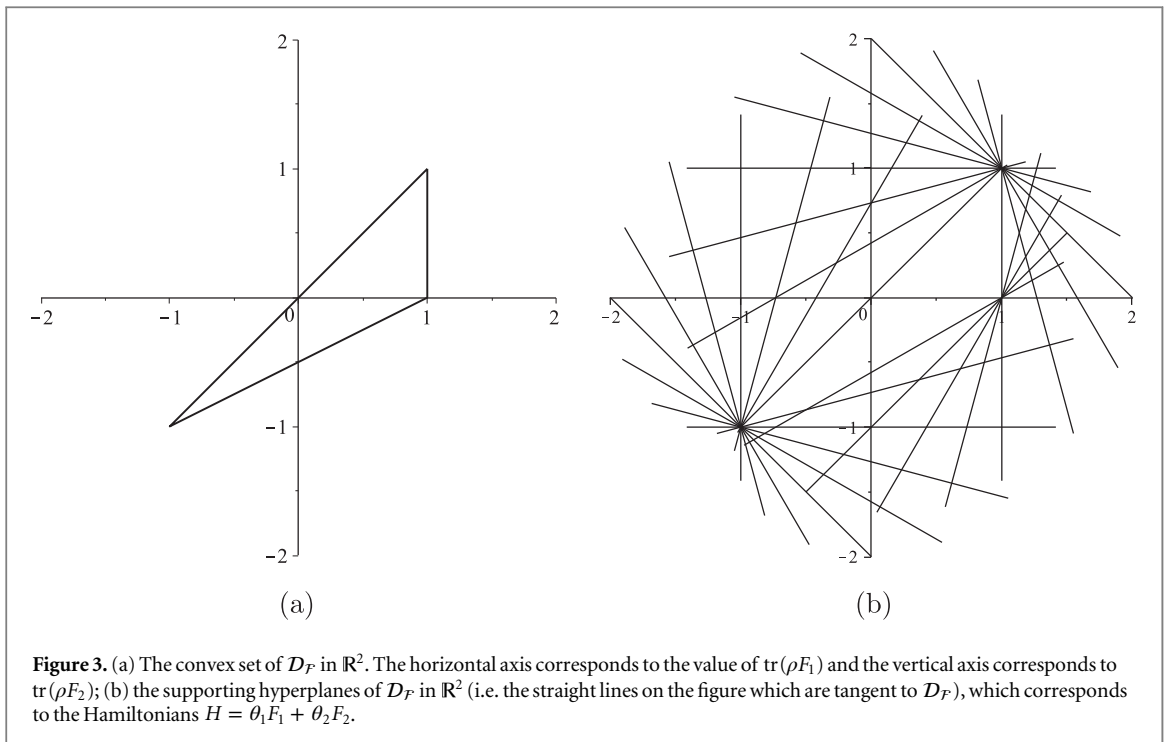
Now this corresponds to the classical situation where  $[F_1, F_2] = 0$ .

The convex set  $\mathcal{D}_{\mathcal{F}}$  is given in figure 3(a). It is a triangle for this example, and a polytope in the general classical case.

Consider the related Hamiltonian  $H = \theta_1 F_1 + \theta_2 F_2$  for some  $\theta_1, \theta_2 \in \mathbb{R}$ , as illustrated as supporting hyperplanes in figure 3(b). Similarly, the ground state of  $H$  is two-fold degenerate for  $\theta_1 < 0, \theta_2 = 0$  (corresponding to the vertical line at  $\alpha_1 = 1$ ) with a basis  $\{|0\rangle, |1\rangle\}$ . For a similar reason, the maximum entropy inference  $\rho^*(\alpha)$  is continuous on the entire line  $[(1, 0), (1, 1)]$  as in the previous example.

If we still consider for any small perturbation  $-F_1 + \epsilon F_2$ , the corresponding ground-state space is non-degenerate: it is  $|1\rangle$  for  $\epsilon < 0$  and  $|2\rangle$  for  $\epsilon > 0$ . So from  $\epsilon < 0$  to  $\epsilon > 0$ , we also see sudden changes of both the measurement results and the ground states.

In the above three examples, the first one is the most interesting and exhibits smooth change in measurement results and discontinuity of the maximum entropy inference  $\rho^*$ . The second and third behave in a similar classical way where a small change in the Hamiltonian will induce a sudden change of measurement results and there is no discontinuity of  $\rho^*$ . We summarize our observations from the three examples in this subsection as below. Although the examples involve two observables only, we state the observation in the more general setting of arbitrarily many observables.



**Observation 1.** Given a set of measurements  $\mathcal{F} = (F_1, F_2, \dots, F_r)$ , and a family of related Hamiltonians  $H$  of the form  $H = \sum_i \theta_i F_i$  with  $\theta_i$  changing with certain parameter. The Hamiltonian  $H$  has two types of ground state level crossing:

- Type I (local type): level-crossing that can be detected by a sudden change of the measurement results.
- Type II (non-local type): level-crossing that can not be detected by a sudden change of the measurement results.

More importantly, only Type II corresponds to discontinuity of the maximum inference  $\rho^*(\alpha)$ .

### 3.2. The example of local measurements

We now give a simple example showing the discontinuity of  $\rho^*$  in a three-qubit system with two-local interactions.

**Example 4.** The three-qubit GHZ state given by

$$|\text{GHZ}_3\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle) \quad (11)$$

is known to be the ground state of a two-body Hamiltonian

$$H = -Z_1 Z_2 - Z_2 Z_3 \quad (12)$$

with  $Z_i$  the Pauli  $Z$  operator acting on the  $i$ th qubit. The ground-state space of  $H$  is two-fold degenerate and is spanned by  $\{|000\rangle, |111\rangle\}$ . Now consider the two-RDMs of the GHZ state

$$\rho^{(2)} = \{\rho_{\{1,2\}}, \rho_{\{2,3\}}, \rho_{\{1,3\}}\}, \quad (13)$$

with  $\rho_{\{i,j\}} = \frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 11|)$  being the two-RDM of qubits  $i$  and  $j$ . We claim that there is discontinuity at  $\rho^{(2)}$ .

To see this, consider a family of perturbations  $H + \epsilon \sum_{i=1}^3 X_i$  of the Hamiltonian  $H$ . For any  $\epsilon \neq 0$ , the ground space is non-degenerate and the unique ground state converges to  $|\text{GHZ}_3\rangle$  when  $\epsilon \rightarrow 0^-$  and to  $(|000\rangle - |111\rangle)/\sqrt{2}$  when  $\epsilon \rightarrow 0^+$ . As the ground state is unique when  $\epsilon \neq 0$  and the Hamiltonian is two-local, the two-RDMs of the ground state determines the state. This means that  $\rho^*$  is pure and coincide with the ground state for all  $\epsilon \neq 0$ . However, at  $\epsilon = 0$ ,  $\rho^*$  is



$$\rho^*(\rho^{(2)}) = \frac{1}{2}(|000\rangle\langle 000| + |111\rangle\langle 111|), \quad (14)$$

and the discontinuity of  $\rho^*$  follows.

It is worth pointing out the similarity in the structure of the above example and example 1, despite their totally different specific form. First notice that  $\frac{1}{\sqrt{2}}(|000\rangle \pm |111\rangle)$  are two eigenstates of  $Z_1Z_2 + Z_2Z_3$  of the same eigenvalue 1. If we complete  $\frac{1}{\sqrt{2}}(|000\rangle \pm |111\rangle)$  to a basis,  $Z_1Z_2 + Z_2Z_3$  will have a 2-by-2 identity block with zero entries to the right and bottom. In that basis, the  $\sum_{i=1}^3 X_i$  also has such a 2-by-2 block proportional to identity and has some non-zero off diagonal entries. In other words,  $Z_1Z_2 + Z_2Z_3$  and  $\sum_{i=1}^3 X_i$  has a rather similar block structure as  $F_1$  and  $F_2$  in example 1.

We generalize the observation 1 in terms of local measurements as follows.

**Observation 1'.** For an  $n$ -particle system, consider the set of all  $k$ -local measurements  $\mathcal{F}$ , which then corresponds to a local Hamiltonian  $H = \sum_j c_j F_j$  with  $F_j \in \mathcal{F}$  acting nontrivially on at most  $k$  particles. There are two kinds of ground state level crossing:

- Type I: level-crossing that can be detected by a sudden change of the  $k$ -RDMs  $\rho^{(k)}$ .
- Type II: level-crossing that can not be detected by a sudden change of the local  $k$ -RDMs  $\rho^{(k)}$ .  
Only Type II corresponds to discontinuity of the maximum entropy inference  $\rho^*(\rho^{(k)})$ .

### 3.3. The example of transverse quantum Ising model

Our next example is an  $n$ -qubit generalization of example 4 and is known as the transverse quantum Ising model.

**Example 5.** The Ising Hamiltonian is given by

$$H(\lambda) = -J \left( \sum_{i=1}^{n-1} Z_i Z_{i+1} + \lambda \sum_{i=1}^n X_i \right), \quad (15)$$

for  $J > 0$ . For any finite  $n$  the discontinuity of  $\rho^*$  determined by the two-RDMs happen at  $\lambda = 0$ . For infinite  $n$ , the discontinuity of  $\rho^*$  happen at  $\lambda = 1$ .

The Hamiltonian  $H(\lambda)$  has a  $\mathbb{Z}_2$  symmetry, which is given by  $X^{\otimes n}$ , i.e.  $[X^{\otimes n}, H(\lambda)] = 0$ . In the limit of  $\lambda = 0$ , the ground state of  $H(0)$  is two-fold degenerate and spanned by  $\{|0\rangle^{\otimes n}, |1\rangle^{\otimes n}\}$ . And in the limit of  $\lambda = \infty$ , the ground state of  $H(\infty)$  is non-degenerate and is given by  $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)^{\otimes n}$ .

In the case of finite  $n$ , the ground space of  $H(\lambda)$  for any  $\lambda > 0$  is non-degenerate. Based on a similar discussion of example 4, we have

$$\lim_{\lambda \rightarrow 0^+} \rho^*(\lambda) = |\text{GHZ}_n\rangle\langle \text{GHZ}_n|, \quad (16)$$

where  $|\text{GHZ}_n\rangle$  is the  $n$ -qubit GHZ state  $\frac{1}{\sqrt{2}}(|0\rangle^{\otimes n} + |1\rangle^{\otimes n})$ . On the other hand, at  $\lambda = 0$ ,  $\rho^*(0)$  has rank 2.

When the two-RDMs of  $\rho^*(0)$  is approached by the two-RDMs of the ground states  $\rho^*(\lambda)$  of  $H(\lambda)$ , the local RDMs of  $\rho^*(\lambda)$  change smoothly, and discontinuity of  $\rho^*(\lambda)$  happens at  $\lambda = 0$ .

In the thermodynamic limit of  $n \rightarrow \infty$ , it is well-known that when  $\lambda$  increases from 0 to  $\infty$ , quantum phase transition happens at the point  $\lambda = 1$  [19]. For  $\lambda \rightarrow 1^+$ ,  $\lambda = 1$  is exactly the point where the ground space of  $H(\lambda)$  undergoes the transition from non-degenerate to degenerate. A discontinuity of  $\rho^*(\lambda)$  happens at  $\lambda = 1$  when  $\lambda \rightarrow 1^+$ , which is a sudden jump of rank from 1 to 2, while the local RDMs of  $\rho^*(\lambda)$  change smoothly.

For  $0 < \lambda \leq 1$ , the two-fold degenerate ground states, although not exactly the same as those two at  $\lambda = 0$ , are qualitatively similar. For the range of  $0 \leq \lambda \leq 1$ , the ground states are all two-fold degenerate. For finite  $n$ , however, in the region of  $0 < \lambda \leq 1$ , an (exponentially) small gap exists between two near degenerate states, and the true ground state does not break the  $\mathbb{Z}_2$  symmetry of the Hamiltonian  $H(\lambda)$ .

This example demonstrates the dramatic difference between the case of finite  $n$  and the case of the thermodynamic limit of infinite  $n$ . It also foretells the difficulty of signaling phase transitions by computing the discontinuity of  $\rho^*$  of finite systems directly. We will propose a solution to this problem in section 4.

## 4. Signaling discontinuity by quantum conditional mutual information

### 4.1. Irreducible correlation and quantum conditional mutual information

We have mentioned the relation between the maximum entropy inference and the theory of irreducible many-body correlations [30]. For an  $n$ -particle quantum state  $\rho$ , denote its  $k$ -RDMs by  $\rho^{(k)}$ . Then its  $k$ -particle irreducible correlation is given by [15, 30]

$$C^{(k)}(\rho) = S\left(\rho^*\left(\rho^{(k-1)}\right)\right) - S\left(\rho^*\left(\rho^{(k)}\right)\right). \quad (17)$$

What  $C^{(k)}$  measures is the amount of correlation contained in  $\rho^{(k)}$  but not contained in  $\rho^{(k-1)}$ .

Consider a partition  $A, B, C$  of the  $n$  particles so that  $A$  and  $C$  are far apart. Define

$$\rho_{ABC}^* = \operatorname{argmax}_{\substack{\sigma_{AB}=\rho_{AB} \\ \sigma_{BC}=\rho_{BC}}} S(\sigma_{ABC}). \quad (18)$$

Then the three-body irreducible correlation of  $\rho_{ABC}$  is given by

$$C^{ABC} = S\left(\rho_{ABC}^*\right) - S(\rho_{ABC}). \quad (19)$$

Note that we do not include the constraint  $\sigma_{AC} = \rho_{AC}$  in the definition of  $\rho_{ABC}^*$ . The reason for this is that the region of  $A$  and  $C$  are chosen to be far apart and, therefore, there will be no  $k$ -local terms in the Hamiltonian that act non-trivially on both  $A$  and  $C$ .

In the discussion on the example of quantum Ising chain, we have observed the difficulty of signaling the discontinuity of  $\rho^*$  in the thermodynamic limit by computations of finite systems. In the following, we propose a quantity that can reveal the physics in the thermodynamic limit by investigating relatively small finite systems.

The quantity we will use is the quantum conditional mutual information

$$I(A : C|B)_\rho = S(\rho_{AB}) + S(\rho_{BC}) - S(\rho_B) - S(\rho_{ABC}). \quad (20)$$

We will also omit the subscript  $\rho$  when there is no ambiguity. Usually, the state  $\rho$  will be chosen to be a reduced state of the ground state of the Hamiltonian. It is known that the quantum conditional mutual information is an upper bound of  $C^{ABC}$  [13, 16]. Namely, we have

$$C^{ABC}(\rho) \leq I(A : C|B)_\rho, \quad (21)$$

which is equivalent to the strong subadditivity [14] for the state  $\rho_{ABC}^*$ . The equality holds when the state  $\rho_{ABC}^*$  satisfies  $I(A : C|B) = 0$ , or is a so-called quantum Markovian state.

We will use the quantum conditional mutual information  $I(A : C|B)$  of the ground state, instead of three-body irreducible correlation  $C^{ABC}$ , to signal the discontinuity and phase transitions in the system. We do this for two reasons. First, it is conjectured that the equality in equation (21) always holds in the thermodynamic limit for gapped systems. In other words, the corresponding  $\rho_{ABC}^*$  of the ground state is always a quantum Markovian state (there are reasons to believe this, see e.g. [8, 16]). Assuming this conjecture,  $I(A : C|B)$  is indeed a good quantity to signal the discontinuity and phase transition in the thermodynamic limit. Second, as it turns out, quantum conditional mutual information performs much better as an indicator when we do computations in systems of small system sizes. Most importantly, it doesn't seem to suffer from the problem  $C^{ABC}$  has in finite systems. For more discussion on the physical aspects of  $I(A : C|B)$ , we refer to [28].

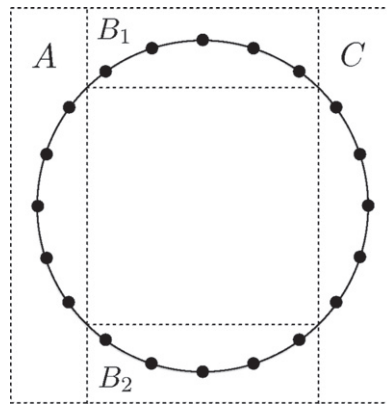
### 4.2. The transverse Ising model

We now illustrate the mutual information approach in one-dimensional systems. First, consider a one-dimensional system with periodic boundary conditions. As we need  $A$  and  $C$  to be large regions far away from each other, the partition  $A, B, C$  can be chosen as in figure 4.

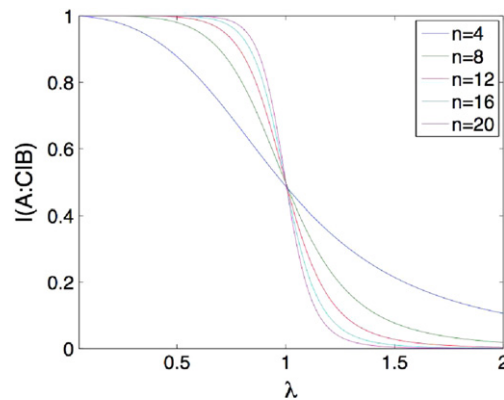
Following the discussions in section 4.1, one can use the quantity  $I(A : C|B)$  to indirectly detect the existence of the discontinuity of  $\rho^*$  and the corresponding phase transition. We have computed  $I(A : C|B)$  for the ground state of the transverse quantum Ising chain  $H(\lambda)$ , with total 4, 8, 12, 16, 20 particles of the system. The results are shown in figure 5, in which  $I(A : C|B)$ 's clearly indicate a phase transition at  $\lambda = 1$  (where the curves intersect). This is consistent with our discussions for the quantum Ising chain with transverse field in section 3.3.

However, the phase transition of the Hamiltonian with a  $Z$  direction magnetic field, given by

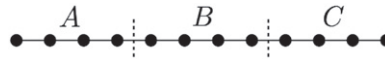
$$H(\lambda_z) = -J \left( \sum_i Z_i Z_{i+1} + \lambda_z \sum_i Z_i \right), \quad (22)$$



**Figure 4.** Each dot represents a particle. The partition of a chain to three parts  $ABC$ , where  $A$ ,  $C$  are disconnected and  $B = B_1 \cup B_2$ .



**Figure 5.**  $I(A : C|B)$  of the Ising model with open periodic boundary condition and the  $A$ ,  $B$ ,  $C$  regions as chosen in figure 4. A similar result is presented in [28], from a different viewpoint.



**Figure 6.**  $A$ ,  $B$ ,  $C$  cutting on a 1D chain.

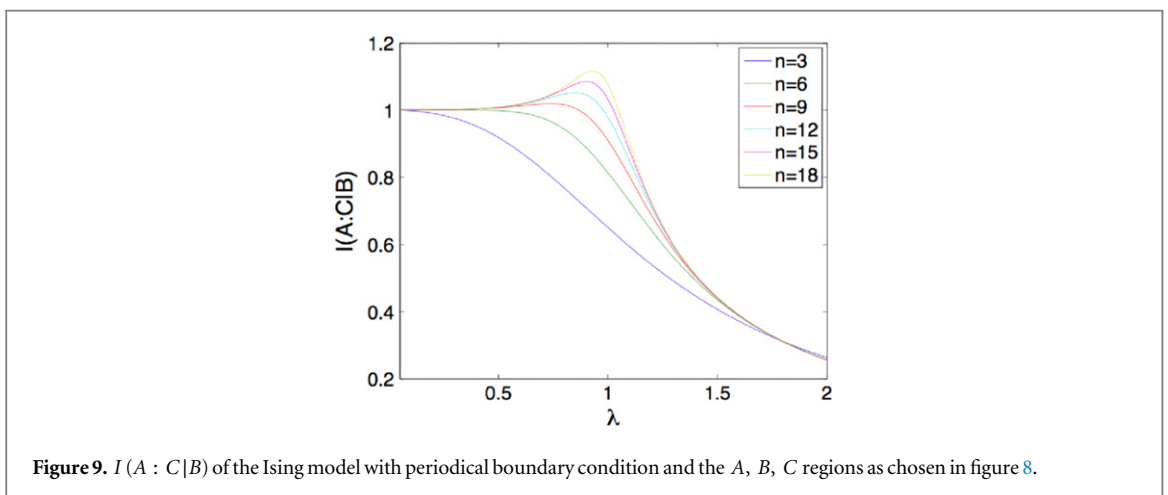
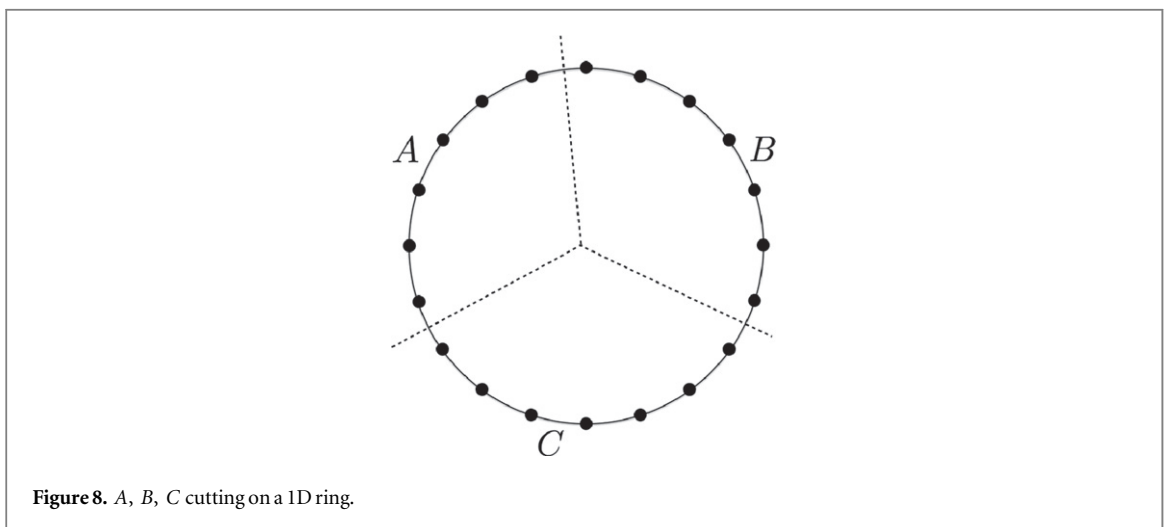
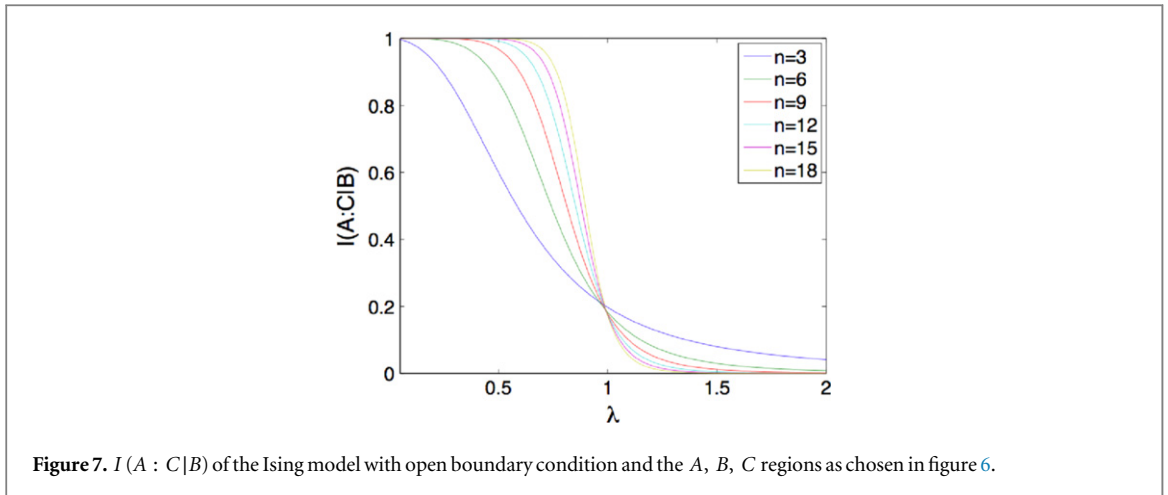
is a *local* transition without discontinuity of  $\rho^*(\lambda_z)$ . That is, when approached on the boundary of  $\mathcal{D}^{(k)}$ , from the direction corresponding to  $\lambda_z \rightarrow 0$ , the local RDMs of  $\rho^*(\lambda_z)$  has a sudden change at the point  $\lambda_z = 0$  (and significantly different for any two points each corresponding to  $\lambda_z < 0$  and  $\lambda_z > 0$ ). If we plot the diagram of  $I(A : C|B)$  for this model, we will not see any transition in the system.

We emphasize that the above approach employs calculations of extremely small systems yet still precisely signals the transition point of the corresponding system in the thermodynamic limit.

#### 4.3. The choice of regions $A$ , $B$ , $C$

It is important to note that the choice of the regions  $A$ ,  $B$ ,  $C$  should respect the locality of the system. If we consider one-dimensional system with open boundary condition, we can choose the  $A$ ,  $B$ ,  $C$  regions as in figure 6. For the transverse Ising model with open boundary condition, this choice will give a similar diagram of  $I(A : C|B)$  as in figure 5, which is given in figure 7. This clearly shows a discontinuity of  $\rho^*$  and a quantum phase transition at  $\lambda = 1$ .

However, if the partition in figure 6 is used for the Ising model with periodical boundary condition, as given in figure 8, the behaviour of  $I(A : C|B)$  will be very different. In fact, in this case  $I(A : C|B)$  reflects nothing but the 1D area law of entanglement, which will diverge at the critical point  $\lambda = 1$  in the thermodynamic limit. For a



finite system as illustrated in figure 9,  $I(A : C|B)$  does not clearly signal the two different quantum phases and the phase transition.

#### 4.4. $I(A : C|B)$ as a universal indicator

From our previous discussions, we observe that to use  $I(A : C|B)$  to detect quantum phase and phase transitions, it is crucial to choose the areas  $A$ ,  $C$  that are *far from each other*. Here ‘far’ is determined by the locality of the system. For instance, on a 1D chain, the areas  $A$ ,  $C$  in figure 6 are far from each other, but in figure 8 are not.

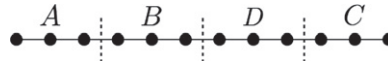


Figure 10.  $A, B, C, D$  cutting on a 1D chain.

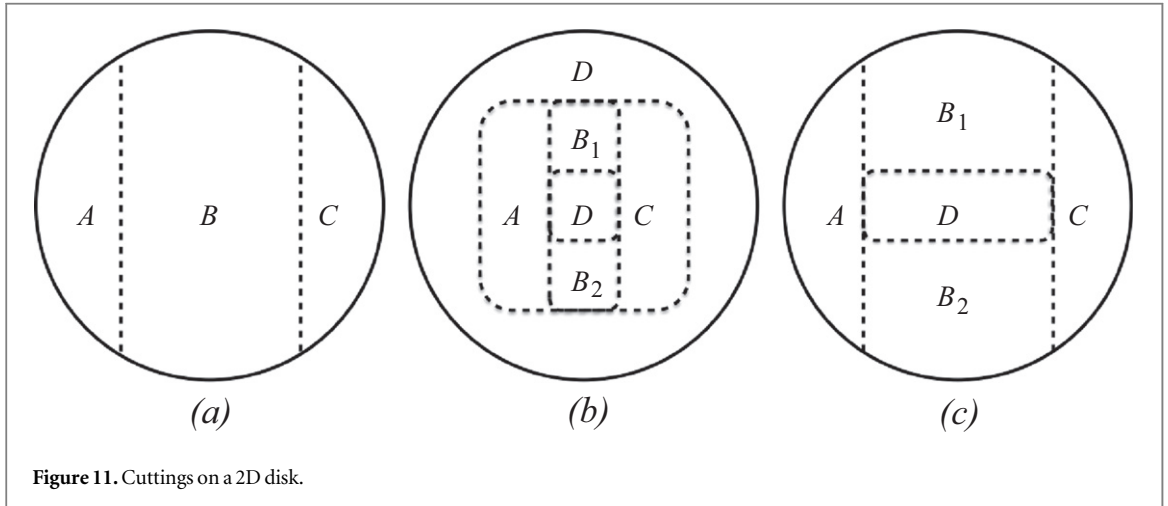


Figure 11. Cuttings on a 2D disk.

If such an areas  $A, C$  are chosen, then for a gapped system, a nonzero  $I(A : C|B)$  of a ground state will then indicates non-trivial quantum order. We have already demonstrated it using the transverse Ising model, where for  $0 < \lambda < 1$ , the system exhibits the ‘symmetry-breaking’ order. In fact, we can also use  $I(A : C|B)$  to detect other kind of non-trivial quantum orders.

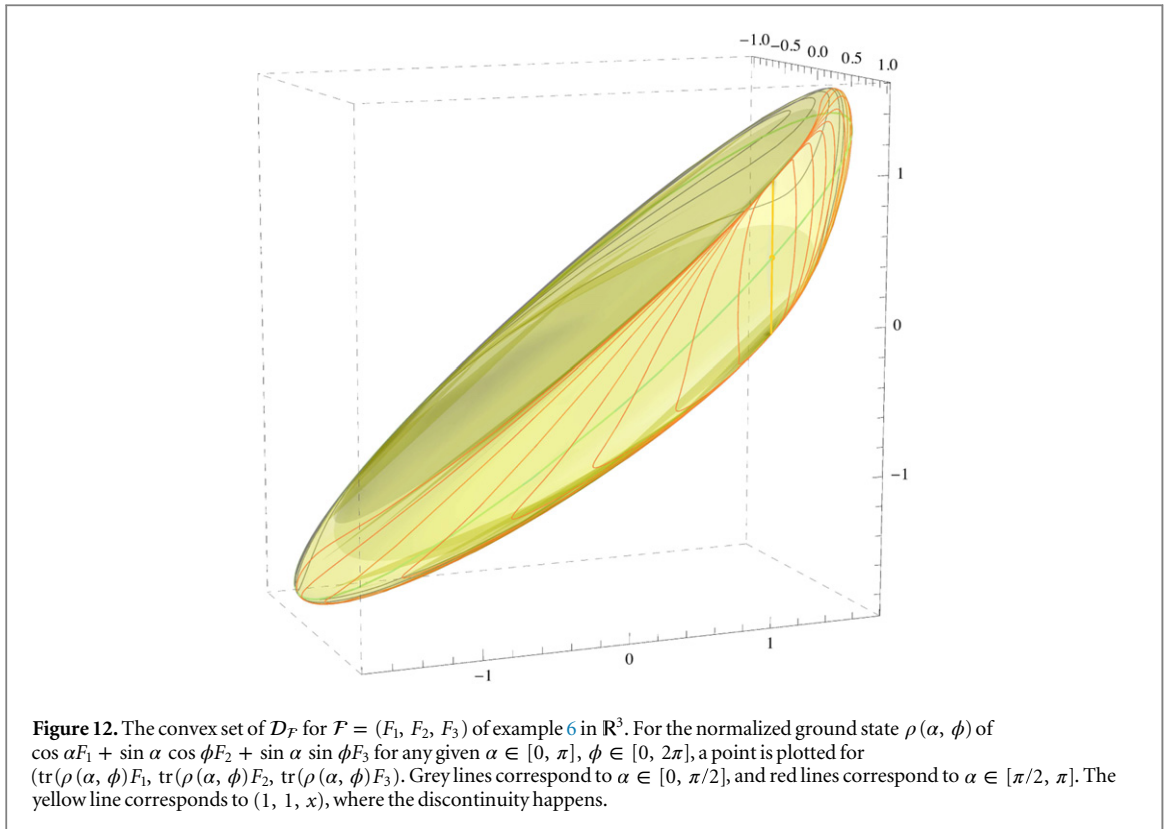
For instance,  $I(A : C|B)$  was recently applied to study the quantum phase transitions related to the so-called ‘symmetry-protected topological (SPT) order’, which also has a ‘nonlocal’ nature despite that the corresponding ground states are only short-range entangled (in the usual sense as discussed in this paper) [29].

It was shown that for a 1D gapped system on an open chain, a non-zero  $I(A : C|B)$  for the choice of the regions  $A, B, C$  as in figure 6 also detects non-trivial SPT order. However, it does not distinguish SPT order from the symmetry-breaking order. In stead, one can use a cutting as given in figure 10, where the whole system is divided into four parts  $A, B, C, D$ , and  $I(A : C|B)$  the detects the non-trivial correlation in the reduced density matrix of the state of  $ABC$ . Under this cutting,  $I(A : C|B)$  is zero for a symmetry-breaking ground state, but has non-zero value for an SPT ground state.

A similar idea also applies to 2D systems. For instance, for a 2D system on a disk with boundary, we can consider three different kinds of cuttings [13, 28, 29], as shown in figure 11. For each of these cuttings, a non-trivial  $I(A : C|B)$  detects different orders of the system. For figure 11(a),  $I(A : C|B)$  detects both symmetry-breaking order and SPT order and topological phase transitions [16]. Figure 11(b) is nothing but the choices of  $A, B, C$  to define the topological entanglement entropy by Levin and Wen [13], which detects topological order. And similarly as the 1D case, figure 11(c) detects SPT order, which distinguishes it from symmetry-breaking order (in this case  $I(A : C|B) = 0$  for symmetry-breaking order) [29].

In this sense, by choosing proper areas  $A, B, C$  with  $A, C$  far from each other, a non-zero  $I(A : C|B)$  universally indicates a non-trivial quantum order in the system. Furthermore, by analyzing the choices of  $A, B, C$ , it also tells which order the system exhibits (symmetry-breaking, SPT, topological, or a mixture of them).

We remark that, for a pure state, the cuttings of figures 4 and 6 give that  $I(A : C|B) = I(A : C)$ . However, this is not the case for a mixed state. Therefore, although one may be able to detect nontrivial quantum order simply using  $I(A : C)$ , in the most general case,  $I(A : C|B)$  is a universal indicator of a non-trivial quantum order but  $I(A : C)$  is not. For instance, the equal-weight mixture of the all  $|0\rangle$  and all  $|1\rangle$  states does not exhibit non-trivial order (i.e. contains no irreducible many-body correlation), hence  $I(A : C|B) = 0$  for the cuttings of figures 4 and 6, but  $I(A : C) \neq 0$ , which in fact indicates the classical correlation in the system.



**Figure 12.** The convex set of  $\mathcal{D}_{\mathcal{F}}$  for  $\mathcal{F} = (F_1, F_2, F_3)$  of example 6 in  $\mathbb{R}^3$ . For the normalized ground state  $\rho(\alpha, \phi)$  of  $\cos \alpha F_1 + \sin \alpha \cos \phi F_2 + \sin \alpha \sin \phi F_3$  for any given  $\alpha \in [0, \pi]$ ,  $\phi \in [0, 2\pi]$ , a point is plotted for  $(\text{tr}(\rho(\alpha, \phi)F_1), \text{tr}(\rho(\alpha, \phi)F_2), \text{tr}(\rho(\alpha, \phi)F_3))$ . Grey lines correspond to  $\alpha \in [0, \pi/2]$ , and red lines correspond to  $\alpha \in [\pi/2, \pi]$ . The yellow line corresponds to  $(1, 1, x)$ , where the discontinuity happens.

## 5. Further properties of the discontinuity

In this section, we further explore the structure associated with the discontinuity of the maximum entropy inference.

### 5.1. Path dependence of discontinuity

We continue our discussion of examples 1–3 in dimension 3, but with more than two observables. The following example illustrates that one may need to choose the right path in order to see the discontinuity of  $\rho^*$ . It is an example that combines examples 1 and 2 together.

**Example 6.** We consider the tuple  $\mathcal{F}$  of 3 operators, with  $F_1, F_2$  the same as given in example 1 and

$$F_3 = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & -1 \end{pmatrix}. \quad (23)$$

In this example,  $\mathcal{D}_{\mathcal{F}}$  is a compact convex set in  $\mathbb{R}^3$ . Consider the point  $\alpha = (1, 1, 0.5)$ . If  $\alpha$  is approached along the line  $[(1, 1, 0), (1, 1, 1)]$ , there is no discontinuity of  $\rho^*(\alpha)$ , similar as the discussion in example 2.

However, if  $\alpha$  is approached from  $\epsilon \rightarrow 0$  in a Hamiltonian  $-F_1 + \epsilon F_2$ , then there is discontinuity of  $\rho^*(\alpha)$ , similar as the discussion in example 1.

The convex set of  $\mathcal{D}_{\mathcal{F}}$  for  $\mathcal{F} = (F_1, F_2, F_3)$  in  $\mathbb{R}^3$  is shown in figure 12. This shows that if one approaches the yellow line (corresponding to  $(1, 1, x)$ ) from a line inside the red area of the surface, then discontinuity of  $\rho^*(\alpha)$  happens. But along the line  $[(1, 1, 0), (1, 1, 1)]$ , there is no discontinuity of  $\rho^*(\alpha)$ .

This example shows that, in general for  $k$  measurements, whether there is discontinuity of  $\rho^*(\alpha)$  at the point  $\alpha \in \mathcal{D}_{\mathcal{F}}$  depends on the direction on the boundary of  $\mathcal{D}_{\mathcal{F}}$  along which  $\alpha$  is approached. If there is a sequence  $\alpha_s$  approaching  $\alpha$  but

$$\rho^*(\alpha_s) \not\rightarrow \rho^*(\alpha), \quad (24)$$

then there is discontinuity of  $\rho^*(\alpha)$ .

The same situation can happen in example 4. If we approach the two-RDM  $\rho^{(2)}$  of the GHZ state using the ground states of  $H + \epsilon \sum_{i=1}^3 Z_i$  instead of  $H + \epsilon \sum_{i=1}^3 X_i$  as in example 4, there will be no discontinuity. And furthermore, for the Hamiltonian  $H + \epsilon_1 \sum_{i=1}^3 X_i + \epsilon_2 \sum_{i=1}^3 Z_i$ , the convex set of  $\mathcal{D}_{\mathcal{F}}$  for  $\mathcal{F} = (F_1, F_2, F_3)$  with  $F_1 = Z_1 Z_2 + Z_2 Z_3$ ,  $F_2 = \sum_{i=1}^3 X_i$ ,  $F_3 = \sum_{i=1}^3 Z_i$  has a similar structure as that in figure 12, as given in figure 1 (c) of [27]. Now consider the situation of the thermodynamic limit, corresponding to the transverse Ising model with also a magnetic field in the  $Z$  direction, i.e. the Hamiltonian

$$H(\lambda_x, \lambda_z) = -J \left( \sum_{i=1}^{n-1} Z_i Z_{i+1} + \lambda_x \sum_{i=1}^n X_i + \lambda_z \sum_{i=1}^n Z_i \right), \quad (25)$$

with  $J > 0$ . The corresponding convex set of  $\mathcal{D}_{\mathcal{F}}$  for  $\mathcal{F} = (F_1, F_2, F_3)$  with

$F_1 = \frac{1}{n-1} \sum_{i=1}^{n-1} Z_i Z_{i+1}$ ,  $F_2 = \frac{1}{n} \sum_{i=1}^n X_i$ ,  $F_3 = \frac{1}{n} \sum_{i=1}^n Z_i$  is quite different, as the line of discontinuity (similar as the line  $(1, 1, x)$  in figure 12) will expand to become a ‘ruled surface’ (see figure 1(b) of [27]), which is nothing but the symmetry-breaking phase [27] (this corresponds to the phase transition at  $\lambda = 1$ ).

Another interesting thing of example 6 is that the discontinuities of  $\rho^*(\alpha)$  do not only happen at the point  $\alpha = (1, 1, 0.5)$ . In fact they can happen at any point  $(1, 1, s)$  with  $(0 < s < 1)$ . This can be done by engineering the Hamiltonian

$$H = -F_1 + \epsilon F_2 + f(\epsilon) F_3, \quad (26)$$

with  $\lim_{\epsilon \rightarrow 0} \frac{f(\epsilon)}{\epsilon} = 0$  for some function  $f(\epsilon)$ . We remark that however, this does not happen in a similar situation of thermodynamic limit. For instance, the Hamiltonian  $H(\lambda_x, \lambda_z)$  discussed above only has one phase transition (discontinuity) point for  $\lambda > 0$  at  $(\lambda = 1)$  that corresponds to zero magnetic field in the  $Z$  direction (see figure 1(b) of [27]).

## 5.2. A necessary condition

Suppose  $\rho^*(\alpha_s) \rightarrow \tilde{\rho}$  when  $\alpha_s \rightarrow \alpha$ , then we must have  $\tilde{\rho} \in \mathcal{L}(\alpha)$ . That is,  $\tilde{\rho}$  returns the measurement results  $\alpha$ . If discontinuity happens at  $\alpha$ , state  $\tilde{\rho}$  is different from  $\rho^*(\alpha)$ . As the maximal entropy inference  $\rho^*$  has the largest range, the range of  $\tilde{\rho}$  is contained in that of  $\rho^*$ . We can then choose a linear combination of  $\rho^*$  and  $\tilde{\rho}$  in  $\mathcal{L}(\alpha)$  that has strictly smaller range than  $\rho^*$ . This then gives us a necessary condition for discontinuity of  $\rho^*(\alpha)$  in finite dimensions. We emphasize, however, that the same claim may not hold in infinite systems.

**Observation 2.** A necessary condition for the discontinuity of  $\rho^*(\alpha)$  at the point  $\alpha$  is that there exists a state  $\tilde{\rho} \in \mathcal{L}(\alpha)$  whose range is strictly contained in that of  $\rho^*(\alpha)$ .

In particular, for local measurements, we have

**Observation 2’.** A necessary condition for the discontinuity of  $\rho^*(\rho^{(k)})$  at the point  $\rho^{(k)}$  is that there exists a state  $\tilde{\rho} \in \mathcal{L}(\rho^{(k)})$  whose range is strictly contained in that of  $\rho^*(\rho^{(k)})$ .

To better understand observation 2’, we would like to examine an example where the condition is not satisfied.

**Example 7.** Consider again a three-qubit system, and the Hamiltonian

$$H = H_{12} + H_{23} \quad (27)$$

as discussed in [4], where  $H_{ij}$  acting nontrivially on qubits  $i, j$  with the matrix form

$$\begin{pmatrix} \frac{2}{9} & 0 & 0 & -\frac{4}{9} \\ 0 & \frac{2}{3} & 0 & 0 \\ 0 & 0 & \frac{2}{3} & 0 \\ -\frac{4}{9} & 0 & 0 & \frac{2}{9} \end{pmatrix}. \quad (28)$$

The ground-state space of the Hamiltonian  $H$  is two-fold degenerate and is spanned by

$$\begin{aligned} |\psi_0\rangle &= \frac{1}{\sqrt{6}}(2|000\rangle + |101\rangle + |110\rangle), \\ |\psi_1\rangle &= \frac{1}{\sqrt{6}}(2|111\rangle + |010\rangle + |001\rangle). \end{aligned}$$

Now take the maximally mixed state

$$\rho^* = \frac{1}{2}(|\psi_0\rangle\langle\psi_0| + |\psi_1\rangle\langle\psi_1|), \quad (29)$$

and its two-RDMs are  $\rho^{(2)}$ .

It is straightforward to check that there does not exist any rank 1 state in the ground-state space with the form  $\alpha|\psi_0\rangle + \beta|\psi_1\rangle$  that has the same two-RDMs as  $\rho^{(2)}$ . Therefore, for  $\rho^*$  ( $\rho^{(2)}$ ), the condition in observation 2' is not satisfied, hence no discontinuity at the point  $\rho^{(2)}$ .

In the previous subsection, we see that discontinuity of  $\rho^*(\alpha)$  at the point  $\alpha \in \mathcal{D}_{\mathcal{F}}$  depends on the direction approaching  $\alpha$ . The next example tells us that one can not conclude the existence of discontinuity by looking at the low dimensional projections of  $\mathcal{D}_{\mathcal{F}}$ .

**Example 8.** Consider the measurement of four operators, with  $F_1, F_2, F_3$  the same as given in example 6 and

$$F_4 = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (30)$$

And let  $\mathcal{F} = (F_1, F_2, F_3, F_4)$ .

Note that the projection of  $\mathcal{D}_{\mathcal{F}}$  to the plane spanned by  $(F_1, F_2)$  is nothing but figure 1(a), whose maximum entropy inference has discontinuity at the point  $(1, 1)$ . However, for the measurements  $\mathcal{F}$ , one can not conclude the existence of points of discontinuity by solely examining the discontinuity at its projections (e.g. the discontinuity for measuring  $(F_1, F_2)$  only). The existence of  $(F_3, F_4)$  does matter.

To see why, for the point  $\alpha = (1, 1, 0.5, 1)$ , the maximum entropy inference is  $\rho^*(\alpha) = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$ . However, there is no rank one state of the form  $\alpha|0\rangle + \beta|1\rangle$  with  $|\alpha|^2 + |\beta|^2 = 1$  that can return the measurement result  $\alpha$ . Then according to observation 2, there is in fact no discontinuity at  $\alpha$ .

### 5.3. A sufficient condition

Notice that the condition in observation 2 is not sufficient. Example 2 provides a counterexample. By studying the examples that do have discontinuity, we find a sufficient condition for the discontinuity of  $\rho^*$ .

**Observation 3.** For a set of observables  $\mathcal{F} = (F_1, \dots, F_r)$ , if:

- the ground state space  $V_0$  of some Hamiltonian  $H_0 = \sum_{i=1}^r c_i F_i$  is degenerate with the maximally mixed state supported on  $V_0$  be  $\rho^*$ , which corresponds to measurement results  $\alpha_i = \text{tr}(\rho^* F_i)$ ;
- there exists a basis  $|\psi_a\rangle$  of  $V_0$  such that

$$\langle\psi_a| F_i |\psi_b\rangle = \delta_{ab} \quad (31)$$

for any  $a \neq b$  and  $F_i \in \mathcal{F}$ ;

- there exists a sequence of

$$\epsilon = (\epsilon_1, \dots, \epsilon_r) \rightarrow (0, \dots, 0), \quad (32)$$

such that the Hamiltonian  $H = H_0 + \sum_{i=1}^r \epsilon_i F_i$  has unique ground states  $|\psi(\epsilon)\rangle$  at any nonzero  $\epsilon$ , and

$$\lim_{\epsilon \rightarrow (0, \dots, 0)} |\psi(\epsilon)\rangle = |\psi\rangle, \quad (33)$$

where  $|\psi\rangle = \frac{1}{\sqrt{m}} \sum_{a=1}^m |\psi_a\rangle$  and  $m$  is the ground state degeneracy of  $H_0$  ( $m > 1$ ); then  $\rho^*(\alpha)$  is discontinuous at the point  $\alpha$ .



**Table 1.** Summary of the relationship between the main concepts discussed in this paper.

Types of quantum phase transitions	Local	Non-local
Discontinuity of $\rho^*(\boldsymbol{\rho}^{(k)})$	No	Yes
Irreducible many-body correlations	No	Yes
Conditional mutual information	Zero	Nonzero

This condition guarantees that the state  $|\psi\rangle$  and the maximally mixed state  $\rho^*$  have the same local density matrices. The discontinuity of maximum entropy inference therefore follows when considering the sequence of reduced density matrices of  $|\psi(\boldsymbol{\epsilon})\rangle$ .

Notice that equation (31) is the quantum error-detecting condition for the error set  $\mathcal{F}$  but without the coherence condition of  $\langle\psi_a|F_j|\psi_b\rangle = c_j$  for  $a = b$  [10], where  $c_j$  is a constant that is independent of  $a$ . We will refer to this condition as the partial error-detecting condition.

For example, for the observables  $\mathcal{F} = (F_1, F_2, F_3)$  discussed in example 6, consider the ground-state space of  $H_0 = -F_1$ , which is degenerate and is spanned by  $\{|0\rangle, |1\rangle\}$ . It is straightforward to check that  $\langle 0|F_i|1\rangle = 0$  for all  $i = 1, 2, 3$ . Furthermore, the Hamiltonian  $H = -F_1 + \epsilon_1 F_2 + \epsilon_2 F_3$  has a unique ground state  $|\psi(\boldsymbol{\epsilon})\rangle$  at any nonzero  $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2) \neq 0$ . And for the sequence that  $\epsilon_2 = 0$  and  $\epsilon_1 \rightarrow 0$ ,  $\lim_{\epsilon_1 \rightarrow 0} |\psi(\epsilon_1, 0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ .

Similarly for local measurements, we have

**Observation 3'.** For a set of  $k$ -local observables  $\mathcal{F} = (F_1, \dots, F_r)$ , if:

- the ground state space  $V_0$  of some Hamiltonian  $H_0 = \sum_{i=1}^r c_i F_i$  is degenerate with the maximally mixed state supported on  $V_0$  be  $\rho^*$ , which corresponds to  $k$ -RDMS  $\boldsymbol{\rho}^{(k)}$ ;
- there exists a basis  $|\psi_a\rangle$  of  $V_0$  such that

$$\langle\psi_a|F_i|\psi_b\rangle = \delta_{ab} \quad (34)$$

for any  $a \neq b$  and  $F_i \in \mathcal{F}$ ;

- there exists a sequence of

$$\boldsymbol{\epsilon} = (\epsilon_1, \dots, \epsilon_r) \rightarrow (0, \dots, 0), \quad (35)$$

such that the Hamiltonian  $H = H_0 + \sum_{i=1}^r \epsilon_i F_i$  has unique ground states  $|\psi(\boldsymbol{\epsilon})\rangle$  at any nonzero  $\boldsymbol{\epsilon}$ , and

$$\lim_{\boldsymbol{\epsilon} \rightarrow (0, \dots, 0)} |\psi(\boldsymbol{\epsilon})\rangle = |\psi\rangle, \quad (36)$$

where  $|\psi\rangle = \frac{1}{\sqrt{m}} \sum_{a=1}^m |\psi_a\rangle$  and  $m$  is the ground state degeneracy of  $H_0$  ( $m > 1$ ); then  $\rho^*(\boldsymbol{\rho}^{(k)})$  is discontinuous at the point  $\boldsymbol{\rho}^{(k)}$ .

For example, for the observables  $\mathcal{F} = (F_1, F_2, F_3)$  with  $F_1 = Z_1 Z_2 + Z_2 Z_3$ ,  $F_2 = \sum_{i=1}^3 X_i$ ,  $F_3 = \sum_{i=1}^3 Z_i$  discussed in example 4, consider the ground-state space of  $H_0 = -F_1$ , which is degenerate and is spanned by  $\{|000\rangle, |111\rangle\}$ . It is straightforward to check that  $\langle 000|F_i|111\rangle = 0$  for all  $i = 1, 2, 3$ . Furthermore, the Hamiltonian  $H = -F_1 + \epsilon_1 F_2 + \epsilon_2 F_3$  has a unique ground state  $|\psi(\boldsymbol{\epsilon})\rangle$  at any nonzero  $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2) \neq 0$ . And for the sequence that  $\epsilon_2 = 0$  and  $\epsilon_1 \rightarrow 0$ ,  $\lim_{\epsilon_1 \rightarrow 0} |\psi(\epsilon_1, 0)\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$ .

These demonstrate an intimate connection between the discontinuity of  $\rho^*(\boldsymbol{\rho}^{(k)})$  and the (partial) quantum error-detecting condition.

## 6. Summary and discussion

We now summarize the main results this paper in table 1. We start from introducing two natural types of quantum phase transitions: a local type that can be detected by a non-smooth change of local observable measurements, and a non-local type which can not. We then further show that the discontinuity the maximum entropy inference  $\rho^*(\boldsymbol{\rho}^{(k)})$  detects the non-local type of transitions. We have done this by examining the convex set  $\mathcal{D}^{(k)}$  of the local reduced density matrices  $\boldsymbol{\rho}^{(k)}$ , where the discontinuity of  $\rho^*(\boldsymbol{\rho}^{(k)})$  only happens on the

**Table 2.** Summary of the choices of the areas of  $A$ ,  $B$ ,  $C$  (in different figures) and the non-trivial indicator  $I(A : C|B)$  for different quantum order. Here ‘yes’ means a non-zero value of  $I(A : C|B)$ .

	Figure 4 or 6 or 11(a)	Figure 11(b)	Figure 10 or 11(c)
Symmetry-breaking order	Yes	No	No
Topological order	No	Yes	No
SPT order	Yes	No	Yes

boundary of the convex set, hence is directly related to the ground states of local Hamiltonians (hence zero temperature physics). And essentially, the discontinuity only happens at the transition points.

We further show that the discontinuity of  $\rho^*(\rho^{(k)})$  is in fact related to the existence of irreducible many-body correlations. This allows us to propose a practical method for detecting the non-local type of transitions by the quantum conditional mutual information of two disconnected parts, which is an analogy of the Levin–Wen topological entanglement entropy [13]. We have demonstrated how the conditional mutual information detects the phase transition in the transverse Ising model and the toric code model, which are both continuous quantum phase transitions.

Based on the connection between irreducible many-body correlation and the quantum conditional mutual information  $I(A : C|B)$ , we have proposed that  $I(A : C|B)$  as a universal indicator of non-trivial quantum order of gapped systems. The crucial part is to choose that the areas  $A$ ,  $C$  that are far from each other, based on the locality of the system. By choosing proper regions to compute  $I(A : C|B)$ , one can indeed further tell the type of the phase transition (symmetry-breaking, topological, SPT, or a mixture of them). We summarize these different indicators in table 2.

We remark that a non-zero  $I(A : C|B)$  even contains information for a gapless system. By choosing different ratios of the lengths (areas) of  $A$ ,  $B$ ,  $C$ , the value  $I(A : C|B)$  of a gapless system could vary, and the dependence of  $I(A : C|B)$  with those ratios is closely related to universal quantities of the system, such as the central charge [28]. We hope that our discussion brings new links between quantum information theory and condensed matter physics.

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## References

- [1] Bardeen J, Cooper L N and Schrieffer J R 1957 Microscopic theory of superconductivity *Phys. Rev.* **106** 162–4
- [2] Bernevig B A, Hughes T L and Zhang S-C 2006 Quantum spin hall effect and topological phase transition in hgte quantum wells *Science* **314** 1757–61
- [3] Castañón O, López-Peña R, Nahmad-Achar E and Hirsch J G 2012 Quantum information approach to the description of quantum phase transitions *J. Phys.: Conf. Ser.* **403** 012003
- [4] Chen J, Ji Z, Kribs D, Lütkenhaus N and Zeng B 2014 Symmetric extension of two-qubit states *Phys. Rev. A* **90** 032318
- [5] Gu S-J 2010 Fidelity approach to quantum phase transitions *Int. J. Mod. Phys. B* **24** 4371–458
- [6] Hastings M B 2010 Locality in quantum systems arXiv:1008.5137
- [7] Jaynes E 1957 Information theory and statistical mechanics *Phys. Rev.* **106** 620–30
- [8] Kim I H 2014 On the informational completeness of local observables arXiv:1405.0137
- [9] Knauf A and Weis S 2012 Entropy distance: new quantum phenomena *J. Math. Phys.* **53** 102206
- [10] Knill E and Laflamme R 1997 Theory of quantum error-correcting codes *Phys. Rev. A* **55** 900
- [11] König M, Wiedmann S, Brüne C, Roth A, Buhmann H, Molenkamp L W, Qi X-L and Zhang S-C 2007 Quantum spin hall insulator state in hgte quantum wells *Science* **318** 766–70
- [12] Laughlin R B 1983 Anomalous quantum hall effect: an incompressible quantum fluid with fractionally charged excitations *Phys. Rev. Lett.* **50** 1395–8
- [13] Levin M and Wen X-G 2006 Detecting topological order in a ground state wave function *Phys. Rev. Lett.* **96** 110405
- [14] Lieb E H and Ruskai M B 1973 Proof of the strong subadditivity of quantum-mechanical entropy *J. Math. Phys.* **14** 1938–41
- [15] Linden N, Popescu S and Wootters W K 2002 Almost every pure state of three qubits is completely determined by its two-particle reduced density matrices *Phys. Rev. Lett.* **89** 207901
- [16] Liu Y, Zeng B and Zhou D L 2014 Irreducible many-body correlations in topologically ordered systems arXiv:1402.4245
- [17] Nagy Á and Romera E 2015 Relative Rényi entropy and fidelity susceptibility *Europhys. Lett.* **109** 60002

- [18] Pankratov O A, Pakhomov S V and Volkov B A 1987 Supersymmetry in heterojunctions: band-inverting contact on the basis of pb1-xsnxte and hg1-xcdxte *Solid State Commun.* **61** 93–96
- [19] Pfeuty P 1970 The one-dimensional Ising model with a transverse field *Ann. Phys., NY* **57** 79–90
- [20] Rodman L, Spitkovsky I M, Szkoła A and Weis S 2015 Continuity of the maximum-entropy inference: convex geometry and numerical ranges approach arXiv:1502.02018
- [21] Romera E and Nagy Á 2013 Density functional fidelity susceptibility and Kullback–Leibler entropy *Phys. Lett. A* **377** 3098–101
- [22] Sachdev S 2007 *Quantum Phase Transitions* (New York: Wiley)
- [23] Weis S 2011 Quantum convex support *Linear Algebr. Appl.* **435** 3168–88
- [24] Wichmann E H 1963 Density matrices arising from incomplete measurements *J. Math. Phys.* **4** 884–96
- [25] Zanardi P, Giorda P and Cozzini M 2007 Information-theoretic differential geometry of quantum phase transitions *Phys. Rev. Lett.* **99** 100603–100603
- [26] Zanardi P and Paunković N 2006 Ground state overlap and quantum phase transitions *Phys. Rev. E* **74** 031123
- [27] Zauner V, Vanderstraeten L, Draxler D, Lee Y and Verstraete F 2014 Symmetry breaking and the geometry of reduced density matrices arXiv:1412.7642
- [28] Zeng B and Wen X-G 2015 Stochastic local transformations, emergence of unitarity, long-range entanglement, gapped quantum liquids, and topological order *Phys. Rev. B* **91** 125121
- [29] Zeng B and Zhou D-L 2014 Topological and error-correcting properties for symmetry-protected topological order arXiv:1407.3413
- [30] Zhou D L 2008 Irreducible multiparty correlations in quantum states without maximal rank *Phys. Rev. Lett.* **101** 180505