Quantum phase transition in a two-dimensional quantum Ising model: Tensor network states and ground-state fidelity

Sheng-Hao Li¹, Guo-Ping Lei²

¹Chongqing Vocational Institute of Engineering, Chongqing 402260, China
²College of Electronic and Information Engineering, Chongqing Three Gorges University, Chongqing 404000, China
shenghaoli@cqu.edu.cn

Abstract. The purpose of this paper is to describe how to describe the phase transition of quantum multibody system from the perspective of the basic concept of quantum information science - fidelity. For systems the traditional way of characterization that undergo a quantum phase transition is Landau's introduction of order and the fluctuation. In particular, for phase transitions caused by spontaneous breaking symmetry, that is, different ground state wave functions are orthogonal to each other. This suggests that, contrary to the ups and downs of traditional expressions, the concept of irrelevant information and vital information can be introduced. By introducing the basic amount of ground lattice fidelity, quantifying irrelevant information and critical information which can identify the quantum phase transition of the system. It is worth emphasizing that no matter the internal order of quantum multibody systems is a traditional symmetry or other novel quantum order, they all can be applied such as topological order, single-grid ground state fidelity. In order to efficiently calculate the single-grid ground state fidelity of quantum multibody systems, tensor network algorithm is needed. This kind of algorithm is the result of the deepening of quantum entanglement in recent years. Quantum entanglement expounds the working principle of real-space renormalization group algorithm, especially density matrix re-grouping algorithm.

1. Introduction

In recent decades, strong correlation electronic systems are one of the key and difficult points of condensed matter physics research, and high temperature superconductors are the most important and most challenging branch of strong correlation electronic system research. The quantum phase transformation is driven by the quantum fluctuation caused by the uncertainty relation, and the phase changed to occur to the change of the control parameter at the absolute zero temperature. The quantum phase transition is characterized by the singularity of the ground state energy. The first order transition is represented by the singularity of the energy first orders partial derivative, while the continuous phase change is expressed as the second order (or higher order) discontinuity. At the singular point, the spectrum is incompetent. So far, quantum transitions that have been extensively studied that can be described by the symmetry spontaneous breaking order of the Landau-Ginzburg-Wilson (LGW) paradigm. Symmetry spontaneous breakage is a unique property that exists only in infinite degrees of freedom system. However, not all phases can be described by symmetric broken order, and the corresponding quantum phase transitions go beyond the LGW paradigm[1-4]. A simple example is the spin chain described by the local Hamiltonian, whose ground state waved function can be represented...
by the matrix multiplication state, but its ground state energy is analytic and thus presents a quantum phase transition beyond the standard paradigm[5].

Quantum information science provides a new perspective for the study of quantum phase transition - its focus is shifted from energy spectrum to wave function. Once the ground state wave function of a quantum multibody system is obtained, the inner order of its intrinsic can be characterized from the perspective of quantum information science. In fact, cross-study of quantum multibody theory and quantum information science has led to a number of striking results, one of which is entangled in the role of characterizing the quantum phase transition. On the other hand, as another basic concept of quantum information science, fidelity has a more fundamental role in the characterization of quantum phase transition. As a measure of the distance between two quantum states, fidelity describes the similarity between the two quantum states. Thus, it is expected that the fidelity exhibits a dramatic change when the system undergoes a quantum phase transition. This suggests that, contrary to the ups and downs of traditional expressions, the concept of irrelevant information and vital information can be introduced. Based on the basic amount of ground-based fidelity[6], the quantified irrelevant information and critical information can be used to identify the unstable and stable fixed points of the renormalized group flow. Thus, regardless of whether the internal order of quantum multibody system is a traditional symmetry broken order or other novel quantum order, such as topological order, single grid ground state fidelity they all can be applied.

Therefore, in order to study the quantum criticality of multi-body system from the perspective of single-grid ground-stated fidelity, it is necessary to develop a numerical algorithm for efficiently generating the ground state wave function of quantum multibody system and calculate the fidelity of single ground. On the other hand, many of the exciting discoveries in the field of condensed matter over the past few decades have shown us the quantum criticality of novel phenomena such as various magnetic ordering, integer and fractional quantum Hall effects and high temperature superconductivity a very rich quantum world. However, the quantum criticality is still one of the most challenging basic problems of the field of condensed matter. The reason for this is that the quantum state space of the multi-body has strong correlation system which shows such rich quantum critical phenomena increases exponentially with the system size. This brings the so-called Exponential wall of divergence. This means that numerical processing is bound to face the choice of state space and cut off it.

In recent years, with the deepening of the understanding of quantum entanglement, people have developed a variety of efficient tensor network algorithm. Since this algorithm does not have a negative sign problem, it is applicable to both the Bose subsystem and the Fermi subsystem and the spinstrapping system. Historically, the tensor network algorithm has been derived from the study of Baxter[7] on the classical lattice statistical model. It can be proved[8], as long as the interaction form is local, the classical lattice statistical model problem can be turned into tensor network research, that is, its parting function can be written as a series of tensor product form.

2. iPEPS tensor network algorithm
The development of the matrix product in the one - dimensional case promotes the thinking of the wave function of the high-dimensional quantum multi - body system. As a natural idea, Tensor Product State (TPS) is expected to be a representation of the high-dimensional quantum system wave function. In the two-dimensional lattice system, from the tensor network structure in the system and the environment boundary we can happily find that the boundary itself represents the size of the system, and each cut the tensor keys to carry their own degrees of freedom. The Projected Entangled-pair State (PEPS)[9] contains two parts: the entangled state and the projection operator. In a V grid system, the performance of Matrix Product State (MPS); in the two-dimensional lattice system, that is, TPS, as shown in Fig 1. PEPS describes the construction of a class of wave functions, the expression can be lattice-dependent, that is, the matrix or tensor in the product can be different. Correspondingly, infinite PEPS (iPEPS) describes a system with translation invariance, the same as the tensor of each grid or each constituent element.
Fig. 1: General form of PEPS construction. (a) The tensor on the square grid multiplied by the state, oblique corresponding to the physical indicators. (b) The PEPS representation of the ground state of the quantum model. (c) Four additional degrees of freedom are introduced for each grid point. Each two adjacent auxiliary degrees of freedom in the graph form a maximum entangled state, represented by a key, with a projection operator $P$ on each grid point.

A two-dimensional quantum grid model is used to solve a two-dimensional quantum grid model. There are two methods: one is the classical simulation, and the two-dimensional quantum model is mapped to the three-dimensional classical statistical model. The quantum model is solved by solving the problem. Dimensional model of the classical model; the second is the quantum simulation, that is, we first find the tensor network state representation of the ground state wave function, so that the calculation of the physical quantity observable value is solved by a two-dimensional classical partition function. The quantum simulation of the tensor network algorithm consists of two steps. One is the solution of the ground state wave function. In general, the tensor network representation of the ground state wave function is always assumed, and then the true ground state wave function is obtained by adiabatic evolution or variational method. For the adiabatic evolution method, as long as the initial wave function is not orthogonal to the true ground state wave function, the ground state wave function can always be obtained by evolution. The second is the solution to the desired value. Once the tensor network state representation of the wave function is obtained, the expected value of the physical observable value can be expressed as the expression of the required physical quantity operator.

A transfer matrix is applied to a random given TPS wave function without increasing the virtual dimension of the wave function, and the maximum eigenstate of the transfer matrix are obtained. This is exactly the idea of iPEPS to solve the ground state of two-dimensional quantum lattice model. In principle, the algorithm can not only deal with two-dimensional quantum wave function real-time and virtual time evolution, but also can deal with three-dimensional classical model. Specifically, for the two-dimensional quantum lattice model, the general steps of iPEPS are: (1) Represent the partition function as a form of quantum transfer matrix. As shown in Fig. 2, the base state of the model is solved into the largest problem of them. (2) The transfer matrix $T$ (which is an infinite tensor network operator) acts on any given PEPS wave function $|\psi_0\rangle$ to obtain a two-dimensional wave function $|\psi_1\rangle = T |\psi_0\rangle$. (3) Using the above solution of the variational equation, we get an optimal low-dimensional approximation of the pair $|\psi_2\rangle \sim |\psi_1\rangle$. (4) Repeat steps (2) - (3) until the wave functions converges gets to a preset accuracy. The convergent wave function $|\psi_c\rangle$ at this time is the ground state wave function of the quantum model.
Fig. 2: Transfer matrix representation in two-dimensional quantum lattice model.

Fig. 3: PEPS wave function representation and Norm form. (i) A PEPS tensor $A_{sudlr}$ with one physical index $s$ and four inner indices; (ii) Local detail of the tensor network $P$ for an iPEPS. (iii) A double tensor $q$ is formed from the tensor $A_{sudlr}$ and its complex conjugate $A^*$; (iv) The TN representation for the norm of a ground-state wave function.

Using the convergence of the ground state wave function $|\phi\rangle = |\psi\rangle$ obtained in the above scheme, the calculation of the physical quantity expected value can be completed $\langle \phi | \hat{o} | \phi \rangle$.

The tensor of the operator $\hat{o}$ is shown in Fig. 2. The meaning of the numerator is that the two ground state tensor network wave functions and the operator's tensor network representation is summed by the physical index, and the denominator is the two ground state tensor network wave function physical index summation. Thus, after the physical index shrinks, the numerator denominator calculations become two two-dimensional tensor mesh shrinkage problems. The denominator's representation $|\phi\rangle$ can be seen in Fig. 3, where the concrete form are the concrete operator that connects the two tensor grids involved in the denominator through physical indicators. For an infinite-size system, it is also possible to use the idea of a transfer matrix to treat the two-dimensional grid as an one-dimensional vertical transfer matrix. The one-dimensional transfer matrix contains an infinite number of lattice points whose matrix dimensions are exponential functions of these lattice dimensions. We cannot give the maximum eigenvalue and eigenvector of the transfer matrix. However, we can use the transfer matrix to evolve any initial wave function that does not intersect with its maximum eigenvector into the largest eigenvector, which is also the result of Vidal et al. For the MPS regularization of the processing ideas [10]. So that the corresponding eigenvalues can be used to derive the grid shrinkage results.

3. Numerical simulation results
Consider a quantum system $S$, the Hamiltonian is $H(h)$, where $h$ is a control parameter that adjusts its size to drive the system to phase change. At zero temperature, the system is in ground state. For a system that undergoes a quantum phase transition, the traditional way of characterization is Landau's
introduction to the order and the fluctuation: at the point of change, the fluctuation is so strong that the order can not survive; when deviating from the transformation point, the presence of the fluctuation is not enough to make the order disappear. In this way, we can quantify the fluctuation and order by introducing (local/nonlocal ) order parameters.

The occurrence of order parameters is equivalent to the orthogonality of two different ground state wave functions. For a system experiencing a quantum phase transition, any two representative ground states \( \phi \) and \( \phi' \) satisfy \( \langle \phi | \phi' \rangle = 0 \), that is, fidelity \( F(\phi, \phi') = |\langle \phi | \phi' \rangle| \) is zero. From the basic assumptions of quantum mechanics on quantum mechanics, two orthogonal states can not be reliably distinguished. In fact, if two non-orthogonal states can be reliably differentiated, then the superluminal communication is allowed. This is contrary to the causality of relativity. According to the traditional phase expression of quantum phase transition and order, whether the two states are in the same phase depends on the quantitative or qualitative difference represented by the order parameter: the orthogonality of the two states in the same phase is derived from the order. The difference between the quantitative differences of the parameters, which is related to the short-range details of the system. The orthogonality of the two states in different phases is derived from the separability of the qualitative differences in the ordered parameters, reflecting the long- behavior. Due to the consideration of universality, the long-range behavior of a system does not depend on its short-range detail, so that any two ground states in the same phase have the same long-range behavior, and their differences are described by short-range details. This means that, from the perspective of quantum information science, the concept of quantum phase transformation can be introduced to introducing critical information and critical information. Critical information/non-critical information is long-range/short-range information embedded in a given ground state. Thus, the same phase of the same state of the same vital information and different irrelevant information, and different phase of the state has a different vital information.

Another description of the quantum phase transition is the renormalization group theory, whose transformation point is characterized by the unstable fixed point of the renormalized group flow, while the ordered state is characterized by a stable fixed point: all of the phases state flows to a stable fixed point. Along the heavy group, high energy degrees of freedom are gradually accumulated, while the low degree of freedom is retained. Thus, irrelevant information and critical information correspond to high energy degrees of freedom and low energy degrees of freedom, respectively.

In order to characterize quantum phase transformation with fidelity, it is necessary to quantify irrelevant information and vital information. We know that the continuous transformation of quantum multibody systems occurs only to thermodynamic limits. However, at the thermodynamic limit, the fidelity of any two different ground states must disappear. Only from this point of view, ground state fidelity lack luster. In order to refine the meaningful physical information, we will system on the different size of the limited lattice on the system fidelity to the size of the scale of \( L \) behavior. Unlike the thermodynamic limit, the fidelity to a finite-size system does not disappear, but decreases with the system size \( L \). That is, fidelity \( F(h, h') \) can be expressed as \( [d(h, h')]^L \) \(^{[11]} \), where \( 0 \leq d(h, h') \leq 1 \), the scale parameter is characterized by the fact that the fidelity varies from \( L \) when approaching the thermodynamic limit. This scale parameter \( d(h, h') \) is defined \( \ln d(h, h') = \lim_{L \to \infty} F(h, h') / L \) under the thermodynamic limit, and its physical representation is the average fidelity of each grid. In fact, the average fidelity of each lattice can be regarded as a partition function of a single grid point of a classical statistical vertex model defined on the same grid. This explains why the single-grid grounded state fidelity can be used to detect the cause of quantum phase transformation.

In this paper, we discuss how to use quantum fidelity to describe the phase transition and the correspondence with the traditional quantum phase transformation. Infinite lateral magnetic field two-dimensional square lattice quantum Ising model with Hamiltonian

\[
H = - \sum_{\langle i, j \rangle} \sigma_i^x \sigma_j^x + \lambda \sum_i \sigma_i^z.
\]
Where the $i$-th lattice has a Pauli operator $\sigma_{\alpha}^i (\alpha = x, z)$ with a spin of $1/2$, and $<i,j>$ denotes that all nearest neighbors on the square grid are the additional lateral magnetic fields $\lambda$ as control parameters. In this case, $\sigma_{x}^i \rightarrow -\sigma_{x}^i$ and $\sigma_{z}^i \rightarrow -\sigma_{z}^i$, the Hamiltonian of the two-dimensional Ising modelling is invariant, indicating that the Hamiltonian of the two-dimensional Ising modelling has a symmetric invariance of the $Z_2$ group. With the change of control parameters $\lambda$, the two-dimensional Ising model undergoes a second-order quantum phase transition.

In Fig. 4, the iPEPS tensor mesh algorithm is used to simulate the infinite two-dimensional square lattice quantum Ising model with spin of $1/2$, and the fidelity graph of the ground lattice is obtained. A two-dimensional fidelity surface in a three-dimensional Euler space can show a pinch point, indicating that there is a continuous phase change. Here, the phase transition point is $\lambda_D$, $D$ is the truncated dimension in the iPEPS tensor network representation, and when the truncation dimension $D$ increases from 2 to 3, Fig. 4 shows little change.

In Fig. 5, the iPEPS tensor grid algorithm is used to simulate the infinite two-dimensional square lattice quantum Ising model with spin of $1/2$. The two-dimensional quantum Ising modelling is obtained by spontaneous symmetry breaking. And the bifurcation of the ground fidelity to the two-point reduced density matrix is the phase transition point. It is obvious that with the increase of the truncated dimension $D$ in the iPEPS algorithm, the critical sub-critical point tends to the true quantum critical point, that is, when $D = 2$, the phase transition point is $\lambda_D = 3.100$, and when $D = 3$, the phase transition point is $\lambda_D = 3.065$, and when $D = 4$, the phase transition point is $\lambda_D = 3.050$. Compare with the Quantum Monte Carlo (QMC) method, we obtain the quantum critical point $\lambda_c \sim 3.044^{[12]}$, which shows that the iPEPS algorithm is reliable under the absolute zero and thermodynamic limits.

![Fig. 4: The ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, as a function of $\lambda_1$ and $\lambda_2$ for two ground states of the two-dimensional quantum Ising model with truncation dimension $D=2$. The fidelity surface clearly indicates that there is a transition point, as a pinch point occur at $\lambda_D = 3.100$. The gray line denotes the normalization $d(\lambda, \lambda) = 1$.](image-url)
Fig. 5: (Upper panel) The ground-state one-site reduced fidelity, $F(\rho_1, \rho_2)$, for quantum Ising model in a transverse field on a square lattice in two spatial dimensions. (Lower panel) The ground-state two-site reduced fidelity, $F(\rho_{12}, \rho_{12})$, for quantum Ising model in a transverse field on a square lattice. Here, we have chosen $\rho_{12}$ as the reference state, with $\lambda_2 = 2.1$ in the $Z_2$ symmetry-broken phase. A phase-transition point occurs as a bifurcation point.

4. Conclusion
This paper briefly introduces the tensor network algorithm which can provide a powerful numerical means to calculate the single-grid ground state fidelity of the quantum multibody system, so that we can determine the ground state phase diagram under the premise that the order of the quantum system is not understood. It should be noted that this applies not only to the LGW paradigm of symmetry to the spontaneous breaking sequence described by the quantum phase transformation, but also to other novel quantum sequences, such as the topological sequence depicted by the phase transition. In addition to the quantum spin lattice system, the tensor network algorithm is equally applicable to the Fermi sub-lattice multi-body system$^{[13,14]}$. Therefore, it can be expected that with the further development of tensor network algorithm, the single-point fidelity theory of quantum phase transition is expected to be applied to all kinds of quantum multi-body systems of condensed matter physics, which deepens our understanding of the quantum world of the state.

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References
[1] Wen X-G, Quantum Field theory of many-body systems, Oxford university press, (2004)
[2] Wen X-G and Wu Y-S, Phys. Rev. Lett., 1993, 70:1501; Senthil T, Marston J B and Fisher M P A, Phys. Rev.B, 1999, 60:4245
[3] Senthil T, Vishwanath A, Balents L, Sachdev S, Fisher M P A, Science, 2004, 303: 1490
[4] Ran Y, Wen X G. Phys. Rev. Lett. 2006, 96: 026802
[5] Wolf M, Ortiz G, Verstraete F, and Cirac J I, Phys. Rev.Lett. 2006, 97: 110403
[6] Zhou H Q, Orus R, Vidal G, Phys. Rev. Lett., 2008, 100:080601
[7] Baxter R J, Exactly Solved Models in Statistical Mechanics (Academic Press, London, 1982)
[8] Murg V, Verstraete F, Cirac J I, Phys. Rev. A, 2007, 75: 033605
[9] Nishino T, Heida Y, Okunishi K, Maeshima N, Akutsu Y, and Gendiar A, Prog. Theor. Phys., 2001, 105: 409
[10] Orus R, Vidal G, Phys. Rev. B, 2008, 78:155117
[11] Zhou H Q, Barjaktarević, J. Phys. A: Math. Theor., 2008, 41: 412001
[12] H. W. J. Blote and Y. Deng, Phys. Rev. E, 2002, 66: 066110
[13] Li S H, Shi Q Q, Zhou H Q, arXiv: 1001.3343
[14] Tagliacozzo L, Vidal G, Phys. Rev. B, 2011, 83:115127