Bell Function Values Approach to Topological Quantum Phase Transitions

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We investigate the relation between Bell function values (BFV) of the reduced density matrix and the topological quantum phase transitions in the Kitaev-Castelnovo-Chamon model. We find that the first order derivative of BFV exhibits singular behavior at the critical point and we propose that it can serve as a good and convenient marker for the transition point. More interestingly, the value of the critical point can be analytically obtained in this approach. Since the BFV serves as a measure of nonlocality when it is greater than the classical bound of the correlation functions, our work has established a link between quantum nonlocality and phase transitions.

Topological phase of some strongly correlated quantum many body systems is a new kind of order that depends on the system topology. It has attracted great interest recently because it can exhibit remarkable phenomena such as quasiparticles with anyonic statistics. An archetypal physical realization of such phase is in the quantum Hall system, which bears many unconventional characteristics, such as fractional statistical behaviors and ground state topological degeneracy that cannot be lifted by any local perturbations. A particular interest in topological ordered states is their robustness against local perturbations which can lead to several consequences such as topological insulators and topological quantum computations.

Not surprisingly, the unconventional properties of topological phase might result in exotic critical phenomena, which cannot be characterized by the Landau-Ginzburg-Wilson spontaneous symmetry-breaking theory where the correlation function of local order parameters plays a crucial role. For example, the quantum phase transition between an Abelian and a non-Abelian topological phase in chiral spin liquid might be characterized by global flux and generalized topological entanglement entropy. More remarkably, for time-reversal invariant anyonic quantum systems, Gils et al., have recently showed that the topological phases could be uniformly described in terms of fluctuations of the two-dimensional surfaces and their topological changes. However, an universal characterization and detection of topological phase and its transitions still pose a big challenge despite a vast amount of prominent works dealing with this problem.

During the past few years, several important concepts in the quantum information field have been borrowed to characterize quantum phase transitions (QPTs) and topological quantum phase transitions (TQPTs), these including entanglement, fidelity, fidelity susceptibility, and discord, etc. A brief review of the progress related to this issue is given in Ref. and references therein. Notwithstanding the great successes in marking QPTs and TQPTs in some physical systems, each approach above has its own disadvantages. Take the fidelity approach for example, to witness the QPTs, one has to find out the exact ground state. However, for most of the physical systems, finding out the exact ground state is very difficult. In addition, it is also a challenge to measure the fidelity in experiment on scalable systems. An alternative choice is to use Bell function values (BFV) as defined in expression below, which indicates the correlations of a quantum system and measures quantum nonlocality when it is greater than the classical bound of the correlation functions. Actually, besides entanglement, quantum nonlocality is also a central nonintuitive phenomena of quantum mechanics and it plays a key role in many quantum information and computation processes, such as quantum key distribution (QKD), nonlocal quantum computation, etc. Naturally, one would ask whether nonlocality can mark QPTs and TQPTs?

In this Letter, we propose the use of BFV as the marker of TQPTs and provide a positive answer to the above question by investigating the relation between BFV of the reduced density matrix and the TQPTs. The motivation for choosing BFV is two-fold: (i) BFV can measure the nonlocality of a quantum system, thus it might establish a connection between nonlocality and TQPTs, which belong to two different aspects; (ii) To get the BFV in an experiment scheme, one only has to do some measurement on the qubits instead of knowing exactly the ground state. Thus, our approach has its advantages in experimental schemes. The discussion here is mainly based on the Kitaev-Castelnovo-Chamon model, which exhibits a second-order TQPT at the critical point. Our results indicate that the first order derivative of BFV...
shows singular behavior at the transition point. More interestingly, through this approach, one can analytically obtain the critical value of the transition point. Finally, using BFV to signal TQPTs and QPTs in other systems is also briefly discussed.

**Bell function values (BFV).**—The famous Bell-Clauser-Horne-Shimony-Holt (Bell-CHSH) inequality for two entangled spin-1/2 (or qubit) particles, which has always provided an excellent test-bed for experimental verification of quantum mechanics against the predictions of local realism, is given by the inequality \[ |I| \leq 2 \] 

where \( I = Q_{11} + Q_{12} + Q_{21} - Q_{22} \) and

\[ Q_{ij} = \int_{\Gamma} \mu(\lambda) X_k(n_{km}^{X}) \lambda d\lambda \]

is the correlation function with \( X_k(n_{km}^{X}) \) denoting the \( m \)-th observable on the \( k \)-th particle (here \( i, j, k, m = 1, 2 \)); \( \Gamma \) is the total space of the hidden variable \( \lambda \) and \( \mu(\lambda) \) is a statistical distribution of \( \lambda \), satisfying \( \int_{\Gamma} \mu(\lambda)d\lambda = 1 \). Quantum mechanically, the above inequality is violated by all pure entangled states of two qubits \[ \rho \] and the expression of the correlation function for any two-qubit state \( \rho \) reads: \[ Q_{ij} = \text{Tr}[(n_{1i}^{X} \cdot \sigma) \otimes (n_{2j}^{X} \cdot \sigma)] \rho \] 

where \( n_{km}^{X} \) are the unit vectors in three-dimensional Hilbert space and \( \sigma \) is the Pauli matrix vector. Based on the Bell-CHSH inequality \[ |I| \leq 2 \], the Bell function values are defined as:

\[ B(\rho) \equiv \max I^Q, \]

where \( I^Q = Q_{11}^Q + Q_{12}^Q + Q_{21}^Q - Q_{22}^Q \) and the maximization is performed over all possible vectors \( n_{km}^{X} \). Generally speaking, for every specific two-qubit quantum state \( \rho \), we need to carry out the procedure of the maximization to obtain its BFV \( B(\rho) \). Fortunately, in Ref. [2], the authors introduced another method to calculate \( B(\rho) \), which can circumvent the tedious maximization. It was proved there that

\[ B(\rho) = 2 \sqrt{v_1 + v_2}, \]

where \( v_1 \) and \( v_2 \) are the two greater eigenvalues of the \( 3 \times 3 \) symmetric matrix \( L_{\rho}^{T} L_{\rho} \), \( L_{\rho} \) is a \( 3 \times 3 \) matrix with elements defined by \( (L_{\rho})_{\sigma\tau} = \text{Tr}[\rho \sigma \otimes \tau] \) where \( \sigma, \tau = 1, 2, 3 \) and \( L_{\rho}^{T} \) is the transpose of \( L_{\rho} \). In the experimental situation, in order to obtain the BFV, the observers of the first (second) qubit should carry out two measurements \( n_{1i}^{X} \cdot \sigma \) and \( n_{2j}^{X} \cdot \sigma \) simultaneously, just the same as in Bell-CHSH inequality testing experiments [2].

**The Kitaev-Castelnovo-Chamon (KCC) Model.**—The physical model we consider in this article was introduced by Castelnovo and Chamon [17], which is a deformation of the Kitaev toric code model [22]. The Hamiltonian of the KCC model with periodic boundary conditions reads:

\[ H = -J_m \sum_{r \in T^2} B_F - J_e \sum_{v \in T^2} A_V + \sum_{v \in T^2} e^{-\beta \sum_{j \in v} \sigma_j^z}, \]

where with \( J_m, J_e > 0, \beta \) is a coupling constant; \( A_V = \prod_{v \in v} \sigma_j^z \) and \( B_F = \prod_{v \in F} \sigma_j^z \) are the vertex and face operators in the original Kitaev toric code model [22]. A brief sketch of this model is shown in Fig. 1. The ground state in the topological sector containing the fully magnetized state \( |0\rangle = |↑↑\cdots↑\rangle \) can be analytically obtained [17]:

\[ \langle G(\beta) \rangle = Z(\beta)^{-\frac{1}{2}} \sum_{g \in G} e^{\beta \sum_j \sigma_j^z} |0\rangle, \]

where \( Z(\beta) = \sum_{g \in G} e^{\beta \sum_j \sigma_j^z} \) is the partition function of the toric code model [22], while when \( \beta \to \infty \), \( \langle G(\beta) \rangle \) becomes the fully magnetized state \( |0\rangle \). At the point \( \beta_c = \frac{1}{2} \ln(\sqrt{2}+1) \) there exists a second-order TQPT where the topological entanglement entropy \( S_{topo} = 1 \) for \( \beta < \beta_c \) changes to \( S_{topo} = 0 \) for \( \beta > \beta_c \) [17].

As shown by Castelnovo and Chamon, there exists a one-to-two mapping between the configurations \( \{g\} = G \) the configurations \( \{\theta\} \) of the classical 2D Ising model [17]. In the mapping, the Hamiltonian of the Ising model has the form \( H_{Ising} = -c \sum_{(r,r')} \theta_r \theta_{r'} \), where \( c \) is a coupling constant and \( \theta_r, \theta_{r'} = +1 \) or \(-1\) depending on whether or not the corresponding vertex operator \( A_V \) is acting on the site \( r \). Thus \( \sigma_j^z = \theta_r \theta_{r'} \) with \( i \) being the edge between the nearest neighboring vertices. An illustration of this mapping is shown in Fig. 1.

**Signaling TQPTs by BFV.**—Since the BFV introduced in expression [2] only account for two-qubit states, we need to calculate the reduced density matrix of two qubit
ward calculations, we arrive at an analytical formula for the derivative of BFV \( \rho_{ij} \) based on the ground state \( |G(\beta)\rangle \) and the symmetry of the Hamiltonian \( H \). It was shown in Ref. [23] that \( \rho_{ij} \) has the following form (details are given in Ref. [17, 24] and references there in):

\[
\rho_{ij} = \frac{1}{4} [I + \langle \sigma_i^z \rangle (\sigma_i^+ + \sigma_i^-) + \langle \sigma_i^+ \sigma_j^- - \sigma_j^+ \sigma_i^- \rangle],
\]

where \( I \) is the \( 4 \times 4 \) identity matrix. Based on the Eq. (3), the BFV can be calculated by using the simplified formula for \( \mathcal{R}(\rho_{ij}) \) in Eq. (3). For convenience and simplicity, we only concentrate on two cases where \( i \) and \( j \) are nearest and next-to-nearest neighbors, respectively. In the thermodynamic limit, the mapping to the 2D Ising model gives that \( \langle \sigma_i^z \rangle = -\coth(2\beta)\pi + (4\tanh^2(2\beta) - 2)\mathcal{X}(\chi)/(2\pi) \), where \( \mathcal{X}(\chi) = \int_0^\pi d\phi (1 - \chi^2 \sin^2 \phi)^{-1/2} \) and \( \chi = 2\sinh(2\beta)/\cosh(2\beta) \). For the calculation of \( \langle \sigma_i^z \rangle \), the equivalence between the 2D Ising model and the quantum 1D XY model yields:

1. For \( i \) and \( j \) the nearest case, \( \langle \sigma_i^z \rangle \) can be calculated using the Bell function values of \( \rho_{ij} \) cannot be greater than 2, the classical bound.

Another interesting consideration here is similar to Ref. [24]: we can calculate the BFV between a local qubit denoted by \( i \) and the rest of the whole lattice by rewriting the ground state as \( |G(\beta)\rangle = \mathcal{P}_+ |\mathcal{P}| |0_i\rangle + \mathcal{P}_- |\mathcal{P}_-| |1_i\rangle \) where \( \mathcal{P}_\pm = (1 \pm (\theta_0, 0, 0, 0))[2], |\mathcal{P}_+\rangle \) and |\mathcal{P}_-\rangle are two orthogonal normalized vectors. Consequently, we can regard \( |G(\beta)\rangle \) as a simple pure two-qubit entangled state. In this case, the BFV has a one-to-one monotonous relation with entanglement for details, see Ref. [24]. However, it is worthwhile to clarify that there is a distinctive difference between the BFV approach and the quantum discord approach. For the quantum discord, its value becomes trivially 0 for the reduced two-qubit state, thus cannot signal the TQPT at the critical point. Nevertheless, as shown in the former paragraphs, the first order derivative of BFV is an excellent marker of the transitions. In addition, the physical meanings of BFV and quantum discord are different. Generally speaking,
quantum discord is a measurement of the ‘quantumness’ of a system. While, BFV measures the nonlocality of the system when it is greater than the classical bound. In this case, \( R(\alpha|\beta) = 2\sqrt{1 + 4\beta^2\beta^2} > 2 \). Thus the BFV \( R(\alpha|\beta) \) can measure the nonlocality of ground state. This establishes a new link between quantum nonlocality and TQPTs.

**Summary and Discussion.** To summarize, based on the KCC model, which exhibits a second-order TQPT at the critical point, we have introduced the BFV approach to TQPTs. Our results show that BFV serves as an accurate marker of the transitions. Since the BFV also serves as a measure of nonlocality, which is a pure quantum phenomenon and cannot be described by any local realism theory, our work has established a new link between quantum nonlocality and phase transitions. Furthermore, experimentally, this approach only involves two measurements on two qubit, thus it might be more convenient to implement in experimental schemes. Actually, the optical lattices and trapped ions might provide suitable experimental test-bed for our results [27].

What is also notable is that this approach is applicable to other models. For instance, for the model recently introduced by Son et al., which is described by a cluster Hamiltonian \( H(\lambda) = -\sum_{i=1}^{N}(\sigma_i^x\sigma_{i+1}^x + \lambda\sigma_i^y\sigma_{i+1}^y) \) and has an exotic phase transition at the critical point \( \lambda = 1 \) [28], our numerical results show that the first order derivative of BFV can explicitly capture the transition. The cluster Hamiltonian above can be simulated in a triangular configuration of an optical lattice of two atomic species [29], thus also leading to the possibility of testing the BFV approach experimentally. To investigate the BFV in QPTs, we have also considered the one dimensional Ising model and XY model. The numerical results show that the first order derivative of BFV exhibits singular behavior at the critical point, too. Thus this approach is useful for both QPTs and TQPTs.

It would be interesting and significant to apply this approach to QPTs and TQPTs in various physical systems, such as quantum spin Hall system, both theoretically and experimentally. It would also be interesting to use BFV based on other Bell inequalities to investigate QPTs and TQPTs. More specifically, studying the BFV of the pure ground states based on multipartite Bell inequalities, such as the famous Mermin-Ardehali-Belinskii-Klyshko (MABK) inequality [20], might shed light on the behavior of the quantum nonlocality of the whole system in QPTs and TQPTs.

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