Scaling of Geometric Quantum Discord Close to a Topological Phase Transition

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Quantum phase transition is one of the most interesting aspects in quantum many-body systems. Recently, geometric quantum discord has been introduced to signature the critical behavior of various quantum systems. However, it is well-known that topological quantum phase transition can not be described by the conventional Landau's symmetry breaking theory, and thus it is unknown that whether previous study can be applicable in this case. Here, we study the topological quantum phase transition in Kitaev’s 1D $p$-wave spinless quantum wire model in terms of its ground state geometric quantum discord. The derivative of geometric quantum discord is nonanalytic at the critical point, in both zero temperature and finite temperature cases. The scaling behavior and the universality are verified numerically. Therefore, our results clearly show that all the key ingredients of the topological phase transition can be captured by the nearest neighbor and long-range geometric quantum discord.

In recent years topological phases have been intensively studied in condensed-matter systems. Their understanding is relevant to topological quantum computation, which provides the paradigm to store and manipulate information in topologically nontrivial systems. The topological states are immune to local noise due to their nonlocal topological nature¹². The progress was impeded by the fact that non-Abelian anyons are known to appear in $p$-wave superconductors⁴. Recently, it has been realized that the $p$-wave pairing can be emulated with $s$-wave pairing provided with spin-orbit coupling and Zeeman splitting⁵. Especially, this provide the possibility of direct simulation⁷ of Kitaev’s 1D $p$-wave spinless quantum wire model⁴, which lead to elementary experimental evidence⁹ for the existence of Majorana fermions. Therefore, these progresses have greatly advanced the field. In addition, the analytic eigenspectra in the 1D Kitaev model have been obtained, and it was shown that this model has one gapless topological phase. But the characters of the topological phase from quantum information approach have never been well studied previously.

Quantum phase transition (QPT), originates from the quantum fluctuations at zero temperature, is characterized by nonanalytical changes in the physical properties of the ground state of a many-body system governed by the variation of a parameter of the system’s Hamiltonian¹⁰. Quantum discord (QD)¹¹ is defined by the difference between two quantum analogues of two classically equivalent expressions of mutual information. The QD has been introduced to analyze the QPT of the spin XY model¹² and much effort has been devoted to various quantum critical systems¹³¹⁴. It is worth to note that other approaches to characterize QPT have also been put forward, such as entanglement¹⁵¹⁶, quantum fidelity¹⁷, fidelity susceptibility¹⁸, geometric phase¹⁹ and Loschmidt Echo²¹. Since the calculation of quantum discord is based on numerical maximization procedure, it does not guarantee exact results and in the literature there are few analytical expressions including special cases. To avoid this difficulty, Dakic et al.²² introduced geometric measure of quantum discord (GMQD) which measures the quantum correlations through the minimum Hilbert-Schmidt distance between the given state and zero discord state. Although quantum discord around a QPT for a fermionic lattice hamiltonian has been studied, they only consider the magnetic phase transition in the transformed picture instead of the physical picture. The Kitaev model is related by the Jordan-Wigner transformation to the transverse field Ising model, however, the Jordan-Wigner transformation is fundamentally non local, the information is not robust to local perturbations in the experimental system. This is because the Jordan-Wigner transformed local perturbations become exactly the non-local sort of term that can mess up topologically protected states. The geometric quantum discord of the ground state is naturally expected to shed some light on the understanding of topological QPT.

Traditionally, QPT can be understood in the frame of Landau’s continuous phase transitions paradigm with local order parameter and long range correlations. However, it has been found that the local order parameters cannot describe all possible orders²³. Therefore, it is interesting to investigate whether this success, describe QPT
with geometric quantum discord (GQD) $D_{GQ}$ can be extended to the purely topological QPT cases. Here, we explore this question taking the topological QPT in Kitaev’s quantum wire model as an example. The present work aims to provide a more general understanding of geometric quantum discord in topological phase transitions. The reason why geometric quantum discord can describe topological phases or determine their boundaries is due to the fact that they depend only on the properties of the ground state of the system. We analyze zero temperature and finite-temperature scaling properties or determine their boundaries is due to the fact that they depend only on the properties of the ground state of the system. In quantum critical phenomena, the most important themes are scaling and universality. In a finite lattice model, it is expected that the anomalies will become clearer and clearer as the size of the lattice increases. The relevant study is the so-called finite-size scaling. The critical features are characterized in term of a critical exponent $\gamma$ defined by $\xi = (t - t_\text{c})^{-\gamma}$ with $\xi$ representing the correlation length. To further understand the relation between GQD and quantum criticality, we calculate the derivative of GQD $dD_{GQ}/dt$ for $\Lambda = 1$ and different lattice sizes around the critical point, as shown in Fig. 2(a). For simplicity, we first look at the case of $\Lambda = 1$, and we will discuss the properties of the family of $\Lambda \neq 1$ later. In fact, there is no real divergence for finite $L$, but the curves exhibit marked anomalies and the height of which increases with lattice size. The

$$H = \sum_{i=1}^{L} \mu c_i^\dagger c_i - \sum_{i=1}^{L-1} \left( t c_i^\dagger c_{i+1} + \Delta c_i^\dagger c_{i+1} + h.c. \right).$$  

Figure 2 | GQD $D_G$ of the ground state (a) and its derivatives $dD_G/dt$ (b) as a function of $t$ around the critical point $t_c = 1$ for different superconducting gap $\Lambda$. The lattice size $L = 1001$. 

**Results**

**The model and topological phase transition.** We consider the typical lattice model of the 1D $p$-wave superconductor, which is described by the $L$-site Hamiltonian

$$H = \sum_{i=1}^{L} \mu c_i^\dagger c_i - \sum_{i=1}^{L-1} \left( t c_i^\dagger c_{i+1} + \Delta c_i^\dagger c_{i+1} + h.c. \right).$$

where $\mu$ is the on-site chemical potential, $t$ is the nearest-neighbor hopping amplitude, $\Delta$ is the $p$-wave superconducting gap, and $c_i^\dagger$ and $c_i$ are fermionic operators that satisfy the anticommutation relations $\{c_i, c_j\} = \delta_{ij}, \{c_i, c_j^\dagger\} = \{c_i^\dagger, c_j\} = 0$. The model has two distinct phases, i.e., topologically trivial and nontrivial phases. Under open boundary condition, the two phases can be distinguished by the presence or absence of zero-energy Majorana bound states at the ends. It is well known that the topologically non-trivial phase of the model is best illustrated for the choice of parameters for $u/t < 2$ for any $\Delta \neq 0$. Without loss of generality, we assume $t$ and $\Delta$ are both real and set $\mu = 2$. Therefore, our choice makes the model possess a critical point at $t = 1$ for any $\Delta \neq 0$.

**GQD close to the phase transition.** To illustrate the intrinsic relation between the geometric quantum discord of ground-state and quantum phase transition in this model. We plot GQD $D_G$ and its derivative $dD_G/dt$ as a function of the Hamiltonian parameters $t$. As shown in Fig. 1(a), given the value of $\Delta$, the GQD increases with increasing the system sizes, the maximum becomes more pronounced. (b) The position of maximum approaches the critical point $t_c = 1$ as $t_m \sim L^{-1/\gamma}$.
position of the peak $t_m$ can be regarded as a pseudo-critical point which changes and tends as $L^{-\nu}$ towards the critical point and clearly approaches $t_c$ as $L \to \infty$. This scaling behavior of $dD_G/dt$ is also clearly shown in in Fig. 2(b).

We now further going to deal with the critical exponent that governs divergence of the correlation length. As shown in Fig. 3(a), the singular behavior of $dD_G/dt$ for the infinite chain can be analyzed in the vicinity of the quantum criticality, and we find the asymptotic behavior as

$$\frac{dD_G}{dt} = \kappa_1 \ln |t-t_c| + \text{const.,} \quad (2)$$

where $\kappa_1 = -0.0638$. On the other hand, As shown in Fig. 3(b), the value of $dD_G/dt$ at the point $t_m$ diverges logarithmically with increasing lattice size as:

$$dD_G|_{t_m} = \kappa_2 \ln L + \text{const.,} \quad (3)$$

where $\kappa_2 = 0.0601$. According to the scaling ansatz, the ratio $|\kappa_1/\kappa_2|$ gives the exponent $\nu$. Therefore, $\nu \sim 1$ is obtained in our numerical calculation for the 1D $p$-wave superconductor model. Furthermore, by proper scaling and taking into account the distance of the maximum of $D_G$ from the critical point, it is possible to make all the data for the value of $F = 10^3 \left[ 1 - \exp \left( \frac{dD_G}{dt} - \frac{dD_G}{dt}|_{t_m} \right) \right]$ as a function of $L^{\nu}(t - t_c)$ for different $L$ collapse onto a single curve. The result for several typical lattice sizes is shown in Fig. 3(c), where we can also extract the critical exponent $\nu = 1$, in the vicinity of the critical point.

**Universality.** As is well known, 1D $p$-wave superconductor with nearest neighbor hopping belongs to the same quantum universality class for non-zero $\Delta$, with the same critical exponents $\nu = 1$. To confirm the universality principle in this model, we need to check the scaling behaviors for different values of the parameter $\Delta$. For instance, from Fig. 3(a) and Fig. 3(b) we get $\kappa_1 = 0.0716$ and $\kappa_2 = -0.0699$ for $\Delta = 0.8$. Moreover, we also verify that, by proper scaling, all data for different $L$ but a specific $\Delta$ and a critical point $t_c = 1$ can collapse onto a single curve. The data for $\Delta = 0.8$ are show in Fig. 3(c). We can extract the same critical exponent $\nu = 1$ from all the above results.

**Extended to finite temperatures.** We would like to further study the relation between the thermal-state $D_G$ and quantum phase transitions at a finite temperature. The derivative of GQD $dD_G/dt$ as a function of $t$ at different temperatures $T$ (including zero temperature) are presented in Fig. 4(a). At zero temperature the...
derivative of $D_G$ shows a singularity at $t_c = 1$, but at nonzero temperature, there are no real divergence. Nevertheless, there are clear anomalies at low temperature, and the height of which increases with the decrease of the temperature. This can be regarded as the precursors of the QPT. What is more, the position of the maximum derivative (pseudocritical point) $t_m$ changes and tends as $T^{-\frac{5}{2}}$ and clearly approaches $t_c$ when $T \to 0$, as shown in Fig. 4(b). Meanwhile, the maximum value of $dD_G/dt$ at the pseudocritical point $t_m$ diverges logarithmically with the decrease of the temperature

$$
\frac{dD_G}{dt}
|_{t_m} = \kappa_3 \ln T + \text{const.}
$$

(4)

Our numerical results, as shown in Fig. 4(c), give $\kappa_3 = 0.0611$. The ratio of the two slopes $(\kappa_3/\kappa_3)$ for a fixed parameter $\Delta$ is equal to the critical exponent $\nu = 1$. Moreover, we also verify that by proper scaling, all data for different temperatures $T$ but a specific $\Delta$ will collapse onto the same curve. The data for $\Delta = 0.8$ and $\Delta = 1.0$ near the critical points $t_c = 1$ are shown in Fig. 4(d). The numerical results agree with the finite-size scaling ansatz and the universality of the above results.

It has also been noted that unlike pairwise entanglement, which is typically short ranged, quantum discord does not vanish even for distant lattice pairs. Fig. 5 shows that quantum discord provides the expected long-range behavior of quantum correlations $L D_G / L = 15$ for 1D Kitaev model exhibiting QPTs. In a topological nontrivial case, one can observe stronger quantum discord. The critical exponent $\nu = 1$ for the correlation length is determined by the two slopes in Fig. 5(c) and Fig. 5(d) for a fixed $\Delta$. Such a behavior close to topological QPT is remarkable, even though quantum discord has been shown to be non-vanishing. Concerning QPTs, long-range quantum discord has been considered as an indicator of the critical point of topological QPT in several systems, having succeeded in this task even in situations where entanglement fails, which may shed some light on the understanding of topological phase transition for the other more complex systems from the viewpoint of quantum discord. Finally further numerical calculation of the quantum discord shows that for 2D Kitaev model exhibiting topological QPTs in the range of $t_x + t_y = 1$, critical exponent $\nu$ also gives exactly the same results with the theoretical results $z = 2, \nu = 1/2$.

**Discussion**

Topological states that are protected from local perturbations need to be supported by quantitative calculations, in particular working with quantum systems of finite sizes. To study the experimental feasibility, we add a random defect perturbation to each hopping amplitude to check the robustness of the topological QPT under the perturbation. Taking the system defects with parameters as given in Fig. 6, the numerical results indicated that the scaling and the critical point of topological QPT are robust against defects. We find topological QPT located in the boundary is robust even the defect amplitude takes $\delta = 0.1$. In summary, we have performed a finite size scaling analysis, whose analytical expression has been extracted from the $D_G$ corresponding to different values of the control parameter near the critical point. This makes it possible to extract the correlation length critical exponent. Finally, our study establishes the connection between the $D_G$ and topological QPT at both zero temperature and nonzero temperature. All key features of the quantum criticality, such as scaling, critical exponent, the universality are presented. We also would like to point out that the results obtained in this paper does not depend on the model. An interesting question is that when added with next-neighbor tunneling, i.e., $H_2 = (\hat{c}_i^\dagger \hat{c}_{i+2} + \Delta \hat{c}_i \hat{c}_{i+2} + h.c.)$, new critical points will appear and this needs further study.

**Added note.** In the revise manuscript we find for the same question, Luo et al.\textsuperscript{24} also investigate the fidelity susceptibility (FS) and the critical exponent of the BdG transformation as a function of the temperature $T$. The curve corresponds to different temperatures $T = 0, 0.01, 0.02$, and 0.04. With the decrease of the temperature, the maximum gets pronounced, and the pseudopoint $t_m$ changes and tends as $T^{-\frac{5}{2}}$ towards the critical point $t_c = 1$ (b). (c) The maximum value of $dD_G/dt$ at the pseudocritical point $t_m$ of this model as a function of temperature $T$. The slope of the line is $-0.0611 (-0.0717)$ for $\Delta = 1(\Delta = 0.8)$. (d) The value of $F = 10^5 \left(1 - \exp\left(dD_G/dt - dD_G/dt|_{t_m}\right)\right)$ as a function of $(t - t_m)/T$ for different temperature.

**Methods**

**Diagonalization of the model hamiltonian.** Under the open boundary condition, the Hamiltonian can be immediately diagonalized

$$
H = \sum_{n=1}^{L_{BDG}} (\hat{h}_n^{\dagger} \hat{h}_n - 1/2),
$$

(5)

by introducing a Bogoliubov-de Gennes (BDG) transformation $\hat{h}_n = \sum_{\alpha} \left(\psi_{\alpha} c_{\alpha,n} + \psi_{\alpha}^\dagger c_{\alpha,n}^\dagger\right)$, where $\psi_{\alpha}$ denotes the quasi-particle energy, and $\psi_{\alpha}$ and $\psi_{\alpha}^\dagger$ can be obtained by solving the corresponding BdG equations. The Bogoliubov-de Gennes matrix is written in blocks as $H_{BDG} = \left(\begin{array}{cc}
\hat{h} - \Delta & -\hat{h} \\
\hat{h} & \hat{h}
\end{array}\right)$ with

$$
\hat{h}_{ij} = \delta_{ij+1} - t \delta_{i,j+1} \quad \text{and} \quad \hat{h}_{ij} = \delta_{ij-1} - t \delta_{i,j-1} \quad \text{in} \quad \Delta = 0.
$$

In order to obtain the $D_G$ in the following, we need to calculate the ground-state correlation functions $\rho^{ij} = \langle \hat{c}_i^\dagger \hat{c}_j \rangle$, $\rho^{ij} = \langle \hat{c}_i^\dagger \hat{c}_j \rangle$, $\rho^{ij} = \langle \hat{c}_i^\dagger \hat{c}_j \rangle$, and $\rho^{ij} = \langle \hat{c}_i^\dagger \hat{c}_j \rangle$, written in terms of the amplitude of the BdG transformation as
Figure 5 | (a)(b) Long-range quantum discord $LD_G$ and its derivatives $dLD_G/dt$ as a function of the parameter $t$. (c) $dLD_G/dt$ against $\ln |t - t_c|$ for evaluating the thermodynamic approaching to the critical point $t_c = 1$. (d) The maximum value of the derivative $dLD_G/dt|_{t=t_c}$ as a function of lattice sizes. The critical exponent $\nu$ for the correlation length is determined by the two slopes in (c) and (d) for a fixed $\Delta$.

Figure 6 | (a)(b) A random defect to each hopping amplitude to check the robustness of the topological QPT under the perturbation in Ising model and 1D Kitaev model.
\[ C_{ij}^{0} = \sum_{n=1}^{3} v_{n,i} v_{n,j}, \quad C_{ij}^{1} = \sum_{n=1}^{3} v_{n,i} v_{n,j}, \quad C_{ij}^{2} = \sum_{n=1}^{3} u_{n,i} u_{n,j}, \quad C_{ij}^{3} = \sum_{n=1}^{3} u_{n,i} u_{n,j}. \]  

(6)

**Computation of \( D_{ij} \):** An arbitrary two-qubit state can be written in Bloch representation:

\[ \rho = \frac{1}{4} \left[ I + \sum_{i=1}^{3} (x_{i} \sigma_{i} \otimes I + y_{i} I \otimes \sigma_{i}) + \sum_{i,j=1}^{3} R_{ij} \sigma_{i} \otimes \sigma_{j} \right] \]  

(7)

where \( x_{i} = Trp(\sigma_{i} \otimes I), y_{i} = Trp(I \otimes \sigma_{i}) \) are components of the local Bloch vectors, \( \sigma_{i}, i \in \{1, 2, 3\} \) are the three Pauli matrices, and \( R_{ij} = Trp(\sigma_{i} \otimes \sigma_{j}) \) are components of the correlation tensor. For two-qubit case, Then a analytic expression of the \( D_{ij} \) is given by:

\[ D_{ij}(\rho) = \frac{1}{4} \left( ||x||^{2} + ||y||^{2} - k_{\text{max}} \right) \]  

(8)

where \( x = (x_{1}, x_{2}, x_{3})^{T} \) and \( k_{\text{max}} \) is the largest eigenvalue of matrix \( K = xx^{T} + RR^{T} \).

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**Author contributions**

C.J.S. conceived the idea, C.J.S., W.W.C., J.B.L., Y.S.C. and T.K.L. performed the numerical calculation, all the authors contribute to the discussion of the content during the whole project. C.J.S. wrote the manuscript with the inputs from all the others.

**Additional information**

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