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Scaling of Geometric Quantum Discord Close to a Topological Phase Transition

SUBJECT AREAS:

QUANTUM
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QUANTUM PHYSICS

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10 December 2013Accepted
10 March 2014Published
26 March 2014Correspondence and
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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 nature^{1,2}. The progress was impeded by the fact that non-Abelian anyons are known to appear in p -wave superconductors^{3,4}. Recently, it has been realized that the p -wave pairing can be emulated with s -wave pairing provided with spin-orbit coupling and Zeeman splitting^{5,6}. Especially, this provide the possibility of direct simulation^{7,8} 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 systems^{13,14}. It is worth to note that other approaches to characterize QPT have also been put forward, such as entanglement^{15,16}, quantum fidelity¹⁷, fidelity susceptibility¹⁸, geometric phase^{19,20} 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

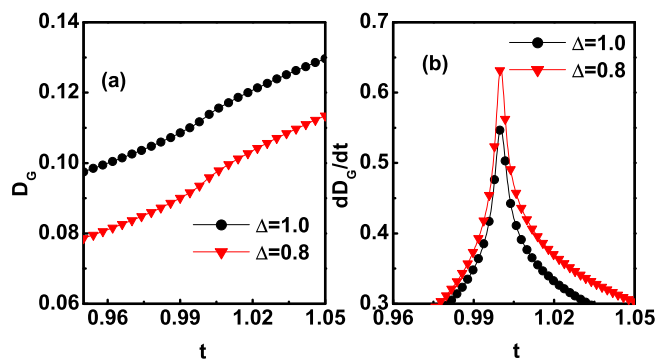


Figure 1 | GQD D_G of the ground state (a) and its derivatives dD_G/dt (b) as a function of t around the critical point $t_c = 1$ for different superconducting gap Δ . The lattice size $L = 1001$.

with geometric quantum discord (GQD) D_G , can be extended to the purely topological QPT cases. Here, we explore this question taking the topological QPT in Kitaev's quantum wire model⁴ 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 parameters, extracted from the D_G of ground state. First, it is found that, in the thermodynamic limit, the derivative of ground-state D_G is nonanalytic at the critical point. A finite size scaling analysis is carried out for model with different lattice sites, and the scaling behavior is confirmed numerically. This allows us to extract the correlation length critical exponent. To confirm the universality, we also perform a finite-temperature scaling analysis for this model, aiming at extracting the correlation length critical exponent from the scaling behaviors of thermal-state D_G . The finite-temperature scaling is manifested when the temperature approaches zero, in analogy with finite-size scaling.

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

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

where μ is the on-site chemical potential, t is the nearest-neighbor hopping amplitude, Δ is the p -wave superconducting gap, and c_i^\dagger and c_i are fermionic operators that satisfy the anticommutation relations $\{c_n^\dagger, c_m\} = \delta_{nm}$, $\{c_n, c_m\} = \{c_n^\dagger, c_m^\dagger\} = 0$. 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 Δ 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 Δ , the GQD increases with increasing the nearest-neighbor hopping strength t . Meanwhile, it is shown in Fig. 1(b) that the derivatives of GQD (dD_G/dt) exhibit sharp peaks around the critical points $t_c = 1$. First, these sharp peaks manifest the nonanalytic property of the GQD at the critical point. Second, this also verified the assertion made by Kitaev⁴ that the critical point will not change with the changing of Δ . This means the GQD of the ground state can signature the criticality in this model, as in the conventional QPT cases.

Finite size scaling. 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 ν defined by $\xi = (t - t_c)^{-\nu}$ with ξ representing the correlation length. To further understand the relation between GQD and quantum criticality, we calculate the derivative of GQD dD_G/dt for $\Delta = 1$ and different lattice sizes around the critical point, as shown in Fig. 2(a). For simplicity, we first look at the case of $\Delta = 1$, and we will discuss the properties of the family of $\Delta \neq 1$ 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

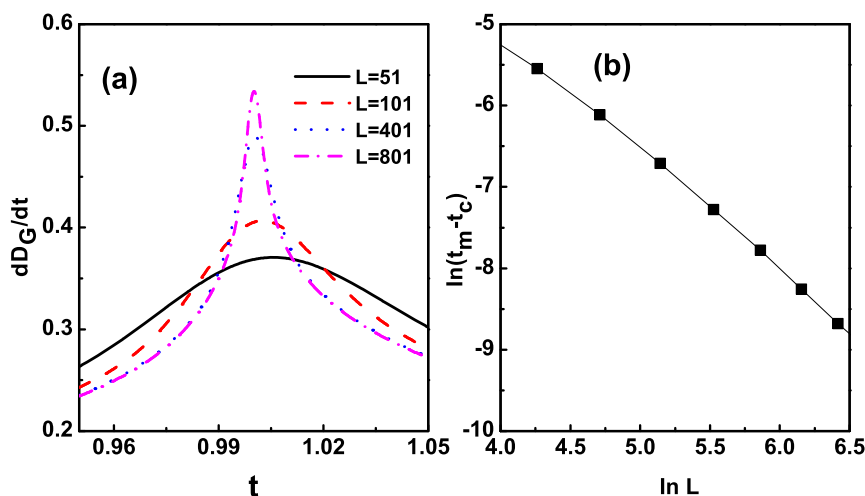


Figure 2 | (a) The derivatives of GQD dD_G/dt as a function of t near the critical point $t_c = 1$ for different system sizes $L = 51, 101, 201, 401, 801, \dots$. With increasing the system sizes, the maximum becomes more pronounced. (b) The position of maximum approaches the critical point $t_c = 1$ as $t_m \sim L^{-1.46}$.



position of the peak t_m can be regarded as a pseudo-critical point which changes and tends as $L^{-1.46}$ towards the critical point and clearly approaches t_c as $L \rightarrow \infty$. 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 $dD_G/d\lambda$ for the infinite chain can be analyzed in the vicinity of the quantum criticality, and we find the asymptotic behavior as

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

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:

$$\left. \frac{dD_G}{dt} \right|_{t_m} \approx \kappa_2 \ln L + \text{const.}, \quad (3)$$

where $\kappa_2 = 0.0601$. According to the scaling ansatz, the ratio $|\kappa_1/\kappa_2|$ gives the exponent ν . 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 $F = 10^3 \left[1 - \exp\left(\frac{dD_G}{dt} - \left. \frac{dD_G}{dt} \right|_{t_m} \right) \right]$ 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 Δ , 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 Δ . 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 Δ 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

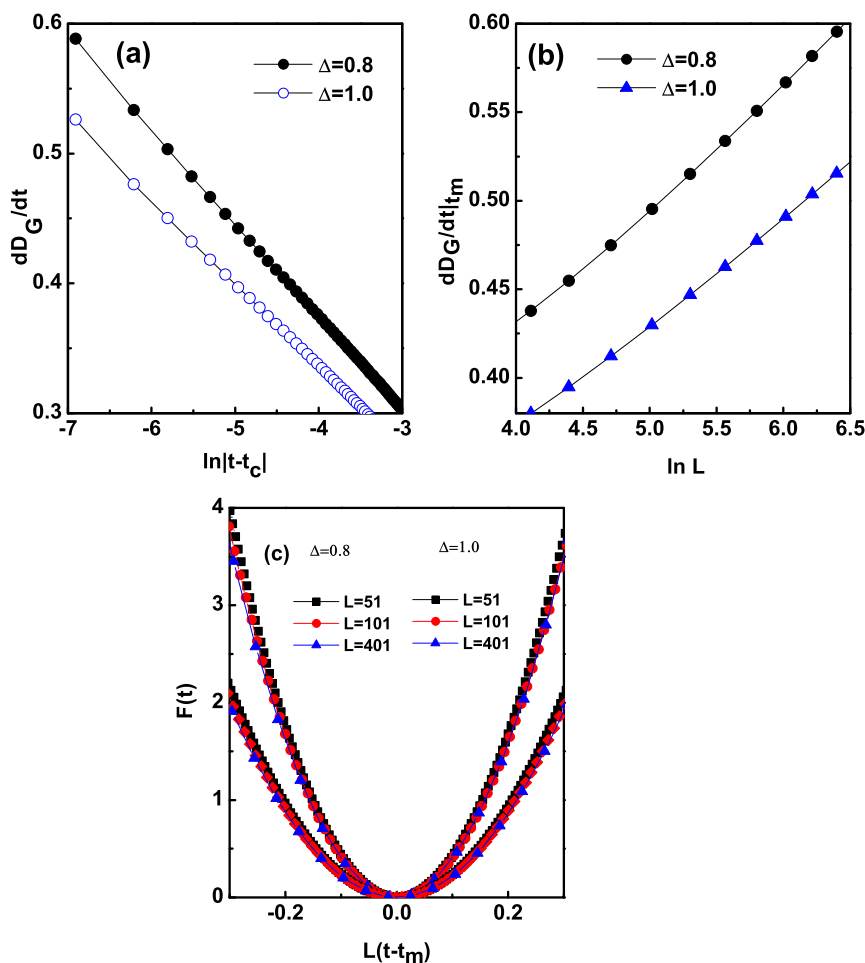


Figure 3 | (a) Plot of dD_G/dt against $\ln|t - t_c|$ for evaluating the thermodynamic approaching to the critical point $t_c = 1$. The line slope close to the critical point is -0.0638 (-0.0716) for $\Delta = 1.0$ ($\Delta = 0.8$). (b) The maximum value of the derivative $dD_G/dt|_{t_m}$ at the pseudocritical point t_m as a function of lattice sizes. The line slope close to the critical point $t_c = 1$ is 0.0601 (0.0699) for $\Delta = 1.0$ ($\Delta = 0.8$). The critical exponent ν for the correlation length is determined by the two slopes in (a) and (b) for a fixed Δ . (c) A finite size scaling analysis is carried out for the value of $F = 10^3 \left(1 - \exp\left(\frac{dD_G}{dt} - \left. \frac{dD_G}{dt} \right|_{t_m} \right) \right)$ as a function of $L(t - t_m)$ for different lattice sizes. All the data from $L = 51$ up to $L = 401$ for a fixed parameter Δ collapse on a single curve. This shows that the system at the critical point is scaling invariant and that the correlation length critical exponent $\nu = 1$.



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 $T^{1.44}$ and clearly approaches t_c when $T \rightarrow 0$, 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

$$\left. \frac{dD_G}{dt} \right|_{t_m} \approx \kappa_3 \ln T + \text{const.} \quad (4)$$

Our numerical results, as shown in Fig. 4(c), give $\kappa_3 = 0.0611$. The ratio of the two slopes (κ_1/κ_3) for a fixed parameter Δ 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 Δ 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

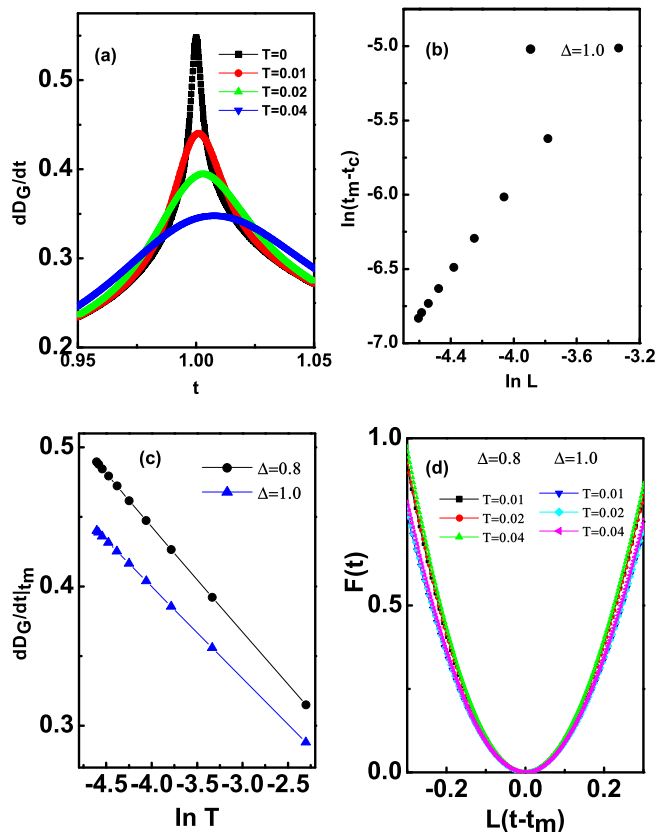


Figure 4 | (a) The derivatives of QGD dD_G/dt as a function of the parameter t . The curve corresponds to different temperatures $T = 0, 0.01, 0.02$, and 0.04 . With the decrease of the temperature, the maximum gets pronounced, and the pseudopoint t_m changes and tends as $T^{1.44}$ towards the critical 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 $F = 10^2(1 - \exp(-dD_G/dt - dD_G/dt|_{t=t_m}))$ as a function of $(t - t_m)/T$ for different temperature.

distant lattice pairs. Fig. 5 shows that quantum discord provides the expected long-range behavior of quantum correlations LD_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 Δ . 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 view 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 ν 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., $H_2 = \lambda_2 (c_i^\dagger c_{i+2} + \Delta c_i c_2 + h.c.)$, new critical points will appear and this needs further study.

Added note. In the revise manuscript we find for the same question, Luo et al²⁴ also investigate the fidelity susceptibility (FS) and the topological phase transition in a two-dimensional spin-orbit coupled (SOC) Fermi superfluid.

Methods

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

$$H = \sum_{n=1}^L \lambda_n (\hat{\eta}_n^\dagger \hat{\eta}_n - 1/2), \quad (5)$$

by introducing a Bogoliubov-de Gennes (BdG) transformation

$\hat{\eta}_n = \sum_{i=0}^{L-1} (u_{n,i} \hat{c}_i + v_{n,i} \hat{c}_i^\dagger)$, where λ_n denotes the quasi-particle energy, and $u_{n,i}$ and $v_{n,i}$ can be obtained by solving the corresponding BdG equations. the Bogoliubovde Gennes matrix is written in blocks as $\mathcal{H}_{BdG} = \begin{pmatrix} \hat{h} & \hat{\Delta} \\ -\hat{\Delta} & -\hat{h} \end{pmatrix}$ with $\hat{h}_{ij} = \delta_{ij} \mu_i - t \delta_{ij+1} - t \delta_{ij-1}$ and $\hat{\Delta}_{ij} = \delta_{ij-1} \Delta - \delta_{ij+1} \Delta$. In order to obtain the D_G in the following, we need to calculate the ground-state correlation functions $C_{ij}^{0,0} = \langle \hat{c}_i \hat{c}_j \rangle$, $C_{ij}^{0,1} = \langle \hat{c}_i \hat{c}_j^\dagger \rangle$, $C_{ij}^{1,0} = \langle \hat{c}_i^\dagger \hat{c}_j \rangle$ and $C_{ij}^{1,1} = \langle \hat{c}_i^\dagger \hat{c}_j^\dagger \rangle$, written in terms of the amplitude of the BdG transformation as

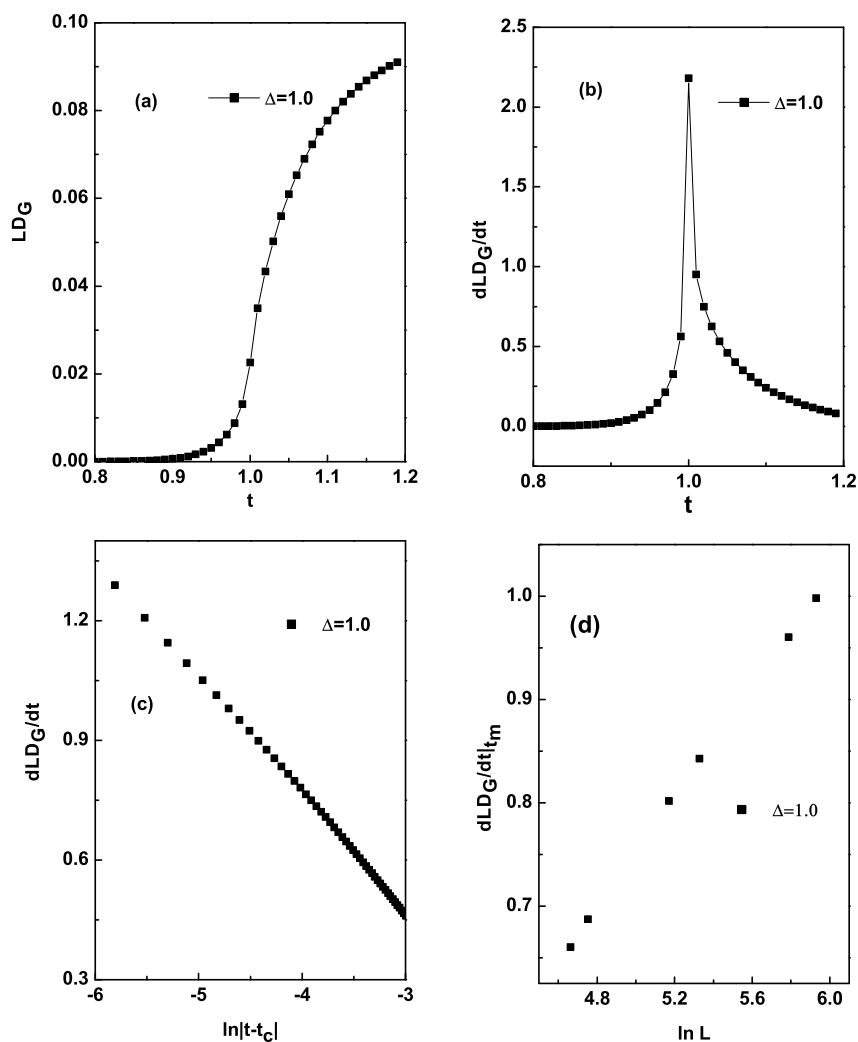


Figure 5 | (a)(b) Long-range quantum discord LD_G and its derivatives dLD_G/dt as a function of the parameter t . (c) dLD_G/dt against $\ln |t - t_c|$ for evaluating the thermodynamic approaching to the critical point $t_c = 1$. (d) The maximum value of the derivative $dLD_G/dt|_{t=t_m}$ at the pseudocritical point t_m as a function of lattice sizes. The critical exponent ν for the correlation length is determined by the two slopes in (c) and (d) for a fixed Δ .

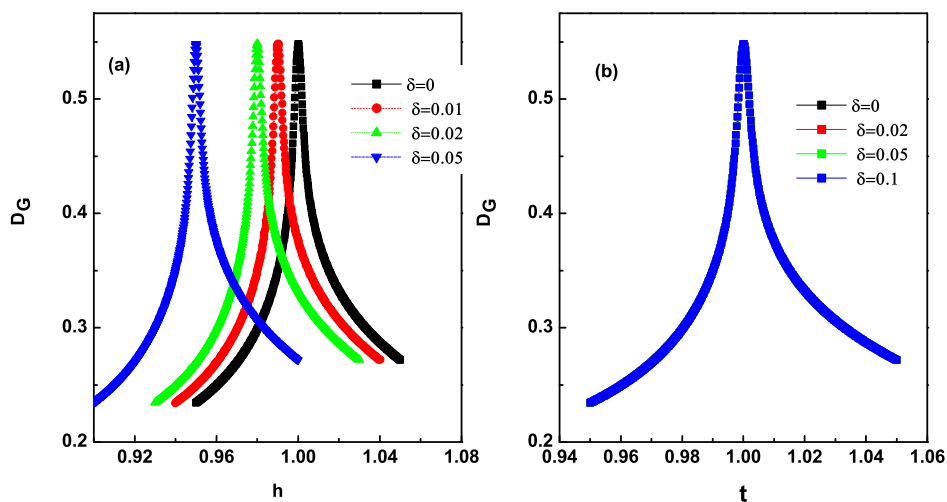


Figure 6 | (a)(b) A random defect to each hopping amplitude to check the robustness of the topological QPT under the perturbation in Ising model and 1D Kitaev model.



$$\begin{aligned}
 C_{ij}^{0,0} &= \sum_{n=1}^L v_{n,i} u_{n,j}, & C_{ij}^{0,1} &= \sum_{n=1}^L v_{n,i} v_{n,j}, \\
 C_{ij}^{1,0} &= \sum_{n=1}^L u_{n,i} u_{n,j}, & C_{ij}^{1,1} &= \sum_{n=1}^L u_{n,i} v_{n,j}.
 \end{aligned}
 \tag{6}$$

Computation of D_G . An arbitrary two-qubit state can be written in Bloch representation:

$$\rho = \frac{1}{4} \left[I + \sum_i^3 (x_i \sigma_i \otimes I + y_i I \otimes \sigma_i) + \sum_{ij=1}^3 R_{ij} \sigma_i \otimes \sigma_j \right]
 \tag{7}$$

where $x_i = \text{Tr}(\rho \sigma_i \otimes I)$, $y_i = \text{Tr}(I \otimes \rho \sigma_i)$ are components of the local Bloch vectors, σ_i , $i \in \{1, 2, 3\}$ are the three Pauli matrices, and $R_{ij} = \text{Tr}(\rho (\sigma_i \otimes \sigma_j))$ are components of the correlation tensor. For two-qubit case, Then an analytic expression of the D_G is given by²²

$$D_G(\rho) = \frac{1}{4} (\|x\|^2 + \|R\|^2 - k_{\max})
 \tag{8}$$

where $x = (x_1, x_2, x_3)^T$ and k_{\max} is the largest eigenvalue of matrix $K = xx^T + RR^T$.

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Acknowledgments

We thank Z.-Y. Xue, D.W. Zhang and F. Mei for useful discussion. C.J.S. is partially supported by the program of Educational Commission of Hubei Province (Grant No. Q20142502).

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

Competing financial interests: The authors declare no competing financial interests.

How to cite this article: Shan, C.-J., Cheng, W.-W., Liu, J.-B., Cheng, Y.-S. & Liu, T.-K. Scaling of Geometric Quantum Discord Close to a Topological Phase Transition. *Sci. Rep.* **4**, 4473; DOI:10.1038/srep04473 (2014).



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