Exact scaling of geometric phase and fidelity susceptibility and their breakdown across the critical points

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It was shown via numerical simulations that geometric phase (GP) and fidelity susceptibility (FS) in some quantum models exhibit universal scaling laws across phase transition points. Here we propose a singular function expansion method to determine their exact form across the critical points as well as their corresponding constants. For the models such as anisotropic XY model where the energy gap is closed and reopened at the special points \((k_0 = 0, \pi)\), scaling laws can be found as a function of system length \(N\) and parameter deviation \(\lambda - \lambda_c\) (where \(\lambda_c\) is the critical parameter). Intimate relations for the coefficients in GP and FS have also been determined. However in the extended models where the gap is not closed and reopened at these special points, the scaling as a function of system length \(N\) breaks down. We also show that the second order derivative of GP also exhibits some intriguing scaling laws across the critical points. These exact results can greatly enrich our understanding of GP and FS in the characterization of quantum phase transitions.

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Ever since its theoretical discovery, geometric phase (GP) has permeated into different branches of physics, including ultracold atoms, quantum computation, condensed matter physics, and even chemistry physics. GP has become a central concept in amounts of investigations in recent decades as an important tool to study the geometric feature of Hamiltonians; especially, it can even be used to characterize topological phase transitions, which are beyond the accessibility of Landau theory of phase transition. Here we propose a singular function expansion method to determine their exact form across the critical points in some quantum models exhibit universal scaling laws across phase transition points. These exact results can provide new insights into the characterization of quantum phase transitions using GP and FS.

Basic Method. We illustrate the basic idea using the following anisotropic XY model,

\[
H = -\sum_{j=-M}^{M} \left( \frac{1 + \gamma}{2} \sigma_j^x \sigma_{j+1}^x + \frac{1 - \gamma}{2} \sigma_j^y \sigma_{j+1}^y + \lambda \sigma_j^z \right),
\]

where \(\lambda\) is the Zeeman field, \(\gamma\) is the anisotropy in \(x\)-\(y\) plane and \(N = 2M + 1\) is the total number of sites. This model reduces to the transverse Ising model when \(\gamma = \pm 1\). To define the geometry phase a circuit of the Hamiltonian is constructed as following,

\[
H_\phi = R_\phi^\dagger H R_\phi,
\]

where \(R_\phi = \prod_{j=-M}^{M} \exp(i\phi \sigma_j^z / 2)\). Hamiltonian \(H_\phi\) can be diagonalized by the standard Jordan-Wigner transformation and Bogoliubov transformation, and the Bogoliubov-de Gennes (BdG) equation reads as

\[
H_{\text{BdG}} = \sum_{k} \Phi_k^\dagger \left( \frac{\epsilon_k}{\Delta_k} \Delta_k^{\star} - \frac{\Delta_k}{\epsilon_k} \right) \Phi_k,
\]

where \(\epsilon_k = \lambda - \cos(k), \Delta_k = -ie^{-2i\phi} \gamma \sin(k)\) and \(\Phi_k^\dagger = (\phi_k, -\phi_{-k})\) in the Nambu basis with \(\phi_k^\dagger\) being the fermion creation operator. The corresponding ground state wave function is obtained exactly using a singular function expansion method to determine their exact form across the critical points.
function is written as
\[ |g\rangle = \prod_{k>0} (\cos(\theta_k/2) + ie^{-i2\phi} \sin(\theta_k/2) e^{i\ell_k} |e^{-}\rangle) |0\rangle, \]
where the relative phase is defined by,
\[ \cos \theta_k = \frac{\epsilon_k}{\xi_k}, \quad \sin \theta_k = \frac{ie^{-2\phi} \Delta_k}{\xi_k}, \]
and (half of) the energy gap \( \xi_k = \sqrt{\chi_k^2 + \Delta_k^2} \). With this ground state the GP is determined [27–29],
\[ \Psi_g = -\sum_{k>0} \frac{\pi}{M} (1 - \cos \theta_k), \]
which can be regarded as summation of all solid-angles for a \(1/2\)-spin in "magnetic field" \(B = (\nabla \Delta_k, 3\Delta_k, \epsilon_k)\). This phase acquired by a closed loop in the parameter space has topological origin [27] and is robust against noise [50, 51]. We are mainly interested in the derivative of the GP across critical points, which can be defined as,
\[ \frac{d\Psi_g}{d\lambda} = \frac{\pi}{M} \sum_{k>0} \frac{1}{\xi_k^2} \left(1 - \frac{\epsilon_k^2}{\xi_k^2}\right). \]

We first consider the scaling of Eq. 6 at the critical point as a function of system length \(N\). In this model the gap is closed at \(k_0 = 0\) (1) when \(\lambda_c = 1\) (-1) and is independent of the anisotropy \(\gamma\). These two points are hereafter defined as special points to discriminate them from the case in the extended models discussed below. Near the critical point when \(\lambda = +1\), \(\lim_{\gamma \to 0} \xi_k = |\gamma| k\), thus we have the following singular function expansion, which is the key mathematical technique used in this work,
\[ \frac{1}{\xi_k} = \chi_k + \mathcal{L}_\lambda(k), \quad \chi_k = \frac{1}{|\gamma|} k. \]

Here \(\mathcal{L}_\lambda(0) = 0\) and \(\mathcal{L}_\lambda(k)\) is finite everywhere in the whole parameter regime. This divergence fully reflects the linear closing and reopening of energy gap across the critical point. The first term is the well-known harmonic number and in the large \(N\) limit, \(\sum_{k=0}^{N} \frac{(1 + \frac{1}{N}(\Gamma - \ln 2 + \ln N))}{\Gamma(1 + \frac{1}{N}(\Gamma - \ln 2 + \ln N))}, \) where \(\Gamma = 0.5772\ldots\) is the Euler-Mascheroni constant. The remained part converges very fast and in the large \(N\) limit can be expressed as an integration,
\[ C = \int_0^\pi dk \frac{1}{\xi_k} \left(1 - \frac{\epsilon_k^2}{\xi_k^2}\right) - \chi_k = \frac{\ln 4 |\gamma|}{|\gamma|} - \frac{1 + \ln \pi}{|\gamma|}. \]

Collecting all these results yields \(\frac{d\Psi_g}{d\lambda}|_{\lambda = \lambda_c} = \alpha_1 \ln N + \beta_1 + \ldots\), where
\[ \alpha_1 = \frac{1}{|\gamma|}, \quad \beta_1 = \frac{\Gamma - \ln 2}{|\gamma|} + \frac{\ln 4 |\gamma|}{|\gamma|} - \frac{1 + \ln \pi}{|\gamma|}. \]

From the harmonic number we see that the next leading term is \(\frac{1}{|\gamma|} \ln N\).

In the thermodynamic limit where the summation of \(k\) can be replaced by an integration over the whole momentum space, we try to study the scaling law of GP as a function of deviation \(\delta \lambda = \lambda - 1\) (for \(\lambda_c = +1\)). We need a slightly different singular function,
\[ \frac{d\Psi_g}{d\lambda}|_{N \to \infty} = \int_0^\pi \left[ (1 - \frac{\chi_k^2}{\xi_k^2} - \chi_k) + \chi_k dk, \right. \]
where \(\chi_k = 1/\sqrt{(\delta \lambda)^2 + (\delta \lambda + \gamma^2) k^2}\). The second part in the above integrand can be computed as,
\[ |\gamma| k dk = -\frac{1}{|\gamma|} \ln |\lambda - 1| + \frac{\ln(2|\gamma|)}{|\gamma|} + O(\lambda - 1). \]
The first integrand in general can not be computed exactly, yet at the critical point (\(\lambda = 1\)), it can be computed exactly (the expression is too complex to be presented here). Gathering all these results together gives
\[ \frac{d\Psi_g}{d\lambda}|_{N \to \infty} = \alpha_2 \ln |\lambda - 1| + \beta_2 + \ldots, \]

\[ \alpha_2 = \frac{1}{|\gamma|}, \quad \beta_2 = \frac{\ln(8|\gamma|^2)}{|\gamma|} - \frac{1}{|\gamma|}. \]

and the next leading term is \((\lambda - 1) \ln |\lambda - 1|\). These next leading terms attribute to the errors in fitting the constants \(\alpha_1\) and \(\alpha_2\) in numerical simulations; and they may become important in the second-order derivative of the GP, see below.

These findings, to the leading orders, are consistent with the numerical results in [28]. We find that in these two scaling laws, \(\alpha_1 = -\alpha_2\) exactly. Notice that \(|\gamma|\) is nothing but just the slope for the closing of energy gap at the critical point, thus \(\alpha_1\) and \(\alpha_2\) is only determined by the inverse of the slope near the critical point, which is the physical meaning of these two constants. The other two \(\beta\)-constants, which are unique functions of \(\alpha\), may have the same or opposite sign depending strongly on the value of \(\gamma\). Moreover, we also have two intriguing limits for these constants. When \(\gamma \to \infty\), all these four constants will approach zero in the manner of \(1/\sqrt{\lambda}\), while on the opposite limit \(\gamma \to 0\), these four constants will approach infinity. In both limits, \(\alpha_1/\beta_1 \sim 1/\ln(\gamma) \sim 0\) and \(\alpha_2/\beta_2 \sim 1/\ln(\gamma) \sim 0\).

This method can also be applied to study the scaling of FS defined as \(|\langle g(\lambda) | g(\lambda + d\lambda) \rangle| = 1 - N \Xi_F d\lambda^2/2\) across the critical point [32, 52]. For Eq. 2, we have
\[ \Xi_F = \frac{1}{4N} \sum_{k>0} \frac{d\theta_k}{d\lambda} = \frac{1}{4N} \sum_{k>0} \frac{1}{\xi_k^2} (1 - \frac{\epsilon_k^2}{\xi_k^2}). \]

This expression is quite similar to Eq. 6 except the \((\gamma k)^{-2}\) divergence at the critical point, for which reason the singular function should be chosen as \(\chi_k = \frac{1}{\gamma k}\). Similarly we first consider the scaling law as a function of system length \(N\), in which the summation of \(k\) gives
\[ \frac{1}{4N} \sum_{k>0} \frac{1}{\gamma k^2} = \frac{N}{96\gamma^2} - \frac{1}{8\pi^2\gamma^2} + \frac{1}{8\pi^2\gamma^2 N} + \ldots. \]
thus \( \alpha_1' = 1/(96\gamma^2) \); and the remained part gives
\[
\frac{1}{8\pi} \int_0^\pi \left[ \frac{1}{8k^2} (1 - \frac{e_k^2}{8k^2}) - \chi_k \right] dk \approx \frac{1}{8\pi^2 \gamma^2} + \frac{\gamma^2 - 3}{64\gamma^3}.\]

Thus we have \( \Xi_F|_{\lambda = \lambda_c} = \alpha_1' N + \beta_1' \), where \( \beta_1' = \frac{\gamma^2 - 3}{64\gamma^3} \).

In the thermodynamic limit, FS as a function of deviation \( \delta \lambda = \lambda - 1 \) is computed similarly with the singular function \( \chi_k = 1/(\delta \lambda^2 + (\delta \lambda + \gamma^2)k^2) \), and we have
\[
\Xi_F = \frac{1}{8\pi} \int_0^\pi \left[ \frac{1}{8k^2} (1 - \frac{e_k^2}{8k^2}) - \chi_k \right] dk + \int_0^\pi \chi_k dk. \tag{15}\]

Again the second integrand can be computed exactly,
\[
\frac{1}{8\pi} \int_0^\pi \xi_k dk = \frac{\tan^{-1}(\pi \sqrt{\lambda - 1 + \gamma^2}/(\lambda - 1))}{8\pi(\lambda - 1)\sqrt{\lambda - 1 + \gamma^2}}
= \frac{\alpha_2'}{|\lambda - 1|} - \frac{1}{8\pi \gamma^2} \frac{\text{sign}(\lambda - 1)}{32\gamma^3} + \cdots, \tag{16}\]

where \( \alpha_2' = 1/(16|\gamma|) \). The first part can also be computed exactly at the critical point, and finally we find
\[
\beta_2' = \frac{\gamma^2 - 3}{64\gamma^3} - \frac{1}{32\gamma^3} \text{sign}(\lambda - 1), \tag{17}\]

thus we find a different scaling law \( \Xi_F|_{N \to} = \alpha_2'/|\lambda - 1| + \beta_2' \), where \( \beta_2' \) has a discontinuous jump across the phase boundary. Notice that the jumping of \( \beta_2' \) can be absorbed to the singular function by assuming \( \alpha_2' (= \alpha_2'(\lambda_c) + \delta \rho_2'/d\lambda)|_{\lambda = \lambda_c} \) to be \( \lambda \)-dependent\,[53], but this will not change our conclusion. Similar to the discussion before, we find that these two constants approach zero when \( \gamma \to \infty \), and infinity when \( \gamma \to 0 \). From this result we can also see that the logarithmic divergence in GP is purely from the linear divergence of the expression at the critical point, and some different scaling laws can be found, for instance in the Dicke model\,[54, 55] and Lipkin-Meshkov-Glick model\,[56–58] where the gaps are closed in a different ways. Thus these coefficients do not directly carry information of the global topology of wave functions.

Coefficients of the divergent terms may be written as,
\[
\alpha_2 = -\alpha_1, \quad \alpha_1' = \frac{1}{96\alpha_1}, \quad \alpha_2' = \frac{1}{16}|\alpha_1|, \tag{18}\]

which is always correct for a system with gap closed and reopened in a linear way at the special points. The latter two equations also indicate the general relation \( \alpha_1' = \frac{8}{3}(\alpha_2')^2 \). Thus these quantities although defined in totally different ways in actually describe the same physics. Besides, from the standard ansatz\,[32, 59, 60],
\[
\Xi_F|_{\lambda = \lambda_c} \sim N^{2/\nu - D}, \quad \Xi_F|_{N \to \infty} \sim |\lambda - \lambda_c|^{D_{\nu - 2}}. \tag{19}\]

For one dimensional system, \( D = 1 \), our analytical results show the critical exponent for the coherent length \( \nu \equiv 1 \) exactly. The same conclusion can be obtained based on scaling of GP, where \( \nu = |\alpha_2|/|\alpha_2| = 1 \).

When both the scaling of size and parameter are taken into account, we can compute the scaling of \( F_1 = \frac{d\psi_2}{dx} \lambda - \frac{\psi_2}{d\lambda} \), and \( F_2 = \Xi_F|_{\lambda - \Xi F}|_{\lambda_c} \) as a function of \( N\gamma(\lambda - \lambda_c) \). These two scaling functions are only determined by the divergent term since \( N\gamma(\lambda - \lambda_c) \ll |\lambda_c| \).

For \( F_1 \) we find
\[
F_1 = \frac{\pi}{2} \sum_{k} \frac{1}{\sqrt{dx^2 + N^2\gamma^2x^2}} - \frac{1}{N|\gamma|} \sum_{n=1}^{\infty} \frac{dx^2}{A_n}, \tag{20}\]

where \( A_n = 6\pi^4 \gamma^3 |\gamma|^3 + 3n|\gamma| dx^2 \) and \( dx = N(\lambda - \lambda_c) \).

Notice that the summation of \( n \) is extended to infinite due to the fast convergence of the above result. After a bit computation we find \( F_1 = \frac{\psi_2(1)|N(\lambda - \lambda_c)|^2}{32\pi^2 |\gamma|^3} \), where \( \psi_2(1) = -2.40411 \) is the polygamma function, thus \( \eta = 1 \). This result is consistent with the numerical finding in\,[28].

The same method can be applied to \( F_2 \) which yields
\[
F_2 = -\frac{(\lambda - \lambda_c)N^{3/2}|\gamma|^2}{1440|\gamma|^3}, \text{ thus } \eta = 3/2. \tag{21}\]

Extended Ising model. We next show that these scaling laws depend strongly on at which point the gap is closed and reopened and they may break down when the gap is not closed at the special points, which can be captured by the following extended Ising model\,[58, 61–64],
\[
H' = -\sum_{j=-M}^{M} (\lambda_1 \sigma_j^z \sigma_{j+1}^z + \lambda_2 \sigma_j^z \sigma_{j-1}^z + \sigma_j^z). \tag{21}\]

This model can still be exactly solved using the same method\,[47–49]. In the fermion picture (Eq. 2) the three-site interaction is equivalent to the next-nearest-neighbor
hopping and pairing determined by \( \lambda_2 \), thus we have
\[
i \Delta_k e^{2i\phi} = \sum_{n=1}^{2} \lambda_n \sin(nk), \quad \epsilon_k = 1 - \sum_{n=1}^{2} \lambda_n \cos(nk). \tag{22}
\]

The closing of energy gap determined by \( \Delta_k = 0 \) and \( \epsilon_k = 0 \) simultaneously yields
\[
\text{Line AC} : k_0 = 0, \quad 1 - \lambda_1 - \lambda_2 = 0, \tag{23}
\]
\[
\text{Line AB} : k_0 = \pi, \quad 1 + \lambda_1 - \lambda_2 = 0, \tag{24}
\]
\[
\text{Line BC} : k_0 = \cos^{-1}(\frac{\lambda_1}{\lambda_2}), \quad \lambda_2 = -1, |\lambda_1| < 2. \tag{25}
\]

The corresponding phase diagram is presented in Fig. 1b. Notice that the BdG equation possesses chiral symmetry \( S = \sigma_s \) at \( \phi = 0 \), where \( \sigma_s \) is the Pauli matrix and \( K \) is the complex conjugate operator, since \( SH_{\text{BdG}}S^\dagger = -H_{\text{BdG}} \). This equation belongs to topological BDI class in one spatial dimension\[65, 66\], which is characterized by the well-defined winding number \( W = \frac{1}{2\pi i} \oint dq g(k) dq \), where \( g = \epsilon_k + \Delta_k \). This model has been studied by Niu et al\[61\] to show the possibility of hosting multiply Majorana fermions in an open chain when \( W = 2 \).

Due to the presence of two parameters in determining the phase boundaries, the divergence of GP and FS depend strongly on how and along which direction the critical boundary is crossed. Consider a line across the critical boundary AC along \( \theta \) direction (see point \( D \) in Fig. 1b and the dashed line is assumed to be \( \lambda_2 = \tan(\theta)\lambda_1 + d \)). Then we find the coordinate of \( D = (\frac{1-d}{1+\tan(\theta)}, \frac{d+\tan(\theta)}{1+\tan(\theta)}) \). With the previous method we have \( (\alpha_2 = 0 \) and \( \alpha_1 < 0) , \)
\[
\alpha_2 = -\alpha_1 = + \frac{|1 + \tan(\theta)|}{|1 + d + 2\tan(\theta)|}, \tag{26}
\]
from which we see that \( \alpha_2 = -\alpha_1 = \infty \) when \( \tan(\theta) = -\frac{d}{1+\tan(\theta)} \); and \( \alpha_2 = -\alpha_1 = 0 \) when along the phase boundary \( (\theta = -\pi/2 \) or \( 3\pi/4) \) since no phases are crossed. When \( \theta = \pi/2 \), we have \( \alpha_2 = -\alpha_1 \equiv \frac{1}{2} \), which is independents of the other parameters. The other two coefficients can also be defined straightforwardly using Eq. 18.

The constants \( \beta_1 \) and \( \beta_2 \) in this extended model can no longer be computed analytically, however, they can still be computed exactly with the technique in Eq. 10 and 15 using numerical methods.

Along the boundary BC, we find \( \frac{d\psi}{d\lambda_1} \propto (1 + \lambda_2) \) and \( \Xi_F|\lambda_1 \propto (1 + \lambda_2) \), thus both \( \frac{d\psi}{d\lambda_1} = 0 \) and \( \Xi_F|\lambda_1 = 0 \) exactly as a function of length \( N \) and deviation \( \delta \lambda \) for the same reason. We next point out that the scaling laws as a function of \( N \) across the phase boundary BC along \( \lambda_2 \) direction is broken-down since the gap is not closed and reopen at the special points. This is different from the previous case where \( k_0 = 0 \) or \( k_0 = \pi \) will not be sampled during the summation of \( k \). A typical result for the GP and FS is presented in Fig. 2, in which we find that at some "magic point" when \( k = 2\pi n/N \to k_0 \), a "pulse" in these two quantities can be found. The analogous features can also be found in other extended models\[58, 62-64\]. The breakdown of this scaling also indicates the failure of Eq. 19 and scaling of \( \frac{d\psi}{d\lambda_1} |\lambda_2 - d\lambda_1, \quad \Xi_F|\lambda_2 - N|\lambda_2 \) as a function of \( N^p|\lambda_2 \).

However, the similar scaling laws can still be found as a function of deviation \( \delta \lambda = \lambda_2 + 1 \) (line BC). In the vicinity of \( k_0 \) the energy gap can be approximated as,
\[
\xi_k^2 \approx a + b(k - k_0) + c(k - k_0)^2, \tag{27}
\]
where \( c = 2 - 2, \cos(2k_0), \quad b = 2\delta \lambda \sin(2k_0) \) and \( a = \delta \lambda^2 \), with \( \cos(k_0) = \lambda_1/2 \) and \( b^2 - 4ac \leq 0 \) for all \( k \). This series expansion is different from the previous ones due to the appearance of linear term \( b \). Notice that when \( k_0 = 0 \) or \( \pi \), the contribution of the numerator in the integrand is always equals to one; however in this case, the numerator then becomes important, and the singular function should be chosen as \( \chi = \frac{\sin^2(k_0)}{\xi_k^2} \) in GP and \( \chi = \frac{\sin^2(k_0)}{\xi_k^2} \) in FS. Thus the final coefficients \( \alpha_i \) are no longer purely determined by the slope \( c \) with these singular function expansions we find
\[
\frac{d\psi}{d\lambda_2} = \alpha_2 \ln |\lambda_2 + 1| + \beta_2, \Xi_F|\lambda_2 = \frac{\alpha'_2}{|\lambda_2 + 1|} + \beta'_2, \tag{28}
\]
\[
\alpha_2 = -\frac{2}{\sqrt{4 - \lambda_2^2}}, \quad \alpha'_2 = \frac{\pi/2 - \tan^{-1}(\lambda_2/\sqrt{4 - \lambda_2^2})}{8\pi}. \tag{29}
\]

The intimate relations in Eq. 18 due to the contribution of the numerator at non-special \( k_0 \) is no longer true (it still holds only when \( \lambda_1 = 0 \)). The above result is correct only when \( \lambda_1 \) is not very close to \( \pm 2 \) (points B, C), in which case the constants \( \beta_2 \) and \( \beta'_2 \) may become singular.

Discussion and Conclusion. Here a general method to obtain the exact scaling laws for GP and FS across the quantum phase transitions is presented. These scaling laws are independent of the choice of singular functions since for different singular functions the divergent behavior near the critical points which determine the scaling
laws are exactly the same. Moreover this method can be applied not only to the first-order derivative of GP but also their higher-order derivatives across the critical point. For instance, for Eq. 1,

$$\frac{d^2\Psi_{\theta}}{dx^2}|_{x=1} = -\frac{3}{2|\gamma|^3} \ln N + \beta_3,$$

(30)

with \( \beta_3 = \frac{3(\ln 2 - (\gamma+3 \ln 2 - 4))}{2|\gamma|^3} - \frac{1}{2|\gamma|} + \cdots \), which has the same form as \( \frac{d\theta}{dx} |_{x=1} \). However for the deviation \( \delta \lambda = \lambda - 1 \), it takes another intriguing form after singular function expansion,

$$\frac{d^2\Psi_{\theta}}{dx^2}|_{N \to \infty} = -\frac{1}{|\gamma|(\lambda - 1)} + \frac{3 \ln(|\lambda - 1|)}{2|\gamma|^3} + \beta_3',$$

(31)

where \( \beta_3' = (3 \ln \frac{\pi^2}{2} + 4)/(2|\gamma|^3) - 1/(2|\gamma|) \). These two singular functions arise from the derivative of the leading term, \( \ln |\lambda - 1| \), and the next leading term, \( \frac{3 \ln(|\lambda - 1|)}{2|\gamma|^3} \). The jumping of constant \( \beta_3' \) is absent[53].

These results also reveal a close relation between the constants \( \beta \) and \( \alpha \). These interesting features, which have been barely discussed in previous literatures, will be presented elsewhere. This method is powerful and can also be adapted to study the singular behaviors in entanglement[52, 67–72] quantum discord and correlation[73–75] and geometric Euler number[59, 76, 77], which will be subject to future investigation. To conclude, these exact results can greatly enrich our understanding of GP and FS in the characterization of quantum phase transitions.

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