Scaling of geometric phase and fidelity susceptibility across the critical points and their relations

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It has been found via numerical simulations that the geometric phase (GP) and fidelity susceptibility (FS) across the quantum critical points exhibit some universal scaling laws. Here we propose a singular function expansion method to find their exact singular forms and the related coefficients across the critical points. For models where the gaps are closed and reopened at special points ($k_0 = 0,\pi$), scaling laws can be found as a function of the system length N and parameter deviation $\lambda - \lambda_c$, where λ_c refers to one of the critical parameters. Although the GP and FS are defined in totally different ways, we find that these two measurements are essentially determined by the same physics, and as a consequence, their coefficients are closely related. Some of these exact relations are found in the anisotropic XY model and extended Ising models. We also show that the constant term in FS may be accompanied by a discontinuous jump across the critical points and, thus, does not have a universal scaling form. These findings should be in contrast to the cases where the gaps are not closed and reopened at the special points, in which some of the above scaling laws may break down as a function of the system length. Finally, we investigate the second-order derivative of GP, which may also exhibit some scaling laws across the critical point. These exact results can greatly enrich our understanding of GP and FS in the characterization of quantum phase transitions and may even find important applications in related physical quantities, such as entanglement, discord, correlation, and quantum Euler numbers, which may also exhibit scaling laws across the critical points.

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I. INTRODUCTION

Ever since its theoretical discovery [1], the geometric phase (GP) has permeated different branches of physics, including ultracold atoms [2–4], quantum computation [5–8], condensed matter physics [9–13], and even chemistry physics [14–16], as an important tool to study the geometric properties of wave functions [17–19]. It can even be used to diagnose topological phase transitions [20–22], which is beyond the accessibility of the Landau theory of phase transition. Across the critical points the derivative of the GP exhibits some universal scaling laws [23–25], which are derived exactly in this paper. In recent years this phase has also been directly measured in experiments [3,26–29], and due to the geometric origin, it is shown to be robust against external perturbation.

The fidelity susceptibility (FS), based on the overlap between two ground-state wave functions, is another way beyond the Landau paradigm to characterize quantum phase transitions [30–44]. This phase is not defined along a closed trajectory in parameter space, thus it is not directly related to the global geometric feature of the ground state. However, since the structures of the ground states in two phases are different in the sense of different order parameters or different topologies, the FS also exhibits some scaling laws across the critical points; see reviews in Refs. [25] and [32]. This work explores the relations between these two quantities in the characterization of quantum phase transitions.

In previous literature, all the scaling laws in various models are exploited by numerical simulations [23–25,30–44], thus our understanding of these laws is still greatly limited. In this paper these scaling laws are obtained exactly using a singular function expansion method, in which the coefficients of the divergent terms, constant terms, and next leading terms are determined analytically. We show that the above two measurements—the GP and FS—for quantum phase transitions are essentially determined by the same physics across the critical points, thus their coefficients also have some intimate relations. We find that the coefficients of the divergent terms reflect only how and in what way the energy gap is closed and reopened during phase transitions, thus they do not carry information about the topological properties of the ground-state wave functions. In the XY model and extended Ising model, the gap is closed and reopened linearly as a function of the momentum k at the critical point, and we find that the coefficients of the divergent terms are purely determined by the slope of this energy gap. The coefficients of the divergent terms are exactly equal to 0 when the GP and FS are calculated along the phase boundaries; otherwise, they will always be nonzero when two phases are crossed. We also find that the constant term in FS may be accompanied by a discontinuous jump across the critical points and, thus, does not have a universal scaling form. When the gap is closed and reopened not at the special points ($k_0 = 0, \pm\pi$), some of the scaling laws may not exist as a function of the system length, thus some of the intimate relations between the coefficients in the GP and FS may break down. This method is powerful and can also be used to study the higher-order derivative of the GP, which may also have some scaling behaviors. The exact relations obtained in this work can provide new insight into the characterization of quantum phase transitions using the GP and FS.

The rest of this paper is organized as follows. In Sec. II, we illustrate our major idea using the anisotropic XY model, in which several general universal scaling laws are derived

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exactly when the critical point is approached along different directions as a function of the system parameters. In Sec. III we investigate the fate of these scaling laws in an extended Ising model, in which the phase boundaries are controlled by two independent parameters. We finally discuss the second-order derivative of the GP and comment on the applicability of our method in other related quantities in Sec. IV.

II. XY MODEL

We first illustrate the basic idea using the anisotropic XY model [45–49],

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

where λ is the Zeeman field, γ is the anisotropy in the x-y plane, and $N=2M+1$ is the total number of sites. This model reduces to the transverse Ising model when $\gamma=\pm1$. To define the geometry phase, a circuit of the Hamiltonian is constructed as follows [23–25]:

$$H_\phi=\mathcal{R}_\phi^\dagger H\mathcal{R}_\phi,\quad \mathcal{R}_\phi=\prod_{j=-M}^{M}\exp\left(\frac{i}{2}\phi\sigma_j^z\right). \quad (2)$$

The above Hamiltonian can be diagonalized by the standard Jordan-Wigner transformation, which transforms the spin model to the p-wave tight-binding model, and then by Bogoliubov transformation [48–50], which transforms the tight-binding model from real space to momentum space. The final Bogoliubov–de Gennes (BdG) equation reads as

$$H_{\mathrm{BdG}}=\sum_k\Phi_k^\dagger\begin{pmatrix}\epsilon_k & ie^{-i2\phi}\Delta_k\\ -ie^{i2\phi}\Delta_k & -\epsilon_{-k}\end{pmatrix}\Phi_k, \quad (3)$$

where $\epsilon_k=\lambda-\cos(k)$, $\Delta_k=-\sin(k)$, and $\Phi_k^\dagger=(c_k^\dagger,c_{-k})$ in the Nambu basis, with $c_k^\dagger$ and c_k being the fermion creation and annihilation operators, respectively. The corresponding ground state is written as

$$|g\rangle=\prod_{k>0}\left(\cos\left(\frac{\theta_k}{2}\right)+ie^{-i2\phi}\sin\left(\frac{\theta_k}{2}\right)c_k^\dagger c_{-k}^\dagger\right)|0\rangle, \quad (4)$$

where the relative phase is defined by

$$\cos\theta_k=\frac{\epsilon_k}{\xi_k},\quad \sin\theta_k=\frac{\Delta_k}{\xi_k}, \quad (5)$$

and the energy gap is defined as $\xi_k=\sqrt{\epsilon_k^2+|\Delta_k|^2}$. With this ground-state wave function the GP is determined [23–25],

$$\Psi_g=-\sum_{k>0}\frac{\pi}{M}(1-\cos\theta_k), \quad (6)$$

which can be regarded as the summation of all solid angles for a spin-$\frac{1}{2}$ electron in a "magnetic field" $\mathbf{B}=(\mathrm{Re}\Delta_k,\mathrm{Im}\Delta_k,\epsilon_k)$[1]. This phase, acquired by a closed loop in the parameter space, has a topological origin [23] and is robust against noise [51,52]. We are mainly interested in the first-order derivative of the GP across the critical points, which reads as

$$\frac{d\Psi_g}{d\lambda}=\frac{\pi}{M}\sum_{k>0}\frac{1}{\xi_k}\left(1-\frac{\epsilon_k^2}{\xi_k^2}\right). \quad (7)$$

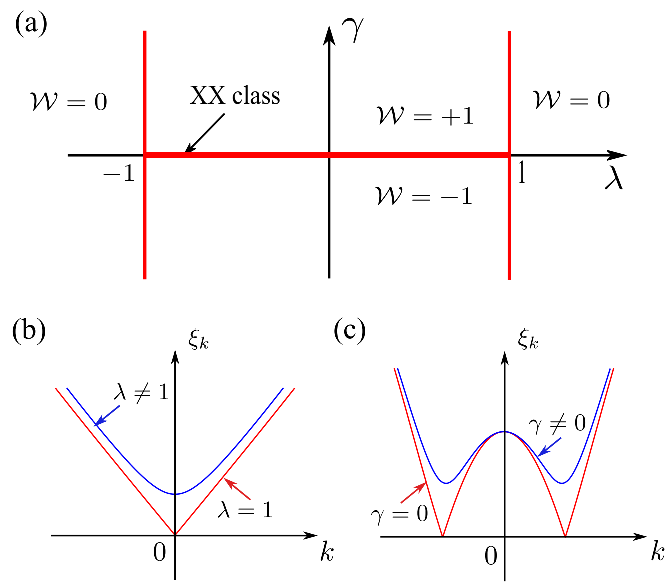

FIG. 1. (a) Phase diagram of the XY model. When $\gamma=0$, the system belongs to the XX universal class. Solid red lines represent the gapless boundaries. In each phase, $\mathcal{W}$ denotes the winding number due to chiral symmetry. (b, c) Typical band gap near $\lambda=\pm1$, $\gamma\neq0$ and $\gamma=0$, $|\lambda|<1$, respectively.

The phase diagram for this model is presented in Fig. 1, which is determined by $\epsilon_k=0$ and $\Delta_k=0$ simultaneously, thus the energy gap is closed ($\xi_k=\sqrt{\epsilon_k^2+|\Delta_k|^2}=0$). There are two cases. When $\lambda_c=\pm1$ the gap is closed and reopened at $k_0=0$ (for $\lambda_c=1$) and $k_0=\pi$ (for $\lambda_c=-1$); see a typical example in Fig. 1(b). Hereafter these two points, $k_0=0,\pi$, are called special points throughout this paper, since their features are totally different from those when the gap is closed and reopened at some other momenta in $(0,\pi)$. These two boundaries are independent of γ, thus the phase transitions are controlled by only a single parameter λ. However, when $\gamma=0$, the pairing term disappears and the XY model reduces to a single-particle model after Jordan-Winger transformation, which is always gapless when $|\lambda|<1$. This boundary is generally called the XX universal class, which contains two gapless points at $k_0=\pm\arccos(\lambda)$ [see Fig. 1(c)]. Note that the BdG equation possesses chiral symmetry $\mathcal{S}=\sigma_x$ at $\phi=0$, where σ_x is the Pauli matrix and $\mathcal{S}H_{\mathrm{BdG}}\mathcal{S}^\dagger=-H_{\mathrm{BdG}}$; this model belongs to the topological BDI class in one spatial dimension [53,54], which is characterized by the winding number

$$\mathcal{W}=\frac{1}{2\pi i}\oint dkq^{-1}dq, \quad (8)$$

where $q=\epsilon_k+i\Delta_k$. The corresponding winding number in each phase is also shown in Fig. 1.

We first consider the scaling law of Eq. (7) at the critical point when $\lambda_c=1$ as a function of the system length N. Near this critical point, $\lim_{k\to0}\xi_k=|\gamma k|$ and $\lim_{k\to0}(1-\frac{\epsilon_k^2}{\xi_k^2})=1$, thus we have the following singular function expansion, which

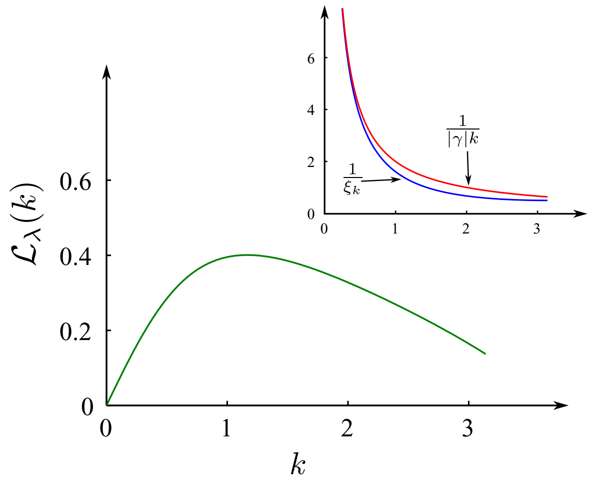

FIG. 2. Basic idea of the singular function expansion method. When the singular function (here $1/\xi_k$, for example) is balanced out by another much simpler singular function ($1/|\gamma k|$), their difference $\mathcal{L}_\lambda(k)$ is general finite in the whole k space. The simpler singular function can be used to determine the divergent term and the corresponding coefficient in GP and FS.

is the key mathematical trick used in this paper:

$$\frac{1}{\xi_k} = \chi_k - \mathcal{L}_\lambda(k), \quad \chi_k = \frac{1}{|\gamma|k}. \tag{9}$$

Here $\mathcal{L}_\lambda(0) = 0$ and $\mathcal{L}_\lambda(k)$ is always finite in the whole parameter space (see Fig. 2). The divergent behavior of χ_k fully reflects the linear closing and reopening of the energy gap as a function of k across the critical point. The first term is the harmonic number and in the large-N limit,

$$\frac{\pi}{M}\sum_{k>0}\frac{1}{|\gamma|k} \to \frac{1}{|\gamma|}\left(1+\frac{1}{N}\right)(\Gamma - \ln 2 + \ln N), \tag{10}$$

where $\Gamma = 0.5772\ldots$ is the Euler-Mascheroni constant. The remaining part converges very rapidly and in the large-N limit it can be expressed as an integration in momentum space:

$$\mathcal{C} = \int_0^\pi dk\left[\frac{1}{\xi_k}\left(1-\frac{\epsilon_k^2}{\xi_k^2}\right) - \chi_k\right] = \frac{\ln(4|\gamma|/\pi) - 1}{|\gamma|}. \tag{11}$$

Thus the constant term is independent of the system length N. Collecting all these results together yields

$$\frac{d\Psi_g}{d\lambda}|_{\lambda=\lambda_c} = \alpha_1 \ln N + \beta_1 + \ldots, \tag{12}$$

where we find analytically that

$$\alpha_1 = \frac{1}{|\gamma|}, \quad \beta_1 = \frac{\Gamma - \ln 2}{|\gamma|} + \frac{\ln 4|\gamma|}{|\gamma|} - \frac{1+\ln\pi}{|\gamma|}, \tag{13}$$

and the next leading term is $\frac{1}{|\gamma|}\frac{\ln N}{N}$.

In the thermodynamic limit ($N \to \infty$), where the summation of k can be replaced with an integration over the momentum space, we try to study the scaling law of the GP as a function of the deviation $\delta\lambda = \lambda - 1$ (for $\lambda_c = +1$). We need a slightly different singular function expansion,

$$\left.\frac{d\Psi_g}{d\lambda}\right|_{N\to\infty} = \int_0^\pi \left[\left(\frac{1}{\xi_k}\left(1-\frac{\epsilon_k^2}{\xi_k^2}\right) - \chi_k\right) + \chi_k\right]dk, \tag{14}$$

where

$$\chi_k = \frac{1}{\sqrt{(\delta\lambda)^2 + (\delta\lambda + \gamma^2)k^2}}. \tag{15}$$

This singular function ensures that the first part of Eq. (14) is always finite when $\delta\lambda$ approaches 0. We may verify easily that

$$\lim_{\delta\lambda\to 0}\lim_{k\to 0}\left(\frac{1}{\xi_k}\left(1-\frac{\epsilon_k^2}{\xi_k^2}\right) - \chi_k\right) = \text{finite}. \tag{16}$$

The second part in the above integral [Eq. (14)] can be evaluated as

$$\int_0^\pi \chi_k dk = -\frac{1}{|\gamma|}\ln|\lambda - 1| + \frac{\ln(2\pi|\gamma|)}{|\gamma|} + \ldots. \tag{17}$$

The first integral in general cannot be computed analytically, yet at the critical point ($\lambda_c = +1$), it can be computed exactly by setting $\delta\lambda = 0$. We find that

$$\begin{aligned}\int_0^\pi dk\left(\frac{1}{\xi_k}\left(1-\frac{\epsilon_k^2}{\xi_k^2}\right) - \chi_k\right) &= \int_0^\pi dk\frac{\gamma^2\sin^2(k)}{((1-\cos(k))^2 + \gamma^2\sin^2(k))^{3/2}} - \frac{1}{|\gamma|k}\\ &= \frac{\ln 4|\gamma| - \ln\pi - 1}{|\gamma|}.\end{aligned} \tag{18}$$

Gathering all these results together gives $\frac{d\Psi_g}{d\lambda}|_{N\to\infty} = \alpha_2\ln|\lambda-1| + \beta_2 + \ldots$, where

$$\alpha_2 = -\frac{1}{|\gamma|}, \quad \beta_2 = \frac{\ln(8\gamma^2)}{|\gamma|} - \frac{1}{|\gamma|}, \tag{19}$$

The next leading term is $\frac{3}{2|\gamma|^2}(\lambda - 1)\ln|\lambda - 1|$, which should be important when considering the second-order derivative of the GP; see the discussion in Sec. IV.

The scaling of the GP along the γ direction at $\gamma = 0$ may also be computed, which we find

$$\left.\frac{d\Psi_g}{d\gamma}\right|_{|\lambda|<1} = \frac{\pi}{M}\sum_{k>0}\frac{\gamma(\lambda - \cos(k))\sin(k)^2}{((\lambda-\cos(k))^2 + \gamma^2\sin(k)^2)^{3/2}} = 0. \tag{20}$$

Note that the geometric phase is a function of γ^2, thus the first-order derivative of the GP with respect to γ will be proportional to γ, which will be 0 exactly when $\gamma = 0$ at the phase boundary.

We are also interested in the first-order derivative of the GP along the phase boundary $\lambda = 1$, which is determined as

$$\begin{aligned}\frac{d\Psi_g}{d\gamma}|_{\lambda=1} &= \int_0^\pi \frac{\gamma(-1+\cos(k))\sin(k)^2}{((1-\cos(k))^2 + \gamma^2\sin(k)^2)^{3/2}}dk\\ &= \frac{2|\gamma|}{\gamma(1-\gamma^2)} - \frac{2\gamma\arcsin(\sqrt{\gamma^2-1})}{(\gamma^2-1)^{3/2}}.\end{aligned} \tag{21}$$

The above result is finite in the whole parameter regime. We also find that $\lim_{\gamma\to 0}\frac{d\Psi_g}{d\gamma}|_{\lambda=1} = 2\text{sgn}(\gamma)$, which changes sign across the phase boundary at $\gamma = 0$. The phase boundaries at $\gamma = 0$ and $|\lambda| < 1$ have similar features. The geometric phase can be computed exactly in this limit [5,24],

$$\Psi_g = -\int_0^\pi\left(1 - \frac{\lambda - \cos(k)}{|\lambda - \cos(k)|}\right)dk = -2\arccos(\lambda), \tag{22}$$

when $\gamma = 0$. Thus the first-order derivative of Ψ_g along the phase boundary can be computed as

$$\frac{d\Psi_g}{d\lambda}|_{N\to\infty} = \frac{2}{\sqrt{1-\lambda^2}}, \tag{23}$$

which is also finite in the parameter regime $\lambda \in (-1,1)$. In the above analysis we compute only the geometric phase along the phase boundary in the thermodynamic limit; the summation of k in a finite system should also be finite. In this regard, the α coefficients (see also the discussion below) can be exactly equal to 0, which is verified to be a rather general conclusion with the model in Sec. III.

These findings, to the leading terms, are quantitatively consistent with the numerical results in [24]. We find that in these two scaling laws, $\alpha_1 \equiv -\alpha_2$ exactly. Note that $|\gamma|$ is nothing but the slope of the energy gap as a function of k during the closing and reopening at the critical point (see Fig. 1), thus α_1 and α_2 are determined only by the inverse of this slope, which is the physical meaning of these two constants. This picture is always correct even for more complicated models as long as the gap is closed and reopened at the special points in a linear manner, and the phase transitions may belong to a different universal class when the gap is closed and reopened in some different ways. For $\lambda_c = \pm 1$, the two β constants should be unique functions of γ and, thus, should be unique functions of α, and the sign of these β constants depends strongly on the value of α. Moreover, we also have two intriguing limits for these constants. When $\gamma \to \infty$, all four constants will approach 0 in the manner of $\frac{1}{|\gamma|}$, while at the opposite limit, $\gamma \to 0$, these four constants will approach ∞. At both limits, $\alpha_i/\beta_i \sim 1/\ln(\gamma)$, $i = 1,2$. This can be understood as follows. When $\gamma \to \infty$, the contribution of the divergent term should be very small and the major contribution to the GP comes from the constant term; however, when $\gamma \to 0$, the system approaches a totally different universal class, in which case the divergent of the constant term β is much faster than the divergent term, thus these two limits are governed by totally different physics.

This method can also be applied to study the scaling of FS, defined as

$$|\langle g(\lambda)|g(\lambda + d\lambda)\rangle| = 1 - N\Xi_F d\lambda^2/2, \tag{24}$$

across the critical point [32,55]. For model 3, we have

$$\Xi_F = \frac{1}{4N}\sum_{k>0}\left(\frac{d\theta_k}{d\lambda}\right)^2 = \frac{1}{4N}\sum_{k>0}\frac{1}{\xi_k^2}\left(1-\frac{\epsilon_k^2}{\xi_k^2}\right). \tag{25}$$

This expression is quite similar to Eq. (7) except the $(\gamma k)^{-2}$ divergence at the critical point; for this reason the singular function should be chosen as $\chi_k = \frac{1}{\gamma^2 k^2}$. Similarly, we first consider the scaling law as a function of the system length N, in which the summation of k gives

$$\frac{1}{4N}\sum_{k>0}\frac{1}{\gamma^2k^2} = \frac{N}{96\gamma^2} - \frac{1}{8\pi^2\gamma^2} + \frac{1}{8\pi^2\gamma^2 N} + \ldots, \tag{26}$$

thus $\alpha_1' = 1/(96\gamma^2)$, and the remaining part gives

$$\frac{1}{8\pi}\int_0^\pi \left[\frac{1}{\xi_k^2}\left(1-\frac{\epsilon_k^2}{\xi_k^2}\right) - \chi_k\right]dk \approx \frac{1}{8\pi^2\gamma^2} + \frac{\gamma^2-3}{64|\gamma|^3}.$$

Collecting these results yields

$$\Xi_F|_{\lambda=\lambda_c} = \alpha_1' N + \beta_1', \quad \text{where} \quad \beta_1' = \frac{\gamma^2-3}{64|\gamma|^3}. \tag{27}$$

In the thermodynamic limit, the FS as a function of the deviation $\delta\lambda = \lambda - 1$ is computed in a similar way with the singular function $\chi_k = 1/(\delta\lambda^2 + (\delta\lambda + \gamma^2)k^2)$, and we have the following singular function expansion:

$$\Xi_F = \frac{1}{8\pi}\left(\int_0^\pi \left[\frac{1}{\xi_k^2}\left(1-\frac{\epsilon_k^2}{\xi_k^2}\right) - \chi_k\right]dk + \int_0^\pi \chi_k dk\right). \tag{28}$$

The second integral can be computed exactly,

$$\begin{aligned}\frac{1}{8\pi}\int_0^\pi \chi_k dk &= \frac{\tan^{-1}(\pi\sqrt{\lambda-1+\gamma^2}/(\lambda-1))}{8\pi(\lambda-1)\sqrt{\lambda-1+\gamma^2}} \\ &= \frac{\alpha_2'}{|\lambda-1|} - \frac{1}{8\pi^2\gamma^2} - \frac{\mathrm{sgn}(\lambda-1)}{32|\gamma|^3} + \ldots,\end{aligned} \tag{29}$$

where $\alpha_2' = 1/(16|\gamma|)$. The first part can also be computed exactly at the critical point, and finally, we have

$$\beta_2' = \frac{\gamma^2-3}{64|\gamma|^3} - \frac{1}{32|\gamma|^3}\mathrm{sgn}(\lambda-1); \tag{30}$$

thus we find a different scaling law, $\Xi_F|_{N\to} = \alpha_2'/|\lambda-1| + \beta_2'$, where β_2' has a discontinuous jump across the phase boundary owing to the appearance of the absolute symbol in the denominator [56] (see numerical simulation in Fig. 3). The jump can be extremely large when $|\gamma|$ is small. This jump has been ignored in previous numerical simulations due to its minor role in the divergent behavior of FS when γ is not small enough and $\lambda - \lambda_c$ approaches 0, thus, differently from the conclusion in Ref. [57], we conclude that the FS across the critical point may not have a universal form. Note that the jump of β_2' can be absorbed into the singular function by assuming α_2' to be a λ dependent parameter [56], that is, $\alpha_2' = \alpha_2'(\lambda_c) + d\alpha_2'/d\lambda|_{\lambda_c}(\lambda-\lambda_c)$. Similarly to the preceding discussion, we find that these two constants approach 0 when $\gamma \to \infty$ and ∞ when $\gamma \to 0$. From this result we can also see that the logarithmic divergence in FS is also purely from the linear closing of the energy gap at the critical point, and some different scaling laws can be found, for instance, in the Dicke model [58,59] and Lipkin-Meshkov-Glick model [60–62], where the gaps are closed and reopened in some different ways. Thus these coefficients do not directly carry information on the global topology of the ground-state wave function.

The coefficients of the divergent terms may be written in a compact way as

$$\alpha_2 = -\alpha_1, \quad \alpha_1' = \frac{1}{96}\alpha_1^2, \quad \alpha_2' = \frac{1}{16}|\alpha_1|, \tag{31}$$

which are always correct for a system with the 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, actually describe the same physics—the slope of the energy gap as a function of k at the critical point. Besides, from the standard scaling ansatz [32,63,64],

$$\Xi_F|_{\lambda=\lambda_c} \sim N^{2/\nu - D}, \quad \Xi_F|_{N\to\infty} \sim |\lambda-\lambda_c|^{D\nu-2}, \tag{32}$$

where ν denotes the critical exponent for the coherent length. For one spatial dimension, $D = 1$, our analytical results show the critical exponent $\nu = 1$ exactly. This quantity can also be obtained from the GP, where $\nu = |\alpha_1/\alpha_2| = 1$.

We may also compute the FS along the phase boundary. When $\lambda = 1$, we have

$$\begin{aligned}\Xi_F|_{\lambda=1} &= \frac{1}{4N}\sum_{k>0}\left(\frac{d\theta_k}{d\gamma}\right)^2 \\ &= \mathrm{sgn}(\gamma)\int_0^{\pi} \frac{(1-\cos(k))\sin(k)}{(1-\cos(k))^2+\gamma^2\sin(k)^2} \\ &= \mathrm{sgn}(\gamma)\frac{2\ln(|\gamma|)}{\gamma^2-1},\end{aligned} \tag{33}$$

which is also finite along the phase boundary. Differently from the GP, this quantity will diverge when the critical point $\gamma = 0$ is reached. Similarly, we can also calculate the FS along the phase boundary at $\gamma = 0$ and $|\lambda| < 1$, which can be written as

$$\Xi_F|_{\gamma=0} = \frac{1}{4N}\sum_{k>0}\frac{\gamma(\lambda-\cos(k))\sin(k)}{(\lambda-\cos(k))^2+\gamma^2\sin(k)^2} = 0, \tag{34}$$

because the phase transition takes place at $\gamma = 0$ in the XX model.

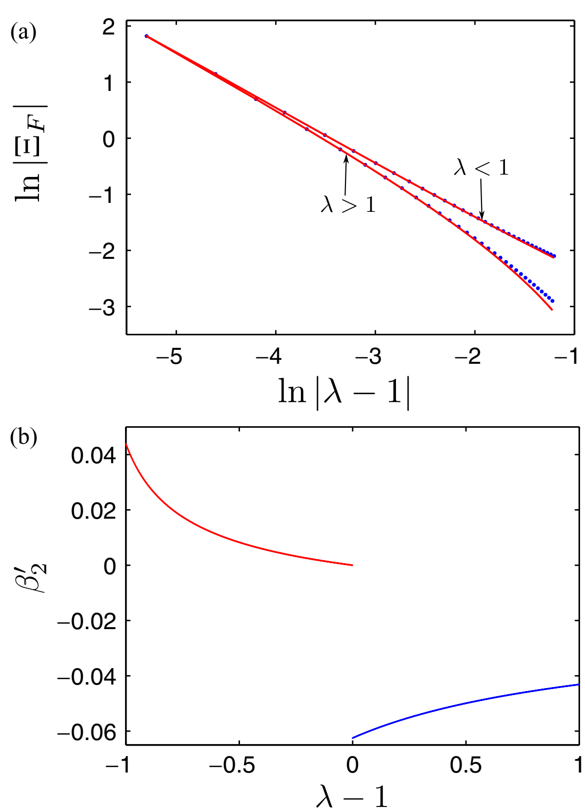

FIG. 3. (a) Fidelity susceptibility Ξ_F across the critical point in the XY model for $\lambda < 1$ and $\lambda > 1$. (b) Jump of β_2' in the two phases, where α_2' is assumed to be a λ independent constant.

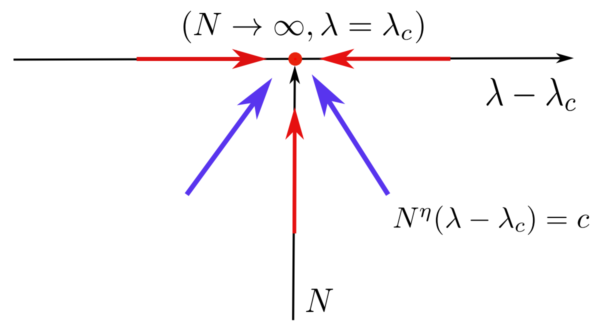

FIG. 4. Scaling laws when approaching the critical point in the thermodynamic limit ($N \to \infty$, $\lambda = \lambda_c$) along different directions. For the red arrows we calculate GP and FS as a function of N and $\lambda - \lambda_c$, while for the blue arrows we compute F_1 and F_2 [defined in Eq. (35)] where both N and λ are variable parameters, keeping $N^\eta(\lambda - \lambda_c)$ a small fixed constant.

These results, together with the GP along the phase boundaries in Eqs. (21)–(23), yield the basic conclusion that the GP and FS along the phase boundaries will always be finite, thus the α coefficients will be nonzero only when two different phases are crossed. This conclusion will also be examined carefully in the extended Ising model in Sec. III.

In the above discussion we have investigated the scaling laws approaching the critical point when either the size N or the parameter $\lambda - \lambda_c$ is fixed; see the red arrows in Fig. 4. It is also interesting to investigate the possible scaling laws when both these parameters are considered variable parameters. We consider the following two scaling functions:

$$F_1 = \frac{d\psi_g}{d\lambda}|_\lambda - \frac{d\psi_g}{d\lambda}|_{\lambda_c}, \quad F_2 = \Xi_F|_\lambda - \Xi_F|_{\lambda_c}. \tag{35}$$

We show that to the leading term these two functions should be unique functions of $N^\eta(\lambda - \lambda_c)$, where η is determined in a very straightforward way. These two scaling functions are determined only by the divergent term since the constant terms are independent of N when the system length is large enough [see the technique first used in Eq. (11), where the summation is replaced with an integration]. For F_1 we find

$$\begin{aligned}F_1 &= 2\pi\sum_k \frac{1}{\sqrt{dx^2+N^2\gamma^2k^2}} - \frac{1}{N|\gamma k|} \\ &= 2\pi\sum_k \frac{N|\gamma k| - \sqrt{dx^2+N^2\gamma^2k^2}}{\sqrt{dx^2+N^2\gamma^2k^2}N|\gamma k|} \\ &\simeq -\sum_{n=1}^{N}\frac{dx^2}{8n^3\pi^2|\gamma|^3} \simeq -\sum_{n=1}^{\infty}\frac{dx^2}{8n^3\pi^2|\gamma|^3},\end{aligned} \tag{36}$$

where $dx = N(\lambda - \lambda_c)$ is treated as a small number and the Taylor expansion to the leading term is carried out separately in the numerator and denominator in the third line. Moreover, the summation of n is extended from N to infinite due to the fast convergence of the series. We then find analytically that

$$F_1 = -\frac{\zeta(3)|N(\lambda-\lambda_c)|^2}{8\pi^2|\gamma|^3}, \tag{37}$$

where $\zeta(n)$ is the zeta function, thus $\eta = 1$ exactly. This result is consistent with the numerical finding in [24] and [57]. The second quantity can be computed in the same way, and we find

$$\begin{aligned} F_2 &= \frac{N}{4}\sum_k \frac{1}{dx^2+N^2\gamma^2k^2} - \frac{1}{(N|\gamma k|)^2} \\ &\simeq -\sum_{n=1}^{\infty}\frac{Ndx^2}{64\pi^4\gamma^4n^4} \simeq -\frac{|(\lambda-\lambda_c)N^{3/2}|^2\zeta(4)}{64\pi^4|\gamma|^4}. \end{aligned} \quad (38)$$

Thus we have $\eta = 3/2$. Let us mention that these results indicate that both F_1 and F_2 are unique functions of $N^\eta(\lambda - \lambda_c)/\gamma^{\eta'}$, where $\eta' = 3/2$ for F_1 and $\eta' = 2$ for F_2.

III. EXTENDED ISING MODEL

For the XY model in Sec. II, the phase transition is controlled by only a single parameter, λ or γ, and we have obtained some general conclusions in regarding the phase transitions across the phase boundaries as well as along the phase boundaries. Unfortunately we do not find the divergent behavior across the phase boundary at $\gamma = 0$ [see Eq. (20)]. Next we examine the validity of these general relations in a more general model, which can be captured by the following extended Ising model [57,62,65–67]:

$$H = -\sum_{j=-M}^{M}\left(\lambda_1\sigma_j^x\sigma_{j+1}^x + \lambda_2\sigma_{j-1}^x\sigma_j^z\sigma_{j+1}^x + \sigma_j^z\right). \quad (39)$$

This model can also be solved exactly using the same method discussed in Sec. II. In the single-particle picture [Eq. (3)] the three-site interaction is equivalent to the next-nearest-neighbor hopping and pairing determined by λ_2, thus we have

$$\Delta_k = \sum_{n=1}^{2}\lambda_n\sin(nk), \quad \epsilon_k = 1 - \sum_{n=1}^{2}\lambda_n\cos(nk). \quad (40)$$

The closing of the energy gap determined by $\Delta_k = 0$ and $\epsilon_k = 0$ simultaneously yields the following three phase boundaries:

$$\text{Line AC:} \quad k_0 = 0, \quad 1-\lambda_1-\lambda_2 = 0; \quad (41)$$

$$\text{Line AB:} \quad k_0 = \pi, \quad 1+\lambda_1-\lambda_2 = 0; \quad (42)$$

$$\text{Line BC:} \quad k_0 = \cos^{-1}\left(\frac{\lambda_1}{2}\right), \quad \lambda_2 = -1, \quad |\lambda_1| < 2. \quad (43)$$

The corresponding phase diagram is presented in Fig. 5. In this model the phase with a large winding number is allowed, which has been reported by Niu *et al.* [65] to host multiple Majorana fermions in an open chain when $\mathcal{W} = 2$.

Due to the presence of two parameters in determining the phase boundaries, the divergence of GP and FS depends strongly on how and along which direction the critical boundary is crossed. Consider a line across the boundary AC along the θ direction (see point D in Fig. 5), with the dashed line 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 ($\alpha_2 > 0$)

$$\alpha_2 = -\alpha_1 = +\frac{|1+\tan(\theta)|}{|1+d+2\tan(\theta)|}, \quad (44)$$

from which we see that $\alpha_2 = -\alpha_1 = \infty$ when $\tan(\theta) = -\frac{d+1}{2}$ and $\alpha_2 = -\alpha_1 = 0$ when along the phase boundary

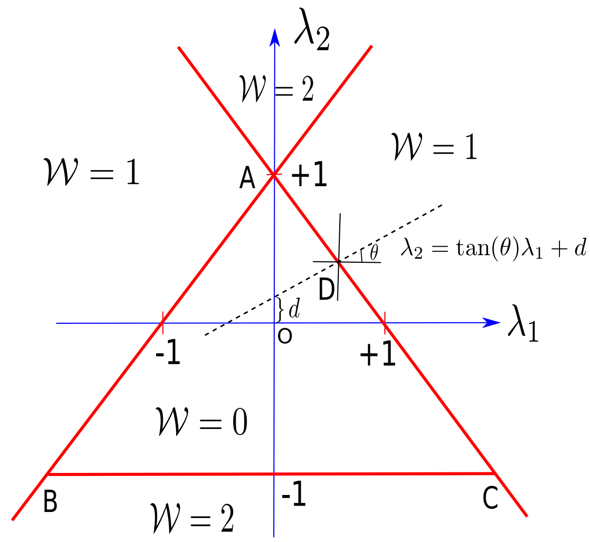

FIG. 5. Phase diagram of the extended Ising model. The different phases are distinguished by the winding number $\mathcal{W}$. Conditions for the phase boundaries determined by the gap closing and reopening are shown in Eqs. (41) to (43).

($\theta = -\pi/4$ 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 independent of the other parameters. The other two coefficients can also be defined straightforwardly using Eq. (31). The constants β_1 and β_2 in this extended model can no longer be computed analytically, however, they can still be computed exactly with the technique in Eq. (11) using numerical methods.

Along the boundary BC, we find

$$\frac{d\psi_g}{d\lambda_1} = -\frac{\pi(1+\lambda_2)}{M}\sum_{k>0}\frac{(\lambda_1+2\lambda_2\cos(k))\sin(k)^2}{\epsilon_k^2+|\Delta_k|^2} \quad (45)$$

and

$$\Xi_F|_{\lambda_1} = \frac{(1+\lambda_2)^2}{4N}\sum_{k>0}\frac{\sin(k)^2}{\epsilon_k^2+|\Delta_k|^2}. \quad (46)$$

In the above two equations we find that when $\lambda_2 = -1$, their results are exactly equal to 0. Thus we find that the conclusions about the GP and FS along the phase boundaries obtained in the XY model (see Sec. II) are also true in this general model; that is, the coefficients of the divergent terms are exactly equal to 0, and the GP and FS are always finite.

We next point out that the scaling laws as a function of N across the phase boundary BC along the λ_2 direction is broken down since the gap is not closed and reopened at special points. A typical result for the GP and FS is presented in Fig. 6, 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. This is different from the previous model, where the critical point at $k_0 = 0$ or $k_0 = \pi$ is not sampled during the summation of k. The analogous features can also be found in other extended models [57,62,66,67] if Δ_k and ϵ_k in the BdG equation can equal 0 simultaneously. The breakdown of this scaling law also indicates the failure of Eq. (32) and the scaling of F_1 and F_2 in Eq. (35).

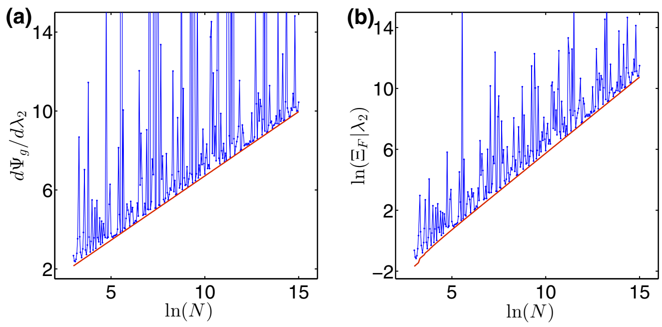

FIG. 6. Breakdown of scaling laws for (a) $\frac{d\Psi_g}{d\lambda_2}$ and (b) $\Xi_F|_{\lambda_2}$ as a function of the system length N across the boundary BC. We set $\lambda_1 = \frac{\sqrt{5}}{2} + \frac{2}{5}$ to avoid the singular point k_0. The solid line is $\alpha_1 \ln(N) + \beta_1$ in (a) and $\alpha_1' N + \beta_2'$ in (b), where $\alpha_1 = |\sin(k_0)|$ and $\alpha_1' = \frac{1}{192}$ are determined using the singular function expansion method. The two β constants are fitted using the lowest bound of the data.

However, similar scaling laws can still be found as a function of the deviation $\delta\lambda = \lambda_2 + 1$ (line BC). In the vicinity of k_0 the gap can be approximated as

$$\xi_k^2 \approx a + b(k - k_0) + c(k - k_0)^2, \tag{47}$$

where $c = 2 - 2\cos(2k_0)$, $b = 2\delta\lambda \sin(2k_0)$, and $a = \delta\lambda^2$, with $\cos(k_0) = \lambda_1/2$ and $b^2 - 4ac < 0$ for $\forall\, k$ when $\delta\lambda \neq 0$. This series expansion is different from the previous ones due to the appearance of the linear term b. Note that when $k_0 = 0$ or π, the contribution of the numerator in the integral is always equal to 1; however, here the numerator then becomes important, and the singular function should be chosen as $\chi_k = \frac{\sin^2(k_0)}{\xi_k}$ for the GP and $\chi_k = \frac{\sin^2(k_0)}{\xi_k^2}$ for the FS. Thus the final coefficients α_i are no longer purely determined by the slope c. With these singular functions we find

$$\frac{d\Psi_g}{d\lambda_2} = \alpha_2 \ln|\lambda_2 + 1| + \beta_2, \tag{48}$$

$$\Xi_F|_{\lambda_2} = \frac{\alpha_2'}{|\lambda_2 + 1|} + \beta_2', \tag{49}$$

where

$$\alpha_2 = -\frac{2}{\sqrt{4 - \lambda_1^2}}, \tag{50}$$

$$\alpha_2' = \frac{\pi/2 - \arctan\left(\lambda_1/\sqrt{4 - \lambda_1^2}\right)}{8\pi}. \tag{51}$$

The intimate relations in Eq. (31) due to the contribution of the numerator at nonspecial k_0 are no longer true. Nevertheless, we still find that α_2 and α_2' are closed related by the following identity due to the same origin of divergence as discussed before:

$$\alpha_2 = -\frac{1}{|\sin(8\pi\alpha_2')|}. \tag{52}$$

The above result is correct only when λ_1 is not very close to ± 2 (points B and C in Fig. 6), in which case some of the constants may approach ∞.

IV. DISCUSSION AND CONCLUSION

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

$$\frac{d^2\Psi_g}{d\lambda^2}\Big|_{\lambda=1} = -\frac{3}{2|\gamma|^3} \ln N + \beta_3, \tag{53}$$

with $\beta_3 = \frac{3(\ln\frac{\pi}{|\gamma|} - (\Gamma + 3\ln 2 - 4))}{2|\gamma|^3} - \frac{1}{2|\gamma|} + \ldots$, which has the same form as $\frac{d\Psi_g}{d\lambda}|_{\lambda=1}$. However, for the deviation $\delta\lambda = \lambda - 1$ in the thermodynamic limit, it takes another intriguing form after singular function expansion,

$$\frac{d^2\Psi_g}{d\lambda^2}\Big|_{N\to\infty} = -\frac{1}{|\gamma|(\lambda - 1)} + \frac{3\ln(|\lambda - 1|)}{2|\gamma|^3} + \beta_3', \tag{54}$$

where $\beta_3' = (3\ln\frac{\pi^2}{2} + 4)/(2|\gamma|^3) - 1/(2|\gamma|)$. The two singular functions in Eq. (54) arise from the derivative of the leading term, $\ln|\lambda - 1|$, and the next leading term, $\frac{3}{2|\gamma|^2}(\lambda - 1)\ln(|\lambda - 1|)$. The jump of constant β_3' is absent [56] due to the lack of an absolute symbol in denominator. We therefore see that although the first-order derivative of the GP as a function of the system length N and deviation $\delta\lambda$ have the same logarithmic divergence, their second-order derivatives take some totally different forms.

The second-order derivative of the GP can be used to calculate the scaling laws across the phase boundary at $\gamma = 0$ in the XY model (see Fig. 1). We note that the GP in Eq. (21) is a function of γ^2 and the phase transition between $\mathcal{W} = 1$ and $\mathcal{W} = -1$ takes place at $\gamma = 0$, thus the first-order derivative of GP, proportional to γ, should be exactly equal to 0. This is different from the extended Ising model, in which the first-order derivative of GP already exhibits divergent behavior. To this end, we compute

$$\frac{d^2\Psi_g}{d\gamma^2}\Big|_{|\lambda|<1} = \int_0^\pi \frac{\left(2\gamma^2\sin(k)^2 - \epsilon_k^2\right)\epsilon_k \sin(k)^2}{\left(\gamma^2\sin(k)^2 + \epsilon_k^2\right)^{5/2}} dk, \tag{55}$$

where $\epsilon_k = \lambda - \cos(k)$ [see Eq. (3)]. When $\gamma = 0$, the singular point takes place at $k_0 = \arccos(\lambda)$ in the form of $\sin(k)^2(\lambda - \cos(k))^3/|\lambda - \cos(k)|^5 = \sin(k)^2\mathrm{sgn}(\lambda - \cos(k))/(\lambda - \cos(k))^2$ when $|\lambda| < 1$. This singular point is removed by the γ term. To compute the scaling law of the above equation with respect to γ, we define the singular function using the method in Eq. (47) as

$$\chi_k = \frac{\sin(k_0)^2}{a + b(k - k_0) + c(k - k_0)^2}, \tag{56}$$

where $a = \gamma^2(1 - \lambda^2)$, $b = 2\gamma^2\lambda(1 - \lambda)$, and $c = 1 - \lambda^2 - \gamma^2 + 2\gamma^2\lambda^2$. We may check that $b^2 - 4ac = -4\gamma^2(1 - \gamma^2)(1 - \lambda^2)^2 < 0$, thus this singular function will always be well defined when $\gamma \neq 0$. Then the above result can be written as

$$\frac{d^2\Psi_g}{d\gamma^2}|_{|\lambda|<1} = -\int_0^{k_0} \chi_k dk + \int_{k_0}^{\pi} \chi_k dk + \text{const.} = \frac{\alpha_4}{|\gamma|} + \beta_4, \tag{57}$$

where

$$\alpha_4 = \frac{\arctan\left(\frac{b-2ck_0}{\sqrt{4ac-b^2}}\right) + \arctan\left(\frac{b+2c(\pi-k_0)}{\sqrt{4ac-b^2}}\right)}{\sqrt{1-\lambda^2}} - \frac{2\arctan\left(\frac{b}{\sqrt{4ac-b^2}}\right)}{\sqrt{1-\lambda^2}}. \tag{58}$$

The corresponding constant β_4 needs to be computed numerically; see our numerical simulation in Fig. 7.

These results also reveal a close relation between the constants β and α, and in the simplest XY model, β can be a unique function of α. Their relations are derived exactly in this paper; they have not been considered in previous literature [5,25,57]. It is quite possible that the β constants may also reveal some important properties of the system during the quantum phase transitions. We, finally, emphasize that this method is powerful and can also be adapted to study the scaling laws of entanglement [55,68–73], quantum discord and correlation [74–76], and geometric Euler number [63,77,78] across the quantum critical points and study relations, which will be investigated in future. These exact results can greatly enrich our understanding of the GP and FS in the characterization of quantum phase transitions.

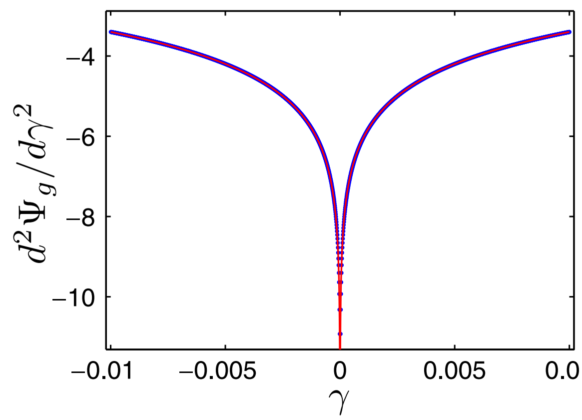

FIG. 7. Second-order derivative of GP as a function of γ for the XY model with $\lambda = 0.5$. The solid red line and open blue symbol represent the results from exact numerical integration and singular function expansion, respectively.

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