Scaling of Geometric Phases Close to the Quantum Phase Transition in the XY Spin Chain

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We show that the geometric phase of the ground state in the XY model obeys scaling behavior in the vicinity of a quantum phase transition. In particular we find that the geometric phase is nonanalytical and its derivative with respect to the field strength diverges at the critical magnetic field. Furthermore, the universality in the critical properties of the geometric phase in a family of models is verified. In addition, since the quantum phase transition occurs at a level crossing or avoided level crossing and these level structures can be captured by the Berry curvature, the established relation between the geometric phase and quantum phase transitions is not a specific property of the XY model, but a very general result of many-body systems.

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The phase factor of a wave function is the source of all interference phenomena and one of most fundamental concepts in quantum physics. Recent considerable interest in this field is motivated by the pioneer work of Berry [1]. Berry discovered that a geometric phase (GP), in addition to the usual dynamic phase, is accumulated on the wave function of a quantum system, provided that the Hamiltonian is cyclic and adiabatic. Since then, the adiabatic GP and its generalizations [2,3] have found many applications to broad fields [4,5], such as condensed matter physics [6–8], atomic, molecular, and optical physics, and quantum computation [9], etc.

Very recently, Carollo and Pachos demonstrated the close relation between GPs and quantum criticality of spin chains [10]. In particular, they showed that a noncontractible GP difference between the ground state and the first excited state exists in the XX model if and only if the closed evolution path circulates a region of criticality. Quantum phase transitions (QPTs) occur for a parameter region where the energy levels of the ground state and the excited state cross or have an avoided crossing, and is certainly one of the major interests in condensed matter physics [11–13] and quantum information [14]. Geometric phase, as a measure of the curvature of Hilbert space, can reflect the energy level structures and can capture certain features of QPTs. However, at least two important problems need to be addressed. (i) The XY model is parametrized by γ and λ [see the definitions below Eq. (1)]. Two distinct critical regions appear in parameter space: the segment $(\gamma, \lambda) = (0, (0, 1))$ for the XX chain and the critical line $\lambda_c = 1$ for the whole family of the XY model [11,15]. The GP difference between the ground state and the first excited states calculated in Ref. [10] can be used as a measure of the presence of the first critical region, but whether this measure remains valid for the second critical region is questionable. The second critical region is clearly more interesting in the sense that second order quantum phase transitions occur there. Whether one can reveal the latter critical region using GP is of significance. (ii) As also noted in Ref. [10], a challenging but also important question warranting further study is whether the typical features of quantum criticality, such as the scaling feature, critical exponents, and universality, etc. have relation to GPs in this many-body system. Answering these questions is certainly significant for a deeper understanding of QPTs, and also from the perspective of GPs. As a consequence, further results that bridge these two interesting areas of research are of great relevance.

In this Letter, we use the XY spin chain as a helpful tool to establish the connection between GPs and QPTs. Instead of using the GP difference between the ground state and the first excited state as a signature of quantum criticality, we focus on the relation between GP of the ground state and quantum criticality in the XY chain. We analyze GPs near the critical point of the XY model and find that the GP is nonanalytical and its derivative with respect to the field strength λ diverges at the critical line described by $\lambda_c = 1$. In particular, the GP obeys scaling behavior in the vicinity of a QPT. Furthermore, universality in the critical properties of GP for a family of models is verified. These results show that the key ingredients of quantum criticality are present in GPs of the ground state. In addition, we show that the relation between GP and QPTs established here is not model dependent, but is valid in a wide variety of systems.

The system under consideration is a spin-1/2 XY chain, which consists of N spins with nearest neighbor interactions and an external magnetic field. The Hamiltonian of the system is given by

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

where $M = (N-1)/2$ for N odd and σ_j^μ $(\mu = x, y, x)$ are the Pauli matrices for the jth spin. We assume periodic boundary conditions for simplicity and choose N odd to

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avoid the subtleties connected with boundary terms. Nevertheless, the differences with other boundary conditions and the even N case are the order to $O(1/N)$ and then negligible in the thermodynamic limit where QPTs occur [14,15]. The parameter λ is the intensity of the magnetic field applied in the z direction, and γ measures the anisotropy in the in-plane interaction. This XY model encompasses two other well-known spin models: it turns into transverse Ising chain for $\gamma = 1$ and the XX (isotropic XY) chain in a transverse field for $\gamma = 0$.

As for quantum criticality in the XY model, we need to distinguish two universality classes depending on the anisotropy γ. The critical features are characterized in term of a critical exponent ν defined by $\xi \sim |\lambda - \lambda_c|^{-\nu}$ with ξ representing the correlation length. For any value of γ, quantum criticality occurs at a critical magnetic field $\lambda_c = 1$. For the interval $0 < \gamma \leq 1$ the models belong to the Ising universality class characterized by the critical exponent $\nu = 1$, while for $\gamma = 0$ the model belongs to the XX universality class with $\nu = 1/2$ [11,15].

To investigate the GP in this system, we introduce a new family of Hamiltonians that can be described by applying a rotation of ϕ around the z direction to each spin, i.e., $H_\phi = g_\phi H g_\phi^\dagger$ with $g_\phi = \prod_{j=-M}^{M} \exp(i\phi\sigma_j^z/2)$ [10]. The critical behavior is independent of ϕ as the spectrum Λ_k (see below) of the system is ϕ independent. This class of models can be diagonalized by means of the Jordan-Wigner transformation that maps spins to one-dimentional spinless fermions with creation and annihilation operation a_j and $a_j^\dagger$ via the relations, $a_j = (\prod_{l<j}\sigma_l^z)\sigma_j^\dagger$ [11,15]. Because of the (quasi) translational symmetry of the system we may introduce Fourier transforms of the fermionic operator described by $d_k = \frac{1}{\sqrt{N}}\sum_j a_j \exp(-i2\pi jk/N)$ with $k = -M, \ldots, M$. The Hamiltonian H_ϕ can be diagonalized by transforming the fermion operators in momentum space and then using the Bogoliubov transformation. The result is given by $H = \sum_k \Lambda_k (c_k^\dagger c_k - 1)$, where the energy spectrum $\Lambda_k = \sqrt{(\lambda - \cos(2\pi k/N))^2 + \gamma^2 \sin^2(2\pi k/N)}$ and $c_k = d_k \cos\frac{\theta_k}{2} - i d_{-k}^\dagger e^{2i\phi} \sin\frac{\theta_k}{2}$ with the angle θ_k defined by $\cos\theta_k = (\cos\frac{2\pi k}{N} - \lambda)/\Lambda_k$.

The ground state $|g\rangle$ of H_ϕ is the vacuum of the fermionic modes described by $c_k|g\rangle = 0$, and can be written as $|g\rangle = \prod_{k=1}^{M} (\cos\frac{\theta_k}{2}|0\rangle_k|0\rangle_{-k} - i e^{2i\phi}\sin\frac{\theta_k}{2}|1\rangle_k|1\rangle_{-k})$, where $|0\rangle_k$ and $|1\rangle_k$ are the vacuum and single excitation of the kth mode, d_k, respectively. The ground state is a tensor product of states, each lying in the two-dimensional Hilbert space spanned by $|0\rangle_k|0\rangle_{-k}$ and $|1\rangle_k|1\rangle_{-k}$. The GP of the ground state, accumulated by varying the angle ϕ from 0 to π, is described by $\beta_g = -\frac{i}{M}\int_0^\pi \langle g|\partial_\phi|g\rangle d\phi$ [10], and is found to be

$$\beta_g = \frac{\pi}{M}\sum_{k=1}^{M}(1 - \cos\theta_k). \tag{2}$$

The term $\beta_k \equiv \pi(1 - \cos\theta_k)$ is a geometric phase for the kth mode, and represents the area in the parameter space enclosed by the loop determined by (θ_k, ϕ). To study the quantum criticality, we are interested in the thermodynamic limit when the spin lattice number $N \to \infty$. In this case the summation $\frac{1}{M}\sum_{k=1}^{M}$ can be replaced by the integral $\frac{1}{\pi}\int_0^\pi d\varphi$ with $\varphi = \frac{2\pi k}{N}$; the GP in the thermodynamic limit is given by

$$\beta_g = \int_0^\pi (1 - \cos\theta_\varphi) d\varphi, \tag{3}$$

where $\cos\theta_\varphi = (\cos\varphi - \lambda)/\Lambda_\varphi$ with the energy spectrum $\Lambda_\varphi = \sqrt{(\lambda - \cos\varphi)^2 + \gamma^2\sin^2\varphi}$.

To demonstrate the relation between GP and quantum phase transitions, we plot GP β_g [the same results were derived in Ref. [10]] and its derivative $d\beta_g/d\lambda$ with respect to the field strength λ as a function of the Hamiltonian parameters λ and γ in Fig. 1. Two particular features are notable: (i) the nonanalytic property of the GP along the whole critical line $\lambda_c = 1$ in the XY model is clearly shown by anomalies for the derivative of GP along the same line; (ii) GP for the XX model under the thermodynamic limit is very special in the sense that, instead of using the GP difference between the ground state and the excited phase as the signature of phase transition [10], a noncontractible GP of the ground state itself also serves the same role [16]. GP under the thermodynamic limit can be obtained explicitly from Eq. (3) for $\gamma = 0$ as $\beta_g = 2\pi - 2\arccos(\lambda)$ when $\lambda \leq 1$ and $\beta_g = 2\pi$ when $\lambda > 1$. However, it appears from Eq. (2) that GP β_g is always trivial for strictly $\gamma = 0$ and every finite lattice size M, since $\theta_k = 0$ or π for every k. The difference between the finite and infinite lattice sizes can be understood from the two limits $N \to \infty$ and $\gamma \to 0$. Assume $\gamma = \epsilon$ with ϵ an arbitrary small but still finite value, then we can still find a solution φ_0 (it implies $N \to \infty$) for $\cos\varphi_0 - \lambda = 0$ but $\Lambda_{\varphi_0} = \epsilon\sqrt{1 - \lambda^2} \neq 0$ for $\lambda \neq 1$. Then a π geometric phase appears for such φ_0 since $\theta_{\varphi_0} = \pi/2$. Thus, a noncontractible GP of the ground state itself is also a witness of QPT [16].

To further understand the relation between GP and quantum criticality, we investigate the scaling behavior of GPs by the finite size scaling approach [13]. We first look at the Ising model. The derivatives $d\beta_g/d\lambda$ for $\gamma = 1$

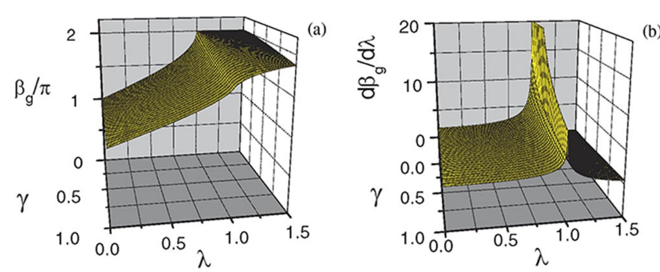

FIG. 1 (color online). (a) Geometric phase β_g of the ground state (b) and its derivative $d\beta_g/d\lambda$ as a function of the Hamiltonian parameters λ and γ. The lattice size $N = 10\,001$. There are clear anomalies for the derivative of geometric phase along the critical line $\lambda_c = 1$.

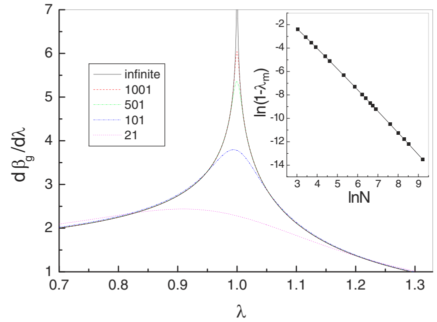

FIG. 2 (color online). The derivatives $d\beta_g/d\lambda$ for the Ising model ($\gamma = 1$) as a function of the Hamiltonian parameter λ. The curves correspond to different lattice sizes $N = 21, 101, 501, 1001, \infty$. With increasing the system sizes, the maximum becomes more pronounced. The inset shows that the position of the maximum changes and tends as $N^{-1.803}$ towards the critical point $\lambda_c = 1$.

and different lattice sizes are plotted in Fig. 2. There is no real divergence for finite N, but the curves exhibit marked anomalies and the height of which increases with lattice size. The position λ_m of the peak can be regarded as a pseudocritical point [13] which changes and tends as $N^{-1.803}$ towards the critical point and clearly approaches λ_c as $N \to \infty$. As shown in Fig. 3(a), the value of $d\beta_g/d\lambda$ at the point λ_m diverges logarithmically with increasing lattice size as:

$$\frac{d\beta_g}{d\lambda}\Big|_{\lambda_m} \approx \kappa_1 \ln N + \text{const}, \tag{4}$$

with $\kappa_1 = 0.3121$. On the other hand, as shown in Fig. 3(b), the singular behavior of $d\beta_g/d\lambda$ for the infinite

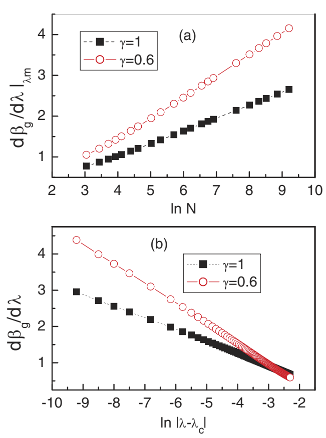

FIG. 3 (color online). (a) The maximum value of the derivative $d\beta_g/d\lambda$ at the pseudocritical point λ_m as a function of lattice sizes. The slope of the line is 0.3121 (0.5234) for $\gamma = 1$ ($\gamma = 0.6$). (b) The derivatives $d\beta_g/d\lambda$ for the thermodynamic limit logarithmically diverge on approaching the critical value. The slope of the line is -0.3123 (-0.5238) for $\gamma = 1$ ($\gamma = 0.6$). The ratio between the two slopes in (b) and (a) for a fixed parameter γ is the critical exponent ν. Here $\nu \sim 1$ is obtained for both $\gamma = 0.6$ and 1, as expected by the concept of universality in the XY model.

Ising chain can be analyzed in the vicinity of the quantum criticality, and we find the asymptotic behavior as

$$\frac{d\beta_g}{d\lambda} \approx \kappa_2 \ln|\lambda - \lambda_c| + \text{const}, \tag{5}$$

with $\kappa_2 = -0.3123$. According to the scaling ansatz in the case of logarithmic divergence [13], the ratio $|\kappa_2/\kappa_1|$ gives the exponent ν that governs the divergence of the correlation length. Therefore, $\nu \sim 1$ is obtained in our numerical calculation for the Ising chain, in agreement with the well-known solution of the Ising model [15]. Furthermore, by proper scaling and taking into account the distance of the maximum of β_g from the critical point, it is possible to make all the data for the value of $F = [1 - \exp(d\beta_g/d\lambda - d\beta_g/d\lambda|_{\lambda_m})]$ as a function of $N^{1/\nu}(\lambda - \lambda_m)$ for different N collapse onto a single curve [13,14]. The result for several typical lattice sizes in the Ising model is shown in Fig. 4, where we can also extract the critical exponent $\nu = 1$.

A cornerstone of QPTs is a universality principle in which the critical behavior depends only on the dimension of the system and the symmetry of the order parameter. The XY model for the interval $\gamma \in (0, 1]$ belongs to the same universality class with critical exponent $\nu = 1$. To verify the universality principle in this model, we check the scaling behavior for different values of the parameter γ. The asymptotic behaviors are also described by Eqs. (4) and (5). For instance, from Fig. 3 we get $\kappa_1 \approx 0.5234$ and $\kappa_2 \approx -0.5238$ for $\gamma = 0.6$. Moreover, we also verify that, by proper scaling, all data for different N but a specific γ can collapse onto a single curve. The data for $\gamma = 0.6$ are shown in Fig. 4. We can extract the same critical exponent $\nu = 1$ from the data shown in both Figs. 3 and 4.

Comparing with the $\gamma \neq 0$ case, the nature of the divergence of $d\beta_g/d\lambda$ at $\gamma = 0$ belongs to a different universality class, and the scaling behavior of geometric phase can be directly extracted from the explicit expression of GP $\beta_g = 2\pi - 2\arccos(\lambda)$ ($\lambda \leq 1$) in the thermodynamic limit. Since $d\beta_g/d\lambda = \sqrt{2}(1-\lambda)^{-1/2}$ ($\lambda \to 1^-$), we can infer the known result that the critical exponent $\nu = 1/2$

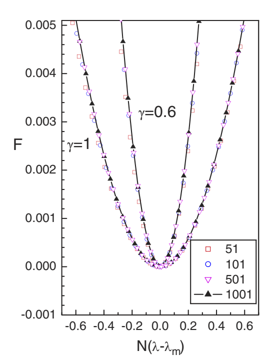

FIG. 4 (color online). The value of $F = [1 - \exp(d\beta_g/d\lambda - d\beta_g/d\lambda|_{\lambda_m})]$ as a function $N(\lambda - \lambda_m)$ for different lattice sizes $N = 51, 101, 501, 1001$. All the data for a fixed parameter γ collapse on a single curve, as expected from the finite size scaling ansatz.

for the XX model. In addition, the dynamical behavior is determined by $\Lambda_{\varphi\to 0} \sim \varphi^z[1 + (\varphi\xi)^{-z}]$, where z is the dynamical exponent in the thermodynamic limit. Then $z = 1$ for $\gamma \in (0, 1]$ and $z = 2$ for $\gamma = 0$ are found by the expansion of Λ_φ in the case $\varphi \to 0$. So we have $z\nu = 1$, which is indeed the case for the XY criticality [11]. Therefore, the above results clearly show that all the key ingredients of the quantum criticality are present in the GPs of the ground state in the XY model.

We now present that the relation between GPs and QPTs addressed above is valid in a general case: quantum phase transition occurs at level crossings or avoided level crossings, and these kinds of level structures usually can be captured by the GP of the ground state. Consider a generic system described by the Hamiltonian $H(\eta)$ with η a dimensionless coupling constant. For any reasonable η, all observable properties of the ground state of H will vary smoothly as η is varied. However, there may be special points denoted as η_c, where there is a nonanalyticity in some property of the ground state at zero temperature, η_c is identified as the position of a QPT. Nonanalytical behavior generally occurs at level crossings or avoided level crossings [11]. On the other hand, we also consider GPs in a generic many-body system where the Hamiltonian can be changed by varying the parameters $\mathbf{R}$ on which it depends. The state $|\psi(t)\rangle$ of the system evolves according to Schrodinger equation $H(\mathbf{R}(t))|\psi(t)\rangle = i\hbar\partial_t|\psi(t)\rangle$. At any instant, the natural basis consists of the eigenstates $|n(\mathbf{R})\rangle$ of $H(\mathbf{R})$ for $\mathbf{R} = \mathbf{R}(t)$, that satisfy $H(\mathbf{R})|n(\mathbf{R})\rangle = E_n(\mathbf{R})|n(\mathbf{R})\rangle$ with energy $E_n(\mathbf{R})$ $(n = 1, 2, 3, \ldots)$. Berry showed that the GP for a specific eigenstate, such as the ground state ($|g\rangle = |1\rangle$) of a many-body system we concern here, adiabatically undergoing a closed path in parameter space denoted by C, is given by $\beta_g(C) = -\iint_C V_g(\mathbf{R})\cdot d\mathbf{S}$, where $d\mathbf{S}$ denotes area element in $\mathbf{R}$ space and $V_g(\mathbf{R})$ is the Berry curvature given by [1]

$$V_g(\mathbf{R}) = \mathrm{Im}\sum_{n\neq g}\frac{\langle g|\nabla_{\mathbf{R}}H|n\rangle\langle n|\nabla_{\mathbf{R}}H|g\rangle}{(E_n - E_g)^2}. \qquad (6)$$

The energy denominators in Eq. (6) show that the Berry curvature usually diverges at the point of parameter space where energy levels are cross and may have maximum values at avoided level crossings. Thus level crossings or avoided level crossings, the two specific level structures related to QPTs, are reflected in the geometry of the Hilbert space of the system and can be captured by GPs of the ground state. “ Moreover, GP and its derivative basically can be written as a function of the derivatives of the ground state energy with respect to the field strength [17]. In this sense it is natural that geometric phase obeys scaling behavior in the vicinity of a QPT. So the connection demonstrated herein is in fact a very general result and not a specific property of the XY model.

In summary, we established the connection between geometric phase of the ground state and QPTs in a generic many-body system. As a typical example, we show in detail that all the key ingredients of quantum criticality, such as scaling features, critical exponents, and universality, etc. are present in the GPs in the XY spin chain.

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Note added.—After this Letter was completed, I got a manuscript [16] where a general connection between Berry phases, topology, and QPTs was rigorously established: a nontrivial and noncontractible GP of the ground state is a signature of QPTs.

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