Scaling of geometric phases close to quantum phase transition in the XY chain

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

PACS numbers: 75.10.Pq, 03.65.Vf, 05.30.Pr, 42.50.Vk

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, 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 geometric phase and its generalizations [2, 3] have found many applications to broad fields [4, 5], such as condensed matter physics [11, 12, 13], atomic, molecular, and optical physics, and quantum computation [6], etc..

Very recently, Carollo and Pachos demonstrated the close relation between geometric phases and quantum criticality of spin chains [10]. In particular they showed that a nontrivial geometric phase 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 usually 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 [7, 8] and quantum information [9]. Geometric phase, as a measure of the curvature of Hilbert space, can reflect the energy level structures and can capture certain features of quantum phase transitions. However, at least two important problems need to be addressed. (i) The XY model is parameterized by $\gamma$ and $\lambda$ (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 nontrivial geometric phase 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 this measure is unlikely to remain valid for the second critical region. Whether one can reveal the latter critical region using geometric phase 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 geometric phases in this many body system. Answering these questions is certainly significant for a deeper understanding of quantum phase transitions, and also from the perspective of geometric phases. So further results that bridge these two interesting areas of research are of great relevance.

In this paper, instead of using the geometric phase difference between the ground state and the first excited state as a signature of quantum criticality, we focus on the relation between geometric phase of the ground state and quantum criticality in the XY chain. We analyse geometric phases near the critical point of the XY model and find that the geometric phase is non-analytical and its derivative with respect to the field strength $\lambda$ diverges at the critical line described by $\lambda_c = 1$. In particular the geometric phase obeys scaling behavior in the vicinity of a quantum phase transition. Furthermore, universality in the critical properties of geometric phase for a family of models is verified. These results show that the key ingredients of quantum criticality are present in geometric phases of the ground state. In addition, we show that the relation between geometric phase and quantum phase transitions 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

$$H = - \sum_{j=-M}^{M} \left( \frac{1+\gamma}{2} \sigma^x_j \sigma^x_{j+1} + \frac{1-\gamma}{2} \sigma^y_j \sigma^y_{j+1} + \lambda \sigma^z_j \right),$$

where $M = (N - 1)/2$ for $N$ odd and $\sigma^\mu_j (\mu = x, y, z)$ are the Pauli matrices for the $j$th spin. We assume periodic boundary conditions. The parameter $\lambda$ is the intensity of the magnetic field applied in the $z$ direction, and $\gamma$ 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 $\gamma$. The critical features are characterized in
term of a critical exponent $\nu$ defined by $\xi \sim |\lambda - \lambda_c|^{-\nu}$
with $\xi$ representing the correlation length. For any value of
the anisotropy $\gamma$, quantum criticality occurs at a criti-
cal magnetic field $\lambda_c = 1$. For the interval $0 < \gamma \leq 1$ the
models belong to the Ising universality class character-
ized by the critical exponent $\nu = 1$, while for $\gamma = 0$ the
model belongs to the XX universality class with $\nu = 1/2$.

To investigate the geometric phase in this system, we
introduce a new family of Hamiltonians that can be
described by applying a rotation of $\phi$ around the $z$ di-
rection to each spin, i.e., $H_\phi = g_\phi g_\phi^\dagger$ with $g_\phi = \prod_{j=-M}^M \exp(i\phi \sigma_j^z/2)$. The critical behavior is inde-
pendent of $\phi$ as the spectrum $\Lambda_k$ (see below) of the system
is $\phi$ independent. This class of models can be diagonal-
ized by means of the Jordan-Wigner transformation that
maps spins to one-dimensional spinless fermions with cre-
atron and annihilation operation $a_j$ and $a_j^\dagger$ via the relations,
$a_j = (\prod_{<j} \sigma_i^z) \sigma_j^z$. Due to 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_{k} a_k \exp(-2\pi i k/N)$ with $k = -M, \cdots, M$.
The Hamiltonian $H_\phi$ can be diagonalized by transform-
ing 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
$\Lambda_k = \sqrt{(\lambda - \cos(2\pi k/N)) + \gamma^2 \sin^2(2\pi k/N)}$
and $c_k = d_k \cos \frac{\theta_k}{2} + id_k^\dagger \sin \frac{\theta_k}{2}$ with the angle $\theta_k$ defined by
cos \theta_k = (\cos \frac{2\pi k}{N} - \lambda)/\Lambda_k$.
The ground state $|g\rangle$ of $H_\phi$ is the vac-
uum of the fermionic modes described by $c_k|g\rangle = 0$, and can be written as $|g\rangle = \prod_{k=1}^M \cos \left[ \frac{\pi}{4} (|0\rangle_k |0\rangle_{-k} - i e^{2i\phi} \sin \frac{\theta_k}{2} |1\rangle_k |1\rangle_{-k}) \right]$, where $|0\rangle_k$ and $|1\rangle_k$ are the vacuum and single excitation of the
$k$th 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 geometric phase of the ground state, accumulated
by varying the angle $\phi$ from $0$ to $\pi$, is described by
$\beta_g = -\frac{\pi}{4} \int_0^\pi \langle g | \partial_\phi |g\rangle d\phi$, and is found to be

$$\beta_g = \frac{\pi}{M} \sum_{k=1}^M \left( 1 - \frac{\cos(2\pi k/N) - \lambda}{\Lambda_k} \right).$$

To study the quantum criticality, we are also 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 $\frac{1}{L} \int_0^L d\varphi$ with $\varphi = \frac{2\pi k}{N}$; the
generic phase in the thermodynamic limit is given by

$$\beta_g = \int_0^\pi \left( 1 - \frac{\cos \varphi - \lambda}{\sqrt{(\cos \varphi - \lambda)^2 + \gamma^2 \sin^2 \varphi}} \right) d\varphi.$$

To demonstrate the relation between geometric phase and quantum phase transitions, we plot geometric phase $\beta_g$ and its derivative $d\beta_g/d\lambda$ with respect to the field strength $\lambda$ as a function of the Hamiltonian parameters $\lambda$ and $\gamma$ in Fig. 1. Two particular features are notable: (i) The non-analytic property of the geometric phase along the whole critical line $\lambda_c = 1$ in the XY model is clearly shown by anomalies for the derivative of geometric phase along the same line; (ii) Geometric phase for the XX model under the thermodynamic limit is very special in the sense that, instead of using the geometric phase difference between the ground state and the excited phase as the signature of phase transition, the geometric phase of the ground state itself also serves the same role. Geometric phase 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 $\lambda > 1$. Thus, a nontrivial geometric phase of the ground state itself is also a witness of quantum phase transition; this fact has also been shown in Ref. [16].

![Fig. 1: (color online). (a) Geometric phase $\beta_g$ of the ground state (b) and its derivative $d\beta_g/d\lambda$ as a function of the Hamiltonian parameters $\lambda$ and $\gamma$. The lattice size $N = 10001$. There are clear anomalies for the derivative of geometric phase along the critical line $\lambda_c = 1$.](image)

To further understand the relation between geometric phase and quantum criticality, we investigate the scaling behavior of geometric phases by the finite size scaling approach. We first look at the Ising model. The derivatives $d\beta_g/d\lambda$ for $\gamma = 1$ 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 $\lambda_m$ of the peak can be regarded as a pseudo-critical point which changes and tends as $N^{-1.803}$ towards the critical point and clearly approaches $\lambda_c$ as $N \to \infty$. As shown in Fig. 3(a), the value of $d\beta_g/d\lambda$ at the point $\lambda_m$ diverges logarithmically with increasing lattice size as:

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

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 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, the ratio \( |\kappa_2/\kappa_1| \) gives the exponent \( \nu \) that governs the divergence of the correlation length. Therefore, \( \nu \approx 1 \) is obtained in our numerical calculation for the Ising chain, in agreement with the well-known solution of the Ising model. Furthermore, by proper scaling and taking into account the distance of the maximum of \( \beta_g \) 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 \( N^{1/\nu}(\lambda - \lambda_c) \) for different \( N \) collapse onto a single curve. 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 quantum phase transitions 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 \( \gamma \in (0, 1] \) belong 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 \( \gamma \). The asymptotic behaviors are also described by Eqs. \( 1 \) and \( 5 \). For instance, from Fig. 3 we get \( \kappa_1 \approx 0.5234 \) and \( \kappa_2 = -0.5238 \) for \( \gamma = 0.6 \). Moreover, we also verify that, by proper scaling, all data for different \( N \) but a specific \( \gamma \) can collapse onto a single curve. The data for \( \gamma = 0.6 \) are show in Fig. 4. We can extract the same critical exponent \( \nu = 1 \) from the data shown in both Fig. 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 geometric phase \( \beta_g = 2\pi - 2\arccos(\lambda) \) (\( \lambda \leq 1 \)) in the thermodynamic limit. Since \( d\beta_g/d\lambda = \sqrt{2(1 - \lambda)}^{-1/2} \), we can infer the known result that the critical exponent \( \nu = 1/2 \) for the XX model. Therefore, the above results clearly show that all the key ingredients of the quantum criticality are present in the geometric phases of the ground state in the XY model.

We now demonstrate that the relation between geometric phase and quantum phase transitions 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 geometric phase of the ground state. Consider a generic system described by the Hamiltonian \( H(\eta) \) with \( \eta \) a dimensionless coupling constant. For any reasonable \( \eta \), all observable properties of the ground state of \( H \) will vary smoothly as \( \eta \) is varied. However, there may be special points denoted as \( \eta_c \), where there is a non-analyticity in some property of the ground state at zero.
temperature, $\eta_c$ is identified as the position of a quantum phase transition. Non-analytical behavior generally occur at level crossings or avoided level crossings. On the other hand, we also consider geometric phases in a generic many-body system where the Hamiltonian can be changed by varying the parameters $R$ on which it depends. The state $|\psi(t)\rangle$ of the system evolves according to Schrodinger equation $H(R(t))|\psi(t)\rangle = i\hbar\partial_t|\psi(t)\rangle$.

At any instant, the natural basis consists of the eigenstates $|n(R)\rangle$ of $H(R)$ for $R = R(t)$, that satisfy $H(R)|n(R)\rangle = E_n(R)|n(R)\rangle$ with energy $E_n(R)$ ($n = 1, 2, 3 \cdots$). Berry showed that the geometric phase 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 $\beta_g(C) = -\int_C V_g(R) \cdot dS$, where $dS$ denotes area element in $R$ space and $V_g(R)$ is the Berry curvature given by:

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

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 quantum phase transitions, are reflected in the geometry of the Hilbert space of the system and can be captured by geometric phases of the ground state. Therefore, the relation between geometric phase and quantum phase transitions demonstrated herein is in fact a very general result and not a specific property of the XY model.

In summary, we established the close relation between geometric phase of the ground state and quantum phase transitions in a general 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 geometric phases in the XY spin chain.

I thank L. M. Duan, H. Fu, J. K. Pachos, and P. Zanardi for helpful discussions and P. Berman for his critical reading of this paper. This work was supported by NSF FOCUS center, the MCTP, the NCET and NSFC under grant No. 10204008.

Note added—After this paper was completed, I got a manuscript where the general relation among Berry phases, topology, and quantum phase transitions in many body systems was independently established.

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