Path-dependent scaling of geometric phase near a quantum multi-critical point

Ayoti Patra, Victor Mukherjee and Amit Dutta

Department of Physics, Indian Institute of Technology Kanpur, Kanpur 208 016, India
E-mail: ayoti@iitk.ac.in, victor@iitk.ac.in and dutta@iitk.ac.in

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Abstract. We study the geometric phase of the ground state in a one-dimensional transverse XY spin chain in the vicinity of a quantum multi-critical point. We approach the multi-critical point along different paths and estimate the geometric phase by applying a rotation in all spins about the z axis by an angle $\eta$. Although the geometric phase itself vanishes at the multi-critical point, the derivative with respect to the anisotropy parameter of the model shows peaks at different points on the ferromagnetic side close to it where the energy gap is a local minimum; we call these points ‘quasi-critical’. The value of the derivative at any quasi-critical point scales with the system size in a power-law fashion with the exponent varying continuously with the parameter $\alpha$ that defines a path, up to a critical value $\alpha = \alpha_c = 2$. For $\alpha > \alpha_c$, or on the paramagnetic side, no such peak is observed. Numerically obtained results are in perfect agreement with analytical predictions.

Keywords: spin chains, ladders and planes (theory), finite-size scaling, quantum phase transitions (theory)

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1. Introduction

Quantum phase transitions (QPT) in quantum many-body systems have been studied extensively in recent years [1]–[3]. The possibility of experimental studies on ultracold atoms trapped in optical lattices, which can, for example, undergo a Mott insulator to a superfluid transition, have opened new avenues to investigate quantum phase transitions [4, 5]. QPTs occur at absolute zero temperature and are associated with a fundamental change in the ground state of the system [1]. A quantum critical point is characterized by a diverging length scale as well as a diverging time scale, namely the relaxation time of the quantum system. This characteristic time scale is the inverse of the minimum energy gap of the underlying quantum Hamiltonian which vanishes at the quantum critical point. Recently, QPTs have also been studied from the viewpoint of quantum information theory. Quantities like concurrence [6], entanglement entropy [7, 8], fidelity susceptibility [9]–[17] and geometric phases [18]–[22] have been studied in the vicinity of quantum critical points, and are found to capture the singularities associated with them. A close relation between geometric phase (GP) and magnetic susceptibility has also been established for the transverse XY chain for QPTs driven by a transverse magnetic field [23]. It is worth mentioning that the ground-state GP in a Heisenberg XY model has been experimentally observed very recently using NMR interferometry [24].

In the present work, we investigate the scaling behavior of GP [25, 26] near a quantum multi-critical point (MCP) generated by the application of rotation on each spin of a quantum spin chain around the z axis. Berry showed that, in addition to the usual dynamic phase, a phase purely of geometric nature is accumulated on the wavefunction of a quantum system under an adiabatic and cyclic change of the Hamiltonian [26]. Quantum critical points are regions of vanishing energy gaps and consequently are accompanied by non-analyticities in various observables of the system. In a quantum critical system, the GP of the ground state of the system, which depends on the energy gap, can capture the associated singularities [18]–[20]. In fact, the GP can also be related to the imaginary part of a general geometric tensor, whose real part on the other hand gives the fidelity susceptibility which is the rate of change of the ground state of the Hamiltonian following an infinitesimal change in its parameters [10, 11, 27, 28].
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We exploit the integrability of a spin-1/2 \( XY \) chain \([29]–[32]\) to investigate the nature of the geometric phase close to the MCP. Recently, it has been shown that a GP difference between the ground and the first excited state exists in an isotropic \( XY \) chain (i.e. the \( XX \) chain) if and only if the closed evolution path circulates a region of criticality \([18]\). In this paper, we use a dynamical scheme so that the MCP is approached along various paths characterized by a parameter \( \alpha \). The non-contractible GP of the ground state is studied following the behavior of the GP and its derivative close to the Ising transition point of an anisotropic \( XY \) chain \([19]\). In the case of an MCP, we find that the derivative of the GP with the anisotropy parameter scales with the chain length in a non-trivial fashion with an exponent depending on the parameter \( \alpha \). Moreover, it does not peak right at the MCP, rather it peaks at points close to the MCP on the ferromagnetic side (which are so-called ‘quasi-critical points’ \([34,35]\)), where the energy gap is a local minima. However, beyond a limiting value of \( \alpha = \alpha_c \) no such peak is observed and the GP as well as its derivative at the MCP is zero for all values of \( \alpha \).

2. The model and the geometric phase

The model we consider is a one-dimensional spin-1/2 \( XY \) model in a transverse field with nearest-neighbor ferromagnetic interactions given by the Hamiltonian \([29,30,32,33]\)

\[
H = -\frac{1}{2} \sum_n [(1 + \gamma) \sigma^x_n \sigma^x_{n+1} + (1 - \gamma) \sigma^y_n \sigma^y_{n+1} + h \sigma^z_n],
\]

where \( \sigma \)s are Pauli spin matrices satisfying the usual commutation relations. The parameter \( h \) is the magnetic field applied in the \( z \) direction and \( \gamma \) measures the anisotropy in the in-plane interactions. The phase diagram of the system, plotted in the \( h-\gamma \) plane, is shown in figure 1 where the vertical bold lines at \( h = \pm 1 \) represent quantum transitions from the ferromagnetic to the paramagnetic phases that belong to the transverse Ising universality class and hence are called the ‘Ising transitions’. The horizontal bold line at \( \gamma = 0 \) with the transverse field lying between 1 and \(-1\) represents transitions between ferromagnetic ordered phases with ordering in the \( x \) and \( y \) directions, respectively \([30,32]\). The points A and B (\( h = \pm 1 \) at \( \gamma = 0 \), respectively) where Ising and anisotropic lines meet are the multi-critical points \([36]\), which are our subject of interest. Analyzing the energy spectrum of the Hamiltonian (1) \([32]\), it can be easily shown that the energy gap scales with the momentum \( k \) as \( k^z (= k) \) at any Ising critical point \( (h = \pm 1, \gamma \neq 0) \) so that the dynamical exponent \( z = 1 \). On the other hand, for the critical mode the gap scales as \( |h - 1|^{\nu z} (= |h - 1|) \) yielding the correlation length exponent \( \nu = 1 \). Similarly, one finds for MCP that \( z = 2 \) and \( \nu = 1/2 \) \([36]\); \( \nu z = 1 \) in either case.

We propose a dynamical scheme that enables us to approach the MCP along the path defined by \([35]\)

\[
h(\gamma) = 1 - |\gamma|^\alpha \text{sgn}(\gamma),
\]

so that the system hits the MCP A at \( h = 1, \gamma = 0 \) (see figure 1). Close to an MCP, the path of approach plays an important role as is also to be shown below in the scaling of any dynamical response; the dynamical scheme (2) in which the path can be changed through tuning the parameter \( \alpha \) therefore facilitates the study of the path-dependent scaling of the GP close to the MCP.

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Figure 1. The phase diagram of a one-dimensional $XY$ model in a transverse field. The vertical bold lines ($h = \pm 1$) denote Ising transitions from the ferromagnetic to the paramagnetic phase. The horizontal bold line stands for the anisotropic phase transition from a ferromagnetic phase with magnetic ordering in the $x$ direction to a ferromagnetic phase with ordering in the $y$ direction. The multi-critical points are at $A$ ($h = 1$, $\gamma = 0$) and $B$ ($h = -1$, $\gamma = 0$). We show different paths for approaching the MCP A corresponding to different values of $\alpha$; path I (path II) is for $\alpha = 1$ ($\alpha = 2$). We show that, for $\alpha < 2$, we observe quasi-critical peaks and there is a continuously varying effective scaling exponent for $d\beta_g/d\gamma$ with the chain length, while for $\alpha > 2$ no peak is observed.

In order to investigate the GP in this system, we introduce a new family of Hamiltonians that can be described by applying a rotation of $\eta$ around the $z$ direction to each spin [18, 19], i.e. $H_\eta = g_\eta H_{\eta}^\dagger$ with $g_\eta = \prod_n \exp[i\eta \sigma_z^n]/2$. For the family of Hamiltonians thus generated, the energy spectrum remains the same, leaving the critical behavior unaltered. The Hamiltonian $H(\eta)$ can be diagonalized by using the Jordan–Wigner transformation which transforms the spin operators into fermionic operators $a_n$ and $a_n^\dagger$ via the relations [29, 37] $a_n = (\prod_{l<n} \sigma_z^l) \sigma^\dagger_n$. Employing a Fourier transformation $d_k = \sum_j [a_j \exp(-i2\pi jk/N)]/\sqrt{N}$ followed by a Bogoliubov transformation, one can recast Hamiltonian (1) to the diagonal form

$$H = \sum_k \Lambda_k (c_k^\dagger c_k - 1),$$

where $\Lambda_k = \sqrt{(h + \cos(2\pi k/N))^2 + \gamma^2 \sin^2(2\pi k/N)}$, $c_k = d_k \cos(\theta_k/2) - d_k^\dagger e^{2i\eta} \sin(\theta_k/2)$ and the angle $\theta_k$ is given by $\cos \theta_k = (\cos(2\pi k/N) + h)/\Lambda_k$.

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 $|1\rangle_k |1\rangle_{-k}$, where $|0\rangle_k$ and $|1\rangle_k$ are the vacuum and the excited state for the $k$th mode $|1\rangle_k |1\rangle_{-k} = d_k^\dagger d_{-k} |0\rangle_k |0\rangle_{-k}$. Under the unitary transformation (i.e. rotation about the $z$ axis), the ground state of the transformed Hamiltonian picks up an additional phase factor and is given by $|g\rangle = \prod_k (\cos(\theta_k/2) |0\rangle_k |0\rangle_{-k} - i e^{2i\eta} \sin(\theta_k/2) |1\rangle_k |1\rangle_{-k})$. The GP of the ground state, accumulated by varying the angle $\eta$ from 0 to $\pi$, is described by $[26] \beta_g = -i/N \int_0^\pi \langle g|\partial_\eta|g\rangle d\eta$, and is

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given by
\[ \beta_g = \frac{\pi}{N} \sum_k (1 - \cos \theta_k). \]  
(3)

This equation in the thermodynamic limit \((N \to \infty)\), where the critical properties are studied, is given by
\[ \beta_g = \int_0^\pi (1 - \cos \theta_\phi) \, d\phi, \]  
(4)

where the summation \(1/N \sum_k\) is replaced by the integral \(1/\pi \int_0^\phi\) with \(\phi = 2\pi k/N\), so that
\[ \cos \theta_\phi = (\cos \phi + h)/\Lambda_\phi \quad \text{and} \quad \Lambda_\phi = \sqrt{(h + \cos \phi)^2 + \gamma^2 \sin^2 \phi}. \]  
(5)

Carollo and Pachos [18] studied the behavior of the GP close to the anisotropic critical point and showed that a non-contractible geometric phase difference between the ground state and the first excited state exists when the Hamiltonian encounters a critical point while passing through an adiabatic cycle. In a subsequent work, Zhu [19] showed that the derivative \(d\beta_g/dh\) as \(h\) is varied shows a peak right at the Ising critical point and diverges logarithmically with the chain length. From the scaling relations \(d\beta_g/dh \sim \kappa_1 \ln N + C_1\) at the critical point \(h = h_c = 1\) and \(d\beta_g/dh \sim \kappa_2 \ln |h - h_c| + C_2\) for an infinite system (where \(C_1\) and \(C_2\) are non-universal constants), the critical exponent \(\nu\) can be obtained from the relation \(\nu = \kappa_2/\kappa_1 = 1\).

3. Results

We study the behavior of the GP in the vicinity of the MCP A (see figure 1) using the dynamical path given in equation (2). Let us first consider the case of \(\alpha = 1\), i.e. a linear path approaching the MCP, and estimate the geometric phase and its derivative using numerical techniques. We observe a series of peaks in the derivative \(d\beta_g/d\gamma\) when plotted against \(\gamma\) close to the MCP on the ferromagnetic side \((\gamma > 0, |h| < 1\) for the path (2)) of it as shown in figure 2. A similar behavior is observed for all values of \(\alpha < 2\) (see figure 3). This is in contrast to the behavior near an Ising critical point where there is only one peak right at the quantum critical point [19] (see figure 4). No such peak is observed on the paramagnetic side \((\gamma < 0, |h| > 1\) and the GP itself becomes trivial at the MCP as seen from equation (3). On the other hand, for \(\alpha > 2\) no peaks are observed close to the MCP (see figure 4), and the case \(\alpha = 2\) shows a limiting behavior to be discussed later (see figure 5). The appearance of the series of peaks in \(d\beta_g/d\gamma\) can be attributed to the existence of quasi-critical points where the energy spectrum attains local minima, to be explained below.

The scaling behavior of the derivative \(d\beta_g/d\gamma\) with the system size for a generic \(\alpha\) can be derived in the following way. From equation (2) we get the spectrum as
\[ \Lambda_\phi = \sqrt{[\cos \phi + (1 - |\gamma|^\alpha \sgn(\gamma))]^2 + \gamma^2 \sin^2 \phi}, \]  
(6)

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Figure 2. The numerically observed variation of $d\beta_g/d\gamma$ with respect to $\gamma$ for $\alpha = 1$ for different chain lengths, $N = 2000$ (blue solid line), $N = 1800$ (red dotted line) and $N = 1500$ (green dashed line). In all cases, a series of peaks is observed on the ferromagnetic side ($\gamma > 0, |h| < 1$) along the path of approach. With increasing $N$ the peak height increases, the peaks shift closer to the MCP and the distance between subsequent peaks decreases.

Figure 3. A similar behavior as in figure 2 for $d\beta_g/d\gamma$ as a function of $\gamma$ is observed for $\alpha = 1.5$.

so that using equation (4) for positive $\gamma$, $d\beta_g/d\gamma$ can be expressed as

$$\frac{d\beta_g}{d\gamma} = -\int_0^\pi \left( \frac{d\cos\theta}{d\gamma} \right) d\phi = \int_0^\pi \left( \frac{\alpha\gamma^{\alpha-1} - A}{\Lambda^2\phi} \right) d\phi,$$

where

$$A = \{\cos\phi + (1 - \gamma^\alpha)\}{[\cos\phi + (1 - \gamma^\alpha)]\alpha\gamma^{\alpha-1} - \gamma\sin^2\phi}.$$

The first term of the integrand dominates over the second term which can be dropped for further calculations. For $\phi \simeq \pi$, the minima in $\Lambda\phi$ occur at points where $\gamma^\alpha \sim \phi^2$ (shown below) so that

$$\frac{d\beta_g}{d\gamma} = \int_0^\pi \frac{\alpha\phi^{(2/\alpha)(\alpha-1)} - A}{\phi^{1/2}(4/\alpha + 2)} d\phi \propto \phi^{2-(4/\alpha)},$$

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Figure 4. Numerically no peak is observed in $d\beta_g/d\gamma$ for $\alpha = 2.5$ which is due to the absence of quasi-critical points along the path. However, a peak is observed corresponding to the Ising critical point at $\gamma = 1.319, h = -1$.

Figure 5. The numerical plot of $d\beta_g/d\gamma$ with $\gamma$ for the marginal case $\alpha = 2$, indicating a peak close to the MCP (left inset) with the peak height saturating to a constant value with $N$ (right inset) as expected from the analytical scaling relation (9). The Ising peak is observed at $\gamma = 1.414$ where $h = -1$.

with $\phi \sim 1/N$. Hence we get the scaling relation

$$
\frac{d\beta_g}{d\gamma} \propto N^{(4/\alpha)-2}.
$$

The scaling relation (9) shows that $d\beta_g/d\gamma$ diverges with the system size for $\alpha < 2$ while for $\alpha = 2$ a saturation is expected. The scaling exponent varies continuously with the path, i.e. with the parameter $\alpha$ up to the limiting value $\alpha = 2$. Figure 6 shows the scaling of $d\beta_g/d\gamma$ with $N$ for $\alpha = 1$ and 1.5, confirming the analytical scaling (9) while no peak is expected for $\alpha > 2$ as numerically observed in figure 4. With increasing $\alpha$, doi:10.1088/1742-5468/2011/03/P03026
The numerical results perfectly match with the scaling relation (9).

Let us now focus on the energy spectrum (6); the energy gap is not minimum at the MCP for $\alpha < 2$, rather it is minimum at the ‘quasi-critical’ points determined by the condition $\cos \phi + (1 - |\gamma|\alpha \text{sgn}(\gamma)) = 0$ or $|\gamma|\alpha \text{sgn}(\gamma) = \phi^2$ if we expand $\phi \simeq \pi$ and rescale $\phi \rightarrow \pi - \phi$. The derivative of the GP shows a peak whenever the energy gap is minimum, i.e. the spectrum hits a ‘quasi-critical’ point resulting in a series of peaks on the ferromagnetic side of the MCP as numerically observed in figures 2 and 3. The condition $|\gamma|\alpha \text{sgn}(\gamma) = \phi^2$ does also imply that, for increasing chain length, the quasi-critical points (and hence the peaks in $d\beta_g/d\gamma$) become closely spaced. Note that, strictly for $N \rightarrow \infty$, the peaks collapse to a single peak: however, for any finite chain there will be multiple peaks. In fact, even in the $N \rightarrow \infty$ limit, the quasi-critical exponents (not the exponents associated with the MCP) will appear in the scaling relation (9) as also observed in the scaling behavior of defect density following a slow quench [35] and that of the fidelity susceptibility [38]. The analysis of equation (6) also shows that no such quasi-critical point exists on the paramagnetic side and hence no peak in $d\beta_g/d\gamma$ is expected. Similarly, for $\alpha > 2$ the minimum in energy gap occurs right at the MCP where the GP and its derivative vanishes and hence no peak appears as shown in figure 4. For $\alpha = 2$ only one peak of $d\beta_g/d\gamma$ is observed close to the MCP and the height of the peak saturates for large $N$ to a constant value as the exponent $(4/\alpha - 2)$ in equation (9) vanishes in the limit at $\alpha \rightarrow 2$ (figure 5). Investigating figures 4 and 5 closely, we observed peaks at the Ising critical points $h = -1$; this peak appears for all values of $\alpha$ and scales logarithmically with $N$ yielding $\nu = 1$ as reported earlier [19].

From equations (4)–(6), one finds that for a finite chain with isotropic interaction ($\gamma = 0$), $\theta_\phi = 0$ or $\pi$ so that $\beta_g = 0$ or $2\pi$ for $h > 1$ whereas for $h \leq 1$, $\beta_g = 2\pi - 2\arccos(h)$ [19, 21]. Additionally, in the thermodynamic limit, for infinitesimally small $\gamma$, we can always find a solution $\phi_0$ such that $\cos \phi_0 + (1 - |\gamma|\alpha \text{sgn}(\gamma)) = 0$ but $\Lambda_{\phi_0} = |\gamma|\sqrt{1 - (1 - |\gamma|\alpha \text{sgn}(\gamma))^2} \neq 0$ (see equation (5)). This leads to $\theta_{\phi_0} = \pi/2$ and a non-trivial geometric phase $\beta_g = \pi$ for $\gamma \rightarrow 0$. 

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The relation between the geometric phase and the transverse magnetization ($M_z$) at zero temperature given by the relation $\beta_k = \pi + \pi M_z$ has been established close to the Ising transition [23]. Close to the MCP $\Lambda$, if one defines an $\alpha$-dependent magnetization $M(\alpha)$ through the derivative $\partial \Lambda_\varphi / \partial h$ for a given path (see equation (2)), it can be shown that $M(\alpha) = M_z + \partial \Lambda_\varphi / \partial \gamma (\partial \gamma / \partial h) = 1/\Lambda_\varphi (h + \cos k) - (2/\alpha) \gamma^{2-\alpha} \sin^2 k$, where the transverse magnetization $M_z$ is related to the geometric phase as discussed in [23]. One can therefore conclude that close to a MCP the derivative of the geometric phase along a path cannot be related to the transverse magnetic susceptibility directly.

4. Conclusion

In this work, the scaling properties of the GP have been studied close to a quantum MCP of a spin-$1/2$ transverse XY spin chain. We show that the scaling of the derivative of the GP depends on the path of approaching the MCP. It shows a peak whenever the system hits a ‘quasi-critical point’, leading to a series of peaks on the ferromagnetic side of the MCP. The peak diverges with the system size with an exponent that varies continuously with path up to a limiting path given by $\alpha = \alpha_c = 2$, where we observe a saturation with $N$. On the paramagnetic side and also for paths beyond the limiting path (i.e. for $\alpha > 2$), the system does not encounter any quasi-critical point, causing the peaks in the derivative to disappear. Clearly, the scaling presented in equation (9) and the limiting value ($\alpha_c = 2$) are established close to an MCP for a transverse XY chain. For a generic MCP, the scaling law and the value of $\alpha_c$ or the position of the peaks are expected to be different as they depend on the spectrum; however, near a generic MCP if quasi-critical points exist, the associated exponents shall dictate the equivalent scaling relations and the limiting path, and the derivative of the GP will show peaks at the quasi-critical points.

We note that, in a recent study, a similar behavior of the fidelity susceptibility, namely occurrence of a series of peaks on the ferromagnetic side of the MCP, has been reported [38]. The fidelity susceptibility has also been found to diverge with the system size with an exponent that continuously varies with the path up to $\alpha = \alpha_c = 2$. Our study therefore points to a deep connection between the scaling of the fidelity susceptibility and the GP close to quantum critical as well as multi-critical points, as was predicted in the study of quantum geometric tensors [10, 11]. Questions may remain on the nature of the quasi-critical points, especially whether they are generic or specific to this particular spin chain. These points may appear in the present model due to the existence of the line of anisotropic critical points with continuously varying ordering wavevectors. However, recent studies including the present work reveal that, in all dynamical responses near a quantum MCP, e.g. defect generation following slow and rapid quenches [34, 35], fidelity susceptibility [38] as well as in the scaling of the GP, these quasi-critical points play a dominant role depending on the path of approach.

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