Geometric phases and criticality in spin chain systems

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A relation between geometric phases and criticality of spin chains is established. As a result, we show how geometric phases can be exploited as a tool to detect regions of criticality without having to undergo a quantum phase transition. We analytically evaluate the geometric phase that correspond to the ground and excited states of the anisotropic XY model in the presence of a transverse magnetic field when the direction of the anisotropy is adiabatically rotated. It is demonstrated that the resulting phase is resilient against the main sources of errors. A physical realization with ultra-cold atoms in optical lattices is presented.

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Since the discovery by Berry [1], geometric phases in quantum mechanics have been the subject of a variety of theoretical and experimental investigations [2]. Possible applications range from optics and molecular physics to fundamental quantum mechanics and quantum computation [3]. In condensed matter physics a variety of phenomena have been understood as a manifestation of topological or geometric phases [4, 5, 6, 7, 8]. An interesting open question is whether the geometric phases can be used to investigate the physics and the behavior of condensed matter systems. Here we show how to exploit the geometric phase as an essential tool to reveal quantum critical phenomena in many-body quantum systems. Indeed, quantum phase transitions are accompanied by a qualitative change in the nature of classical correlations and their description is clearly one of the major interests in condensed matter physics [3, 10]. Such drastic changes in the properties of ground states are often due to the presence of points of degeneracy and are reflected in the geometry of the Hilbert space of the system. The geometric phase, which is a measure of the curvature of the Hilbert space, is able to capture them, thereby revealing critical behavior. This provides the means to detect, not only theoretically, but also experimentally the presence of criticality without having to undergo a quantum phase transition.

In this letter we analyze the XY spin chain model and the geometric phase that corresponds to the XX criticality. Since the XY model is exactly solvable and still presents a rich structure it offers a benchmark to test the properties of geometric phases in the proximity of a quantum phase transition. Indeed, we observe that, an excitation of the model obtains a non-trivial Berry phase if and only if it circulates a region of criticality. The generation of this phase can be traced down to the presence of a conical intersection of the energy levels located at the XX criticality. This geometric interpretation reveals a relation between the critical exponents of the model. The insights provided here shed light into the understanding of more general systems, where analytic solutions might not be available. A physical implementation is proposed with ultra-cold atoms superposed by optical lattices [11, 12]. It utilizes Raman activated tunneling transitions as well as coherent drive of the system via Bragg scattering. The independence of the generated phase from the number of atoms, its topological nature and its resilience against control errors makes the proposal appealing for experimental realization.

Consider the one dimensional spin-1/2 XY model, with N spins, in a transverse magnetic field. This chain has nearest neighbor interactions with Hamiltonian given by

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

where $M = (N - 1)/2$ for $N$ odd. In particular, we are interested in the Hamiltonian that can be obtained by applying a rotation of $\phi$, around the z-direction, to each spin

$$H(\phi) = g(\phi) H g(\phi) \quad \text{with} \quad g(\phi) = \prod_{l=-M}^{M} e^{i \sigma_l^x \phi / 2}. \quad (1)$$

The family of Hamiltonians that is parameterized by $\phi$ is clearly isospectral and, therefore, the critical behavior is independent from $\phi$. This is reflected in the symmetric structure of the regions of criticality shown in Figure 1. In addition, due to its bilinear form, $H(\phi)$ is $\pi$-periodic in $\phi$. The Hamiltonian $H(\phi)$ can be diagonalized by a standard procedure, which can be summarized in the following three steps: (i) the Jordan-Wigner transformation, which converts the spin operators into fermionic operators via the relations, $a_i = (\prod_{m<c} \sigma_m^z) (\sigma_i^x + i \sigma_i^y) / 2$; (ii) their Fourier transformation, $d_k = \frac{1}{\sqrt{N}} \sum_i a_i e^{-i \pi k / N}$, with $k = -M, \ldots, M$; and (iii) the Bogoliubov transformation, which defines the fermionic operators, $b_k = d_k \cos \frac{\delta_k}{2} - id_k^* e^{2i \phi} \sin \frac{\delta_k}{2}$, where the angle $\theta_k$ is defined by $\cos \theta_k = \epsilon_k/\Lambda_k$ with $\epsilon_k = \cos \frac{2\pi k}{N} - \lambda$ and $\Lambda_k = \sqrt{\epsilon_k^2 + \gamma^2 \sin^2 \frac{2\pi k}{N}}$. These
and the relative one between the ground and excited state (c).

The geometric phase corresponding to the ground state (b)
and the relative one between the ground and excited state (c)
as a function of the path parameters $\lambda$ and $\gamma$. Values of the
geometric phase corresponding to the loops $C_1$, $C_2$ and $C_3$ in
(a) are also indicated.

procedures diagonalize the Hamiltonian to a form
\[ H(\phi) = \sum_{k=-M}^{M} \Lambda_k b_k^\dagger b_k. \] (2)

The ground state of $H(\phi)$ is the vacuum $|g\rangle$ of the
fermionic modes, $b_k$, given by
\[ |g\rangle = \prod_{k>0} \left( \cos \frac{\theta_k}{2} |0\rangle_k |0\rangle_{-k} - i e^{i2\phi} \sin \frac{\theta_k}{2} |1\rangle_k |1\rangle_{-k} \right), \] (3)

where $|0\rangle_k$ and $|1\rangle_k$ are the vacuum and single excitation
of the $k$-th mode, $d_k$, respectively. The regions of criticality
which appear when the ground and first excited states become degenerate are shown for this model in Figure (a). The XX model, which corresponds to $\gamma = 0$, has criticality region along the line between $\lambda = 1$ and $\lambda = -1$. The region of the Ising model phase transition are the two planes at $\lambda = 1$ and $\lambda = -1$. The interesting paths of evolution for generating a Berry phase are those for which the state of the system can evolve around a region of criticality. Here we shall focus on the criticality region corresponding to the XX model, which can be encircled by adiabatically varying the angle $\phi$ from 0 to $\pi$. The corresponding Berry phase of ground and first excited states can be evaluated as a function of $\lambda$ and $\gamma$.

Using the standard formula it is easy to show that the
Berry phase of the ground state $|g\rangle$ is given by
\[ \varphi_g = -i \int_0^\pi \langle g | \frac{\partial}{\partial \phi} | g \rangle = \sum_{k>0} \pi (1 - \cos \theta_k). \] (4)

This result can be understood by considering the form of $|g\rangle$, which is a tensor product of states, each lying in the
two dimensional Hilbert space spanned by $|0\rangle_k |0\rangle_{-k}$ and
$|1\rangle_k |1\rangle_{-k}$. For each value of $k(> 0)$, the state in each of
these two-dimensional Hilbert spaces can be represented as a Bloch vector with coordinates $(2\phi, \theta_k)$. A change in the parameter $\phi$ determines a rotation of each Bloch vector about the $z$ direction. A closed circle will, therefore, produce an overall phase given by the sum of the individual phases as given in Figure (b) and illustrated in Figure (c). It is worth noticing that when $\gamma$ is small, the overall phase is strongly dependent on the exact values of $\lambda$ and $\gamma$ due to the (large) proportionality factor $M$.

On the other hand, when $\gamma \gg \lambda$, each pair of $k$ and $-k$ states from $|g\rangle$ contributes almost equally to the overall Berry phase (see Figure (b)). In this case, we obtain $\varphi_g/M \approx \pi$ which makes effectively the dependence of the overall Berry phase on the parameters $\gamma$, $\lambda$ much weaker.

Of particular interest is the relative geometric phase between the first excited and ground states given by the difference of the Berry phases acquired by these two states. The first excited state is given by $|e_k\rangle \equiv b_k^\dagger |g\rangle$, i.e. it is the single excitation of the $b$ fermionic field, with $k_0$ corresponding to the minimum value of the energy $\Lambda_k$.

The relative geometric phase then becomes
\[ \varphi_{eg} \equiv \varphi_e - \varphi_g = -i \int \langle g | b_k \frac{\partial}{\partial \phi} b_k^\dagger | g \rangle. \] (5)

If the parameter $\phi$ is adiabatically changed from 0 to $\pi$, we obtain $\varphi_{eg} = -\pi (1 - \cos \theta_{k_0})$ which, in the thermodynamical limit ($N \rightarrow \infty$), takes the form
\[ \varphi_{eg} = \left\{ \begin{array}{ll}
-\pi + \frac{\pi \lambda}{\sqrt{(1-\gamma^2)(1-\gamma^2-\lambda^2)}} & \text{for } |\lambda| > 1 - \gamma^2 \\
0 & \text{for } |\lambda| < 1 - \gamma^2.
\end{array} \right. \] (6)

As can be seen from Figure (c), the most interesting behavior of $\varphi_{eg}$ is obtained in the case of $\gamma$ small compared to $\lambda$. In this case $\varphi_{eg}$ behaves as a step function, giving either $\pi$ or 0 phase, depending on whether $|\lambda| < 1$ or $|\lambda| > 1$, respectively. This behavior is precisely determined from whether the corresponding loop encloses a critical point or not and can be used as a witness of its presence. In particular, in the $|\lambda| < 1 - \gamma^2$ case the first term corresponds to a purely topological phase, while the second is a geometric contribution.

This is related to a more general property: a non-trivial Berry phase is generated when the closed loop in the parameter space is spanned in the vicinity of a degeneracy point. The topological nature of this phase is evident in the case of a loop contracting to a point. If, in this limit, the Berry phase remains non-vanishing, then the contraction point identifies the position of the degeneracy. As a critical point is also a point of degeneracy it is apparent that this procedure can be used to locate the criticality of an Hamiltonian.

To better understand the properties of the relative geometric phase in our model, let’s focus on the region of
parameters with $\gamma \ll 1$, i.e. for a loop around the region of criticality which contracting to a point. In this case, it can be shown that the Hamiltonian, when restricted to its lowest energy modes $d_{k\alpha}$ and $d_{-k\alpha}$, can be casted in a real form and, for $|\lambda| < 1$, its eigenvalues present a conical intersection centered at $\gamma = 0$. It is well known that when a closed path is taken within the real domain of a Hamiltonian, a topological phase shift $\pi$ occurs only when a conical intersection is enclosed. In the present case, the conical intersection corresponds to a point of degeneracy where the XX criticality occurs and it is revealed by the topological term in the relative geometric phase $\varphi_{eg}$. It is worth noticing that the presence of a conical intersection indicates that the energy gap scales linearly with respect to the coupling $\gamma$ when approaching the degeneracy point. This implies that the critical exponents of the energy, $z$, and of the correlation length, $\nu$, satisfy the relation $z\nu = 1$ which is indeed the case for the XX criticality [10].

From an experimental point of view, this method of obtaining a geometric phase is robust against relevant sources of errors. The most significant one originates from undesired transitions induced by the time dependence of the Hamiltonian. In any adiabatic process the occurrence of these transitions is hindered primarily by the presence of a finite energy separation between neighboring levels. However, as in many condensed matter systems, these energy separations may decrease quite rapidly as the thermodynamical limit is approached. In fact, in this model, the gaps between the energies of the lowest excited states scale typically as $N^{-2}$, which might substantially reduce the applicability of the adiabatic approximation in a truly many-body setup. However, in the adiabatic evolution proposed here, all the transitions between closely separated energy levels are prohibited due to symmetry reasons. It is apparent form equation 11 that the adiabatic evolution is generated by the Hamiltonian term $H \propto \sum_k \sigma_k^z = \sum_k d_k^\dagger d_k$, which preserves the excitations in each fermionic mode, $d_k$. In fact, the excitations $|e_k\rangle = b_k^\dagger |g\rangle$ of model 11 are also eigenstates of $H$. Therefore, the only allowed transitions induced by $H$ are between the ground state and the doubly excited states $b_k^\dagger b_{-k}^\dagger |g\rangle$. The corresponding finite energy gap $2\Delta_k$ is then sufficient to adiabatically prevent these unwanted transitions, even in the thermodynamical limit. Moreover, this symmetry constraint guarantees the viability of the adiabatic approximation also when energy level crossings occur between singly excited states $|e_k\rangle$.

Another important feature of this model is the behavior of the phase under errors in the initial preparation. The smooth dependence of the geometric phase on the momentum $\chi = 2\pi k/N$, insures that a small deviation $\delta = \chi - \chi_0$ from the value $\chi_0 = 2\pi k_0/N$ (corresponding to first excited state, i.e. the minimum of the function $\Delta(\chi)$) does not drastically affect the interference pattern. Indeed a perturbation analysis shows that states with a small momentum difference, $\delta$, from $\chi_0$ acquire geometric phases with values shifted by an amount proportionally to $\delta$. In particular, due to the independence of the function $\Delta(\chi)$ from the system size, $N$, the spread of the geometric phase only depends on $\delta$ and remains unchanged in the thermodynamical limit. Naturally, this effect is accompanied by a reduction of the visibility and a shift in the value of the measured phase, which, however, only depend on the preparation and measurement accuracies and does not depend on the system size.

This construction, apart from its theoretical interest, offers a possible experimental method to detect critical regions without the need to cross them, which undermines the ability to identify the state of the system due to the presence of degeneracy. In particular, we shall implement this model with optical lattices. To this end, consider two bosonic species labelled by $\sigma = a, b$ that can be given by two hyperfine levels of an atom. Each one can be trapped by employing two in-phase one dimensional optical lattices. The tunneling of atoms between neighboring sites is described by $V = -\sum_{\sigma}(J_\sigma a^\dagger_{\sigma l}a_{\sigma(l+1)} + H.c.)$. When two or more atoms are present in the same site, they experience collisions given by $H^{(0)} = \sum_{\sigma,l} \frac{U_{\sigma l}}{2} a^\dagger_{\sigma l} a_{\sigma l} a^\dagger_{\sigma l} a_{\sigma l}$. We shall consider the limit $V \ll U$ where the system is in the Mott insulator regime [13] with one atom per lattice site. In this regime, the effective evolution is obtained by adiabatic elimination of the states with a population of two or more atoms per site, which are energetically unfavorable. Hence, to describe the Hilbert space of interest, we can employ the pseudospin basis of $|\uparrow\rangle \equiv |n^a_l = 1, n^b_l = 0\rangle$ and $|\downarrow\rangle \equiv |n^a_l = 0, n^b_l = 1\rangle$, for lattice site $l$, and the effective evolution can be expressed in terms of the corresponding Pauli operators. It is easily verified that when the tunneling coupling of both atomic species is activated, the following exchange interaction is realized between neighboring sites [12 14 15],

$$H_1 = -\frac{J_{ab}}{U_{ab}} \sum_l (\sigma^x_l \sigma^x_{l+1} + \sigma^y_l \sigma^y_{l+1}).$$

(7)

In order to create an anisotropy between the $x$ and $y$ spin directions, we activate a tunneling by means of Raman couplings [12 15]. Application of two standing lasers $L_1$ and $L_2$, with zeros of their intensities at the lattice sites and with phase difference $\phi$, can induce tunneling of the state $|\uparrow\rangle \equiv (e^{-i\phi/2}|a\rangle + e^{i\phi/2}|b\rangle)/\sqrt{2}$. The resulting tunneling term is given by $V_c = J_c \sum_l (c^\dagger_l c_{l+1} + H.c.)$, where $c_l$ is the annihilation operator of $|\uparrow\rangle$ state particles. The tunneling coupling, $J_c$, is given by the potential barrier of the initial optical lattice superposed by the potential reduction due to the Raman transition. The resulting evolution is dominated by an effective Hamiltonian given, up to a readily compensated Zeeman term, by

$$H_2 = \frac{1}{2} \frac{J^2}{U_{ab}} \sum_l g(\phi) \sigma^x_l \sigma^x_{l+1} g^\dagger(\phi).$$

(8)
where \( g(\phi) \) was defined in \((1)\). Combining the rotationally invariant Heisenberg interaction \( H_1 \) with \( H_2 \) gives the rotated XY Hamiltonian described by equation \((1)\), where the parameter \( \gamma \) is given by \( J_z^2/(2U_{ab}) \) and \( \epsilon = (2J_aJ_b + J_z^2/2)/U_{ab} \) is the overall energy scale multiplying the Hamiltonian \((1)\).

At this point we would like to generate and measure the relative phase between the ground and excited states. To create the first spin chain excitation, \( |e_{k_0}| \), in the optical lattice setup we employ two-photon Bragg spectroscopy \((13)\). The use of a two-photon process allows for an accurate energy resolution of the state we want to excite, which is crucial considering that the energy gap, \( \Lambda_{k_0} \), is small compared to the tunneling and collisional couplings \((14)\). For example, an amplitude modulation of the axial lattice potential, \( V_x(x, t) = [V_{x,0} + A_{\text{mod}} \sin(2\pi \nu_{\text{mod}} t)] \sin^2(kx) \), can be employed \((20)\) with a frequency that satisfies the resonant Bragg condition, \( \nu_{\text{mod}} = \Lambda_{k_0} \). This will activate a coherent energy population transfer from the ground state to the excited one with a transition amplitude proportional to the modulation amplitude, \( A_{\text{mod}} \). Such an experimental technique has already been employed to study the atom-number excitations in an optical lattice near its criticality between the superfluid and the Mott insulator regime \((20)\). To detect the Berry phase of the excited state, one can initially create the superposition \(|g\rangle + |e_{k_0}\rangle\) with an appropriately timed lattice modulation with frequency \( \nu_{\text{mod}} = \Lambda_{k_0} \). The Berry phase procedure is then applied to generate a phase difference of \( \pi \) between the ground and the excited states giving \(|g\rangle - |e_{k_0}\rangle\). Applying the same modulation procedure as before will finally result in the state \(|e_{k_0}\rangle\). To distinguish between the states \(|g\rangle\) and \(|e_{k_0}\rangle\) one can measure the corresponding spin-spin correlators, e.g., by atomic scattering of fast atoms off the lattice \((17)\).

To conclude, we have presented a method that theoretically, as well as experimentally, enables the detection of regions of criticality through the geometric phase, without the need for the system to experience phase transitions. The latter is experimentally hard to realize as the adiabaticity condition breaks down and the state of the system is no longer faithfully represented by the ground state. The origin of the geometric phase can be ascribed to the existence of degeneracy points in the parameter space of the Hamiltonian. Hence, a criticality point can be detected by performing a looping trajectory around it and detecting whether or not a non-zero Berry phase has been generated. For the case of the XY model the topological nature of the resulting phase pinned to the value, \( \varphi_{\text{eg}} \approx \pi \), is revealed by its resilience with respect to small deformations of the loop. Topological phases are inherently resilient against control errors, a property that can be proved to be of a great advantage when considering many-body systems. Such a study can be theoretically performed on any system which can be analytically elaborated such as the case of the cluster Hamiltonian \((11)\), or exploited numerically when analytic solutions are not known. The generalization of these results to a wide variety of critical phenomena and their relation to the critical exponents is a promising and challenging question which deserves extensive future investigation.

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