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Quantized Berry phases for a local characterization of spin liquids in frustrated spin systems

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Abstract

Recently, by using quantized Berry phases, a prescription for a local characterization of *gapped* topological insulators has been given (Hatsugai 2006 *Preprint* cond-mat/0603230). It requires that the ground state is gapped and is invariant under some anti-unitary operation. A spin liquid which is realized as a unique ground state of the Heisenberg spin system with frustrations is a typical target system, since pairwise exchange couplings are always time-reversal invariants even with frustrations.

As for a generic Heisenberg model with a finite excitation gap, we locally modify the Hamiltonian by a continuous $SU(2)$ twist only at a specific link and define the Berry connection by the derivative. Then the Berry phase evaluated by the entire many-spin wavefunction is used to define the local topological order parameter at the link. We numerically apply this scheme for several spin liquids and show its physical validity. For example, it implies that the Haldane phase of the $S = 1$ chains is characterized by uniform π quantized Berry phases.

(Some figures in this article are in colour only in the electronic version)

1. Topological orders

In a modern condensed matter physics, the concept of symmetry breaking has a fundamental importance. At a sufficiently low temperature, most classical systems show some ordered structure which implies that the symmetry at high temperature is lost or reduced. This is the spontaneous symmetry breaking which is usually characterized by using a *local* order parameter as an existence of the long-range order. States of matter in a classical system are mostly characterized by this order parameter with the symmetry breaking. Even in a quantum system, the local order parameter and the symmetry breaking play similar roles and they form a foundation of our physical understanding. Typical examples can be ferromagnetic and Néel orders in spin systems.

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Recent studies have revealed that this symmetry breaking may not always be enough to characterize some of important quantum states [2, 3]. Low dimensionality of the system and/or geometrical frustrations that come from the strong correlation can prevent the formation of local order. Especially with a quantum fluctuation, it may happen that a quantum ground state without any explicit symmetry breaking is realized even at zero temperature. Such a state is classified as a quantum liquid which mostly has an energy gap (this may not always be the case). Typical examples of these quantum liquids are the Haldane spin chain and the valence bond solid (VBS) states [4, 5]. Also some of the frustrated spin systems and spin–Peierls systems can belong to this class [6–8]. To characterize these quantum liquids, a concept of a topological order can be useful [2, 3]. It was proposed to characterize quantum Hall states which are typical quantum liquids with energy gaps. There are many clearly different quantum states but they do not have any local order parameter associated with symmetry breaking. Then topological quantities such as the number of degenerate ground states and the Chern numbers as the Hall conductance are used to characterize the quantum liquids. We generalize the idea of using topological quantities such as the Chern numbers for the characterization of generic quantum liquids [3]. This is a global characterization. When we apply this to spin systems with time-reversal (TR) symmetry, the Chern number vanishes in most cases. Recently we proposed an alternative for a system with TR invariance using the quantized Berry phases [1]. Although the Berry phases can take any values generically, the TR invariance of the ground state guarantees a quantization of the Berry phases which enables us to use them as local topological order parameters. In the present paper, we use them for several spin systems with frustrations and verify the validity. Although the geometrical frustration affects the standard local order substantially, it does not bring any fundamental difficulties for the topological characterizations, as shown later. The quantized Berry phase should be quiteuseful for characterizations for general quantum liquids [1].

Finally we mention the energy spectra of systems with classical or topological orders. There can be interesting differences between the standard order and the topological order. As for energy spectra, we have two situations when the symmetry is spontaneously broken. If the spontaneously broken symmetry is continuous, there exists a gapless excitation as a Nambu–Goldstone mode. On the other hand, the symmetry is discrete, the ground states are degenerate and above these degenerate states, there is a finite energy gap. Note that when the system is finite (with periodic boundary condition), the degeneracy is lifted by the small energy gap, $e^{-L^d/\xi}$ [9], where L, d and ξ are a linear dimension of the finite system, dimensionality and a typical correlation length. For the topological ordered states with energy gaps, we may expect degeneracy of the ground states depending on the geometry of the system (topological degeneracy). When the system is finite, we expect edge states generically [10]. This implies that the topological degeneracy is lifted by energy gaps of the order $e^{-L/\xi}$.

2. Local order parameters of quantum liquids

After the discovery of the fractional quantum Hall states, quantum liquids have been recognized to exist quite universally in a quantum world where quantum effects cannot be treated as a correction to the classical description and the quantum law itself takes the wheel that determines the ground state. The resonating valence bond (RVB) state which is proposed for a basic platform of the high-T_C superconductivity is a typical example [11]. The RVB state by Anderson can be understood as a quantum mechanical collection of *local* spin singlets. When it becomes mobile under the doping, the state is expected to show superconductivity. Original ideas of this RVB go back to Pauling's description of benzene compounds where the quantum mechanical ground state is composed of *local bonding states (covalent bonds)* where the basic

variables to describe the state are not electrons localized at sites but the bonding states on links [12]. This is quite instructive. That is, in both of Anderson's RVB and Pauling's RVB, the basic objects to describe the quantum liquids are quantum mechanical objects such as a *singlet pair* and a *covalent bond* [1]. The 'classical' objects such as small magnets (localized spins) and electrons at the site never play major roles. The constituents of the liquids themselves do not have a classical analogue and are purely quantum mechanical objects. Based on this view point, it is natural to characterize these quantum objects, the singlet pairs and the covalent bonds, as working variables of the *local* quantum order parameters. This is to be compared with the conventional order parameter (a magnetic order parameter is defined by a local spin as a working variable). From these observations, we proposed to use quantized Berry phases to define local topological order parameters [1]. (We only treat here the singlet pairs as the topological order parameters. As for the local topological description by the covalent bonds, see [1].) For example, there can be many kinds of quantum dimer states for frustrated Heisenberg models, such as column dimers, plaquette dimers, etc. As is clear, one cannot find any classical local order parameters to characterize them. However, our topological order parameters can distinguish them as different phases not by just a crossover.

3. Quantized Berry phases for the topological order parameters of frustrated Heisenberg spins

Frustration among spins prevent them from forming a magnetic order and their quantum ground states tend to belong to quantum liquids without any symmetry breaking. Since they do not have any local order parameters, even if they have apparent different physical behaviours, it is difficult to make a clear distinction as a phase not just as a crossover. We apply the general scheme in [1] to classify these frustrated spin systems. Defining quantized Berry phases as 0 or π, the spin liquids are characterized locally, reflecting their topological order. We can distinguish topological phases which are separated by local quantum phase transitions (local gap closings).

We consider the following spin 1/2 Heisenberg models with general exchange couplings, $H = \sum_{ij} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$. *We allow frustrations among spins.* We assume that the ground state is *unique and gapped*. To define a local topological order parameter at a specific link $\langle ij \rangle$, we modify the exchange by making a local $SU(2)$ twist θ only at the link as

$$J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \to J_{ij} \left(\tfrac{1}{2} (\mathrm{e}^{-\mathrm{i}\theta} S_{i+} S_{j-} + \mathrm{e}^{\mathrm{i}\theta} S_{i-} S_{j+}) + S_{iz} S_{jz} \right).$$

Writing $x = \mathrm{e}^{\mathrm{i}\theta}$, we define a parameter-dependent Hamiltonian $H(x)$ and its normalized ground state $|\psi(x)\rangle$ as $H(x)|\psi(x)\rangle = E(x)|\psi(x)\rangle$, $\langle\psi|\psi\rangle = 1$. Note that this Hamiltonian is invariant under the time-reversal (TR) Θ_{T}, $\Theta_{\mathrm{T}}^{-1} H(x) \Theta_{\mathrm{T}} = H(x)$.[1] Also note that by changing $\theta : 0 \to 2\pi$, we define a closed loop C in the parameter space of x. Now we define the Berry connection as $A_\psi = \langle\psi|\mathrm{d}\psi\rangle = \langle\psi|\frac{\mathrm{d}}{\mathrm{d}x}\psi\rangle \, \mathrm{d}x$. Then the Berry phase along the closed loop C is defined as $\mathrm{i}\gamma_C(A_\psi) = \int_C A_\psi$ [13]. In addition to the system being gapped, we further assume that *the excitation gap is always finite* (for $^\forall x$), to ensure the regularity of the ground state [3]. This may not always be true, since the gap can collapse by local perturbation as an appearance of localized states (edge states) [10]. Note that by changing a phase of the ground state as $|\psi(x)\rangle = |\psi'(x)\rangle \mathrm{e}^{\mathrm{i}\Omega(x)}$, the Berry connection gets modified as $A_\psi = A'_\psi + \mathrm{i}\,\mathrm{d}\Omega$ [13, 3]. This is a gauge transformation. Then the Berry phase, $\boldsymbol{\gamma}_C$, also

[1] The TR is defined as $\Theta_{\mathrm{T}} = K \otimes_j (\mathrm{i}\sigma_{jy})$, as the anti-unitary operation (K: complex conjugation). It operates for a state $|G\rangle = \sum_{J=\{\sigma_1,\ldots,\sigma_N\}} C_J |\sigma_1, \sigma_2, \ldots, \sigma_N\rangle$, ($\sigma_i = \pm 1$) as $\Theta_{\mathrm{T}}|G\rangle = \sum C_J^* (-)^{\sum_{i=1}^N (1+\sigma_i)/2} | -\sigma_1, \ldots, -\sigma_N\rangle$. Then spins get transformed as $^\forall j$, $\boldsymbol{S}_j \to \Theta_{\mathrm{T}}^{-1} \boldsymbol{S}_j \Theta_{\mathrm{T}} = -\boldsymbol{S}_j$ and $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$ is a TR invariant.

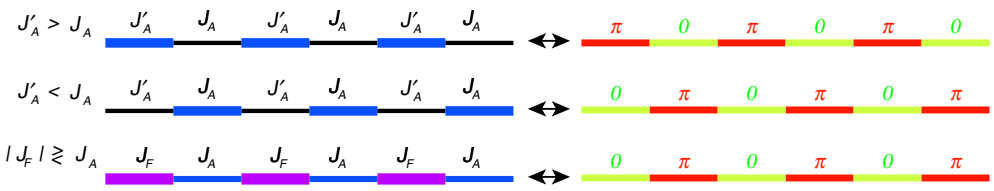

Figure 1. One-dimensional Heisenberg models with alternating exchange interactions with periodic boundary condition (left). Numerically evaluated quantized Berry phases (right). $J_{\mathrm{A}}, J_{\mathrm{A}'} > 0$ and $J_{\mathrm{F}} < 0$. The results are independent of the system size.

changes generically. This implies that the Berry phase is not well defined without specifying the phase of the ground state (gauge fixing). It can be fixed by taking a single-valued reference state $|\phi\rangle$ and a gauge-invariant projection into the ground state $P = |\psi\rangle\langle\psi| = |\psi'\rangle\langle\psi'|$ as $|\psi_\phi\rangle = P|\phi\rangle/\sqrt{N_\phi}$, $N_\phi = \|P|\phi\rangle\|^2 = |\eta_\phi|^2$, $\eta_\phi = \langle\psi|\phi\rangle$ [3, 1]. We here require the normalization, N_ϕ, to be finite. When we use another reference state $|\phi'\rangle$ to fix the gauge, we have $|\psi_\phi\rangle = |\psi_{\phi'}\rangle e^{\mathrm{i}\Omega}$, $\Omega = \arg(\eta_\phi - \eta_{\phi'})$. Due to this gauge transformation, the Berry phase gets modified as $\gamma_C(A_{\psi_\phi}) = \gamma_C(A_{\psi_{\phi'}}) + \Delta$, $\Delta = \int_C \mathrm{d}\Omega$. Since the reference states $|\phi\rangle$ and $|\phi'\rangle$ are single-valued on C, the phase difference Ω is just different by $\Delta = 2\pi M_C$ with some integer M_C. Generically this implies that the Berry phase has a gauge-invariant meaning just up to the integer as

$$\gamma_C \equiv -\mathrm{i}\int_C A, \qquad \mathrm{mod}\ 2\pi.$$

By the TR invariance, the Berry phase get modified as $\gamma_C(A_\psi) = \sum_J C_J^* \mathrm{d}C_j = -\sum_J C_J \mathrm{d}C_j^* = -\gamma_C(A_{\Theta\psi})$ since $\sum_J |C_J|^2 = 1$ [1]. Therefore to be compatible with the gauge ambiguity, the Berry phase of the unique TR-invariant ground state, $|\psi\rangle \propto \Theta|\psi\rangle$, satisfies $\gamma_C(A_\psi) \equiv -\gamma_C(A_\psi)(\mathrm{mod}\ 2\pi)$. Then it is required to *be quantized* as

$$\gamma_C(A_\psi) = 0, \pi \qquad (\mathrm{mod}\ 2\pi).$$

These quantized Berry phases have a topological stability since any small perturbations cannot modify them unless the gauge becomes singular. Here we note that the Berry phase of the singlet pair for the two-site problem is π [1]. Now let us take any dimer covering of all sites $\mathcal{D} = \{\langle ij\rangle\}$ and assume that the exchange interaction is nonzero only on these dimer links; then the Berry phases, π, pick up the dimer pattern $\mathcal{D}$. Now imagine an adiabatic process to include the interactions across the dimers. Due to the topological stability of the quantized Berry phase, they cannot be modified unless the dimer gap collapses. This dimer limit presents a non-trivial pattern of a quantized Berry phase and shows the usefulness of the quantized Berry phases as *local order parameters of singlet pairs*. To show the validity of the concept, we diagonalized the Heisenberg Hamiltonians numerically by the Lanzcos method and obtained the quantized Berry phases.

The first numerical examples are Heisenberg chains with alternating exchanges. When the exchanges are both antiferromagnetic as $J_{\mathrm{A}} > 0$ and $J'_{\mathrm{A}} > 0$, it is a spin–Peierls or dimerized chain. In this case, the Berry phases are π on the links with the strong exchange couplings and 0 on the one with the weak couplings (figure 1). This is expected from the adiabatic principle and the quantization[2]. When one of them is negative as $J_{\mathrm{A}} > 0$ and $J_{\mathrm{F}} < 0$, the calculated Berry phases are π for the antiferromagnetic links and 0 for the ferromagnetic ones. This is independent of the ratio $J_{\mathrm{A}}/J_{\mathrm{F}}$. Since the strong ferromagnetic limit is equivalent to

[2] As for the gapped phase of the $S = \frac{1}{2}$ antiferromagnetic XXZ model with Ising anisotropy, there occurs a local gap closing. We need to use the non-Abelain Berry phase [1, 14].

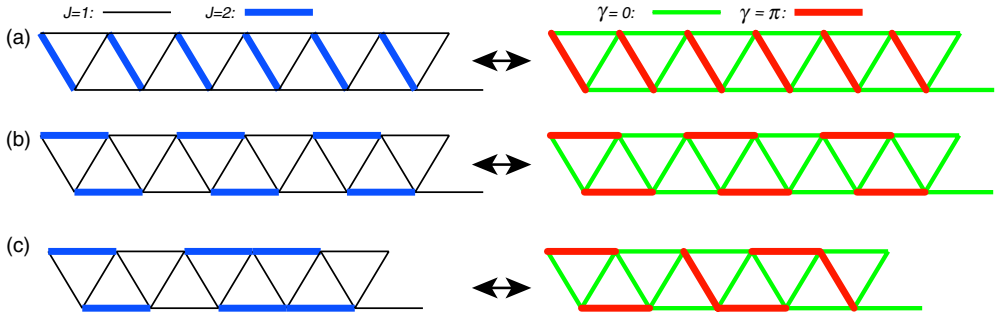

Figure 2. One-dimensional Heisenberg models with NN and NNN exchanges (left) with periodic boundary condition. Numerically evaluated quantized Berry phases (right). (a)–(c) Three different exchange configurations of $J = 1$ and $J' = 2$.

the spin 1 chain, this means that the quantized Berry phases of the spin 1 chain (Haldane phase) are given by the uniform π s. Further analysis on the $S = 1$ systems will be published elsewhere [14]. The next numerical examples are spin chains with nearest-neighbour (NN) and next-nearest-neighbour (NNN) exchanges as ladder of triangles (figure 2). These are typical systems with frustrations. (a) and (b) are two different but specific configurations in which one may adiabatically connect the system with different dimer coverings by the strong coupling bonds. In these cases, the quantized Berry phases are π for the strong coupling links and 0 for the remaining links. This is consistent with the adiabatic principle. We note here that it is difficult to make a qualitative difference between the two quantum liquids by conventional methods. However, we have made a clear distinction between them as two different topological phases. The present scheme is not only valid for these simple situations but is also useful for the generic situation. For example, as for a system in the figure 2(c), we cannot use the adiabatic principle simply. However, the quantized Berry phases show non-trivial behaviours and this makes a clear distinction that the phase (c) is topologically different from the ones in (a) and (b) as an independent phase not just as a crossover. A local quantum phase transition separates them by the gap closing. As is now clear, the present scheme is quite powerful in making a local characterization of topological quantum insulators.

Acknowledgments

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