Topological identification of location of spin-singlet pairs and edge states

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Abstract. Quantized Berry phases proposed as a new tool for exploring gapped quantum liquids at zero temperature which do not exhibit symmetry breaking are applied to identify location of spin-singlet pairs in the open boundary conditions. In the $S = 1/2$ Heisenberg chain with bond alternation, a relation between the Berry phases and the edge state is studied. The results agree with the picture of the nonlocal singlet of free spins at the open boundaries with the exponentially small effective coupling. Discrepancy between the Berry phases of the periodic and open boundary conditions indicates relocation of the local singlets.

Without spontaneous symmetry breaking, many important phases with strong quantum fluctuation form a novel class of matter as quantum liquids. Typical examples of the quantum liquids are many of integer and fractional quantum Hall states, where a topological invariant known as the Chern number has been discussed theoretically and observed experimentally. Spin analog of the quantum liquids is the spin liquid, which includes the Haldane integer spin chain[1] and the $S = 1/2$ Heisenberg chain with bond alternation mapped exactly onto the $S = 1$ Heisenberg chain when one of alternating bonds is ferromagnetic and strong[2].

To classify phases, not only correlation functions corresponding to the phases but also the string order parameter[3], entanglement entropy or concurrence[4], and Lieb-Schulz-Mattis twist operators[5] have been studied. In addition, the topological quantities such as the Chern numbers and the quantized Berry phases have been studied. Quantized Berry phases[6] have been used to classify quantum phases in gapped systems. It has the advantage that the value is invariant against small perturbations such as randomness unless the gap closes. In other words, it is topologically protected due to the finite gap.

Quantized Berry phases[6] can be used as a new tool for exploring gapped systems which do not exhibit symmetry breaking and are related to edge states through the bulk-edge correspondence[7]. In previous study on the spin-1/2 two-leg ladder with four-spin ring exchange, we have demonstrated that quantized Berry phases[8] and entanglement[9] are useful tool to classify the phases. Reflecting the bulk-edge correspondence as in the Kennedy triplet[10] in the VBS phase, $S = 1$ three-fold degenerated low-lying states in the bulk gap have exponentially small excitation energy under the open boundary condition(OBC). Moreover, existence of these edge states depends on the type of OBCs.[9] Motivated by them, to clarify the boundary-dependent edge states, we evaluate the quantized Berry phases of the edge states with the OBC.
For simplicity, we limit ourselves to the spin 1/2 chain.

Here we describe the definition of Berry phase in detail. The following explanation is limited to Abelian Berry phase for a unique ground state while one can use the non-Abelian Berry phase for degenerated ground states. The Berry phase $\gamma$ is defined for an one-parameter dependent Hamiltonian $H(\phi)$ by considering the parameter $\phi$ as time. The adiabatic time ($\phi$) evolution of the ground state $|gs(\phi)\rangle$ satisfies $H(\phi)|gs(\phi)\rangle = E(\phi)|gs(\phi)\rangle$. Assuming the periodicity $H(2\pi) = H(0)$, $|gs(0)\rangle$ and $|gs(2\pi)\rangle$ must be the same state except for the phase factor $\gamma$. It is theoretically defined as $\gamma = -i \int_0^{2\pi} A(\phi)\ d\phi (mod 2\pi)$ with the Berry connection $A(\phi) = \langle gs(\phi)|\partial_{\phi}|gs(\phi)\rangle$. To obtain $\gamma$ numerically, there is a useful expression. Discretizing the integral of $\phi$ into $M$ points[11] we obtain the Berry phase as $\gamma = \lim_{M \to \infty} \gamma_M$ with $\gamma_M = - \sum_{m=1}^M \text{arg} \langle gs(\phi_m)|gs(\phi_{m+1})\rangle (mod 2\pi)$ and $\phi_m = 2\pi m/M$. The periodicity $|gs(\phi_{M+1})\rangle = |gs(\phi_1)\rangle$ is imposed. It can be shown that $\gamma$ does not depend on the phase of $|gs(\phi_m)\rangle$. Then, we can replace the adiabatic state $|gs(\phi_m)\rangle$ by a ground state of $H(\phi_m)$.

The Berry phase depends on how the parameter $\phi$ is introduced to the Hamiltonian with the periodicity $H(2\pi) = H(0)$. Since we want to detect a spin singlet by Berry phases in the present paper, $\phi$ is introduced as a twisted spin exchange. [6,8,12,13] To detect a spin singlet, The twisted spin exchange on a specified link $i,j$ is introduced by replacing $S_i^+ S_j^- + S_i^- S_j^+ \rightarrow e^{i\delta} S_i^+ S_j^- + e^{-i\delta} S_i^- S_j^+$. On the other links, $\phi$ is not introduced. Spin twist $\phi$ introduces a magnetic flux penetrating the spin system. For a spin chain with the periodic boundary condition (PBC), i.e., a spin ring, the spin twist $\phi$ is identical to a flux penetrating the spin ring. In general, the spin twist introduces fluxes in local plaquettes. After calculation of $\gamma_{i,j}$ on every link $(i,j)$, we can obtain a texture pattern of the Berry phases which reflects the property of the ground state. Since each Berry phase is defined by a local spin twist, it has been used as a local order parameter. In this calculation, we can use local gauge transformation especially for the spin ring[13]. For the spin $S$ ring, the gauge transformation tells us the relation

$$\gamma_{i,i+1} = \gamma_{i,i-1} + 2\pi S (mod 2\pi).$$

(1)

The Berry phase is quantized due to an anti-unitary symmetry generally. The anti-unitary symmetry in the present case is the time-reversal symmetry. Then, the quantized Berry phase for identification of spin singlet is defined.

Let us consider the dimerized anti-ferromagnetic Heisenberg spin 1/2 chain,

$$H = \sum_{i=1}^{L_b} \left(1 + (-1)^i \delta\right) S_i \cdot S_{i+1},$$

(2)

where $L_b = L - 1$ for the OBC. For the PBC, $L_b = L$ and $S_{L+1} = S_1$. For both conditions, we assume the number of sites $L$ is even. The quantized Berry phase $\gamma$ of Eq.2 with the PBC has been studied[12]. We obtain $\gamma = \pi$ for the strong coupling links and $\gamma = 0$ for the weak coupling links except for $\delta = 0$. See Fig.1 (a) and (b). In the gapless case ($\delta = 0$), the Berry phase becomes undefined. As an advantage, the transition around $\delta = 0$ is clear because $\gamma_{i,i+1}$ are step functions of $\delta$. Another advantage is that the decoupled models ($\delta = \pm 1$) are easily obtained because $\gamma$ cannot change unless the gap closes. That is, Berry phases obtained for $\delta > 0$ (or $\delta < 0$) are the same as for $\delta = 1$ ($\delta = -1$). The Berry phase of the decoupled models is easily understood because the decoupled model is summation of two-site Heisenberg Hamiltonians which give $\pi$-Berry phase corresponding the singlet state.

Here we proceed the quantized Berry phase with the OBC. We obtain $\gamma_{L,1} = 0$ and Eq.(1). Note that no $\phi$ dependence is introduced by spin twist on the link $(L, 1)$ due to the OBC, which means the Berry phase $\gamma_{L,1} = 0$. Since $L$ is even, the result of spin 1/2 chain is $\gamma_{2k-1,2k} = \pi$ and $\gamma_{2k,2k+1} = 0$. It does not depend on the parameter of the Hamiltonian $\delta$. See Fig1 (c) and...
(d). Compared with the result of the PBC, that of the OBC is the same if \( \delta > 0 \), and different if \( \delta < 0 \). The discrepancy between the results of the PBC and OBC means that for the OBC in the limit \( L \rightarrow \infty \) the system for \( \delta < 0 \) has a topological change, that is, emergence of the Kennedy triplet[10]. Due to the four-fold degenerated edge states, the Berry phase becomes undefined in the limit \( L \rightarrow \infty \). We can define a new Berry phase \( \gamma^s \) only for a singlet state by projecting out the Kennedy triplet. \( \gamma^s \) can be defined even in the limit \( L \rightarrow \infty \). In the following, we shall describe the definition of \( \gamma^s \) and its meaning.

Let us define a new Berry phase \( \gamma^s \) for a singlet state chosen from four-fold degenerated edge states. When degenerated edge states exist in the thermodynamic limit, the gap closes and the Berry phase becomes undefined. To define a Berry phase, we begin with the fact that spin twist Hamiltonian \( H(\phi) \) for the OBC can be written by the gauge transformation \( U(\phi) \) as \( H(\phi) = U^{-1}(\phi) H U(\phi) \). Here, \( U \) is unitary and is written as \( U(\phi) = \prod_{k=1}^{L} e^{i(S^- S^+_k) \phi} \) if spin twist \( \phi \) is introduced on the link \((l, l+1)\). Then, the ground state is written as \( |gs(\phi)\rangle = U(\phi)|s_i\rangle \) for the OBC, the ground state is written as \( |gs(\phi)\rangle = U(\phi)|s_i\rangle \) and defines the Berry phase for the singlet state \( \gamma^s \). Since the ground state for finite system-size is also the singlet state, \( \gamma \) defined for finite system-size with using exponentially small gap is equals to \( \gamma^s \) defined with the bulk gap.

We have shown the validity of \( \gamma \) defined for finite system-size with using exponentially small gap between the singlet ground state and the Kennedy triplet for the OBC. The result is different from that of \( \gamma \) for the PBC and \( \delta < 0 \), which is well-defined due to the bulk gap. See Fig 1 (a) and (c). What it means is that the spin singlet of the boundaries is relocated. Conceptually we may consider that the local spin singlet located on the link \((L, 1)\) with the PBC is transformed into the nonlocal spin singlet located on the whole chain \( i = 1, 2, \ldots, L \) when we adopt the OBC. The former singlet gives the \( \pi \) Berry phase only on the link \((L, 1)\). The latter gives the \( \pi \) Berry phase on all links except absent link \((L, 1)\) for the OBC. We shall describe the detail as follows.

For the PBC and \( \delta < 0 \), it is easy to consider the Berry phase in the decoupled case \( \delta = -1 \), where the ground state is \( |gs\rangle = |s_{L,1}\rangle|s_{2,3}\rangle \ldots |s_{L-2,L-1}\rangle \), where \( |s_{i,j}\rangle = |s_{i,j}(0)\rangle \), and \( |s_{i,j}(\phi)\rangle = (|1_j\rangle|1_j\rangle - e^{i\phi}|1_j\rangle|1_j\rangle)/\sqrt{2} \). Even if we introduce the spin twist \( \phi \) on the link \((2k-1, 2k)\), the ground state does not depend on \( \phi \) and the Berry phase becomes zero. On the other hand, if we introduce it on the link \((2k, 2k+1)\), \( \phi \) dependence of \(|gs\rangle \) comes from \(|gs_{2k,2k+1}\rangle \) and \( \gamma_{2k,2k+1} = \pi \). For the OBC, the ground state is believed to be the same as that for the PBC. However, the effective coupling between \( L \)-th spin and 1-st spin is antiferromagnetic for even \( L \) and exponentially small as \( J \exp(-L/\xi)|S_L \cdot S_1| \), where \( \xi \) is the correlation length. [14] When we consider the spin twist \( \phi \) on the link between the boundaries, the effective coupling term is also spin twisted by \(-\phi\), which can be proved easily because \(|gs(\phi)\rangle \) with the OBC is written by the gauge transformation \( U(\phi) \) and \(|gs\rangle \) as described above. \( \phi \) dependence of \(|gs\rangle \) comes from \(|s_{L,1}(\phi)\rangle \) for the link \((2k-1, 2k)\) and \(|s_{L,1}(\phi)\rangle|s_{2k,2k+1}(\phi)\rangle \) for the link \((2k, 2k+1), k \neq L/2 \). After the summation of the Berry phases as shown in Fig 2, we obtain \( \gamma_{2k-1,2k} = \pi \) and \( \gamma_{2k,2k+1} = 0 \). This result is obtained from the nonlocal singlet picture and agrees with that of the gauge transformation.

In conclusion, we have studied a relation between the quantized Berry phase with the OBC and the edge states. In a dimerized Heisenberg chain, the relation is exactly shown. We emphasize that the quantized Berry phase has been used only with the PBC because the bulk properties is focused while the OBC plays a role of an local impurity. However, our previous study[9] with using decoupled models obtained from the quantized Berry phases with the PBC.

\(^1\) The result is also numerically checked by Mathematica for \( L = 4 \).
reveals the Kennedy-triplet type excitation of a spin 1/2 two-leg ladder with four-spin ring exchange. In this ladder model, existence of the Kennedy triplet depends on the shape of boundary. There is a Kennedy triplet if there are free spins on both edge due to the shape of boundary. To study the boundary dependent edge states, we can use quantized Berry phases with the OBC. Finally, we comment on the our numerical calculation of the spin 1/2 two-leg ladder with four-spin ring exchange. In the dominant vector chirality phase (a model parameter θ in Ref.[9] is 0.7π and the number of spins is small up to 2 × 5), the relocation of the local singlets is observed when the system has the Kennedy-triplet type excitation. That is, the boundary dependent edge states comes from recombination of boundary spins on both edge. The detail of the numerical result will be reported elsewhere.

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