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Topological identification of a spin- $\frac{1}{2}$ two-leg ladder with four-spin ring exchange

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A spin- $\frac{1}{2}$ two-leg ladder with four-spin ring exchange is studied by quantized Berry phases, used as local-order parameters. Reflecting local objects, nontrivial (π) Berry phase is founded on a rung for the rung-singlet phase and on a plaquette for the vector-chiral phase. Since the quantized Berry phase is topologically invariant for gapped systems with the time-reversal symmetry, topologically identical models can be obtained by the adiabatic modification. The rung-singlet phase is adiabatically connected to a decoupled rung-singlet model and the vector-chiral phase is connected to a decoupled vector-chiral model. Decoupled models reveal that the local objects are a local singlet and a plaquette singlet, respectively.

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I. INTRODUCTION

The recent progress in the multiple-spin exchange interactions is attracting much attention. It has been found to be important in several materials such as two-leg ladder compound $\text{La}_x\text{Ca}_{14-x}\text{Cu}_{24}\text{O}_{41}$,¹⁻⁴ two-dimensional antiferromagnet La_2CuO_4 ,^{5,6} magnetism of two-dimensional quantum solids, e.g., solid ^3He films,⁷ and Wigner crystals.⁸ Four-spin ring exchange plays an essential role in several models to give rise to exotic phases due to its frustration, e.g., the vector-chirality phases,⁹ nematic orderings,¹⁰ and octapolar order.¹¹

Especially, the two-leg ladder model with the multiple-spin exchange interactions has been studied extensively.¹²⁻¹⁹ To clarify its rich phases, not only correlation functions corresponding to phases but also entanglement concurrence,²⁰ entanglement entropy,^{21,22} and string order^{14,23} are useful to characterize the phases. As such a novel order parameter, which is beyond the Ginzburg-Landau symmetry-breaking description, there is an order parameter based on the topological invariants corresponding to the topological order.²⁴

Recently, Berry phases²⁵ have been used in order to detect the topological order and the quantum order.²⁶⁻²⁸ The Berry phases are quantum quantities based on the Berry connection which is defined by the overlap between the two states with infinitesimal difference and do not have any corresponding classical analogs. Then, one can define it even though there is no classical-order parameter. The advantage of the Berry phase is that it quantizes to 0 or π even in the finite-sized systems in any dimension when the system has the time-reversal invariance. It has been successfully applied to several quantum systems such as generalized valence bond solid states,²⁹ dimerized Heisenberg models,^{28,30} and t - J model.³¹ For these systems, the nontrivial (π) Berry phase on a link reveals a singlet on the link, which is a pure quantum object due to two-spin exchange.

In this paper, we extend the quantized Berry phase to be sensitive to the effect of four-spin ring exchange and apply it to a $S=1/2$ spin ladder with a ring-exchange interaction as an alternative to correlation functions, entanglement, and string order. According to the phase diagram,¹⁴ there are two

first-order transitions from the ferromagnetic phase. One is transition to the *run-g-singlet* phase. The other is that to the *dominant collinear spin* phase, which connects to the *dominant vector-chirality* phase through crossover at a self-dual point.¹⁷ These two phases are the singlet phases with short-range order and have dominant correlation of collinear spin and vector chirality, respectively. The rung-singlet phase includes the spin ladder with only two-spin exchange interactions and the dominant vector-chirality phase includes that with only four-spin exchange interactions. These three phases have a unique ground state with finite gap, while the other phases including the ferromagnetic phase do not have finite gap under the translational symmetry. Moreover, through the spin-chirality duality transformation, the gap in the dominant vector-chirality phase of the original Hamiltonian is smoothly connected to that in the rung-singlet phase of the transformed Hamiltonian.¹² Although it is believed that the ground state of the rung-singlet phase is well approximated by the product of local rung singlets, there is no simple picture for the dominant vector-chirality phase. To clarify it, we discuss the adiabatic connection of the Hamiltonian to a simple model, i.e., a topologically equivalent model.

II. DEFINITION OF THE BERRY PHASE

Let us start with the definition of Berry phase²⁵ in a quantum spin system. For the parameter-dependent Hamiltonian $H(\phi)$, the Berry phase γ of the ground state is defined as $i\gamma = \int_0^{2\pi} A(\phi) d\phi \pmod{2\pi}$, where $A(\phi)$ is the Abelian Berry connection obtained by the single-valued normalized ground state $|\text{gs}(\phi)\rangle$ of $H(\phi)$ as $A(\phi) = \langle \text{gs}(\phi) | \partial_\phi | \text{gs}(\phi) \rangle$. This Berry phase is quantized to 0 or π if $|\text{gs}(\phi)\rangle$ is a gapped ground state and the Hamiltonian $H(\phi)$ is invariant under the anti-unitary operation Θ , i.e., $[H(\phi), \Theta] = 0$. It has a remarkable property that the Berry phase has topological robustness against the small perturbations unless the energy gap between the ground state and the first excited state closes. We note that the Berry phase is undefined if the energy gap vanishes while varying the parameter ϕ . Then, we limit ourselves to the rung-singlet phase and the dominant vector-

chirality (collinear spin) phase, which have finite gap. To calculate the Berry phase numerically,³² we use $\gamma = \lim_{M \rightarrow \infty} \gamma_M$, where γ_M is defined by discretizing the parameter space of ϕ into M points as $\gamma_M = -\sum_{m=1}^M \arg C(\phi_m)$, $\phi_m = 2\pi m/M$, where $C(\phi_m)$ is defined by $C(\phi_m) = \langle \text{gs}(\phi_m) | \text{gs}(\phi_{m+1}) \rangle$ with $\phi_{M+1} = \phi_1$. In general, M can be a very small number.³³

To study a local structure of the quantum system, such as a local singlet, we use a local spin twist on a specified link i, j as the parameter ϕ .²⁸ Under this local spin twist on a link i, j the term $S_i^+ S_j^- + S_i^- S_j^+$ in the Hamiltonian is replaced with $e^{i\phi} S_i^+ S_j^- + e^{-i\phi} S_i^- S_j^+$, where $S_i^\pm = S_i^x \pm iS_i^y$. Although previous studies^{26–29,31} deal with the spin twist only for the two-body terms, we extend the twist to the four-spin exchange interactions. Since the Hamiltonian is written by $H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{ijkl} K_{ijkl} (\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l)$, the local spin twist for a selected link i, j is introduced for all the term $\mathbf{S}_i \cdot \mathbf{S}_j$ in the Hamiltonian. As described below, the extended Berry phase can detect not only the local singlet but also the plaquette singlet.

The quantized Berry phase is considered as a link variable. Then each link is labeled as one of three labels: “0 bond,” “ π bond,” or “undefined.” Especially, we shall calculate the leg Berry phase γ_l , the rung Berry phase γ_r , and the diagonal Berry phase γ_d . The quantization of the Berry phase is guaranteed by the time-reversal symmetry Θ of the quantum spin system.²⁶

III. MODELS AND THE RESULTS

A. $S=1/2$ spin ladder model with four-spin exchange

The $S=1/2$ spin ladder model with four-spin ring exchange is described by the following Hamiltonian:

$$H_{\text{cyc}} = J \left[\sum_{i=1}^{N/2} \sum_{\alpha=1,2} S_{i,\alpha} \cdot S_{i+1,\alpha} + \sum_{i=1}^{N/2} S_{i,1} \cdot S_{i,2} \right] + K \sum_{i=1}^{N/2} (P_i + P_i^{-1}) \quad (1)$$

with the ring exchange

$$P_i + P_i^{-1} = S_{i,1} \cdot S_{i,2} + S_{i+1,1} \cdot S_{i+1,2} + S_{i,1} \cdot S_{i+1,1} + S_{i,2} \cdot S_{i+1,2} + S_{i,1} \cdot S_{i+1,2} + S_{i,2} \cdot S_{i+1,1} + 4(S_{i,1} \cdot S_{i,2}) \times (S_{i+1,1} \cdot S_{i+1,2}) + 4(S_{i,1} \cdot S_{i+1,1})(S_{i,2} \cdot S_{i+1,2}) - 4(S_{i,1} \cdot S_{i+1,2})(S_{i,2} \cdot S_{i+1,1}), \quad (2)$$

where $S_{i,\alpha}$ are the spin- $\frac{1}{2}$ operators on the site (i, α) and N is the total number of sites. The periodic boundary condition is imposed as $S_{N/2+i,\alpha} = S_{i,\alpha}$ for all of the models in this paper. We set the parameters as $J = \cos \theta$ and $K = \sin \theta$. Figure 1 shows Berry phases on local links of $N=16$ ladder obtained numerically by the exact diagonalization method. Three kinds of Berry phases, γ_l on the leg link $(i, 1) - (i, 2)$, γ_r on the rung link $(i, 1) - (i, 2)$, and γ_d on the diagonal link $(i, 1) - (i+1, 2)$, are calculated and turn out to be translational symmetric. Nontrivial (π) Berry phases obtained for finite-size systems identified two different phases: one is the rung-singlet phase and the other is the dominant vector-chirality

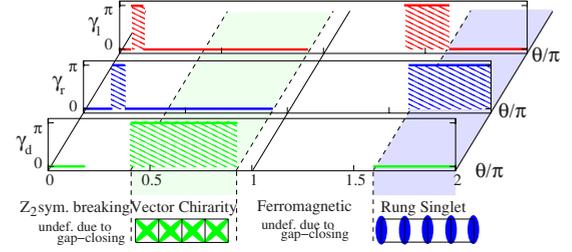


FIG. 1. (Color online) Leg, rung, and diagonal Berry phases γ_l , γ_r , and γ_d of the $S=1/2$ periodic $N=16$ ladder model with four-spin ring exchange as a function of θ ($J = \cos \theta$, $K = \sin \theta$) with the schematic pictures of corresponding phases. Berry phases are zero, π (shaded region), or undefined (region without data).

phase including the dominant collinear spin phase. These three phases have a spin gap in thermodynamic limit.^{12,14} The crossover between the dominant vector-chirality phase and the dominant collinear spin phase is not found. It is neither found by the entanglement²⁰ nor by the Lieb-Schulz-Mattis twist operator.¹⁴ In the dominant collinear spin phase, collinear spin-spin correlations are dominant, which means that spins on the same leg exhibit ferromagnetic correlations.¹⁴ It will be identified by another kind of Berry phase or another type of entanglement.

Berry phases in the other phases are also obtained in Fig. 1 but become undefined due to gap closing in the thermodynamic limit, such as in the ferromagnetic phase and around the self-dual point $\theta = \arctan(1/2) \sim 0.14\pi$. The staggered dimer and scalar-chirality phases around the self-dual point are Z_2 symmetry-breaking phase with twofold degeneracy in the thermodynamic limit.²⁰ In a $N=16$ system, there is a finite-size gap in the $S_z=0$ sector of H_{cyc} for most values of θ and we can obtain the Berry phase. However, results around the self-dual point in Fig. 1 shows the numerical instability, i.e., Berry phase becomes undefined. Note that we can define non-Abelian Berry phase to avoid the numerical instability with using the gap above the twofold degenerated ground states in the thermodynamic limit around the self-dual point. The transition point θ_c between the rung-singlet phase and Z_2 symmetry-breaking phase is about 0.1π ,^{12,14} while Fig. 1 shows $\theta_c < 2\pi$. To clarify this difference, we shall study the Berry phase at $\theta=0$.

Before studying the model at $\theta=0$, let us now interpret the phases by the adiabatic modification in order to obtain a decoupled model with the same Berry phases. We shall calculate the ϕ dependence of the energy gap to see whether the gap closes or not during the adiabatic modification since the Berry phase remains the same if the gap does not close during the adiabatic modification.

1. Rung-singlet phase

We consider the adiabatic modification from $H_{\text{cyc}}|_{\theta=1.8\pi}$ in the rung-singlet phase to the completely decoupled model which has the Heisenberg-type coupling only on the rung bonds,

$$H_{\text{RS}} = \sum_{i=1}^{N/2} S_{i,1} \cdot S_{i,2}. \quad (3)$$

These two models are connected by adiabatic parameter α as $H(\alpha) = (1-\alpha)H_{\text{cyc}} + \alpha H_{\text{RS}}$.

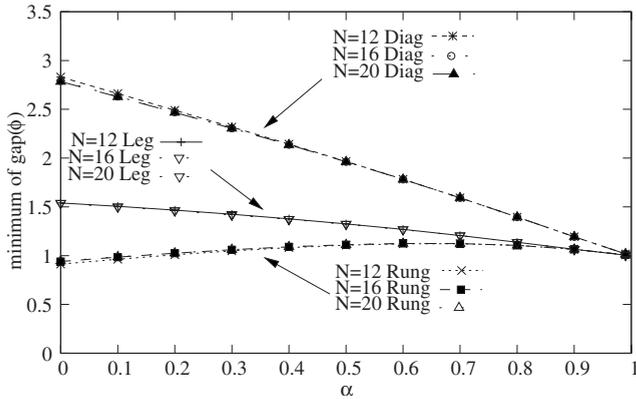


FIG. 2. Minimum gaps for twist ϕ on a leg, rung, and diagonal links of the $S=1/2$ periodic ladder model with four-spin ring exchange as a function of adiabatic parameter α for $H(\alpha)=(1-\alpha)H_{\text{cyc}}|_{\theta=1.8\pi}+\alpha H_{\text{RS}}$. Several data are plotted for $N=8, 12, 16$, and 20.

As shown in Fig. 2, the minimum gap through the twist ϕ does not close. It means not only that the gap of $H_{\text{cyc}}|_{\theta=1.8\pi}$ adiabatically connects to the singlet-triplet gap but also that these two models with the same Berry phases are topologically identical. This adiabatic connection is consistent with the fact that the ground state is well approximated by the product of local rung singlets and is identified by entanglement concurrence of two spins on a rung.²⁰

2. Vector-chirality phase

The dominant vector-chirality phase is characterized by correlations of the vector-chirality order parameters $\mathbf{S}_{i,\alpha} \times \mathbf{S}_{i+1,\alpha}$ and $\mathbf{S}_{i,1} \times \mathbf{S}_{i,2}$,¹⁴ while entanglement concurrence of two spins on a diagonal bond fails to capture this phase around $J/K=1$ ($\theta=\pi/2$) point.²⁰ Motivated by the vector-chirality order parameter, we consider the adiabatic modification from $H_{\text{cyc}}|_{\theta=0.8\pi}$ in the dominant vector-chirality phase to a decoupled model as follows:

$$H_{\text{DVC}} = \sum_{i=1}^{N/4} (\mathbf{S}_{2i,1} \times \mathbf{S}_{2i,2}) \cdot (\mathbf{S}_{2i+1,1} \times \mathbf{S}_{2i+1,2}). \quad (4)$$

We call its ground state as the ‘‘dimerized vector-chiral state’’ since it minimizes the local operator $(\mathbf{S}_{2i,1} \times \mathbf{S}_{2i,2}) \cdot (\mathbf{S}_{2i+1,1} \times \mathbf{S}_{2i+1,2}) = (\mathbf{S}_{2i,1} \cdot \mathbf{S}_{2i+1,1})(\mathbf{S}_{2i,2} \cdot \mathbf{S}_{2i+1,2}) - (\mathbf{S}_{2i,1} \cdot \mathbf{S}_{2i+1,2})(\mathbf{S}_{2i,1} \cdot \mathbf{S}_{2i+1,2})$. This operator is used as an order parameter in previous studies and a classical spin configuration corresponds to a 90° spin structure.¹⁵ The ground state is the product of plaquette singlet states.³⁴ Moreover, through the duality transformation,¹² H_{DVC} is mapped to the summation of $\tilde{\mathbf{S}}_{2i,1} \cdot \tilde{\mathbf{S}}_{2i,2} + \tilde{\mathbf{S}}_{2i+1,1} \cdot \tilde{\mathbf{S}}_{2i+1,2} - \tilde{\mathbf{S}}_{2i,1} \cdot \tilde{\mathbf{S}}_{2i+1,2} - \tilde{\mathbf{S}}_{2i,2} \cdot \tilde{\mathbf{S}}_{2i+1,1}$. This transformed model is identified as the rung-singlet phase by the Berry phase.

Figure 3 shows the minimum energy gap through the twist ϕ of $H(\alpha)=(1-\alpha)H_{\text{cyc}}|_{\theta=0.8\pi}+\alpha H_{\text{DVC}}$ in the adiabatic deformation. Three kinds of gaps agree with untwisted gap $\phi=0$ and have system-size dependence. Since the gap does not close during the modification in $N=20$ system at least, we identify that the nontrivial diagonal Berry phase γ_d exhibits

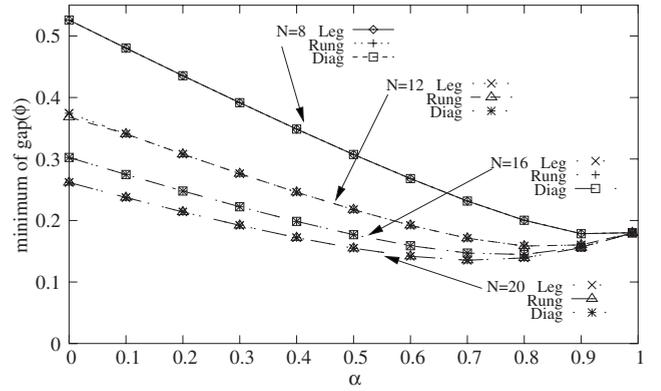


FIG. 3. Minimum gaps for twist ϕ on a leg, rung, and diagonal links of the $S=1/2$ periodic ladder model with four-spin ring exchange as a function of adiabatic parameter α for $H(\alpha)=(1-\alpha)H_{\text{cyc}}|_{\theta=0.8\pi}+\alpha H_{\text{DVC}}$. Several data are plotted for $N=8, 12, 16$, and 20.

the decoupled vector-chiral state. Although the gap in the thermodynamic limit at $\alpha=0$ is subtle in Fig. 3, the density-matrix renormalization-group (DMRG) method has shown a small gap which smoothly connects to a finite gap in the rung-singlet phase of the transformed Hamiltonian.¹² We should note that the Hamiltonian H_{DVC} breaks the translational symmetry although the original Hamiltonian does not. In other words, although the gap does not close by the twist of diagonal bond in *oddth* plaquette, it does for the diagonal bond in *eventh* plaquette. In this sense, the ground state of $H_{\text{cyc}}|_{\theta=0.8\pi}$ is *locally* identical to the vector chiral state.

B. $S=1/2$ spin ladder model without four-spin exchange

Although the rung-singlet phase is thought to include $\theta=0$,¹⁴ Fig. 1 shows that the rung-singlet phase does not include $H_{\text{cyc}}|_{\theta=0}$ ($K/J=0$). To clarify it, we study a $S=1/2$ spin ladder model *without* four-spin exchange,

$$H_{\text{lad}} = J_l \sum_{i=1}^{N/2} \sum_{\alpha=1,2} \mathbf{S}_{i,\alpha} \cdot \mathbf{S}_{i+1,\alpha} + J_r \sum_{i=1}^{N/2} \mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2}, \quad (5)$$

where J_l and J_r are parametrized as $J_l = \sin \theta$ and $J_r = \cos \theta$, respectively. We consider the antiferromagnetic case of $0 \leq \theta < \pi/2$ in this paper to concentrate on $H_{\text{lad}}|_{\theta=\pi/4} = H_{\text{cyc}}|_{\theta=0}$. Note that $H_{\text{lad}}|_{\theta=0} = H_{\text{RS}}$. On the other hand, $H_{\text{lad}}|_{\theta=\pi/2}$ is the model of decoupled two chains, which has gapless excitation in the thermodynamic limit.

Figure 4 shows the θ dependence of the Berry phases on local links of H_{lad} at $N=16$ except for the gapless point $\theta=\pi/2$. $\gamma_d=0$ is trivial because there is no diagonal interaction. Although the gap of untwisted Hamiltonian $\phi=0$ is smoothly connecting,³⁵ the gap of twisted Hamiltonian $\phi=\pi$ for γ_r closes at $\theta \sim 0.233\pi < \pi/4$ and γ_r changes. We denote the $\gamma_r=0$ phase for $\theta > \pi/4$ as rung* phase, which implies the limitation of the localized rung-singlet picture and encourages us to use another picture such as the resonating valence bond theory.³⁶ It is consistent with very strong quantum fluctuations introduced on the product singlet ground state³⁷ and with ‘‘nonperturbative’’ (in J_r/J_l) behavior

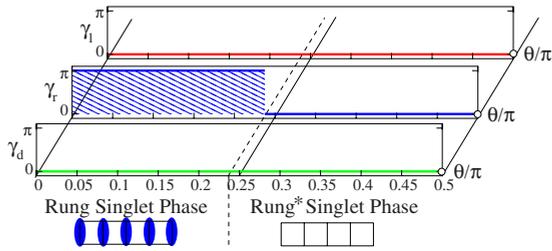


FIG. 4. (Color online) Leg, rung, and diagonal Berry phases γ_l , γ_r , and γ_d of the $S=1/2$ periodic $N=16$ ladder model without a four-spin interaction as a function of θ ($J_r = \cos \theta$, $J_l = \sin \theta$) with the schematic pictures of corresponding phases. Berry phases are zero, π (shaded region), or undefined (region without data).

obtained numerically.³⁵ To clarify the phase which has no π bond, we need further discussion while considering another kind of spin twist, because the twist should correspond to a local structure of the model. It should be emphasized that the rung* phase results from the quantum phase transition of the twisted Hamiltonian ($\phi = \pi$) for γ_r and is not contradicting previous studies for untwisted Hamiltonian.

IV. CONCLUSION

In conclusion, we have shown that the quantized Berry phases are useful to classify the phases of spin chains with four-spin ring exchange. In the dominant vector-chirality

phase, which comes from the ring-exchange interaction, the Berry phase on each diagonal link is used as a plaquette variable and becomes a nontrivial value (π), while the Berry phase has been used as a link variable in previous study. The Berry phase is also useful to clarify the phase boundary from the finite-size systems since it is quantized even in the finite-size systems. The property of the phase is revealed through the adiabatic deformation into a decoupled model: the rung-singlet phase (and the vector-chirality phase) corresponds to a product of rung singlets (plaquette singlets). These two phases are connecting through the duality transformation. The other phases of this model will be detected by the Berry phase with another kind of twist or the non-Abelian Berry phase for twofold-degenerated ground states.

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