Berry's phase under the Dzyaloshinskii-Moriya interaction

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In this paper, we study the Dzyaloshinskii-Moriya (DM) anisotropic XX spin-chain model in the presence of an external homogeneous magnetic field. We found that the Berry phase of the system varies interestingly with small and large amounts of DM interaction and the magnetic field. In addition, we also considered the concurrence (i.e., the amount of entanglement) of the system, and the relationship between the concurrence and the Berry phase. Finally, we calculate the Berry phase of thermal states and verify that the results are consistent with that of the pure states.

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I. INTRODUCTION

To account for the weak magnetism of antiferromagnetic crystals, such as MnCO₃, CoCO₃, and spin arrangement in antiferromagnets of low symmetry, Dzyaloshinskii and Moriya [1,2] independently proposed an extended superexchange mechanism interaction [3] by considering a term proportional to spin-orbit coupling. In megnetoelectric multiferroics, such as perovskites, one observes the presence of spin canting, typically about 0.5°, leading to weak ferromagnetism with a modest remanent magnetization [4]. Such canting has been attributed to the Dzyaloshinskii-Moriya (DM) interaction.

Recently, magnetic molecules such as Mn_{12} or V_{15} have attracted much interest [5]. These nanomagnets have been used to study explicit real-time quantum dynamics, e.g., tunneling of the magnetization and quantum decoherence. Experiments can directly probe the magnetization dynamics of the individual molecules arising from the weak intermolecular interactions. A likely candidate for such interaction is precisely the DM interaction. Indeed, several low-spin ground-state systems such as the polyoxovanadate $K_6[V_{15}As_6O_{42}]\cdot 9H_2O$ could also have DM interactions.

Quantum entanglement has been regarded as a useful resource for quantum information processing. In Ref. [6], the concurrence of the thermal state of a two-qubit Heisenberg chain under DM interaction was studied and it was shown that DM interaction could enhance the concurrence of the thermal state. Moreover, teleportation in the presence of DM interaction has higher resulting fidelity. In Ref. [7], two-qubit entanglement for the most general XYZ Heisenberg magnet under DM interaction was studied.

In this paper, we consider an XX chain with DM interaction in an applied magnetic field of the form

$$H = \sum_{\langle i,j \rangle} \left[J(S_i^x S_j^x + S_i^y S_j^y) + \vec{D}_{ij} \cdot \vec{S}_i \times \vec{S}_j \right] + \vec{B} \cdot \vec{S}_1, \tag{1}$$

where the sum is taken over the nearest-neighbor sites, the spin operator $\vec{S} = (S^x, S^y, S^z)$, the vector \vec{D}_{ij} is the DM vector, and \vec{B} is the orientation of the magnetic field, which is applied only to the first site as in [8,9]. Note that their Hamiltonian differs from ours in which they consider a special case

of XY interaction. For simplicity, we shall choose DM vector so that it is aligned to the z-component, parametrize the vector \vec{B} by B_0 (sin $\theta \cos \phi$, sin $\theta \sin \phi$, cos θ) and set the spin-spin coupling term J to 1.

This paper is organized as follows: in Sec. II, we calculate the geometric (berry) phase for the eigenvectors of the two-particle Hamiltonian. In Sec. III, we consider the thermal state for the system and apply the formalism in Ref. [10] to obtain the geometric phase of the thermal state with changes in the azimuthal angle and temperature. In Sec. IV, we discuss and summarize the results.

II. GEOMETRIC PHASE

We consider two sites under the Hamiltonian in Eq. (1). There are four eigenstates, $(|E_1\rangle,|E_2\rangle,|E_3\rangle,|E_4\rangle)$ corresponding to the four eigenvalues: $E_1 = -\sqrt{P+Q}$, $E_2 = -\sqrt{P-Q}$, $E_3 = \sqrt{P-Q}$, and $E_4 = \sqrt{P+Q}$. (Note that $P = 2 + B^2 + 2D^2$, $Q = 2\sqrt{(1+D^2)(1+D^2+B^2\sin^2\theta)}$ and B and D corresponds to the magnitude of the applied magnetic field and the DM interaction, respectively.) Note that $P \ge Q$ and that $E_1 \le E_2 \le E_3 \le E_4$. Thus, E_1 corresponds to the ground state, $|E_2\rangle$ corresponds to the first excited state, and so forth.

For each eigenvector $|E_i\rangle$, we consider the situation in which the external magnetic field undergoes adiabatic evolution in the azimuthal angle ϕ for a closed loop at a fixed polar angle θ . The dynamical phase of the system is zero, and the total phase of the system is equal to the geometric (Berry) phase [11]. Thus the geometric (Berry) phase is given by

$$\gamma_j = i \int_0^{2\pi} \langle E_j | \frac{d}{d\phi} | E_j \rangle d\phi. \tag{2}$$

We repeat this calculation for different values of the polar angle, θ .

Due to the symmetry inherent in the eigenstates, it turns out that the eigenstates $|E_1\rangle$ and $|E_4\rangle$ (and $|E_2\rangle$ and $|E_3\rangle$) yield the same Berry phase as one adiabatically evolves the parameter ϕ around a closed path. The graph of the Berry phase against the polar angle θ for the eigenstate $|E_1\rangle$ (or $|E_4\rangle$) for different values of the B field and with the DM interaction set to unity is shown in Fig. 1.

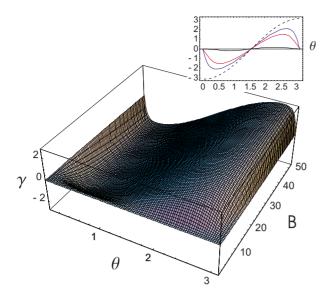


FIG. 1. (Color online) Geometric phase for the ground state $|E_1\rangle$ (or the highest excited state, $|E_4\rangle$) with different values of the external magnetic field and with constant DM interaction, D=1. The inset shows the cross-sectional plots for different values of B. The dashed plot in the inset is the limit of the variation of Berry phase with θ for $B\to\infty$.

As shown in Fig. 1, an increase in the external magnetic field can substantially increase the amount of the Berry phase. Moreover, the Berry phase assumes the value of $-\pi\cos\theta$ in the large B limit, i.e., $B\to\infty$ independent of the value of D. In Fig. 2, we plotted the Berry phase for the ground state $|E_1\rangle$ as a function of θ and D for a fixed B=1. In this case, we see that the Berry phase goes rapidly to zero as D increases. Thus in order for Berry phase to be observed, it is essential that the DM interaction is kept small. At B=1, a large DM interaction will wash away any variation of the Berry phase with the polar angle.

We plot the graph of the Berry phase against the polar angle θ for the eigenstate $|E_2\rangle$ (or $|E_3\rangle$) for different values of the *B* field and with the DM interaction set to unity in Fig. 3. In the large *B* limit, the Berry phase is given by $-\pi\cos\theta$. Unlike the case of the ground state (or highest excited state), the Berry phase could be nontrivial for the low magnetic

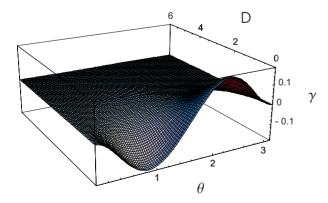


FIG. 2. (Color online) Geometric phase for the eigenstate $|E_1\rangle$ (or $|E_4\rangle$) with different DM interaction and with the magnitude of the external magnetic field set to B=1.

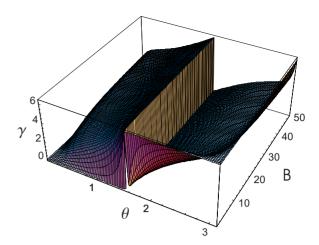


FIG. 3. (Color online) Geometric phase for the eigenstate $|E_2\rangle$ ($|E_3\rangle$) with different magnetic field strength *B* under constant DM interaction. D=1.

field if one confines the evolution to a polar angle near $\theta = \frac{\pi}{2}$. Figure 4 shows the variation of the Berry phase with θ and D for fixed B=1. We see that for a large DM interaction, the Berry phase is zero except for a tiny range of values near the polar angle $\theta = \frac{\pi}{2}$. Note that the Berry phase in Fig. 3 and Fig. 4 has been plotted from 0 to 2π instead of $-\pi$ to π for the other cases. If one plots the Berry phase for the range $-\pi$ to π , the same surface generates a curve of discontinuities which is due to the fact that the Berry phase for the eigenstates $|E_2\rangle$ (or $|E_3\rangle$) is not continuous in the $-\pi$ to π domain. In addition, we can also better observe the behavior of the Berry phase in the limit of large B and D, respectively.

Since we consider a bipartite system, we could compute the concurrence for the four eigenstates. It turns out that there are exactly two different sets of concurrence; the pairs $\{|E_1\rangle, |E_4\rangle\}$ and $\{|E_2\rangle, |E_3\rangle\}$ have the same concurrence for all B, D, θ , and ϕ . Fortunately, the concurrence does not change with ϕ . Thus, one could vary θ and plot the geometric phase (as ϕ varies from 0 to 2π with concurrence.) Figure 5(a) shows the parametric plots of the geometric phase of $|E_1\rangle$ (or $|E_4\rangle$) as a function of concurrence for various values of B

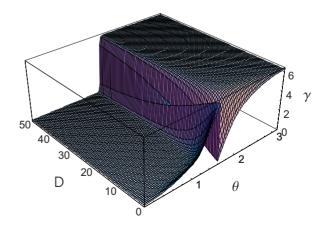
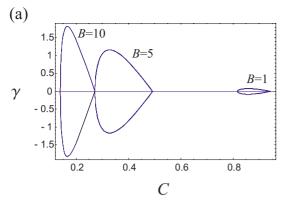


FIG. 4. (Color online) Geometric phase for the eigenstate $|E_2\rangle$ ($|E_3\rangle$) with different DM interaction and with the magnitude of the external magnetic field set to B=1.



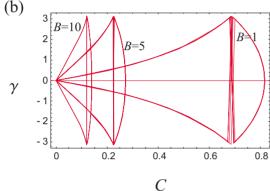


FIG. 5. (Color online) Geometric phase for the eigenstate as a function of concurrence. In (a), we show the result for $|E_1\rangle$ and $|E_4\rangle$ and in (b), we show the result for $|E_2\rangle$ and $|E_3\rangle$ for D=1 and B=1,5,10.

=1,5, and 10 at a fixed value of D=1 as θ is varied. As noted earlier, the geometric phase increases for larger values of B field even though the state becomes less entangled since the magnetic field is applied only to the first site.

Figure 5(b) shows the parametric plots of the geometric phase of $|E_2\rangle$ (or $|E_3\rangle$) as a function of concurrence for different magnetic fields. In this case, the range of the Berry phase remains the same as the magnetic field is increased.

Moreover, whereas the concurrence for the pair $\{|E_1\rangle, |E_4\rangle\}$ vanishes at some point, which is not the case for the other set of eigenstates, $\{|E_2\rangle, |E_3\rangle\}$. For the latter, there is always a range of concurrence (C_{\min}, C_{\max}) such that C_{\min} goes to zero as B increases.

III. THERMAL STATE

The thermal state of the two-particle system is given by

$$\varrho = \frac{\exp(-\beta H)}{\operatorname{Tr}[\exp(-\beta H)]},\tag{3}$$

where $\beta = \frac{1}{kT}$ is the inverse temperature. For a mixed state, the geometric phase is no longer a well-defined concept. One typical way of analyzing the geometric phase of a mixed state is to purify the state to a larger space and consider the geometric phase of the purified state. In this paper, we follow the argument in Ref. [10] in which we explicitly derive an expression for the geometric phase of a mixed state under kinematic consideration.

Consider a quantum system with mixed state $\rho(t)$ given by

$$\rho(t) = \sum_{k=1}^{N} \omega_k(t) |\phi_k(t)\rangle \langle \phi_k(t)|, \tag{4}$$

where $\omega_k(t)$ and $|\phi_k(t)\rangle$ are the eigenvalues and eigenvectors, respectively, of the system's density operator $\rho(t)$. The eigenvalues are real and assumed to be nondegenerate, i.e., $\omega_k(t) \neq \omega_{k'}(t)$ if $k \neq k'$.

To introduce the notion of mixed state geometric phase in nonunitary evolution, we first begin by lifting the mixed state to a pure state in a larger system. The mixed state $\rho(t)$ can be purified as

$$|\Psi(t)\rangle = \sum_{k=1}^{N} \sqrt{\omega_k(t)} |\phi_k(t)\rangle \otimes |a_k\rangle, \quad t \in [0, \tau],$$
 (5)

where $|\Psi(t)\rangle \in \mathcal{H}_s \otimes \mathcal{H}_a$ is a purification of the density operator of $\rho(t)$ in the sense that $\rho(t)$ is the partial trace of $|\Psi(t)\rangle\langle\Psi(t)|$ over the ancilla. The relative phase between $|\Psi(\tau)\rangle$ and $|\Psi(0)\rangle$ reads

$$\alpha(\tau) = \arg\left(\sum_{k=1}^{N} \sqrt{\omega_k(0)\omega_k(\tau)} \langle \phi_k(0) | \phi_k(\tau) \rangle\right).$$
 (6)

Since both $\{|\phi_k(0)\rangle\}$ and $\{|\phi_k(t)\rangle\}$ are orthonormal bases of the same Hilbert space \mathcal{H}_s , there exists, for each $t \in [0, \tau]$, a purification dependent unitary operator V(t) such that

$$|\phi_k(t)\rangle = V(t)|\phi_k(0)\rangle,\tag{7}$$

where V(0)=I, I being the identity operator on \mathcal{H}_s . Explicitly, we may take $V(t)=|\phi_1(t)\rangle\langle\phi_1(0)|+\cdots+|\phi_N(t)\rangle\langle\phi_N(0)|$. As shown in Ref. [10], the relative phase is given by

$$\alpha(\tau) = \arg\left(\sum_{k=1}^{N} \sqrt{\omega_k(0)\omega_k(\tau)} \langle \phi_k(0)|V(\tau)|\phi_k(0)\rangle\right).$$
 (8)

We may naturally take $\alpha(\tau)$ as the relative phase between the purifications of the nonunitarily connected initial and final states of s.

At this stage, $\alpha(\tau)$ depends on how we purify the state, and we need to remove this dependence. So we first notice that $\alpha(\tau)$ becomes the standard geometric phase of the pure entangled state $|\Psi(t)\rangle$, $t\in[0,\tau]$ when the evolution satisfies the parallel transport condition $\langle \Psi(t)|\dot{\Psi}(t)\rangle=0$. However, this single condition is insufficient for mixed states as it only specifies one of the N undetermined phases of V(t), and the resulting pure state geometric phase remains strongly dependent upon the purification. Instead, the essential point to arrive at the geometric phase is to realize that there is an equivalence set \mathcal{S} of unitarities $\tilde{V}(t)$ of the form

$$\widetilde{V}(t) = V(t) \sum_{k=1}^{N} e^{i\theta_k(t)} |\phi_k(0)\rangle \langle \phi_k(0)|, \qquad (9)$$

where $V(t) \in \mathcal{S}$ fulfills V(0) = I, but is otherwise arbitrary and $\theta_k(t)$ are real time-dependent parameters such that $\theta_k(0) = 0$. Thus, the parallel transport conditions read

B = 5: D = 1

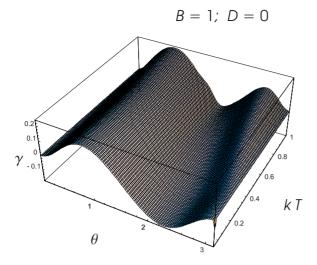


FIG. 6. (Color online) Geometric phase for the thermal state ϱ as a function of azimuthal angle θ and temperature kT for B=1 and no DM interaction (i.e., D=0). Note that we have plotted the geometric phase in the principal range between $-\pi$ and π .

$$\langle \phi_k(0) | \tilde{V}^{\dagger}(t) \tilde{\dot{V}}^{\parallel}(t) | \phi_k(0) \rangle = 0, \quad k = 1, \dots, N.$$
 (10)

This is satisfied, provided that for each k,

$$\theta_k(t) = i \int_0^t \langle \phi_k(0) | V^{\dagger}(t') \dot{V}(t') | \phi_k(0) \rangle dt'. \tag{11}$$

Substituting this result into Eq. (9) and replacing $V(\tau)$ in Eq. (8) by $\tilde{V}(\tau)$, we obtain

$$\gamma = \arg \left(\sum_{k=1}^{N} \sqrt{\omega_{k}(0) \omega_{k}(\tau)} \langle \phi_{k}(0) | \phi_{k}(\tau) \rangle e^{-\int_{0}^{\tau} \langle \phi_{k}(t) | \dot{\phi}_{k}(t) \rangle dt} \right). \tag{12}$$

Using Eq. (12), we numerically compute the geometric phase for the thermal state. In Fig. 6, we evaluate the geometric phase of the thermal state for B=1 and without any DM interaction (i.e., D=0). In Fig. 7, we compute the geometric phase for B=5 and D=1, a system with nontrivial DM interaction. We note that the presence of DM interaction provides significantly different behavior for larger values of temperature. At low temperature, we expect that the thermal state reduces to the eigenstate with the least eigenvalue, namely, $|E_1\rangle$. The results in Figs. 6 and 7 are indeed consistent with the geometric phase associated with $|E_1\rangle$ in the previous section, except that in the previous section, we have plotted the geometric phase in the interval $[0,2\pi)$ whereas in this section we have replaced the principal values of the geometric phase in the interval $[-\pi, \pi)$. In the limit $T \rightarrow 0$, we recovered the previous results in Sec. II.

Therefore, it shows that the method used to calculate the Berry phase of a mixed state as discussed earlier is indeed accurate as it corresponds to the scenario whereby only pure states were considered.

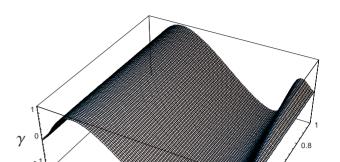


FIG. 7. (Color online) Geometric phase for the thermal state ϱ as a function of azimuthal angle θ and temperature kT for B=5 and DM interaction D=1.

 θ

IV. CONCLUSION

In summary, we study how the Berry phase changes in a system of XX chain with DM interaction in an applied magnetic field. The Berry phase in the system does indeed depend on the amount of DM interaction and also the external magnetic field. However, from Figs. 1 and 2, it seems to suggest that large DM interaction tends to wash out the Berry phase while large magnetic field produces a larger range of Berry phase. We then investigated the dependence of the Berry phase with concurrence with the DM interaction set to unity and found that the concurrence decreases with increasing magnetic field. It can also be concluded that the amount of entanglement is high when the magnetic field is comparable to the DM interaction with both set to unity. Finally, we investigated the Berry phase of thermal states using Eq. (11) and found that the DM interaction and magnetic field again plays a part in the determination of the Berry phase. The mixed state results (when T=0) were checked to be consistent with the earlier part (ground state), whereby only pure states were considered. We can conclude that the treatment used to calculate the Berry phase of a mixed state is sound. In the future, we hope to study a system which produces some nontrivial subsystems so that we can investigate if the addition of these values yield the Berry phase of the system.

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