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Mean-field Berry phase of an interacting spin-1/2 system

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Abstract – We study a long-range interacting spin-1/2 system in the mean-field perspective, and obtain an analytical expression for its Berry phase. The magnetic-like flux interpretation of the Berry phase shows that the source and sink of the magnetic-like field are, respectively, located at the disk-shaped level-crossing region, where the first-order quantum phase transition occurs, and its boundary, where the continuous quantum phase transition occurs. From the asymptotic distribution of the field at the infinity, we find that the source and sink as a whole can be seen as a disk-shaped monopole with a negative magnetic charge. The analogues of this monopole and its exotic field can generally exist in other interacting spin systems.

Introduction. – Since Berry's pioneer work [1], various geometric phases have been widely studied [2,3]. A classical textbook paradigm of the adiabatic geometric phase, or the Berry phase (BP), comes from the single spin-1/2 system. According to the quantum adiabatic theorem [4], when a slowly rotating external magnetic field is applied, a single spin-1/2 system, which is initially in an energy eigenstate, will remain in this eigenstate, and thus will evolve with the field simultaneously. After a complete period, the system will acquire a BP. This BP can be interpreted as either a half solid angle or the flux of a magnetic-like field in the parameter space. In the latter interpretation, the magnetic-like field originates from the monopole located at the level-crossing point. For various theoretical and practical purposes, this paradigm has been generalized to the nonisolated spin-1/2 system [5], the spin-1/2 system in a classical fluctuating field [6], etc. Recently, the relation between geometric phases and quantum phase transitions (QPTs) is proposed [7]. Since the mean-field analysis is the most simple and effective method to investigate phase transitions, this relation naturally motivates us to generalize the paradigm to an interacting spin-1/2 system in the mean-field perspective.

In this letter, we analytically calculate the BP of a long-range interacting spin-1/2 system in the mean-field perspective. This mean-field BP reduces to the BP of the single spin-1/2 system when the interaction vanishes. The magnetic-like flux interpretation of the BP shows that the source and sink of the relevant magnetic-like field are, respectively, located at the disk-shaped level-crossing region, where the first-order QPT occurs, and its boundary, where the continuous QPT occurs. Specifically, one part of the field originates from the level-crossing region and ends at its boundary, while the other part comes from the infinity and ends at its boundary too. The shape of the interface between these two parts reflects the critical property of the system. From the asymptotic distribution of the field at the infinity, we find that the source and sink as a whole can be seen as a disk-shaped monopole with a negative magnetic charge. We emphasize that all these results generalize the above textbook paradigm to the interacting spin-1/2 system, and the analogues of the disk-shaped monopole and its exotic magnetic-like field can generally exist in other interacting spin systems.

Model. – We consider a long-range interacting spin-1/2 system in an adjustable external magnetic field $\mathbf{R} = (x, y, z) = (\rho\cos\phi, \rho\sin\phi, z)$. In appropriate units, its Hamiltonian takes the form

$$H = \sum_{i=1}^{N} \mathbf{R}\cdot\boldsymbol{\sigma}_i + \frac{K}{N}\sum_{i\neq j=1}^{N} \sigma_i^z\sigma_j^z, \qquad (1)$$

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where $\boldsymbol{\sigma}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$ is the Pauli matrix vector of the i-th spin, K is the reduced interaction constant, and $N \gg 1$ is the spin number. Expressing the state of the system as $|\Psi\rangle = |\psi\rangle^N$ and applying the mean-field approximation to the Hamiltonian (1), we obtain the mean-field Hamiltonian $H_m = \mathbf{G}\cdot\boldsymbol{\sigma}$, where $\mathbf{G} = \mathbf{R} + (0, 0, K\langle\psi|\sigma^z|\psi\rangle)$. Then the Schrödinger equation $i\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle = H|\Psi\rangle$ reduces to the mean-field Schrödinger equation $i\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = H_m|\psi\rangle$. Inserting $|\psi\rangle = (\cos\frac{\alpha}{2}, \sin\frac{\alpha}{2}e^{i\beta})^T e^{-i\lambda}$ into this equation yields

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = -2\rho\sin(\beta - \phi), \tag{2}$$

$$\frac{\mathrm{d}\beta}{\mathrm{d}t} = 2z + 2K\cos\alpha - 2\rho\cot\alpha\cos(\beta - \phi), \tag{3}$$

$$\frac{\mathrm{d}\lambda}{\mathrm{d}t} = z + K\cos\alpha + \rho\tan\frac{\alpha}{2}\cos(\beta - \phi). \tag{4}$$

For a fixed K, eqs. (2) and (3) connect the projective Hilbert space spanned by (α, β) with the parameter space spanned by (ρ, ϕ, z). If we introduce the mean spin vector $\mathbf{s} = (s_x, s_y, s_z) = \langle\psi|\boldsymbol{\sigma}|\psi\rangle = (\sin\alpha\cos\beta, \sin\alpha\sin\beta, \cos\alpha)$, eqs. (2) and (3) can be expressed as the following compact form:

$$\frac{\mathrm{d}\mathbf{s}}{\mathrm{d}t} = 2\mathbf{G}\times\mathbf{s}. \tag{5}$$

We now assume that the point $(\bar{\alpha}, \bar{\beta})$ is a fixed point of the projective Hilbert space, *i.e.*, $\frac{\mathrm{d}}{\mathrm{d}t}\bar{\alpha} = 0$ and $\frac{\mathrm{d}}{\mathrm{d}t}\bar{\beta} = 0$. At this point, eqs. (2) and (3), respectively, become

$$\bar{\beta} = \phi \quad \text{or} \quad \bar{\beta} = \phi + \pi, \tag{6}$$

$$z + K\cos\bar{\alpha} = \pm\rho\cot\bar{\alpha}, \tag{7}$$

where the upper sign is for $\bar{\beta} = \phi$, and the lower sign for $\bar{\beta} = \phi + \pi$. Likewise, eq. (5) becomes $\bar{\mathbf{G}}\times\bar{\mathbf{s}} = 0$, where $\bar{\mathbf{s}} = (\bar{s}_x, \bar{s}_y, \bar{s}_z) = (\sin\bar{\alpha}\cos\bar{\beta}, \sin\bar{\alpha}\sin\bar{\beta}, \cos\bar{\alpha})$ and $\bar{\mathbf{G}} = \mathbf{R} + (0, 0, K\cos\bar{\alpha})$. Because the fixed point of the projective Hilbert space corresponds to the eigenstate of H_m, eqs. (6) and (7) actually determine all eigenstates of H_m. Furthermore, from eqs. (6) and (7), we also find that the eigenvalue corresponding to the eigenstate $|\bar{\psi}\rangle = (\cos\frac{\bar{\alpha}}{2}, \sin\frac{\bar{\alpha}}{2}e^{i\bar{\beta}})^T$ can be expressed as

$$\mu = \langle\bar{\psi}|H_m|\bar{\psi}\rangle = \pm\frac{\rho}{\sin\bar{\alpha}}, \tag{8}$$

where the sign convention is the same as in eq. (7).

When $z = 0$, the eigenstates and eigenvalues of H_m are shown in table 1. Here we stress that the eigenstates $|3\rangle$ and $|4\rangle$ exist only when $\rho < |K|$. From table 1, we can find the ground-state, *i.e.*, the eigenstate with the minimum μ. For the ferromagnetic interaction case where $K < 0$, the disk-shaped region determined by $z = 0$ and $\rho < |K|$ is the level-crossing region where the eigenstates $|3\rangle$ and $|4\rangle$ serve as the degenerate ground states and the first-order QPT occurs [8,9]. Outside this region, the eigenstate $|2\rangle$ serves as the ground state instead of eigenstates $|3\rangle$ and $|4\rangle$. When ρ crosses the boundary of this region determined by $z = 0$ and $\rho = |K|$ from the outside to the inside, $\bar{s}_z$ of the ground state changes continuously from zero to a nonzero value, and thus can be used as the order parameter to indicate the continuous QPT occurs at the boundary. Actually, similar QPTs occur widely in interacting spin systems [8–10]. When $z \neq 0$, the eigenstates and eigenvalues of H_m can be numerically obtained from eqs. (6), (7), and (8), and no other QPT is found. In general, we can analytically prove that H_m has two eigenstates when $K^{2/3} < \rho^{2/3} + z^{2/3}$, and has four eigenstates when $K^{2/3} > \rho^{2/3} + z^{2/3}$.

Table 1: Eigenvalues and eigenstates of H_m when $z = 0$.

Eigenstate	$\bar{s}_z = \cos\bar{\alpha}$	$\bar{\beta}(K>0)$	$\bar{\beta}(K<0)$	μ
$\|1\rangle$	0	ϕ	ϕ	ρ
$\|2\rangle$	0	$\phi+\pi$	$\phi+\pi$	$-\rho$
$\|3\rangle$	$-\sqrt{1-\rho^2/K^2}$	ϕ	$\phi+\pi$	K
$\|4\rangle$	$\sqrt{1-\rho^2/K^2}$	ϕ	$\phi+\pi$	K

Mean-field Berry phase. – Now we consider that the external field $\mathbf{R}$ changes with time, and use the dimensionless adiabatic parameter $\epsilon \sim |\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{R}|$ to measure its rate of change. Furthermore, we assume that ϵ is small enough so that, according to the adiabatic evolution condition in mean-field models [11], the system, which is initially in an eigenstate of H_m, can remain in this eigenstate, and thus can evolve with $\mathbf{R}$ simultaneously. When $\mathbf{R}$ returns to its initial value, the system will acquire a mean-field BP γ. Here we note that, because H_m includes α and thus is state dependent, γ cannot be expressed in the conventional form, *i.e.*, $\gamma \neq -i\oint_L\langle\bar{\psi}|\nabla|\bar{\psi}\rangle\cdot\mathrm{d}\mathbf{R} = \frac{1}{2}\oint_L(1-\cos\bar{\alpha})\mathrm{d}\phi$, where L is the evolution loop of the system in the parameter space. To obtain the expression for γ, we need to use the method introduced in ref. [12] to separate the γ-related term from the expression for $\frac{\mathrm{d}}{\mathrm{d}t}\lambda$. To proceed, we first note that, because the adiabatic parameter ϵ is small but finite, the system will fluctuate around the eigenstate during the evolution. This means that $\alpha = \bar{\alpha} + \delta\alpha$ and $\beta = \bar{\beta} + \delta\beta$, where $\delta\alpha \sim \delta\beta \sim O(\epsilon)$. Then, from eqs. (4), (7), and (8), we obtain

$$\frac{\mathrm{d}\lambda}{\mathrm{d}t} = \mu + \left[\frac{\mu}{2\cos^2(\bar{\alpha}/2)} - K\right]\sin\bar{\alpha}\delta\alpha + O(\epsilon^2), \tag{9}$$

where the zeroth-order term μ has been completely separated out. Integrating this term over the evolution time, we obtain the corresponding dynamical phase. Furthermore, from eqs. (3), (7), and (8), we obtain

$$\frac{\mathrm{d}\bar{\beta}}{\mathrm{d}t} = \frac{2\mu - 2K\sin^2\bar{\alpha}}{\sin\bar{\alpha}}\delta\alpha + O(\epsilon^2). \tag{10}$$

Here we note that $\frac{\mathrm{d}}{\mathrm{d}t}\delta\beta \sim O(\epsilon^2)$. Combining eqs. (9) and (10) yields

$$\frac{\mathrm{d}\lambda}{\mathrm{d}t} = \mu + \frac{1}{2}\left[1 - \frac{\cos\bar{\alpha}}{1-(K/\mu)\sin^2\bar{\alpha}}\right]\frac{\mathrm{d}\bar{\beta}}{\mathrm{d}t} + O(\epsilon^2), \quad (11)$$

where the first-order term, *i.e.*, the γ-related term, has been completely separated out. Integrating this term over the evolution period and using eq. (6), we find the mean-field BP

$$\gamma = \frac{1}{2}\oint_L \left[1 - \frac{\cos\bar{\alpha}}{1-(K/\mu)\sin^2\bar{\alpha}}\right]\mathrm{d}\phi. \quad (12)$$

Since the above derivation does not involve any restrictions on the eigenstate and the evolution loop L, eq. (12) is a general analytical expression for the mean-field BP of the system. In contrast to the previous result [13], eq. (12) includes the accumulative effect of the fluctuation during the evolution.

When $K=0$, *i.e.*, the interaction vanishes, eq. (12) obviously reduces to the expression for the BP of the single spin-1/2 system. When $K \neq 0$, the correctness of eq. (12) can be confirmed by a numerical calculation if we consider γ as the difference between the total phase and the dynamical phase in the adiabatic limit. For simplicity, we can assume that $\phi = 2\pi t/T$ with ρ and z fixed. Under this assumption, the numerical calculation consists of the following steps: i) solve $\bar{\beta}$ and $\bar{\alpha}$ from eqs. (6) and (7) and substitute $\bar{\alpha}$ into eq. (8) to obtain μ; ii) integrate eqs. (2), (3), and (4) from 0 to T with the initial values $\alpha_0 = \bar{\alpha}$, $\beta_0 = \bar{\beta}$ and $\lambda_0 = 0$ to obtain λ; iii) compare the result of eq. (12) with the approaching value of $(\lambda - \mu T)$ at large T.

The integrand in eq. (12) diverges when

$$\mu = K\sin^2\bar{\alpha}. \quad (13)$$

From eqs. (7), (8), and (13), we obtain that

$$K^{2/3} = \rho^{2/3} + z^{2/3}, \quad (14)$$

$$\mu = K^{1/3}\rho^{2/3}, \quad (15)$$

$$\cos\bar{\alpha} = -z^{1/3}/K^{1/3}, \quad (16)$$

where eq. (14) determines the divergence-related region in the parameter space, eqs. (15) and (16) determine the divergence-related μ and eigenstate as the functions of the parameters. Here we stress that eqs. (14), (15), and (16) apply to all eigenstates of H_m. From the previous description about eigenstates, we know that the divergence-related region determined by eq. (14) is exactly the region where the number of the eigenstates changes. This indicates that the behavior of γ reflects the property of the eigenstate faithfully.

From the derivation of eq. (12), we can see that the BP γ is closely related to the fluctuation $\delta\alpha$. Substituting eqs. (6) and (13) into eq. (10), we find that, at the divergence-related region, a slow change of ϕ will lead to an infinite fluctuation $\delta\alpha$. For the present mean-field model, an infinite fluctuation around the ground-state arises only when the continuous QPT occurs. Therefore, the divergence of the ground-state BP γ_g can be seen as the consequence of the quantum criticality. Here and below, the subscript g refers to the ground state.

Magnetic-like flux interpretation. – From the form of eq. (12), we find that the mean-field BP γ is not proportional to any solid angle, and thus has no solid angle interpretation. In spite of this, we can always interpret γ as the flux of a magnetic-like field in the parameter space as long as the field takes the appropriate form. This magnetic-like flux interpretation actually serves as the differential formulation for γ. In the following we perform the interpretation of the ground-state BP γ_g, and reveal the relation between this interpretation and the QPTs of the system.

We first define the vector potential $\mathbf{A}_g$ satisfying $\oint_L \mathbf{A}_g \cdot \mathrm{d}\mathbf{R} = \gamma_g$. Because $\bar{\beta}_g = \phi + \pi$, we have

$$\mathbf{A}_g = \left(\frac{1}{2\rho} - \frac{\cos\bar{\alpha}_g}{2\rho + 2K\sin^3\bar{\alpha}_g}\right)\hat{\mathbf{e}}_\phi. \quad (17)$$

Here we stress that $\mathbf{A}_g$ is independent of the evolution loop L. Then we define the magnetic-like field $\mathbf{B}_g$ satisfying $\mathbf{B}_g = \nabla \times \mathbf{A}_g - \boldsymbol{\delta}_g$, where $\boldsymbol{\delta}_g$ denotes the contribution from the Dirac string. A direct calculation gives

$$\mathbf{B}_g = \left(U\frac{\partial\bar{\alpha}_g}{\partial\rho} + V\right)\hat{\mathbf{e}}_z - \left(U\frac{\partial\bar{\alpha}_g}{\partial z}\right)\hat{\mathbf{e}}_\rho, \quad (18)$$

where

$$\frac{\partial\bar{\alpha}_g}{\partial z} = \frac{\rho\cos^2\bar{\alpha}_g}{(z+K\cos\bar{\alpha}_g)^2 + K\rho\sin\bar{\alpha}_g\cos^2\bar{\alpha}_g}, \quad (19)$$

$$\frac{\partial\bar{\alpha}_g}{\partial\rho} = -\frac{(z+K\cos\bar{\alpha}_g)\cos^2\bar{\alpha}_g}{(z+K\cos\bar{\alpha}_g)^2 + K\rho\sin\bar{\alpha}_g\cos^2\bar{\alpha}_g}, \quad (20)$$

$$U = \frac{3K\sin^2\bar{\alpha}_g\cos^2\bar{\alpha}_g + K\sin^4\bar{\alpha}_g + \rho\sin\bar{\alpha}_g}{2(\rho + K\sin^3\bar{\alpha}_g)^2}, \quad (21)$$

$$V = -\frac{K\sin^3\bar{\alpha}_g\cos\bar{\alpha}_g}{2\rho(\rho + K\sin^3\bar{\alpha}_g)^2}. \quad (22)$$

Besides, from the distribution of $\mathbf{A}_g$ at the large $\mathbf{R}$ limit, we find that there is a Dirac string along the positive z-axis.

Because the real antiferromagnetic ground state of the original system cannot be described under the present mean-field approximation, in the following we focus on the ferromagnetic interaction case where $K<0$. Without loss of generality we take $K=-1$. Then the field line distribution of $\mathbf{B}_g$ (see fig. 1) shows that the source and sink of $\mathbf{B}_g$ are, respectively, located at the disk-shaped level-crossing region and its boundary. Specifically, one part of $\mathbf{B}_g$ originates from the level-crossing region and ends at its boundary, while the other part comes from the infinity and ends at its boundary too. From eq. (7) and

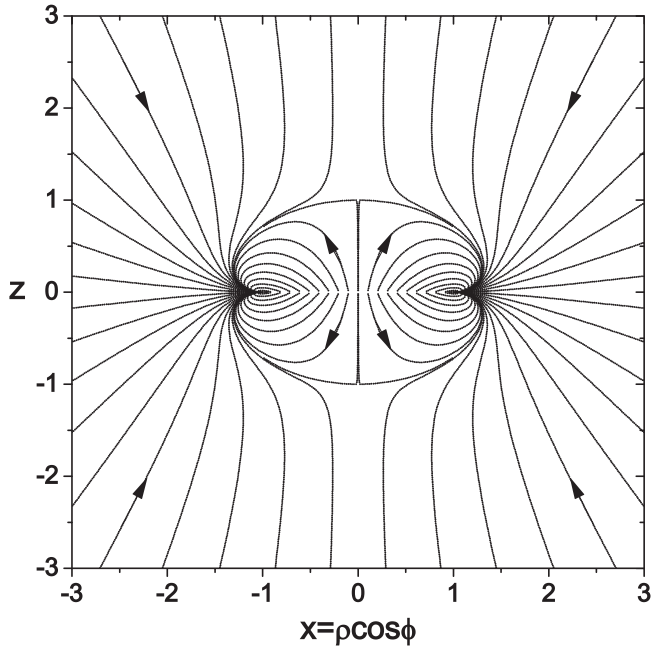

Fig. 1: The field line distribution of $\mathbf{B}_g$ in the (x,z)-plane when $K=-1$. The arrows indicate the direction of $\mathbf{B}_g$.

the condition that $\gamma_g = 2\pi$ or 0 with the evolution loop L azimuthally symmetric, we find that the interface between these two parts, which we call the flux-free surface, is determined by $\rho = \sqrt{1-|z|}(1+\sqrt{|z|})$.

At the large $\mathbf{R}$ limit, the interaction between the spins can be ignored. Then the distribution of $\mathbf{B}_g$ is the field distribution of the point-like monopole with the elementary magnetic charge $(-1/2)$. This asymptotic distribution indicates that the source and sink of $\mathbf{B}_g$ as a whole can be seen as a disk-shaped monopole located at the region of the QPTs. Actually, similar deformed monopoles have been noticed recently [14]. From the distribution of $\mathbf{B}_g$ near the level-crossing region, we find that the surface-density of the magnetic charge on this region is

$$\sigma_g = \frac{1}{4\pi(1-\rho^2)^{3/2}}, \tag{23}$$

where $\rho < 1$. When $\rho \to 1$, eq. (23) gives $\sigma_g \sim (1-\rho)^{-\Lambda}$ with the critical exponent $\Lambda = 3/2$. The surface-density σ_g, together with the total magnetic charge of the monopole, determines $\mathbf{B}_g$ completely. Therefore, we can say that σ_g is the central quantity in the differential formulation for γ_g, and Λ is the corresponding central critical exponent. Since the BP can provide the key ingredients of the criticality in principle [7], it is promising and challenging to investigate the relation between Λ and other critical exponents.

Because the ground-state is twofold degenerate on the level-crossing region, any evolution loop L on this region corresponds to two different γ_g's. It is easy to show that their difference $\Delta\gamma_g = 4\pi Q_g^L (\text{modulo } 2\pi)$, where Q_g^L is the magnetic charge enclosed by L. This indicates that the magnetic charge of the monopole originates from the phase difference $\Delta\gamma_g$. From eq. (23), we find that the charge on the level-crossing region is divergent. Combining this divergence with the distribution of $\mathbf{B}_g$ at the large $\mathbf{R}$ limit, we find that the negative charge on the boundary of this region must be divergent too.

Discussion and conclusion. – From the previous results, we can easily see that both the disk-shaped monopole and the exotic distribution of $\mathbf{B}_g$ are the natural consequences of the physical properties of the system. These properties include i) the asymptotic behavior of the system at the large $\mathbf{R}$ limit; ii) the degeneracy of the ground state; iii) the criticality which leads to the divergent γ_g. Because the similar properties exist in many interacting spin systems, the analogues of the disk-shaped monopole and its exotic magnetic-like field also exist generally in these systems.

On the other hand, the structure of the monopole and the distribution of $\mathbf{B}_g$ reflect the properties of the system naturally. In particular, the shape of the flux-free surface reflects the critical property of the system. Roughly speaking, both the external field $\mathbf{R}$ and the interaction between the spins affect γ_g, and the flux-free surface is located at the region where their effects on γ_g cancel each other out. In essence, the criticality of the system is exactly the consequence of the competition between $\mathbf{R}$ and the interaction. Therefore, the shape of the flux-free surface can reflect the critical property of the system. This provides the possibility to measure the criticality by the BP without having the system undergo the QPT.

In conclusion, we have studied a long-range interacting spin-1/2 system in the mean-field perspective, and obtained an analytical expression for its BP. The magnetic-like flux interpretation of the BP gives an exotic magnetic-like field and a relevant disk-shaped monopole, which are closely related to the QPTs of the system. We emphasize that this result visualizes the relation between the BP and the QPTs, and may have many prospective applications in the study of QPTs.

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