Spin tunneling, Berry phases, and doped antiferromagnets

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(Received 10 December 1992; revised manuscript received 8 January 1993)

Interference effects between Berry-phase factors in spin-tunneling systems have been discussed by several groups in the context of quantum magnets. I point out that similar effects appear in the semiclassical analysis of the two-dimensional doped antiferromagnet. As a consequence, the sign of the dispersion of a spin polaron in the t-J model depends on the spin size s through a phase factor $e^{i2\pi s}$. Thus we arrive at a semiclassical interpretation of the ground-state momentum for the single hole. It agrees with numerical diagonalizations of the t-J model for $s=\frac{1}{2}$, and predicts a difference between integer- and half-odd-integer-spin cases.

Interference effects between Berry-phase factors in spin-tunneling systems have been discussed in recent papers by Loss, DiVincenzo, and Grinstein[1] (LDG) and von Delft and Henley (vDH).[2] As physical realizations, LDG proposed tunneling of magnetic clusters, and vDH proposed an anisotropic spin Hamiltonian and the Heisenberg antiferromagnet on the *kagomé* lattice. In these examples, for certain spin sizes s, the classical ground-state degeneracies are not lifted by tunneling processes.

This paper points out that Berry phases in spin tunneling are important in another interesting system: the two-dimensional doped antiferromagnet, as described by the t-J model. This model is often used for the cuprate superconductors near the antiferromagnetic phase. We shall see that the Berry phases of Refs. 1 and 2 effect the possible ground-state momenta of the single hole. This helps to explain the results of exact diagonalizations of the t-J Hamiltonian on finite clusters.[3]

In Ref. 4, the hole in the antiferromagnet has been cast as a spin-tunneling problem. First the t-J model was extended to $s > \frac{1}{2}$. Its energy Green function is given by a spin coherent states path integral

$$G(E) = \int dt \int \mathcal{D}\Omega \exp\left[i \int_0^t dt' \left(\sum_i \left(s - \frac{\rho_i}{2} \right) (1-\cos\theta_i)\dot{\phi}_i - H[\Omega] + E \right) \right] \tag{1}$$

where Ω_i is a unit vector at site i, which is parametrized by $[\cos\theta_i(t'), \phi_i(t')]$. The classical Hamiltonian is

$$H = \frac{J}{2} \sum_{\langle i,j \rangle} \Omega_i \Omega_j (1-\rho_i)(1-\rho_j) - E^{\text{hole}}[\Omega; t], \tag{2}$$

where $\langle i,j \rangle$ denotes nearest neighbors on the square lattice, and t is the hole hopping parameter. In the large s limit, the path integral (1) can be expanded about the classical paths between the end-point configurations. Also in that limit, $E^{\text{hole}}[\Omega]$ and $\rho[\Omega]$ are simply the ground-state energy and density of the adiabatic single-particle Hamiltonian:

$$H^{\text{hole}}_{i,j} = t \sqrt{\frac{1+\Omega_i \Omega_j}{2}}\, \delta_{\langle i,j \rangle} + H^{\text{NNN}}, \tag{3}$$

where $\delta_{\langle i,j \rangle}$ is unity for nearest neighbors i,j and zero elsewhere. H^{NNN} is the next-nearest-neighbor hopping, which is less important in the parameter regime of interest.

To gain more intuition as to the properties of $E^{\text{hole}}[\Omega]$, let us consider a five-site polaron in a Néel state, where the spins are ordered in the $\pm\bar{\Omega}$ directions. The central spin of the polaron at site a points in the arbitrary direction Ω_a. Neglecting H^{NNN} one obtains, by diagonalizing (3),

$$E^{\text{hole}} = -t\sqrt{2(1+\Omega_a \bar{\Omega})}\,, \qquad \rho_i = \begin{cases} 1/2, & i=a, \\ 1/8, & \langle i,a \rangle, \\ 0, & \text{elsewhere}, \end{cases} \tag{4}$$

which shows that E^{hole} is ferromagnetic, and is minimized by a flipped spin at site a: $\Omega_a = \bar{\Omega}$.

The semiclassical expansion of (1) has been carried out in Ref. 4. Here we quote the results relevant to tunneling effects: For $1 < t/J < 4.1$, the classical ground state of (2) is the five-site polaron (one flipped spin at site a). Translational invariance is restored by *spin-tunneling paths*, and the polaron acquires a disperion relation

$$\epsilon_{\mathbf{k}} = \sum_j e^{i\mathbf{k}\cdot\mathbf{j}} \Gamma_{ij}, \tag{5}$$

where the tunneling rates Γ_{ij} describe the motion of the polaron's center from site i to j under the classical energy barrier. It was also shown that conservation of total magnetization requires Γ_{ij} to vanish for i,j on different sublattices.[4] The dominant hopping processes are

the second- and third-nearest neighbors (Γ_{ab} and Γ_{ac}, respectively). Hoppings to larger distances are supressed exponentially at large s. Thus the semiclassical band structure of the polaron is given by

$$\epsilon_{\mathbf{k}} \simeq 2\Gamma_{ab}\left[\cos(k_x+k_y)+\cos(k_x-k_y)\right] +2\Gamma_{ac}\left[\cos(2k_x)+\cos(2k_y)\right]. \quad (6)$$

In Ref. 6 a general expression for the tunneling matrix element in multidimensions was derived:

$$\Gamma_{12} = \langle\Psi_1|[\Sigma_1]G(E_0)[\Sigma_2]|\Psi_2\rangle, \quad (7)$$

where E_0 is the classical ground-state energy and $[\Sigma_i]$ are current operators, which are defined with respect to appropriately chosen surfaces in configuration space Σ_i, which enclose the minima of H. Ψ_i is a restricted harmonic oscillator wave function, for the spin waves about a polaron at site i. For the purpose of evaluating the leading order term, and the associated Berry phases, suffices it to note that in Eq. (1) the Green function is an off-diagonal matrix element of the propagator between two different classical ground states. Thus, the tunneling necessarily involves paths which connect between translated polaron configurations. The leading order $\exp(-s\bullet)$ of Γ_{12} is determined by *"instantons"* (classical paths in imaginary time). The Gaussian fluctuations about the instantons, the surface integrations of $[\Sigma]$, and the normalization of Ψ_i are higher order in $1/s$ and contribute to the magnitude of the preexponential (see Ref. 6).

In analogy to normal tunneling of a particle in a double well, in the absence of Berry phases the signs of Γ_{ij} are negative. In the following we shall find that the tunneling matrix elements are multiplied by overall Berry-phase factors which yield

$$\Gamma_{ij} = -e^{i2\pi s}|\Gamma_{ij}|. \quad (8)$$

Proving Eq. (8) requires only general knowledge of the tunneling path. In order to fix our notations we shall discuss the particular hopping process from site a to c. The result however can easily be seen to hold for any other hopping (provided, as we have mentioned, that it is between sites on the same sublattice). Consider a local Néel order which points in the $\hat{x}$ direction. The bonds which share the hole density are marked by dashed lines. These bonds experience the competition between the ferromagnetic interaction due to E^{hole}, and the antiferromagnetic coupling of the Heisenberg term. Since the action must be minimized, the tunneling path does not involve appreciable motion of the background spins, i.e., those which do not need to rotate between the initial and final configurations. The dominant contribution to Γ_{ac} is given by the simultaneous rotation of spins a and c, as depicted in Fig. 1. We parametrize the instanton by the angle φ. To satisfy classical energy conservation ($H[\Omega]-E=0$), we complexify the z components of the spins,

$$\cos\theta_i \rightarrow -i\tilde{\mu}_i, \quad (9)$$

where $\tilde{\mu}_i$ are real. Following Ref. 2 (see also Refs. 5 and 6), we note that two instanton paths contribute equal magnitudes to Γ, and are described by clockwise and anticlockwise rotations of φ in the xy plane. Using Eq. (1) and summing over both rotations we obtain

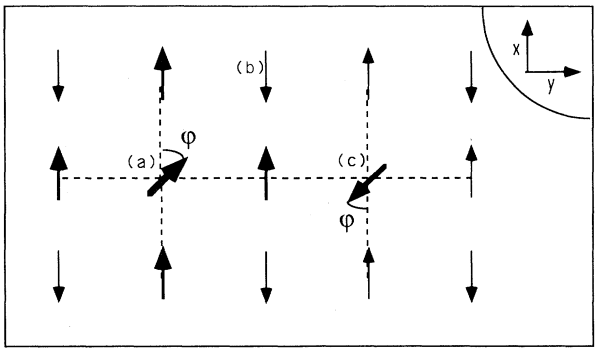

FIG. 1. Tunneling path (instanton) describing the translation of a polaron from site a to c. The background spins are ordered in the $\pm\hat{\mathbf{x}}$ directions. The path is parametrized by the azimuthal angle φ of the rotating spins. This rotation gives rise to a nontrivial Berry phase. Thick arrows represent large hole densities at the sites. Dashed lines highlight the bonds for which the hole t hopping term is nonzero.

$$\Gamma_{ac} = -\mathcal{N}\exp\left(-\int_0^{\pi}d\varphi\sum_i\left(s-\frac{\rho_i}{2}\right)\mu_i\frac{d\phi_i}{d\varphi}\right)\sum_{\pm}e^{i\Upsilon^{\pm}}. \quad (10)$$

$\mathcal{N}$ is the positive fluctuation prefactor,[2] and the Berry phases are

$$\Upsilon^{\pm} = \int_0^{\pm\pi}d\varphi\sum_i\left(s-\frac{\rho_i}{2}\right)\frac{d\phi_i}{d\varphi} = \pm 2\pi s-\int_0^{\pm\pi}d\varphi\sum_i\frac{\rho_i}{2}\frac{d\phi_i}{d\varphi}. \quad (11)$$

The factor of 2π in the first term describes the total rotation of ϕ_a and ϕ_c. Other spins retrace their paths, and their contribution to that term vanishes. The sum over two orientations yields

$$-\sum_{\pm}e^{i\Upsilon^{\pm}} = -2e^{i2\pi s}\cos\left[\sum_i\int_0^{\pi}d\varphi\frac{\rho_i}{2}\frac{d\phi_i}{d\varphi}\right], \quad (12)$$

which yields Eq. (8). Q.E.D.

Thus for half-odd-integer spins, the ground-state momenta $\bar{\mathbf{k}}$, as given by the minima of Eq. (6), depends on the ratio $\Gamma_{ab}/(2\Gamma_{ac})$. For $\Gamma_{ab}>2\Gamma_{ac}>0$ one obtains

$$\bar{\mathbf{k}} = (\pm\pi,0),(0,\pm\pi) \quad (13)$$

and for $2\Gamma_{ac}>\Gamma_{ab}>0$,

$$\bar{\mathbf{k}} = (\pm\pi/2,\pm\pi/2). \quad (14)$$

This is a semiclassical interpretation of the numerical results of Ref. 3, which found that cases (13) and (14) are realized for $s = \frac{1}{2}$ in different regimes of t/J. For integer s, however, Eqs. (6) and (8) predict the ground state to be at $\mathbf{k} = (0,0)$ or $\mathbf{k} = (\pi,\pi)$. The latter prediction, to my knowledge, has not yet been checked numerically.

I thank C. Henley and A. Garg for helpful conversations. The hospitality of the Aspen Center for Physics is gratefully acknowledged. This work was partially supported by the U.S.-Israeli Binational Science Foundation, the Fund for the Promotion of Research at the Technion, and NSF DMR-9213884.

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[1] D. Loss, D.P. DiVincenzo, and G. Grinstein, Phys. Rev. Lett. **69**, 3232 (1992).

[2] J. von Delft and C.L. Henley, Phys. Rev. Lett. **69**, 3236 (1992).

[3] See, e.g., E. Dagotto, R. Joynt, A. Moreo, S. Bacci, and E. Gagliano, Phys. Rev. B **41**, 9049 (1990), and references therein.

[4] A. Auerbach and B.E. Larson, Phys. Rev. Lett. **66**, 2262 (1991).

[5] A. Garg and G.H. Kim, Phys. Rev. B **45**, 12 921 (1992).

[6] A. Auerbach and S. Kivelson, Nucl. Phys. **B257**, 799 (1985), see Eq. (3.8).