Geometric (Berry) phases and statistical transmutation in the two-dimensional systems of strongly correlated electrons

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Focusing on the hole-doped two-dimensional systems of strongly correlated electrons, we examine geometric phases acquired by electronic wave functions as a result of polaron transport around a closed loop. For this study we apply the Lanczos exact diagonalization method to Holstein-Hubbard, Holstein-\(tJ\), and Holstein-\(tJ_x\) models in order to reveal various aspects of geometric phases. We demonstrate that transverse spin fluctuations are responsible for the generation of nontrivial geometric phases. From the exchange symmetry of polarons we find that the statistical transmutation of polarons occurs depending on the strength of electron correlations.

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I. INTRODUCTION

Since the discovery of high temperature superconductivity in copper oxides, attempts have been made to identify the nature of charge carriers in these materials. There are some experimental evidences that polaronic charge carriers exist in both the superconducting state and the normal state. Photoinduced absorption measurements in La\(_2\)CuO\(_4\) and YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) indicate that self-localized structural distortions are present around photoexcited charge carriers. A recent experiment demonstrated that Sr-induced local lattice distortions occur in La\(_2\)-Sr\(_x\)CuO\(_4\) in association with holes donated by the Sr atoms. In order to investigate the nature of the polaronic charge carriers, we study geometric phases acquired by the electronic wave functions after the transport of a polaron around a closed loop.

A quantum object (a subsystem of fast degrees of freedom) acquires a geometric (Berry) phase in an environment where a parameter (a subsystem of slow degrees of freedom) is slowly transported around a closed circuit in a parameter space. Thus quantum subsystems with two widely separated energy scales (between slow and fast degrees of freedom) exhibit geometric phases. In this paper we investigate the geometric phases acquired by the electronic wave functions as a result of polaron transport around a closed loop in a hole-doped two-dimensional system of strongly correlated electrons, e.g., the copper oxide plane in high \(T_c\) superconductors. In addition, we investigate the statistical transmutation of polarons by studying the exchange symmetry of polarons varying with the strength of electron correlations.

II. VARIOUS GEOMETRIC (BERRY) PHASES BASED ON MODEL HAMILTONIANS

We first study the geometric phases varying with the strength of antiferromagnetic electron correlations and of electron-phonon coupling. For this study we introduce the Holstein-Hubbard model Hamiltonian for the hole-doped two-dimensional systems of square lattice,

\[
H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{c.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - g \sum_i u_i n_i \\
+ \frac{K}{2} \sum_i (x_i^2 + y_i^2), \tag{1a}
\]

with the Holstein coordinate \(u_i\),

\[
u_i = \frac{1}{4} (x_{i,x,i_y} - x_{i_x,i_y} + y_{i_x,i_y} - y_{i_x,i_y}) . \tag{1b}
\]

Here \(c_{i\sigma}^\dagger (c_{i\sigma})\) is the creation (annihilation) operator of an electron with spin \(\sigma\) at a copper site \(i\) \((i = (i_x, i_y))\), and \(n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}\) is the electron number operator. \(x_i\) and \(y_i\) denote the displacements of oxygen atoms in the unit cell of CuO\(_2\) plane. \(t\) represents the on-site Coulomb repulsion energy (correlation strength); \(g\), the electron-lattice coupling constant and \(K\), the spring constant. In our calculations the magnitude of the Holstein coordinate \(u_i\) is normalized to unity, \(|u_i| = 1\) when a polaron is formed around copper site \(i\) as a result of hole doping. The energy of the polaron is then given by \(-g\).

Now for the study of geometric phases varying with the Heisenberg coupling constant \(J\) and the electron-phonon coupling constant \(g\), Hamiltonians of interest are the Holstein-\(tJ\) model,

\[
H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{c.c.}) + J \sum_i S_i \cdot S_j - g \sum_i u_i n_i \\
+ \frac{K}{2} \sum_i (x_i^2 + y_i^2) , \tag{2}
\]

and the Holstein-\(tJ_x\) model,

\[
H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{c.c.}) + J_z \sum_i S_i^z S_j^z - g \sum_i u_i n_i \\
+ \frac{K}{2} \sum_i (x_i^2 + y_i^2) . \tag{3}
\]

Here \(\hat{c}_{i\sigma} = c_{i\sigma} (1 - n_{i,-\sigma})\) is the electron annihilation operator at site \(i\), which excludes double occupation.
\( S_i = \frac{1}{2} \gamma c_{\alpha i} \sigma_{\alpha \beta} c_{\beta i} \) is the electron spin operator. The Holstein-\( t \)-\( J_z \) Hamiltonian takes into account only the spin \( z \)-component interaction.

The lattice distortions are treated in the adiabatic limit. The electronic wave functions (the fast degree of freedom) varying with lattice distortions are obtained from the application of Lanczos exact diagonalization method\(^8\) to a tilted \( \sqrt{10} \times \sqrt{10} \) lattice with periodic boundary conditions.\(^9\) The propagation of the local lattice distortion (polaron hopping) is described by

\[
\psi_i(\tau) = \psi_{\mathbf{r} \tau} + (\psi_{\mathbf{r} + \mathbf{a}_i} - \psi_{\mathbf{r} \tau}) \tau
\]

with \( \tau \) being the dimensionless time lapse with \( 0 \leq \tau \leq 1 \) for polaron hopping between adjacent lattice sites. For instance, the lattice distortion occurs at copper site \( A \) at \( \tau = 0 \) and moves to an adjacent copper site \( B \) at \( \tau = 1 \). For this process, a closed path in the parameter space \( \{ u_\mathbf{r} \} \) can be defined. We compute the geometric phase factors, \( e^{i\gamma n(C)} \) acquired by the electronic wave function after polaron transport around a closed path \( C \) during time \( T \), by using

\[
e^{i\gamma n(C)} = \lim_{N \to \infty} \prod_{k=1}^{N} (\langle n(u(\tau_k)) | n(u(\tau_{k-1})) \rangle).
\]

Here \( \langle n(u(\tau_k)) \rangle \) is the electronic eigenfunction for a given lattice distortion \( u(\tau_k) \) at time \( \tau_k \). \( \tau_k \) is a \( k \)th discretized time lapse between the initial time \( \tau_0 = 0 \) and the final time (period) \( \tau_N = T \). Eq. (6) is derived under the condition that \( \langle n(u(\tau_k)) \rangle \) is a single-valued complex wave function, that is, \( \langle n(u(0)) \rangle = \langle n(u(T)) \rangle \). On the other hand, all the electronic wave functions obtained from the diagonalization of the model Hamiltonians above are real-valued. In such cases, geometric phases in the form of double-valued real wave functions can be defined. Using the local gauge transformation in parameter space \( u \), the double-valued real wave function, \( | n(u) \rangle_c \), can be converted into a single-valued complex wave function \( | n(u) \rangle_c \),

\[
| n(u) \rangle_c = e^{-i\theta(u)} | n(u) \rangle_c
\]

with \( \theta(u) \), a differentiable function and \( \theta(u(T)) - \theta(u(0)) = \pi \) (see Appendix for details). By introducing the above expression into Eq. (6), one can now obtain the geometric phases of interest.

**III. COMPUTED BERRY PHASES AND STATISTICAL TRANSMUTATION**

First, by using the Holstein-Hubbard model we consider the Berry phase acquired by the electronic wave function as a result of polaron hopping around a closed path. Two types of closed paths, a triangular path and a square path, are displayed in Figs. 1(a)–(b). For simplicity, for the nearest neighbor hopping we chose the identical value of hopping integral to the one used for the nearest neighbor hopping. The electronic wave function is predicted to gain a geometric phase by \( \pi \) (the geometric phase factor of \(-1\)) for polaron hopping around the smallest possible closed path, that is, the triangular path [Fig. 1(a)]. On the other hand, the electronic wave function with the polaron transported around the square path [Fig. 1(b)] is predicted to gain a phase angle by \( 2\pi \), thus leaving the phase factor of the electronic wave function unchanged. The geometric phase of \( 2\pi \) can be understood from the decomposition of the square path into two triangular paths, as shown in Fig. 2. The geometric phase factor of \(+1\) for the square path results from the product of two identical geometric phase factors of \(-1\) for the decomposed triangular paths.

**FIG. 1.** Geometric phase factors based on the Holstein-Hubbard model for (a) a triangular loop and (b) a square loop. The horizontal axis denotes the Coulomb correlation strength \( U \) and the vertical axis, the electron-lattice coupling constant \( g \). The energy unit is \( t = 1 \).

**FIG. 2.** The decomposition of a square path into two triangular paths.

By using both the Holstein-\( t \)-\( J_z \) model and the Holstein-\( t \)-\( J_x \) model, we now examine the geometric phases which result from the transport of a single polaron. They are shown in Figs. 3(a)–(b) and Figs. 3(a)–(b). The predicted geometric phase factor for the case of the triangular path [Fig. 3(a)] is in agreement with that of Schützler et al.\(^9\) For large \( U \) values, say, \( U = 8t \) both the Holstein-\( t \)-\( J_z \) model and the Holstein-Hubbard model yield identical geometric phase factors for both the triangular path and the square path, as are shown in Figs. 3(a)–(b) and Figs. 3(a)–(b). Such direct comparison between the two model Hamiltonians is valid only for large \( U \) values. This is because the \( t \)-\( J \) model is equivalent to the Hubbard model Hamiltonian corresponding to large \( U \) values. On the other hand, the Holstein-\( t \)-\( J_z \) model yields a trivial geometric phase factor of \(+1\) for the triangular path [Fig. 3(a)], while the Holstein-\( t \)-\( J_z \) model Hamiltonian gives rise to the nontrivial geo-
metric phase factor of $-1$. It is of note that only the $t$-$J$ (but not the $t$-$J_z$) Hamiltonian allows transverse spin fluctuations. Thus we discover from comparison of the two Hamiltonians that the generation of the nontrivial geometric phase factor of $-1$ is caused by the transverse spin fluctuations (or spin flip-flop fluctuations) which comes from interactions involving the $x$- and $y$-component (but not the $z$-component) spins, that is, $J \sum_{(ij)}(S_{ix}S_{ix} + S_{iy}S_{iy}) = \frac{1}{2} J \sum_{(ij)}(S_{i+}S_{j-} + S_{i-}S_{j+})$. The nontrivial geometric phases are also predicted by the Holstein-Hubbard model Hamiltonian, in agreement with the Holstein-$t$-$J$ model Hamiltonian, as is shown in Fig. 1(a).

![Fig. 3](image)

FIG. 3. Geometric phase factors based on the Holstein-$t$-$J$ model for (a) a triangular loop and (b) a square loop. The horizontal axis denotes the Heisenberg exchange interaction $J$ and the vertical axis, the electron-lattice coupling constant $g$. The energy unit is $t = 1$.

![Fig. 4](image)

FIG. 4. Geometric phase factors based on the Holstein-$t$-$J_z$ model for (a) a triangular loop and (b) a square loop. The horizontal axis denotes the Ising interaction $J_z$ and the vertical axis, the electron-lattice coupling constant $g$. The energy unit is $t = 1$.

Now we investigate the exchange symmetry of two polarons based on the Holstein-Hubbard model. The numeral label for the square path in Fig. 5 indicates the consecutive order of polaron hopping. Interestingly enough, there exist both trivial and nontrivial geometric phase factors. After the two polarons are exchanged, the electronic wave function is seen to acquire a trivial geometric phase factor of +1 for the case of weak electron correlations ($U \lesssim 1$). This is in sharp contrast with the nontrivial geometric phase factor of $-1$ for the case of intermediate electron correlations ($2 \lesssim U \lesssim 4$). A reentrant behavior of the trivial geometric phase factor of +1 occurs for the case of strong antiferromagnetic electron correlations ($U \gtrsim 6$). It is thus proper to state that polarons behave as hard core bosons in the case of weakly and strongly correlated electrons, while they act as fermions in the intermediate region of electron correlations. Such statistical transmutation of polarons can be mapped into the Jordan-Wigner transformation for the two-dimensional lattice,

$$a_i a_i^\dagger = \delta_{ij} - e^{i\delta} a_j a_i \ . \tag{7}$$

We find that the predicted phase angle $\delta$ depends on $U$, the strength of electron correlation (Coulomb repulsion). That is, $\delta = \pi$ for small and large $U$ values, indicating that polarons behave as bosons and $\delta = 0$ for intermediate $U$ values, indicating that they act as fermions.

![Fig. 5](image)

FIG. 5. Geometric phase factors based on the Holstein-Hubbard model for two-polaron exchange around a square path. The numeral label for the path indicates the consecutive order of polaron hopping. The axes are the same as in Fig. 1.

We examine the exchange symmetry of polarons in different aspect. For the case of weak electron correlations (or free electron limit, $U \lesssim 1$) the predicted exchange symmetry indicates a bosonic nature of polarons with the absence of fictitious magnetic flux line. This is depicted in Fig. 5(a). As correlation (repulsive interaction) between electrons increases, a change of the geometric phase is predicted. That is, for the case of intermediate correlations it can be stated that the polarons hop around a fictitious flux of an elementary flux unit (fluxon), thereby exhibiting a fermionic nature (see a solid line in Fig. 5(b)). For the case of strong antiferromagnetic electron correlations, the exchange of the two polarons indicates the presence of two fictitious flux quanta, as is depicted in Fig. 5(c). Then the statistical transmutation of boson to a composite boson occurs. By composite boson we mean that the boson remains as a boson with the acquired phase of $2\pi$. In short the number of fictitious flux quanta is seen to vary with the strength of electron correlation and allows the statistical transmutation.

![Fig. 6](image)

FIG. 6. Exchange of two polarons. Open circles denote polarons, and each vertical solid line represents a fictitious flux line of one flux quantum (flux unit).
IV. CONCLUSION

By applying the Lanczos exact diagonalization method to Holstein-Hubbard, Holstein-J, and Holstein-Jz model Hamiltonians, we have examined the different aspects of geometric phases acquired by electronic wave functions during the transport of a single polaron around a triangular loop. We find that the nontrivial geometric phase factor of $-1$ is caused by the presence of transverse spin fluctuations. Further by examining the exchange symmetry of polarons based on the Holstein-Hubbard model we discover the statistical transmutation of polarons which varies with the strength of antiferromagnetic electron correlation. It is interesting to note that polarons behave as bosons in the hole-doped two-dimensional system (background) of weakly and strongly correlated electrons and as fermions in the background of intermediate correlation strength. In the future it remains to examine how the statistical transmutation for the exchange of polarons occurs as a function of electron correlation and whether there exists a possibility of anyonic exchange of polarons occurs as a function of electron correlation. It is interesting to note that polarons behave as bosons in the hole-doped two-dimensional system (background) of weakly and strongly correlated electrons and as fermions in the background of intermediate correlation strength. In the future it remains to examine how the statistical transmutation for the exchange of polarons occurs as a function of electron correlation and whether there exists a possibility of anyonic exchange of polarons occurs as a function of electron correlation. It is interesting to note that polarons behave as bosons in the hole-doped two-dimensional system (background) of weakly and strongly correlated electrons and as fermions in the background of intermediate correlation strength.

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APPENDIX:

For the case of multi-valued real wave functions here we prove the Berry phase to be $\gamma(C) = \theta(R(T)) - \theta(R(0))$ by introducing a local gauge transformation in the parameter space, $R(=u)$. The Berry phase $\gamma_n(C)$ is a geometric contribution to the total phase change for the final state of $|\psi(T)\rangle = \exp[i\gamma_n(C)] \exp \left\{ \frac{-i}{\hbar} \int_0^T dt E_n(R(t)) \right\} |\psi(0)\rangle$ where $T$ is the time period. For a subsystem of fast degrees of freedom coupled to a subsystem of slow degrees of freedom the Berry phase is obtained from

$$\gamma_n(C) = i \int \langle n; R|\nabla_R|n; R \rangle \cdot dR,$$  

(A1)

as is well known.

The equation of motion for the subsystem of fast degrees of freedom is given by

$$H(R(t))|n; R(t)\rangle = E_n(R(t))|n; R(t)\rangle,$$  

(A2)

where $R(t)$ is the slowly varying parameter. To obtain the nontrivial (non-zero) Berry phase in Eq. (A1), the eigenstate $|n; R(t)\rangle$ should be complex, non-degenerate, and single-valued. The gauge potential

$$A(R) = i\langle n; R|\nabla_R|n; R \rangle,$$  

(A3)

vanishes for the case of the real eigenstates $|n; R\rangle$.

It is obvious that the nontrivial (nonzero) ‘magnetic field’ $B(R) = \nabla \times A(R)$ cannot be defined for the case of real eigenstates $|n; R(t)\rangle$, since the gauge potential $A(R)$ vanishes. However, by using the following gauge transformation it is possible to define the nonvanishing Berry phase:

$$|n; R\rangle_c = e^{-i\theta(R)}|n; R\rangle_r.$$  

(A4)

Indeed, this is the local gauge transformation in the parameter space $R$, which provides the gauge invariance of the Schrödinger equation, Eq. (A2). Using Eq. (A4) in Eq. (A1) we readily obtain the Berry phase $\gamma(C)$,

$$\gamma_n(C) = \theta(R(T)) - \theta(R(0))$$  

(A5)

or using the notation used for the parameter space in Section 7.

$$\gamma_n(C) = \theta(u(T)) - \theta(u(0)).$$  

(A6)

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