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Effect of Interstitial Coulomb Interaction on the Occurrence of a Gapless Superconducting Phase of Hubbard Fermions on a Triangular Lattice

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Abstract—The concentration dependence of the position of nodal points of a superconducting order parameter is investigated using the *t–J–V* model for a triangular lattice with regard to the exchange and Coulomb interactions in two coordination spheres. The conditions for a topological quantum transition are established.

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INTRODUCTION

The discovery of superconductivity in Na_xCoO_2 sodium cobaltite upon intercalation with water [1] has evoked great interest in studying the Cooper instability and properties of the superconducting phase in this system. The experimental data on spin–lattice relaxation [2] and the measured specific heat [3] and Knight shift show that the system exhibits antiferromagnetic correlations, and the superconducting order parameter (SOP) is anisotropic and spin-singlet. This means that a phase with chiral symmetry $d_{x^2-y^2} + id_{xy}$ of the SOP can occur in sodium cobaltite. The question of whether there is a gap in the Fermi excitation spectrum in such a superconducting phase acquires fundamental importance. As was mentioned in [4], for the pairing potential observed only for nearest neighbors, the superconducting phase with SOP symmetry $d + id$ has a gap over the entire range of concentration x, contradicting the experimental data. As was shown in [4], the pairing potential for the second coordination sphere yields only a gapless superconducting phase with the required SOP symmetry.

For the superconducting phases studied in [4] to satisfy the system of self-consistency equations, however, we must consider interactions in the first coordination sphere. This was done in [5], where additional conditions for the occurrence of a gapless superconducting phase were established.

In this work, we investigate the effect of Coulomb interaction between electrons located on both the nearest and next-to-nearest sites.

MODEL

Let us describe a system using the *t–J–V* model associated with the upper Hubbard band. In the representation of Hubbard operators [6, 7], the Hamiltonian of the model is written as

$$H = \sum_{f\sigma}(\varepsilon-\mu)X_f^{\sigma\sigma} + \sum_f(2\varepsilon+U-2\mu)X_f^{22} + \sum_{fm\sigma} t_{fm}X_f^{2\bar{\sigma}}X_m^{\bar{\sigma}2} + \sum_{f\neq m,\sigma} J_{fm}\left(X_f^{\uparrow\downarrow}X_m^{\downarrow\uparrow} - X_f^{\uparrow\uparrow}X_m^{\downarrow\downarrow}\right) + \frac{1}{2}\sum_{f\neq m} V_{fm}\left(\hat{n}_f - \langle\hat{n}_f\rangle\right)\left(\hat{n}_m - \langle\hat{n}_m\rangle\right). \quad (1)$$

Here, the first two terms describe the one- and two-electron states on sites of the triangular lattice in the atomic representation, ε is the energy of the one-electron state, μ is the chemical potential of the ensemble, and U is the energy of Hubbard repulsion. Nondiagonal Hubbard operators describe the transition between single-site states. The third term of the Hamiltonian corresponds to the hopping of an electron with spin σ from site m to site f in the upper Hubbard band. The transitions from two-electron state $|2\rangle$ to the one-electron state with opposite spin $|\bar{\sigma}\rangle$ and, vice versa, from state $|\bar{\sigma}\rangle$ to state $|2\rangle$ occur on sites m and f, respectively. The amplitude of the probability of such electron hopping is determined by parameter t_{fm}. The fourth term of the Hamiltonian corresponds to the exchange interaction of the *t–J* model in the Hubbard operator representation [8]; J_{fm} is the integral of exchange coupling of ions in the one-electron states on sites f and m. The last term of the Hamiltonian reflects the presence of charge fluctuations in the system under the action of the Coulomb repulsion of electrons on sites f and m; V_{fm} is a parameter reflecting the intensity of these fluctuations.

To describe the superconducting phase, we use the diagram technique for Hubbard operators [7]. The derivation of the equation for a chiral SOP in the t–J–V model was described in detail in [5], so we present only the final self-consistency equation for the order parameter in the superconducting phase,

$$\Delta(p) = \frac{1}{N}\sum_q \left(J_{p+q} + J_{p-q} - V_{p-q}\right)\Delta(q)\frac{\tanh(E_q/2T)}{2E_q}. \quad (2)$$

Here, $E_q = \sqrt{\xi_q^2 + |\Delta(q)|^2}$ is the excitation spectrum in the superconducting phase, $\xi_q = \varepsilon + (N_2 + N_\sigma)t_q - \mu$ is the Hubbard fermion spectrum, and N_i are the occupancies of the one-site states with two electrons (N_2) and one electron with spin projection σ (N_σ).

CHIRAL $d + id$ SUPERCONDUCTING PHASE

If we consider the interaction from only the first two coordination spheres, Fourier images J_q and V_q on a triangular lattice have the form

$$\begin{aligned} J_q &= 2J_1\left[\cos(q_y) + 2\cos\left(\frac{\sqrt{3}q_x}{2}\right)\cos\left(\frac{q_y}{2}\right)\right] \\ &+ 2J_2\left[\cos\left(\sqrt{3}q_x\right) + 2\cos\left(\frac{\sqrt{3}q_x}{2}\right)\cos\left(\frac{3q_y}{2}\right)\right], \\ V_q &= 2V_1\left[\cos(q_y) + 2\cos\left(\frac{\sqrt{3}q_x}{2}\right)\cos\left(\frac{q_y}{2}\right)\right] \\ &+ 2V_2\left[\cos\left(\sqrt{3}q_x\right) + 2\cos\left(\frac{\sqrt{3}q_x}{2}\right)\cos\left(\frac{3q_y}{2}\right)\right]. \end{aligned} \quad (3)$$

We seek the solution to the equation for the SOP with $d + id$ symmetry in the form

$$\Delta_2(q) = 2\Delta_{21}^0\varphi_{21}(q) + 2\Delta_{22}^0\varphi_{22}(q), \quad (4)$$

where the chiral basis functions

$$\begin{aligned} \varphi_{21}(q) &= \cos q_y - \cos\left(\frac{\sqrt{3}q_x}{2}\right)\cos\left(\frac{q_y}{2}\right) \\ &+ i\sqrt{3}\sin\left(\frac{\sqrt{3}q_x}{2}\right)\sin\left(\frac{q_y}{2}\right), \\ \varphi_{22}(q) &= \cos\sqrt{3}q_x - \cos\left(\frac{\sqrt{3}q_x}{2}\right)\cos\left(\frac{3q_y}{2}\right) \\ &- i\sqrt{3}\sin\left(\frac{\sqrt{3}q_x}{2}\right)\sin\left(\frac{3q_y}{2}\right) \end{aligned} \quad (5)$$

correspond to the first and second coordination spheres [4].

The system of equations for finding the temperature dependence of the chiral parameter is

$$\begin{aligned} &(1 - A_{11})\Delta_{21}^0 - A_{12}\Delta_{22}^0 = 0, \\ &-A_{21}\Delta_{21}^0 + (1 - A_{22})\Delta_{22}^0 = 0. \end{aligned} \quad (6)$$

In these equations, functions A_{ij} are defined as

$$\begin{aligned} A_{11} &= \frac{2J_1 - V_1}{N}\sum_q \cos\left(\frac{\sqrt{3}}{2}q_x + \frac{1}{2}q_y\right) \\ &\times\left[\cos\left(\frac{\sqrt{3}}{2}q_x + \frac{1}{2}q_y\right) - \cos q_y\right]\frac{\tanh(E_q/2T)}{E_q}, \\ A_{12} &= \frac{2J_1 - V_1}{N}\sum_q \cos\left(\frac{\sqrt{3}}{2}q_x + \frac{1}{2}q_y\right) \\ &\times\left[\cos\left(\frac{\sqrt{3}}{2}q_x - \frac{3}{2}q_y\right) - \cos\sqrt{3}q_x\right]\frac{\tanh(E_q/2T)}{E_q}, \\ A_{22} &= \frac{2J_2 - V_2}{N}\sum_q \cos\left(\sqrt{3}q_x\right) \\ &\times\left[\cos\left(\sqrt{3}q_x\right) - \cos\left(\frac{\sqrt{3}}{2}q_x + \frac{3}{2}q_y\right)\right]\frac{\tanh(E_q/2T)}{E_q}, \\ A_{21} &= \frac{2J_2 - V_2}{N}\sum_q \cos\left(\sqrt{3}q_x\right) \\ &\times\left[\cos q_y - \cos\left(\frac{\sqrt{3}}{2}q_x + \frac{1}{2}q_y\right)\right]\frac{\tanh(E_q/2T)}{E_q}. \end{aligned} \quad (7)$$

EFFECT OF COULOMB CORRELATIONS

To describe the topological features of the superconducting phase, we use index $Q = \frac{1}{8\pi}\sum_\Delta \vec{m}_1[\vec{m}_2 \times \vec{m}_3]$ [4], where summation is performed over all triangular plaquettes. Vectors $\vec{m}_1$, $\vec{m}_2$, and $\vec{m}_3$ are calculated in the vertices of these plaquettes and $\vec{m} = \left\{\frac{Re\Delta_2(q)}{E_q}, \frac{-Im\Delta_2(q)}{E_q}, \frac{\xi_q}{E_q}\right\}$ [9]. The Q value reflects the topological structure of the superconducting phase and is related to the position of nodal points $\Delta_2(q)$. A topological quantum transition occurs if the Fermi contour crosses the normal phase of the nodal points upon variation in concentration (Fig. 1).

Allowing for the Coulomb correlations can lead to a topological transition upon variation in electron concentration x. When the two invariants are considered, the zero position depends on the ratio between amplitudes Δ_{21}^0 and Δ_{22}^0 of the complex parameter $\Delta_2(q) = 2\Delta_{21}^0\varphi_{21}(q) + 2\Delta_{22}^0\varphi_{22}(q)$. In [5], we considered possible scenarios of the evolution of a system of nodal points upon variation in electron concentration as a

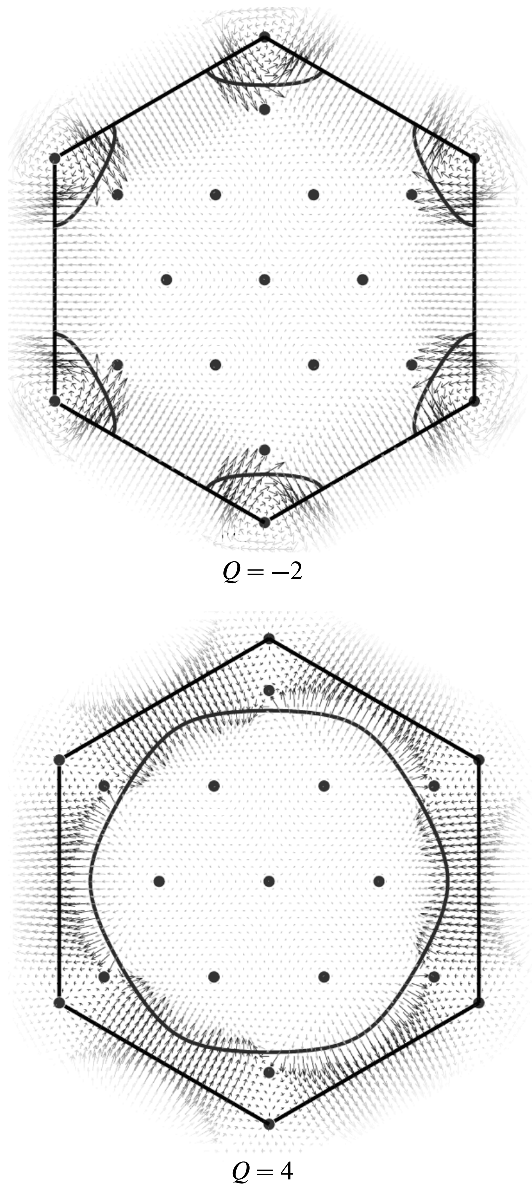

Fig. 1. Behavior of vector $\vec{m}$ at different positions of nodal points of the SOP and Fermi surface.

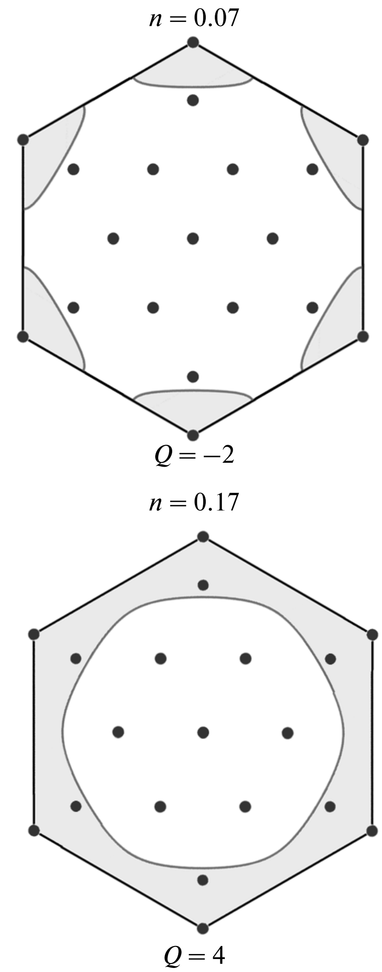

Fig. 2. Position of nodal points at different concentrations for system parameters of $t_1 = 1$, $t_2 = t_3 = 0$, $J_1 = 0.3$, $J_2 = 0.2$, $V_1 = 0.35$, and $V_2 = 0.1$.

function of the ratio between the intensities of interaction in the first $(2J_1 - V_1)$ and second $(2J_2)$ coordination spheres.

When Coulomb repulsion V_2 is switched on, the intensity of interaction in the second coordination sphere is already specified by parameter $(2J_2 - V_2)$. At weak V_2 $(V_2 \leq J_2)$, the range of parameters in which the topological quantum transition can be observed will then change.

When $V_2 \geq 2J_2$, the superconducting phase is completely suppressed or the main contribution to the SOP is made by invariant $\varphi_{21}(q)$ with no nodal points inside the band; the superconducting phase will consequently have a gap.

CONCLUSIONS

It was shown for a *t–J–V* model on a triangular lattice that the Coulomb repulsion of electrons on next-to-nearest sites narrows the range of parameters at which a gapless superconducting phase can occur.

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