Journal of Magnetism and Magnetic Materials 440 (2017) 129–132

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Effect of the three-center terms on the chiral superconducting d-wave pairing of the Hubbard fermions on the triangular lattice

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ARTICLE INFO

Keywords:
Superconductivity
Chiral order parameter
Triangular lattice

ABSTRACT

Using the diagram technique for the Hubbard operators an integral equation that determines the order parameter of the superconducting phase $\Delta(p)$ was obtained in the framework of t–J–V and t–J^*–V models on triangular lattice. It is shown that there are two scenarios of formation of superconducting phase with gapless spectrum at the critical concentration of carriers x_c. The effect of three-center terms on implementation of this phase was also considered.

1. Introduction

Layered materials with a triangular lattice (e.g., sodium cobaltite Na_xCoO_2) constantly attract the attention of researchers. These materials are of interest because of their non-trivial structure of magnetic ordering in the case of the antiferromagnetic exchange coupling between the neighboring spins. This feature is related to the frustrated nature of the exchange Hamiltonian for a triangular lattice, and, as a consequence, the induction of strong quantum fluctuations.

The discovery of superconductivity with $T_c = 5$ K in the water intercalated Na_xCoO_2 near x=0.3 [1] increased significantly the flow of research of the properties of the superconducting phase, as well as the study of the nature of Cooper instability in 2D triangular lattice systems. Particular attention was paid to the symmetry of the superconducting order parameter (SOP) (see reviews [2–4]). Since the symmetry of the triangular lattice allows the implementation of the chiral $d_{x^2-y^2} + id_{xy}$ SOP, it becomes an important to answer the question on the presence (or the absence) of a gap in the spectrum of the Fermi excitations of such a superconducting phase.

It is known that the single-orbital Hubbard model [5] can be used as a minimal model of the electronic structure of the CoO_2 plane. In the regime $U \gg |t|$ (U is the Hubbard repulsion of electrons at one site, t is the hopping integral) it is advisable to pass to the effective Hamiltonian. As efficient models are the t–J [6] and t–J^* models [7] obtained with accuracy up to terms of the second order in the parameter $|t|/U$. The superconducting phase with a complex order parameter within the t–J model on a triangular lattice was considered in [8–10]. However, in these works the interaction between fermions was taken into account only within the first coordination sphere. In this case, the nodal point of SOP is located only in the center of the Brillouin zone and at its borders, and the spectrum is gapful at all levels of doping. The paper [11] has been shown that at the accounting of the interactions on the next-nearest sites, the nodal point of the complex order parameter are within the Brillouin zone and at a certain concentration (when the Fermi surface the normal state intersects the nodal points of SOP) spectrum of the superconducting phase becomes gapless, and is characterized by six Dirac's points. In the work [12] it was considered the concentration dependence of the position of the nodal points of the SOP and conditions for the implementation of the superconducting phase with gapless spectrum were found in the framework of t–J–V model with taking into account the interactions between the electrons in the two coordination spheres. In this paper we study the effect of the three-center terms on the conditions of implementation of such a phase.

2. Formulation of models

Let us consider an ensemble of the Hubbard fermions in the framework of t–J–V and t–J^*–V models. The Hamiltonian of the t–J^* model differs from the Hamiltonian of t–J model in that it consists of the three-center term $H_{(3)}$ (6). In the representation of the Hubbard operators [13,14], the Hamiltonians take the form

$$H_{t-J} = H_0 + H_T + H_J, \tag{1}$$

$$H_{t-J^*} = H_0 + H_T + H_J + H_{(3)}, \tag{2}$$

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http://dx.doi.org/10.1016/j.jmmm.2016.12.085
Received 27 October 2016; Received in revised form 9 December 2016; Accepted 20 December 2016
Available online 23 December 2016
0304-8853/

where

$$H_0 = \sum_{f\sigma} (\varepsilon - \mu) X_f^{\sigma\sigma} + \sum_f (2\varepsilon + U - 2\mu) X_f^{22} \tag{3}$$

$$H_T = \sum_{fm\sigma} t_{fm} X_f^{2\bar{\sigma}} X_m^{\bar{\sigma}2}, \tag{4}$$

$$H_J = \frac{1}{2} \sum_{fm\sigma} J_{fm} (X_f^{\bar{\sigma}\sigma} X_m^{\sigma\bar{\sigma}} - X_f^{\bar{\sigma}\bar{\sigma}} X_m^{\sigma\sigma}), \tag{5}$$

$$H_{(3)} = - \sum_{\substack{fmg\sigma \\ (f \neq g)}} \frac{t_{fm} t_{mg}}{U} (X_f^{2\bar{\sigma}} X_m^{\bar{\sigma}\sigma} X_g^{\sigma 2} - X_f^{2\bar{\sigma}} X_m^{\sigma\sigma} X_g^{\bar{\sigma}2}). \tag{6}$$

H_0 describes the one-site energy of electrons, H_T and H_J are kinetic and exchange terms, respectively, $H_{(3)}$ describes the correlated hoppings. When taking into account the Coulomb repulsion between the electrons located on the neighboring sites in the Hamiltonians (1) and (2), the term H_V

$$H_V = \frac{1}{2} \sum_{f\delta} V (\hat{n}_f - \langle \hat{n}_f \rangle) \cdot (\hat{n}_{f+\delta} - \langle \hat{n}_{f+\delta} \rangle) \tag{7}$$

occurs and we get Hamiltonians of t–J–V and t–J^*–V models. The Hamiltonians are written in terms of the Hubbard operators for the upper Hubbard subband. Here ε is the energy of one-electron state, μ is the chemical potential of the ensemble. The operator describing the number of electrons at the site f is given by the expression $\hat{n}_f = X_f^{\uparrow\uparrow} + X_f^{\downarrow\downarrow} + 2X_f^{22}$.

The diagram technique for the Hubbard operators [14] is used to describe the superconducting phase. The equation for SOP in framework of the t–J–V model was obtained in [12]. In the mean-field approximation, the components of anomalous mass operator are determined by three graphs shown in Fig. 1. Here the thin lines correspond to the bare Green's functions and thick lines show the generalized ones. Indices near these lines determine the root vectors [13]. The wavy lines in two upper diagrams correspond to the exchange interaction, and the dashed line in lower diagram corresponds to the Coulomb repulsion of electrons. Diagrams arising from the accounting of kinetic term do not contribute to the SOP with $d + id$ type of symmetry, and therefore are not presented here. Self-consistent equation for the order parameter $\Delta(p)$ obtained within t–J–V model has the form

$$\Delta(p) = \frac{1}{N} \sum_q (J_{p+q} + J_{p-q} - V_{p-q}) \Delta(q) \frac{\tanh(E_q/2T)}{2E_q}, \tag{8}$$

where $E_q = \sqrt{\xi_q^2 + |\Delta(q)|^2}$ is the spectrum of the Hubbard fermions in superconducting phase, $\xi_p = \varepsilon + U + \frac{1+x}{2} t_p - \mu$ is the spectrum in normal phase measured from the chemical potential (contributions from the exchange and interstitial Coulomb interaction are dispersionless and are not affected to the Fermi contour, and therefore they are not shown here), $x = n - 1$ is the concentration of one-site states with two electrons.

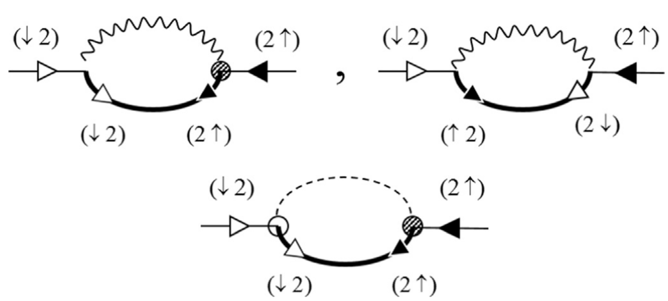

Fig. 1. One-loop diagrams for the mass operator for the t–J–V model.

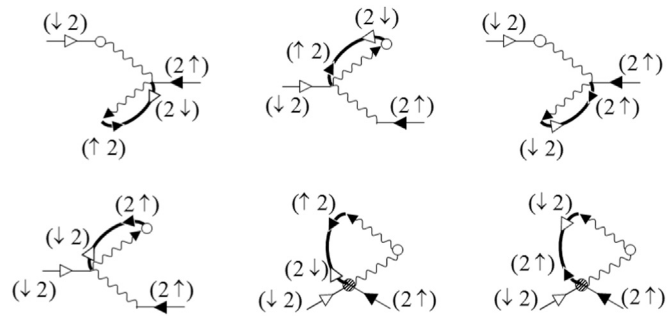

Fig. 2. One-loop diagrams for the mass operator resulting from $H_{(3)}$ term.

Account for correlated hoppings (6) leads to an additional term in the expression for the spectrum in the normal phase

$$\tilde{\xi}_p = \varepsilon + U + \frac{1+x}{2} t_p + \frac{1-x^2}{4} t_p^2 - \mu. \tag{9}$$

Additionally, several new diagrams for the mass operator occur (Fig. 2). As a result, the equation for the order parameter with the $d + id$-type symmetry in the framework of the t–J^*–V model takes the form

$$\Delta(p) = \frac{1}{N} \sum_q \left(\frac{1-x}{2} (J_{p+q} + J_{p-q}) - V_{p-q} \right) \times \Delta(q) \frac{\tanh(\widetilde{E}_q/2T)}{2\widetilde{E}_q}, \tag{10}$$

where $\widetilde{E}_q = \sqrt{\tilde{\xi}_q^2 + |\Delta(q)|^2}$. The comparison (8) and (10) shows that term H_3 leads to a renormalization of the pairing interaction due to the exchange processes. Near the bottom of band, the renormalization reduces pairing in two times and decreases it to zero with an increasing carrier concentration.

Solution of Eqs. (8) and (10) for the superconducting gap with $d + id$ symmetry can be written in the form of the superposition

$$\Delta_d(q) = 2\Delta_{d1}^0 \varphi_{d1}(q) + 2\Delta_{d2}^0 \varphi_{d2}(q), \tag{11}$$

where $\varphi_{d1}(q)$ and $\varphi_{d2}(q)$ are the complex basis functions corresponding to the first and second coordination spheres of the lattice. The expressions for the basic functions and the Fourier transforms of the interaction integrals are given in works [12,11].

Substitution of Eq. (11) into (8) or (10) leads to a system of two algebraic equations for the amplitudes Δ_{d1}^0 and Δ_{d2}^0

$$\begin{aligned} &(1 - A_{11})\Delta_{d1}^0 - A_{12}\Delta_{d2}^0 = 0, \\ &- A_{21}\Delta_{d1}^0 + (1 - A_{22})\Delta_{d2}^0 = 0. \end{aligned} \tag{12}$$

Functions A_{ij} are defined as

$$\begin{aligned} A_{11} &= (\alpha J_1 - V) \frac{1}{N} \sum_q \cos\left(\frac{\sqrt{3}}{2} q_x + \frac{1}{2} q_y\right) \times \left[\cos\left(\frac{\sqrt{3}}{2} q_x + \frac{1}{2} q_y\right) - \cos q_y\right] L_q, \\ A_{12} &= (\alpha J_1 - V) \frac{1}{N} \sum_q \cos\left(\frac{\sqrt{3}}{2} q_x + \frac{1}{2} q_y\right) \times \left[\cos\left(\frac{\sqrt{3}}{2} q_x - \frac{3}{2} q_y\right) - \cos\sqrt{3} q_x\right] L_q, \\ A_{22} &= \alpha J_2 \frac{1}{N} \sum_q \cos(\sqrt{3} q_x) \times \left[\cos(\sqrt{3} q_x) - \cos\left(\frac{\sqrt{3}}{2} q_x + \frac{3}{2} q_y\right)\right] L_q, \\ A_{21} &= \alpha J_2 \frac{1}{N} \sum_q \cos(\sqrt{3} q_x) \times \left[\cos q_y - \cos\left(\frac{\sqrt{3}}{2} q_x + \frac{1}{2} q_y\right)\right] L_q, \end{aligned} \tag{13}$$

where $L_q = \tanh(E_q/2T)/E_q$ and $\alpha = 2$ for the t–J–V model, and $L_q = \tanh(\widetilde{E}_q/2T)/\widetilde{E}_q$, $\alpha = 1 - x$ for the t–J^*–V model.

The system (12) describes the temperature dependence of $\Delta_d(q)$, and ordering temperature T_c determines by the existence of non-trivial solutions of the equation

$$(1 - A_{11})(1 - A_{22}) - A_{12}A_{21} = 0 \tag{14}$$

when $\Delta_d(q) = 0$. The solutions of this equation for both models show that the renormalization of the exchange interaction caused by the inclusion of the three-center terms, leading to a decrease in both the critical temperature and the implementation of the superconducting phase. The inclusion of the Coulomb correlations also leads to suppression of the pairing interaction.

3. Influence of Coulomb correlations on the evolution of nodal points

The importance of the Coulomb correlations is related, in particular, to the additional possibility of the formation of a gapless spectrum phase with an increase in the number of carriers. It is known that the formation of a gapless spectrum superconducting phase with a complex order parameter occurs when the Fermi surface intersects nodal point of $\Delta_d(q)$. The presence of the real and imaginary parts in the $\Delta_d(q)$ complicates this condition. In Ref. [11] it was shown that if there is only one basic function corresponding to the second coordination sphere, then zeros of $\Delta_d(q)$ are located inside the Brillouin zone.

When taking into account the interactions of the two coordination spheres the situation may change qualitatively, because the position of zeros of the two basic functions depend on the ratio of the amplitudes of Δ^0_{d1} and Δ^0_{d2} of the complex parameter $\Delta_d(q) = 2\Delta^0_{d1}\varphi_{d1}(q) + 2\Delta^0_{d2}\varphi_{d2}(q)$ (see. Fig. 3).

t–J–V model: Let us consider first the conditions of the formation of the phase with gapless spectrum in the framework of the *t–J–V* model. Fig. 4 shows the location of the nodal points of $\Delta_d(q)$ in the Brillouin zone and the Fermi contour for various system parameters. Fig. 4a corresponds to the case when the intersite Coulomb interaction is not taken into account. With an increase x the ratio $\Delta^0_{d1}/\Delta^0_{d2}$ is changed. This causes a shift of the nodal points to the center of the Brillouin zone stronger than a shift of the Fermi contour. As a result, changes in the concentration of fermions in this mode do not generate phase with gapless spectrum. This is one of the essential features associated with the superposition nature of the chiral order parameter.

When taking into account the Coulomb correlations the situation can be changed dramatically. In particular, there is a range of parameters ($V \sim J_1$), for which the mutual dynamics of the nodal points and the Fermi contour changes qualitatively (Fig. 4b). In this case, the nodal points move relatively slow and the Fermi contour manages "catch up" nodal point. At the critical concentration, the system of nodal points of $\Delta_d(q)$ located on the Fermi contour.

Thus, the Coulomb correlations between the Hubbard fermions from the first coordination sphere not only suppress tendency to pairing, but also can significantly affect the dynamics of the nodal points by modifying the partial amplitudes Δ^0_{d1} and Δ^0_{d2}, and initiate the superconducting phase with the gapless spectrum.

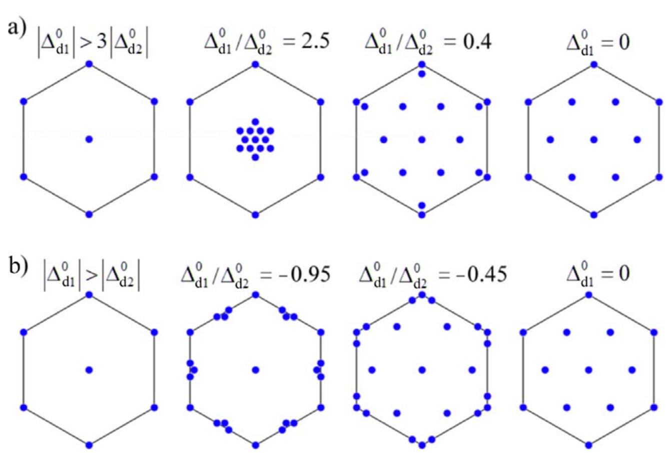

Fig. 3. The dependence of the position of nodal points of SOP with $d + id$ symmetry type at different ratios between the amplitudes Δ^0_{d1} and Δ^0_{d2} with coincide (a) and opposite (b) signs.

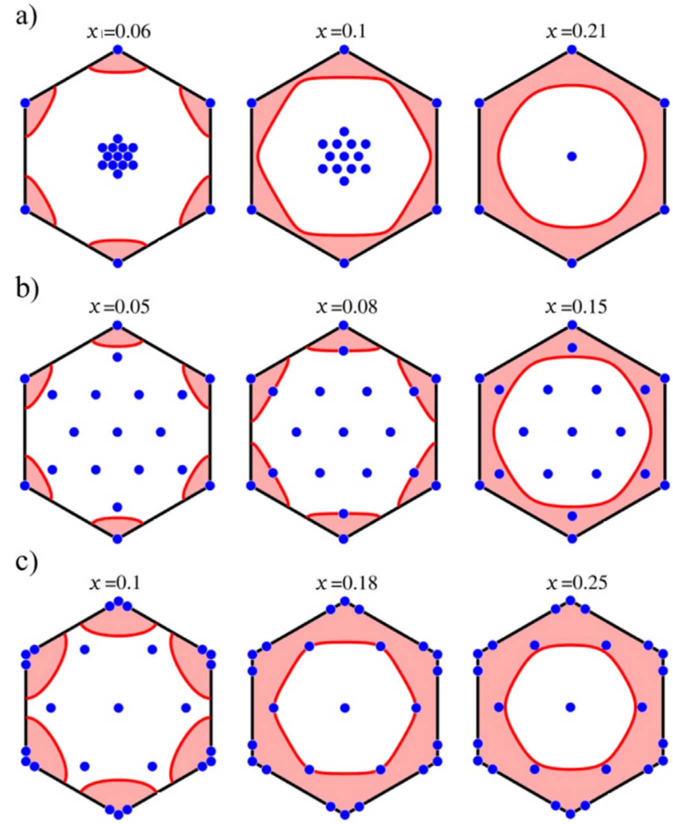

Fig. 4. Nodal points of $\Delta_d(q)$ and the Fermi contour for the *t–J–V* model calculated for the model parameters $J_1 = 0.3$; $J_2 = 0.2$ and (a) $t_2 = t_3 = 0$, V=0, (b) $t_2 = t_3 = 0$, V=0.3, (c) $t_2 = 0.2$, $t_3 = 0.15$, $V = 10$ (all parameters in the units of $|t_1|$).

In the case $V \gg J_1$, the system of nodal points becomes close to the system defined by only the second basic function. In this case, the concentration behavior of the system corresponds to the scenario described in [11], and the increase in the Coulomb interaction results only in reducing both the transition temperature and the implementation of the superconducting phase, but does not affect the position of the nodal points. In Fig. 4c the model parameters are chosen in such a way that for large values of V superconducting phase exists at the critical concentration.

t–J–V model*: As we mentioned in Section 2, an account for the three-center terms results in the renormalization of the pairing interaction. This renormalization leads to a decrease in the critical temperature and the implementation of the superconducting phase. In the absence of the Coulomb correlations (Fig. 5a), the behavior of the system does not differ qualitatively from the behavior of the *t–J* model. But if the intersite repulsion of electrons is taking into account, the transition in the gapless spectrum phase (Fig. 5b) occurs at $V \sim \frac{1}{2}J_1$. In contrast to the *t–J–V* model, in the framework of the *t–J*–V* model the second scenario of formation of phase with gapless spectrum (when $V \gg J_1$) is not implemented, because the superconductivity is destroyed at the concentrations less than the critical.

4. Conclusion

The main results of the paper are as follows:

(1) Using the diagram technique for the Hubbard operators we obtain an integral equation for the SOP within the *t–J–V* and *t–J*–V* models on the triangular lattice.

(2) It is shown that for system of the Hubbard fermions interacting at the nearest and next-nearest sites, the formation of the superconducting phase with gapless spectrum can be implemented in two qualitatively different scenarios.

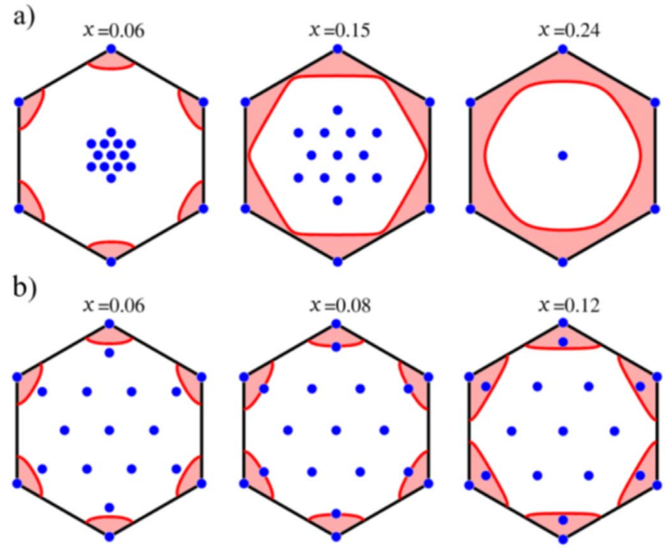

Fig. 5. Nodal points of $\Delta_d(q)$ and the Fermi contour for the t–J^*–V model excluding intersite correlations at V=0 (a), and their account V=0.15 (b). $J_1 = 0.3$; $J_2 = 0.2$; $t_2 = t_3 = 0$ (all parameters in the units of $|t_1|$).

According to the first scenario [11], which can be implemented in case of the strong Coulomb correlations, $V \gg J_1$, the system of the nodal points of SOP is determined almost by the second basic function $\varphi_{d2}(q)$ and the position of the zeros in the Brillouin zone is practically unchanged with an increase in concentration.

The second scenario is implemented when the value of V is comparable to the J. In this case, the formation of zeros of SOP involved both basis functions, and the strong dynamics of the nodal points takes place under changes of concentration.

(3) It is shown that the second scenario of the formation of a phase with gapless spectrum within the t–J–V model is implemented at $V \sim J_1$, while for t–J^*–V model it is implemented at $V \sim \frac{1}{2}J_1$ because of renormalization of the exchange interaction by three-center terms.

(4) We found the parameters of the model, in which the formation of a gapless spectrum phase within t–J–V model takes place in the first scenario. But within t–J^*–V model this scenario is not implemented due to the fact that the superconductivity is destroyed at concentrations less than critical ones.

Acknowledgments

The reported study was funded by the Russian Foundation for Basic Research, project no. 16-02-00073 and by Russian Foundation for Basic Research, Government of Krasnoyarsk Territory, Krasnoyarsk Region Science and Technology Support Fund to the research project no. 16-42-240435.

References

[1] K. Takada, H. Sakurai, E. Takayama-Muromachi, F. Izumi, R.A. Dilanian, T. Sasaki, Nature 422 (2003) 53.
[2] Y. Yanase, M. Mochizuki, M. Ogata, J. Phys. Soc. Jpn. 74 (2005) 430.
[3] M. Ogata, J. Phys.: Condens. Matter 19 (2007) 145282.
[4] N.B. Ivanova, S.G. Ovchinnikov, M.M. Korshunov, I.M. Eremin, N.V. Kazak, Phys. Usp. 52 (2009) 789.
[5] J. Hubbard, Proc. R. Soc. Lond. Ser. A 276 (1963) 238.
[6] N.M. Plakida, High-Temperature Superconductivity, Springer, Berlin, 1995.
[7] V.V. Val'kov, T.A. Val'kova, D.M. Dzebisashvili, S.G. Ovchinnikov, JETP Lett. 75 (2002) 378.
[8] G. Baskaran, Phys. Rev. Lett. 91 (2003) 097003.
[9] B. Kumar, B.S. Shastry, Phys. Rev. B 68 (2005) 104508.
[10] M. Ogata, J. Phys. Soc. Jpn. 72 (2003) 1839.
[11] S. Zhou, Z. Wang, Phys. Rev. Lett. 100 (2008) 217002.
[12] V.V. Val'kov, T.A. Val'kova, V.A. Mitskan, JETP Lett. 102 (2015) 361.
[13] R.O. Zaitsev, Sov. Phys. JETP 41 (1975) 100.
[14] R.O. Zaitsev, Diagram Methods in Theory of Superconductivity and Ferromagnetism, URSS, Moscow, 2004 [in Russian].