The triplet superconductivity in square lattices and its optimal doping dependence

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Abstract

In this work, we study the p-wave superconductivity in a square lattice within a Hubbard model, in which a second-neighbour correlated hopping $D_{t_3}$ is included. An infinitesimal distortion of the right angles in the square lattice is considered, which leads to second correlated hoppings $D_{t_3} \pm \delta t$ in the $\hat{x} \pm \hat{y}$ directions, respectively. This study is carried out by means of the BCS formalism and we found a triplet superconducting ground state even though $V=0$. The optimal electron density for the critical temperature and the superconducting gap is analyzed as a function of the parameters of the model. Finally, the single-particle excitation gap is also calculated for different electron densities.

Keywords: D. Superconductivity; A. Superconductors

1. Introduction

It has been proposed that the Sr$_2$RuO$_4$ exhibits a spin-triplet or p-wave superconductivity [1], in contrast to the d-wave pairing found in many cuprates [2]. In fact, Sr,RuO$_4$ is structurally similar to the first cuprate superconductor, (La, Sr)$_2$CuO$_4$, and its electrons in the RuO$_2$ planes are expected to play the most important role for the superconductivity [1]. It is accepted that the so-called $\gamma$ band plays the dominant role in the superconducting transition, and the pairing on the other two bands, $\alpha$ and $\beta$, is induced passively through the inter-orbit couplings [3]. Furthermore, a structural distortion has been observed at the surface of the Sr$_2$RuO$_4$ [4], although it is not clear its occurrence in the bulk. In order to describe the electron dynamics on the RuO$_2$ planes, a single-band Hubbard model is considered [3,5] and, in the vicinity of the Fermi level, the LDA band structure can be reasonably well described by a square-lattice single $\gamma$-band tight-binding model with first- and second-neighbour hoppings $t_0=0.4$ and $t'_0=-0.12$ eV, respectively, [6]. On the other hand, it has been reported that the Hubbard model could lead to an anisotropic superconducting gap if a second-neighbour correlated hopping ($D_{t_3}$) is included, in addition to the on-site $U$ and nearest-neighbour $V$ repulsions [7]. In this paper, we study the effects of a structural distortion on the p-wave superconducting state as well as the electron density dependence of the critical temperature and superconducting gap. By considering a small distortion in the right angles of a square lattice, the degeneracy of the $k_x \pm k_y$ oriented p-wave superconducting states is broken favouring one of the p-wave states in competition with the s- and d-wave superconducting states. Moreover, the existence of an optimal doping in the superconducting state is analyzed in terms of the expectation value of the potential energy of the system. Finally, we calculated the single-particle excitation energy gap for different values of the electron concentration.

2. The model

We start from a Hubbard model in which first- ($\Delta t$) and second-neighbour ($\Delta t_3$) correlated-hopping interactions are considered in addition to the on-site ($U$), and nearest-neighbour ($V$) Coulomb interactions. This model has lead to s- and d-wave hole-superconducting ground states without negative $U$ and $V$ [7,8], hence this Hubbard Hamiltonian can be written as [9,10]
\[
H = -t_0 \sum_{\langle ij \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} - t_0' \sum_{\langle ij \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \times \sum_{\langle ij \rangle} n_i n_j + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \sum_i n_i n_j + \Delta t \times \sum_{\langle ij \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma}(n_{i,-\sigma} + n_{j,-\sigma}) + \Delta t_\delta \sum_{\langle ij \rangle, \langle jk \rangle, \langle ki \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} n_j,
\]

where \(c_{i,\sigma}^\dagger(c_{i,\sigma})\) is the creation (annihilation) operator with spin \(\sigma = \downarrow\) or \(\uparrow\) at site \(i\), \(n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}\), \(n_i = n_{i,\uparrow} + n_{i,\downarrow}\), \(\langle ij \rangle\) and \(\langle jk \rangle\) denote, respectively, the nearest-neighbour and the next-nearest-neighbour sites.

Let us consider a square lattice with lattice parameter \(a\). In order to break the degeneracy of p-wave pairing states, we will further consider a small distortion of the right angles in the square lattice, which leads to changes in the second-neighbour interactions, such as \(t'\) and \(\Delta t\) terms in Eq. (1), and their new values are \(t'_0 = t_0' \pm \delta\) and \(\Delta t'_3 = \Delta t_3 \pm \delta_3\), where \(\pm\) refers to the \(x\) or \(y\) direction. Performing a Fourier transform,

\[
c_{k,\sigma} = \frac{1}{\sqrt{N_s}} \sum_j e^{i k \cdot R_j} c_{j,\sigma},
\]

and

\[
c_{k,\sigma}^\dagger = \frac{1}{\sqrt{N_s}} \sum_j e^{i k \cdot R_j} c_{j,\sigma}^\dagger,
\]

the Hamiltonian [Eq. (1)] in the momentum space becomes

\[
H = \sum_{k, \sigma} \epsilon_0(k)c_{k,\sigma}^\dagger c_{k,\sigma} + \frac{1}{N_s} \times \sum_{k'k'q} V_{k'k'q} c_{k+q,\sigma}^\dagger c_{k',-q,\sigma} + \frac{1}{N_s} \times \sum_{k'k'q} W_{k'k'q} c_{k+q,\sigma}^\dagger c_{k',-q,\sigma} + \frac{1}{N_s} \times \sum_{k'k'q} W_{k'k'q} c_{-k,\sigma}^\dagger c_{k'+q,\sigma} + \frac{1}{N_s} \times \sum_{k'k'q} W_{k'k'q} c_{-k,\sigma}^\dagger c_{k'-q,\sigma},
\]

where \(N_s\) is the total number of sites,

\[
\epsilon_0(k) = -2t_0[\cos(k_xa) + \cos(k_ya)] - 2t_0' \cos(k_x + k_y) - 2t'_0 \cos(k_x - k_y),
\]

\[
V_{k'k'q} = U + V \beta(k - k') + \Delta t_\delta \gamma(k + q) + \Delta t_3 \gamma(k + q) + \beta(k' + q) + \beta(-k' + q) + \Delta t_\delta \gamma(k + q, k') + \gamma(-k + q, -k' + q) + \Delta t_3 \gamma(k + q, k') + \gamma(-k + q, -k' + q),
\]

and

\[
W_{k'k'q} = \frac{V}{2} \beta(k - k') + \Delta t_\delta \gamma(k + q, k' + q) + \Delta t_3 \gamma(k + q, k' + q).
\]

where \(\beta(k) = 2[\cos(k_xa) + \cos(k_ya)]\), \(\gamma(k, k') = 2 \cos[a(k_x + k'_x)] + 2 \cos[a(k'_y - k_y)]\), and \(2q\) is the wave vector corresponding to the centre of mass of pairs. Notice that \(V_{kk'q}\) and \(W_{kk'q}\), respectively, contribute to antiparallel and parallel spin pairings, and their main contributions come from \(q = 0\) terms.

Within the standard BCS formalism, a normal Hartree–Fock decoupling of the interaction terms in Eq. (4) leads to the following reduced Hamiltonian for pairs with parallel spins \([11,12]\),

\[
H - \mu N = H_1 + H_2
\]

where

\[
H_1 = \sum_{k, \sigma} \left[\epsilon(k) - \mu\right] c_{k,\sigma}^\dagger c_{k,\sigma},
\]

\[
H_2 = \frac{1}{N_s} \sum_{k, k', \sigma} W_{kk'q} c_{k,\sigma}^\dagger c_{k',-q,\sigma} c_{k',\sigma} c_{k,\sigma},
\]

\[
\mu \text{ is the chemical potential, } N \text{ is the number of electrons, and }
\]

\[
\epsilon(k) = \left(\frac{U}{2} + 4V\right)n + 2(t_0 + n\Delta t)[\cos(k_xa) + \cos(k_ya)] + 2(t'_0 + 2n\Delta t_3)[\cos(k_x + k_y) + 2(t'_0 + 2n\Delta t_3)[\cos(k_x - k_y)],
\]

being \(n\) the density of electrons per site. Notice that the single-electron dispersion relation \(\epsilon(k)\) is now modified by adding terms \(n\Delta t, 2n\Delta t_3\) and \((U/2 + 4V)n\) to the hoppings \(t_0, t'_0\) and the self-energy, respectively.

At finite temperature \(T\), the equations that determine the superconducting gap \(\Delta(k)\) and the chemical potential \(\mu\) for the case of parallel spins are \([7]\),

\[
\Delta_k = -\frac{1}{N_s} \sum_k W_{kk'0} \frac{\Delta k'}{2E_{k'}} \tanh \left(\frac{E_{k'}}{2k_b T}\right),
\]

and

\[
n - 1 = -\frac{1}{N_s} \sum_k \frac{\epsilon(k') - \mu}{E_{k'}} \tanh \left(\frac{E_{k'}}{2k_b T}\right),
\]

where the single-particle excitation energy \(E_k\) is

\[
E_k = \sqrt{(\epsilon(k) - \mu)^2 + \Delta_k^2}.
\]
and the p-wave superconducting gap is given by $\Delta_k = \Delta_p \{ \sin(k_x a) \pm \sin(k_y a) \}$. It is worth mentioning that for the case of $(|\uparrow\uparrow| + |\downarrow\downarrow|)/\sqrt{2}$ pairs, the same Eqs. (15) and (16) are obtained except that $V_{kk'/0}$ replaces $W_{kk'/0}$, hence the Eq. (15) can be written as

$$1 = -\frac{(V + 4\delta_3)}{N_S} \sum_k (\sin^2 ak_x \pm \sin ak_y \sin ak_y) \times \frac{1}{E_k} \tanh \left( \frac{E_k}{2k_B T} \right).$$

where $\delta_3 = (\Delta_{t1}^2 - \Delta_t^2)/2$. Notice that, for given $n$ and $T$, Eqs. (16) and (18) have to be solved simultaneously for $\mu$ and $\Delta_p$. In particular, the critical temperature $T_c$ is determined by $\Delta_p(t_c) = 0$. For the case of triplets with $(|\uparrow\downarrow| + |\downarrow\uparrow|)/\sqrt{2}$ and $q = 0$, the terms $U$ and $\Delta_t$ in Eq. (7) are even functions in the $k'$ space and $\Delta_k = \Delta_p \{ \sin(k_x a) \pm \sin(k_y a) \}$ is odd, and then the sum over the first Brillouin zone of the product of them is zero. Furthermore, the terms $V$ and $\Delta_{t1}^2$ reduce to those of $W_{kk'/0}$, except for a factor of 2. However, due to the sum over the spin index $\sigma$ in the third term of Eq. (4), it turns out that triplets with antiparallel spins obey the same Eqs. (16) and (18).

In order to analyze the doping dependence of the superconducting gap and critical temperature, we studied the average potential energy ($W_T$) given by [12]

$$W_T = \langle H_z \rangle = \frac{1}{2} \int \frac{dk_x dk_y}{BZ} \left( W_{kk'} - W_{k-k'} u_k u_k v_{k} d k_x dk_y dk'_x dk'_y \right)$$

where $\langle \ldots \rangle$ indicates the ground state expectation value, with the functions $u_k$ and $v_k$ given by

$$u_k = \left( \frac{1}{2} - \frac{\epsilon(k) - \mu}{2E_k} \right)^{1/2} \quad \text{and} \quad v_k = \left( \frac{1}{2} + \frac{\epsilon(k) - \mu}{2E_k} \right)^{1/2}.$$

Replacing the expression for the electron-electron interaction (Eq. (7)), $W_T$ becomes

$$W_T = \frac{V}{16\pi^4} \int \frac{dk_x dk_y dk'_x dk'_y}{BZ} \left[ \sin(k_x a) \sin(k'_x a) + \sin(k_y a) \sin(k'_y a) \right] \times \frac{1}{E_k} \left[ \left( \frac{\epsilon(k) - \mu}{E_k} \right)^2 \right]^{1/2} \left[ \left( \frac{\epsilon(k') - \mu}{E_k} \right)^2 \right]^{1/2} - \frac{3\delta_3}{4\pi^2} \times \left[ \int \frac{dk_x dk_y dk'_x dk'_y}{BZ} \left[ \sin(k_x a) \sin(k'_x a) + \sin(k_y a) \sin(k'_y a) \right] \right] \times \frac{1}{E_k} \left[ \left( \frac{\epsilon(k) - \mu}{E_k} \right)^2 \right]^{1/2} \left[ \left( \frac{\epsilon(k') - \mu}{E_k} \right)^2 \right]^{1/2}.$$

where each integral is performed over the first Brillouin zone (BZ).

3. The results

For the strong coupling limit, i.e. $t_0$, $t'_0 \rightarrow 0$, analytical solutions of Eqs. (15) and (16) have been obtained for the low density regime ($n \rightarrow 0$), and they are

$$\frac{\Delta_p}{\delta_3} = 2\sqrt{2} \left( \frac{9n}{4} \right), \quad \text{and} \quad \frac{k_B T_c}{\delta_3} = \frac{1 - n}{\tanh^{-1}(1 - n)}.$$

In Fig. 1(a) and (b), numerical results of $\Delta_p/\delta_3$ and $T_c/\delta_3$ versus $n$ are, respectively, shown for arbitrary $\delta_3$ and $U$, and the rest of parameters equal to zero, where the analytical solutions are indicated by dashed lines. Notice that in this limit $\Delta_p/\delta_3$ and $T_c/\delta_3$ are functions of $n$ only.

Fig. 2(a)–(c) show $T_c$, $\Delta_p$ and $W_{rt}$, respectively, for $V = \Delta_t = \delta = 0$, $t_0 = 0.4$, $t'_0 = -0.12$ eV, $\delta = 0.15$ eV and $\Delta_{t1} = 0.3$ eV (circles), 0.2 eV (up triangles), and 0 (down triangles) as a function of $n$. We can observe the existence of an optimal electron density ($n_{op}$), given by $n_{op} = 0.52$, 0.55, and 0.61 for $T_c(n)$; $n_{op} = 0.528$, 0.592 and 0.64 for $\Delta_p(n)$; and $n_{op} = 0.524$, 0.592 and 0.64 for $W_{rt}(n)$, respectively. Notice that for the three systems shown, the optimal doping for $\Delta_p$ is shifted to higher carrier concentrations with respect to the optimal doping for $T_c$, which is due to the slight change of the chemical potential ($\mu$) when $T$ changes from $T_c$ to 0 K. However, the optimal electron density for $W_{rt}$ is essentially the same as $\Delta_p$. Moreover, for

![Fig. 1. Numerical results (solid lines) of p-channel (a) superconducting gap ($\Delta_p$) and (b) critical temperature ($T_c$) versus the electron concentration ($n$), for arbitrary $\delta$ and $U$, and the other are taken parameters equal to zero, in comparison with the analytical solutions (dashed lines) valid for $n \rightarrow 0$.](image-url)
fixed $t_0 > 0$ and $t'_0 < 0$, $n_{op}$ shifts to higher densities when $\Delta_3$ or $\delta_3$ diminish as shown in Fig. 3, where $T_c$ is plotted as a function of $n$, for $V = \Delta_1 = \Delta_3 = 0$, $t_0 = 0.4$ eV, $t'_0 = -0.12$ eV, and $\delta_3 = 0.06$ eV. In this case, $n_{op} \approx 0.875$ and the maximum critical temperature is about 2 K.

On the other hand, the influence of the kinetic energy on the location of $n_{op}$ is important, since if it is diminished, $T_c$ and $\Delta_p$ increase and $n_{op}$ moves to a greater value. In general, it has been seen that, for $t_0 = 0.4$ and $t'_0 = -0.12$ eV, by increasing $\Delta t$, $n_{op}$ shifts towards 1, and $T_c$ and $\Delta_p$ decrease but if $\Delta t$ or $\delta_3$ increase, $n_{op}$ moves towards 0 and $T_c$ and $\Delta_p$ increase.

However, for $t_0 < 0$ the effect is inverse for $\Delta t$ and $\Delta_3$, respectively, the diminished of $\delta_3$ act always with a decreasing for $T_c$ and $\Delta_0$ and $n_{op}$ shifting to 1.

In Fig. 4(a)–(c), the angular dependence of the single-particle excitation gap $[\Delta_p(\theta)]$ is shown for a system with $V = \Delta t = \delta = 0$, $t_0 = 0.4$, $t'_0 = -0.12$ eV, $\Delta_3 = 0.2$ eV, arbitrary $U$ and $n = 0.5, 0.55$ and 0.6, respectively. The polar angle is given by $\theta = \tan^{-1}(k_y/k_x)$ and $\Delta_0$ is defined as the minimum value of $E_k$ given by Eq. (17), with $\Delta_k = \Delta_p[\sin(k_x a) + \sin(k_y a)]$, and we have measured the energy from the $(\pi, \pi)$ point since the minimum is located there. Notice that $\Delta_0$ changes its form when $n$ grows from a $p$-wave spectrum to an $f$-wave one, in analogy to that previously found for the $d$-wave case, where both $d_{x^2-y^2}$- and $d_{xy}$-symmetry single-particle excitation energy gaps are predicted, depending on the hole density [13].

4. Conclusions

In summary, we have studied the electron concentration dependence of the $p$-wave superconducting state in a distorted square-lattice by means of a Hubbard model, in which first- and second neighbour correlated hoppings are considered. For the dilute limit, we have been able to obtain an analytical solution. Additionally, we have shown the correspondence between the minimum of the potential energy and the maximum of the
superconducting gap and critical temperature. We have also shown the key participation of the second correlated hoppings $\Delta t^G_2$ in the formation of a p-wave superconducting state. The results also show that the optimal carrier concentration $n_{op}$ for $\Delta_p$ coincide with that of the superconducting gap $W_T$. Finally, this model predicts the existence of both p- and f-wave single-particle excitation energy gaps depending on the electron density.

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