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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 Δt_3 is included. An infinitesimal distortion of the right angles in the square lattice is considered, which leads to second correlated hoppings $\Delta t_3 \pm \delta_3$ 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_2RuO_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_2RuO_4 is structurally similar to the first cuprate superconductor, $(La,Sr)_2CuO_4$, 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 γ band plays the dominant role in the superconducting transition, and the pairing on the other two bands, α and β, is induced passively through the inter-orbit couplings [3]. Furthermore, a structural distortion has been observed at the surface of the Sr_2RuO_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 γ-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 (Δt_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- (Δt) and second-neighbour (Δt_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]

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$$H = -t_0 \sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} - t'_0 \sum_{\langle\langle i,j\rangle\rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \times \sum_{\langle i,j\rangle} n_i n_j + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \frac{V}{2} \sum_{\langle i,j\rangle} n_i n_j + \Delta t \times \sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} (n_{i,-\sigma} + n_{j,-\sigma}) + \Delta t_3 \sum_{\langle i,l\rangle,\langle j,l\rangle,\langle\langle i,j\rangle\rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} n_l, \quad (1)$$

where $c^{\dagger}_{i,\sigma}(c_{i,\sigma})$ is the creation (annihilation) operator with spin $\sigma = \downarrow$ or $\uparrow$ at site i, $n_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$, $n_i = n_{i,\uparrow} + n_{i,\downarrow}$, $\langle i,j\rangle$ and $\langle\langle i,j\rangle\rangle$ 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 Δt_3 terms in Eq. (1), and their new values are $t'_{\pm} = t'_0 \pm \delta$ and $\Delta t_3^{\pm} = \Delta t_3 \pm \delta_3$, where $\pm$ refers to the $x \pm y$ direction. Performing a Fourier transform,

$$c_{\mathbf{k},\sigma} = \frac{1}{\sqrt{N_s}} \sum_j e^{i\mathbf{k}\cdot\mathbf{R}_j} c_{j,\sigma}, \quad (2)$$

and

$$c^{\dagger}_{\mathbf{k},\sigma} = \frac{1}{\sqrt{N_s}} \sum_j e^{i\mathbf{k}\cdot\mathbf{R}_j} c^{\dagger}_{j,\sigma}, \quad (3)$$

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

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_0(\mathbf{k}) c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{1}{N_s} \times \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{\mathbf{k}k'q} c^{\dagger}_{\mathbf{k}+\mathbf{q},\uparrow} c^{\dagger}_{-\mathbf{k}+\mathbf{q},\downarrow} c_{-\mathbf{k}'+\mathbf{q},\downarrow} c_{\mathbf{k}'+\mathbf{q},\uparrow} + \frac{1}{N_s} \times \sum_{\mathbf{k},\mathbf{k}',(5)\mathbf{q},\sigma} W_{\mathbf{k}k'q} c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma} c^{\dagger}_{-\mathbf{k}+\mathbf{q},\sigma} c_{-\mathbf{k}'+\mathbf{q},\sigma} c_{\mathbf{k}'+\mathbf{q},\sigma}, \quad (4)$$

where N_s is the total number of sites,

$$\varepsilon_0(\mathbf{k}) = -2t_0[\cos(k_x a) + \cos(k_y a)] - 2t'_+ \cos(k_x + k_y) - 2t'_- \cos(k_x - k_y), \quad (5)$$

$$V_{\mathbf{k}k'q} = U + V\beta(\mathbf{k}-\mathbf{k}') + \Delta t[\beta(\mathbf{k}+\mathbf{q}) + \beta(-\mathbf{k}+\mathbf{q}) + \beta(\mathbf{k}'+\mathbf{q}) + \beta(-\mathbf{k}'+\mathbf{q})] + \Delta t_3^{+}[\gamma(\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}) + \gamma(-\mathbf{k}+\mathbf{q},-\mathbf{k}'+\mathbf{q})] + \Delta t_3^{-}[\zeta(\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}) + \zeta(-\mathbf{k}+\mathbf{q},-\mathbf{k}'+\mathbf{q})], \quad (6)$$

and

$$W_{\mathbf{k},\mathbf{k}',\mathbf{q}} = \frac{V}{2}\beta(\mathbf{k}-\mathbf{k}') + \Delta t_3^{+}\gamma(\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}) + \Delta t_3^{-}\zeta(\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}). \quad (7)$$

being

$$\beta(\mathbf{k}) = 2[\cos(k_x a) + \cos(k_y a)], \quad (8)$$

$$\gamma(\mathbf{k},\mathbf{k}') = 2\cos[a(k_x + k'_y)] + 2\cos[a(k'_x + k_y)], \quad (9)$$

$$\zeta(\mathbf{k},\mathbf{k}') = 2\cos[a(k_x - k'_y)] + 2\cos[a(k'_x - k_y)], \quad (10)$$

and 2q is the wave vector corresponding to the centre of mass of pairs. Notice that $V_{\mathrm{kk'q}}$ and $W_{\mathrm{kk'q}}$, 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

$$H_1 \equiv \sum_{\mathbf{k},\sigma} [\varepsilon(\mathbf{k}) - \mu] c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}, \quad (11)$$

$$H_2 \equiv \frac{1}{N_s} \sum_{\mathbf{k},\mathbf{k}',\sigma} W_{\mathbf{k}k'0} c^{\dagger}_{\mathbf{k},\sigma} c^{\dagger}_{-\mathbf{k},\sigma} c_{-\mathbf{k}',\sigma} c_{\mathbf{k}',\sigma}, \quad (12)$$

μ is the chemical potential, N is the number of electrons, and

$$\varepsilon(\mathbf{k}) = \left(\frac{U}{2} + 4V\right) n + 2(t_0 + n\Delta t)[\cos(k_x a) + \cos(k_y a)] + 2(t'_+ + 2n\Delta t_3^{+})\cos(k_x + k_y) + 2(t'_- + 2n\Delta t_3^{-})\cos(k_x - k_y), \quad (13)$$

being n the density of electrons per site. Notice that the single-electron dispersion relation $\varepsilon(\mathrm{k})$ is now modified by adding terms $n\Delta t$, $2n\Delta t_3^{\pm}$ 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 (Δ_{k}) and the chemical potential (μ) for the case of parallel spins are [7],

$$\Delta_{\mathbf{k}} = -\frac{1}{N_s} \sum_{\mathbf{k}'} W_{\mathbf{k}k'0} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2k_B T}\right), \quad (14)$$

and

$$n - 1 = -\frac{1}{N_s} \sum_{\mathbf{k}'} \frac{\varepsilon(\mathbf{k}') - \mu}{E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2k_B T}\right), \quad (15)$$

where the single-particle excitation energy ($\mathrm{E_k}$) is

$$E_{\mathbf{k}} = \sqrt{(\varepsilon(\mathbf{k}) - \mu)^2 + \Delta^2_{\mathbf{k}}}. \quad (16)$$