Magnetic-field influence on anisotropic *p*- and *d*-wave superconductivity

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ABSTRACT

Based on the BCS formalism, we propose a unified description of the anisotropic *p*- and *d*-wave superconducting states by using a local interacting electron model with a unique second-neighbour correlated-hopping interaction. In this work, we study the dependence of both *p*- and *d*-channel critical temperatures (T_c) on the electron concentration (n), as well as the angular dependence of single-particle excitation energy gaps (Δ_0), which can be measured by the angle-resolved photoemission spectroscopy (ARPES) and the tunnelling spectroscopy. The effects of an external magnetic field on T_c and Δ_0 in anisotropic superconductors are also investigated within the rigid band-shift approximation.

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1. Introduction

In the last two decades, the observation of *d*-wave pairing in cuprate superconductors has motivated the research of models beyond the standard BCS theory [1]. The recent discovery of the *p*-wave spin-triplet superconductivity in Sr_2RuO_4 [2] has highly enhanced this research. The two-dimensional nature present in both systems could be essential for understanding their anisotropic superconductivity. A considerable number of experiments, including angle-resolved photoemission spectroscopy (ARPES) [3] and phase-sensitive ones [4], have suggested a $d_{x^2-y^2}$ symmetry superconducting gap in many cuprate superconductors [5]. Likewise, quantum interference measurements have established the odd-parity superconductivity in Sr_2RuO_4 [6].

From theoretical point of view, three-band Hubbard models have been proposed to describe the dynamics of carriers on CuO_2 [7] and RuO_2 [8] planes. The electronic states close to the Fermi energy can be reasonably well described by a single-band tight-binding model on a square lattice with second-neighbour hoppings [9,10]. Recently, we have found that a small correlated second-neighbour interaction can lead to *d*-wave superconductivity [11] and a *p*-wave superconducting ground state could be induced by a small distortion of the square-lattice right angles within a generalized Hubbard model [12]. It would be worth mentioning that a structural distortion has been observed at the surface of Sr_2RuO_4 [13], although it is not proved its occurrence in the bulk. In this work, we study the effects of an external magnetic field on the critical temperature (T_c) and on the single-particle excitation energy gap (Δ_0) by using a single-band electronic Hamiltonian with a second-neighbour correlated-hopping interaction (Δt). This correlated hopping describes the interaction between an electronic charge at site *l* and a bond charge located between sites *i* and *j*, which are mutually second neighbours and are also first neighbours of site *l*. In spite of its generally small strength in comparison with density–density interactions, the correlated hopping is always present in real solids and can lead to anisotropic superconducting ground states [11,12], which are not sensitive to the onsite Coulomb repulsion.

2. The model

We start from the following Hamiltonian,

$$\hat{H} = t \sum_{\substack{\langle i,j \rangle \\ \sigma}} c_{i,\sigma}^{\dagger} c_{j,\sigma} + t' \sum_{\substack{\langle\langle i,j \rangle\rangle \\ \sigma}} c_{i,\sigma}^{\dagger} c_{j,\sigma} + \Delta t$$
$$\times \sum_{\substack{\langle\langle i,j \rangle\rangle, \sigma \\ \langle i,l \rangle, \langle j,l \rangle}} c_{i,\sigma}^{\dagger} c_{j,\sigma} n_l - \mu_B B \sum_i (n_{i,\uparrow} - n_{i,\downarrow}) \quad (1)$$

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 $\langle\langle ij \rangle\rangle$ denote, respectively, nearest-neighbor and next-nearest-neighbor sites. In Eq. (1), the last term represents the change in energy due to an external magnetic field (B), where $\mu_B \simeq 5.788 \times 10^{-5}$ eV/Tesla is the Bohr magneton. We further consider an electron–electron interaction shell of width (W) around the chemical potential (μ),

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as in the BCS theory [14], *i.e.*,

$$\Delta t(\varepsilon_\sigma(k)) = \begin{cases} \Delta t_3, & \text{if } |\varepsilon_\sigma(k) - \mu| \leq W \\ 0, & \text{other cases} \end{cases} \quad (2)$$

where $\varepsilon_\sigma(\boldsymbol{k}) = \langle \boldsymbol{k}, \sigma | \hat{H} | \boldsymbol{k}, \sigma \rangle$ is the single-electron energy, being $|\boldsymbol{k}, \sigma\rangle$ the Bloch states. In addition, for Sr_2RuO_4 a small distortion of the right angles in the square lattice is included, in consequence, the second-neighbour hopping (t') and interaction (Δt) parameters change, respectively, to $t'_\pm \equiv t' \pm \delta$ and $\Delta t_\pm \equiv \Delta t \pm \delta$, where

$$\delta(\varepsilon_\sigma(\boldsymbol{k})) = \begin{cases} \delta_3, & \text{if } |\varepsilon_\sigma(k) - \mu| \leq W \\ 0, & \text{other cases} \end{cases} \quad (3)$$

and $\pm$ refers to the $\hat{x} \pm \hat{y}$ directions.

Performing a Fourier transform with

$$c_{\boldsymbol{k},\sigma} \equiv \frac{1}{\sqrt{N_S}} \sum_j e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j} c_{j,\sigma}, \quad (4)$$

where N_S is the total number of sites, and after a standard Hartree–Fock decoupling of the interaction term in Eq. (1), the Hamiltonian can be rewritten in the momentum space as

$$\hat{H} = \sum_{\boldsymbol{k},\sigma} \varepsilon_\sigma(\boldsymbol{k}) c_{\boldsymbol{k},\sigma}^\dagger c_{\boldsymbol{k},\sigma} + \frac{1}{N_S} \sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} c_{\boldsymbol{k}+\boldsymbol{q},\uparrow}^\dagger c_{-\boldsymbol{k}'+\boldsymbol{q},\downarrow}^\dagger c_{-\boldsymbol{k}'+\boldsymbol{q},\downarrow} c_{\boldsymbol{k}+\boldsymbol{q},\uparrow}$$
$$+ \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} W_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} c_{\boldsymbol{k}+\boldsymbol{q},\sigma}^\dagger c_{-\boldsymbol{k}'+\boldsymbol{q},\sigma}^\dagger c_{-\boldsymbol{k}'+\boldsymbol{q},\sigma} c_{\boldsymbol{k}+\boldsymbol{q},\sigma} \quad (5)$$

where

$$\varepsilon_\sigma(\boldsymbol{k}) = -\sigma\mu_B B + 2(t'_+ + 2n \Delta t_+) \cos(k_x a + k_y a) + 2(t'_-$$
$$+ 2n \Delta t_-) \cos(k_x a - k_y a) + 2t[\cos(k_x a) + \cos(k_y a)], \quad (6)$$

$$V_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} = \Delta t_+ [\gamma(\boldsymbol{k}+\boldsymbol{q}, \boldsymbol{k}'+\boldsymbol{q}) + \gamma(-\boldsymbol{k}+\boldsymbol{q}, -\boldsymbol{k}'+\boldsymbol{q})]$$
$$+ \Delta t_- [\zeta(\boldsymbol{k}+\boldsymbol{q}, \boldsymbol{k}'+\boldsymbol{q}) + \zeta(-\boldsymbol{k}+\boldsymbol{q}, -k'+\boldsymbol{q})], \quad (7)$$

and

$$W_{k,k',q} = \Delta t_+ \gamma(k+q, k'+q) + \Delta t_- \zeta(k+q, k'+q), \quad (8)$$

being

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

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

a is the lattice constant and $2\boldsymbol{q}$ is the wave vector of the pair centre of mass.

Applying the BCS formalism [14] to Eq. (5) for $\boldsymbol{q} = 0$, we obtain the following two coupled integral equations for the d-channel superconductivity,

$$\begin{cases} 1 = \dfrac{1}{N_S} \sum_{k,\sigma} \dfrac{\Delta t(\varepsilon_\sigma(\boldsymbol{k}))[\cos(k_x a) - \cos(k_y a)]^2}{E_\sigma(\boldsymbol{k})} \tanh\left(\dfrac{E_\sigma(\boldsymbol{k})}{2k_B T}\right) \\ n - 1 = -\dfrac{1}{2N_S} \sum_{k,\sigma} \dfrac{\varepsilon_\sigma(\boldsymbol{k}) - \mu}{E_\sigma(\boldsymbol{k})} \tanh\left(\dfrac{E_\sigma(\boldsymbol{k})}{2k_B T}\right) \end{cases}, \quad (11)$$

where

$$E_\sigma(\boldsymbol{k}) = \sqrt{[\varepsilon_\sigma(\boldsymbol{k}) - \mu]^2 + \Delta^2(\boldsymbol{k})}, \quad (12)$$

and

$$\Delta(\boldsymbol{k}) = \Delta_d[\cos(k_x a) - \cos(k_y a)]. \quad (13)$$

Eq. (11) determine the d-wave superconducting gap (Δ_d) and μ for a given temperature (T), electron density (n), and external magnetic field (B). For the case of p-channel superconductivity, there

Table 1
Parameters used for the calculations.

Symmetry	d-Wave	p-Wave
t (eV)	−1.0	0.4
t' (eV)	0.3	−0.12
Δt_3 (eV)	0.1	0.1
δ_3 (eV)	0	0.08
W (eV)	0.1	0.1

are three possible spin functions for the pairs, *i.e.*, $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, and $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$. In this paper, we only analyze the last spin function corresponding to pairs with null total spin projection. Assuming that $\Delta(\mathbf{k}) = \Delta_p[\sin(k_x a) \pm \sin(k_y a)]$, the first equation in (11) is replaced by

$$1 = \pm\frac{1}{N_S} \sum_{\boldsymbol{k},\sigma} \frac{\delta(\varepsilon_\sigma(\boldsymbol{k}))[\sin(k_x a) \pm \sin(k_y a)]^2}{E(\boldsymbol{k})} \tanh\left(\frac{E(\boldsymbol{k})}{2k_B T}\right), \quad (14)$$

which together with the second equation in (11) determine the p-wave superconducting properties. In general, the critical temperature (T_c) is obtained by taking $\Delta_\alpha = 0$, for $\alpha = p$ or d. It would be worth mentioning that this simplified model without attractive second-neighbor density–density interactions has the advantage of avoiding the phase separation [11] and giving rise to both p- and d-wave superconductivities within the standard BCS formalism.

3. Results

The Hamiltonian parameters of single-electron terms (t and t') in Eq. (1) have been calculated by means of the density functional theory (DFT) [9,10], while those corresponding to interaction and distortion are estimated to give reasonable p- and d-channel critical temperatures. The specific parameters used in this work are summarized in Table 1. Numerical calculations of Eqs. (11) and (14) are carried out, in order to determine the dependence of T_c and Δ_α on the electron density per unit cell (n) and magnetic-field strength (B). Fig. 1 shows the T_c of (a) d-wave (open squares) and (b) p-wave (open triangles) superconducting states as functions of n. Note that the maximum $k_B T_c = 0.01|t|$ for d-channel superconductivity is located at $n = 0.52$, while for the p-channel the maximum $k_B T_c = 0.00025|t|$ is found at $n = 0.54$. This non-monotonic behavior of T_c on n agrees with the experimental observations [15]. In fact, the optimal critical temperatures are very close to those obtained in
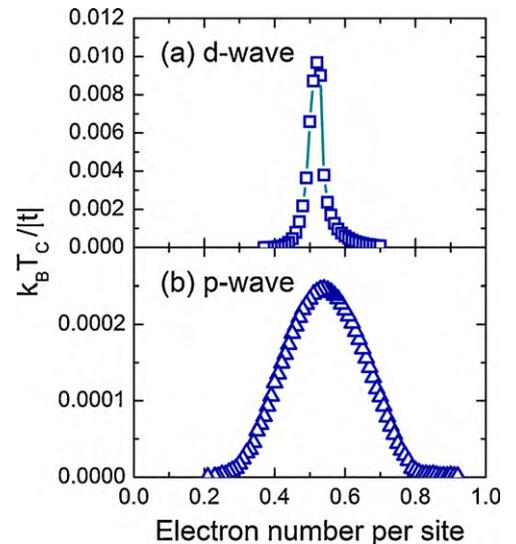
Fig. 1. (a) d-Wave and (b) p-wave superconducting critical temperature (T_c) versus the electron concentration per unit cell (n) in the absence of external magnetic field.

Fig. 2. Critical temperature (T_c) as a function of the magnetic-field strength for (a) d-wave and (b) p-wave superconducting states with $n = 0.52$ and $n = 0.54$, respectively.

BiSrCaCu$_2$O$_x$ [16] and Sr$_2$RuO$_4$ [2]. However, the optimal electronic densities have not been unambiguously determined by experiments, since such obtained from Hall-effect measurements does not correspond to those calculated by the doping concentration [17].

In Fig. 2, the dependence of T_c on B is plotted for (a) d-wave and (b) p-wave superconducting states with optimal densities $n = 0.52$ and $n = 0.54$, respectively. Notice that both T_c decreases as B grows, as expected from Eq. (1), since the main effect of B is to change the relative electron populations of spin-up and spin-down states, which reduces the Cooper pairs number and in consequence T_c. Therefore, T_c is zero when the external magnetic-field strength is higher than the critical field value, which is estimated to be around 200 Tesla for cuprate superconductors [18].

Fig. 3 shows the angular dependence of the single-excitation energy gap $[\Delta_0(\theta)]$, which is defined as the minimum value of $E_\sigma(\mathbf{k})$ in $\mathbf{k}$ direction [12], for (a) d-wave and (b) p-wave superconducting states with optimal densities $n = 0.52$ and $n = 0.54$, respectively. The blue thick lines correspond to $B = 0$, the red thin lines to $\mu_B B = 0.02|t|$, and the magenta dashed lines to $\mu_B B = 0.05|t|$, where the polar angle is given by $\theta = \tan^{-1}(k_y/k_x)$. For the p-wave case, $\Delta_0(\theta)$ is calculated around $\mathbf{k} = (\pi,\pi)$, where the minimum of the single-electron band $[\varepsilon_\sigma(\mathbf{k})]$ is located. Observe that the effects of an external magnetic field are essentially to reduce Δ_0 as well as T_c, preserving the superconducting gap symmetries within the rigid band-shift approximation.

4. Conclusions

The results of this study make known that, by means of the standard BCS formalism, a simple second-neighbour correlated-hopping interaction can induce p- and d-wave anisotropic superconductivities and their critical temperatures as functions of the electron concentration show a non-monotonic behaviour, in qualitative agreement with d-channel experiment results. The calculated single-excitation energy gap (Δ_0) can be measured by ARPES and the existence of nodes could depend on the electron concentration, as discussed in Ref. [19]. By using the rigid band approximation, the effects of an external magnetic field on the anisotropic superconductivity have been analyzed and the results reveal a significant diminution of the critical temperature and Δ_0. It is important to note that the calculated upper critical field is of the same order of magnitude for d-wave superconductors, but for triplet superconductors this model overestimates its value in comparison with the expected one [2,20]. Finally, there is no distinction of the magnetic-field orientation within this simple rigid band-shift analysis. A more sophisticated treatment of the magnetic-field effects on anisotropic superconductivity would be carried out through the Peierls substitution and the Bogoliubov–de Gennes equations [21], where screening currents can be introduced if the applied magnetic field is perpendicular to the planes. This approach is currently under study.

Fig. 3. Angular dependence of the single-excitation energy gap (Δ_0) for (a) d-wave and (b) p-wave superconducting states with, respectively, $n = 0.52$ and $n = 0.54$, when the external magnetic-field strength $B = 0$ (blue thick lines), $\mu_B B = 0.02|t|$ (red thin lines) and $\mu_B B = 0.05|t|$ (magenta dashed lines). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

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