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Superconducting gap symmetry determined by the electron density

Luis A. Pérez[a,*], J. Samuel Millán[b], Chumin Wang[c]

[a]*Instituto de Física, Universidad Nacional Autónoma de México (UNAM), A.P. 20-364, C.P. 01000, México D.F., México*
[b]*Facultad de Ingeniería, UNACAR, C.P. 24180, Cd. del Carmen, Campeche, México.*
[c]*Instituto de Investigaciones en Materiales, UNAM, A.P. 70-360, C.P. 04510, México D.F., México*

Abstract

In this work, a comparative study of pairing and superconducting states in square lattices with s-, p- and d-symmetries is performed within the BCS formalism and a generalized Hubbard model, in which correlated-hopping interactions are considered in addition to the repulsive Coulomb interactions. The two-particle analysis reveals the importance of the van Hove singularity in the formation of pairs and then the two-particle states with different pairing symmetry have their maximum binding energies at the same hopping strength. This feature is confirmed by the superconducting critical temperature (T_c) calculation at the low-density regime. However, a different picture is found for the high-density regime, i.e., the maxima of the s- and d-channel T_c split from the expected value and no p-wave superconducting state is found. This study suggests that the three superconducting symmetries can be analyzed within a single framework.

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The discovery of d-symmetry pairing in the cuprate superconductors [1] and a probably p-wave spin-triplet superconducting state in Sr_2RuO_4 [2] has enhanced the search of microscopic models being able to describe different anisotropic superconducting states in a single framework. In particular, the essentially two-dimensional behavior, present in both mentioned systems, could be basic for understanding their peculiar properties. Three-band Hubbard models have been proposed to describe the dynamics of the carriers on the planes and the electronic states close to the Fermi energy can be reasonably well described by a single-band tight-binding square lattice with second-neighbor hoppings [3,4]. Recently, we have found that the second-neighbor correlated-hopping interaction (Δt_3) is essential in the $d_{x^2-y^2}$-wave superconductivity [5] and that a further small distortion of the right angles in such square lattices leads to p-wave superconductivity [6]. In this work, we start from a single-band Hubbard model, in which first (Δt) and second (Δt_3) neighbor correlated-hopping interactions are considered in addition of the on-site (U) and nearest-neighbor (V) Coulomb interactions. The corresponding Hamiltonian can be written as

$$\hat{H} = -t \sum_{<i,j>,\sigma} c^{+}_{i\sigma} c_{j\sigma} - t' \sum_{\ll i,j\gg,\sigma} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \frac{V}{2} \sum_{<i,j>} n_i n_j + \Delta t \sum_{<i,j>,\sigma} c^{+}_{i\sigma} c_{j\sigma} \left(n_{i-\sigma} + n_{j-\sigma}\right) + \Delta t_3 \sum_{\ll i,j\gg,\sigma,<i,l>,<j,l>} c^{+}_{i\sigma} c_{j\sigma} n_l, \tag{1}$$

where $c^{+}_{i\sigma}(c_{i\sigma})$ is the creation (annihilation) operator with spin $\sigma = \downarrow$ or $\uparrow$ at site i, $n_{i,\sigma} = c^{+}_{i\sigma} c_{i\sigma}$, $n_i = n_{i,\uparrow} + n_{i,\downarrow}$, $<i,j>$ and $\ll i,j \gg$ denote first- and second-neighbor sites, $-t$ and $-t'$ are the first- and second-neighbor hopping parameters, respectively. When an electron–hole transformation is made in Eq. (1), the hopping parameters for holes are given by $t_h \equiv t - 2\Delta t$ and $t'_h \equiv t' - 4\Delta t_3$ instead of $-t$ and $-t'$ for electrons, as done in Ref. [7]. In order to break the degeneracy of p-wave pairing states, we further consider a small distortion of the right angles in the square lattice with lattice parameter a, which leads to changes in the second-neighbor interactions and their new values are

*Corresponding author. Tel.: +52 55 56225183; fax: +52 55 56225008.
E-mail address: lperez@fisica.unam.mx (L.A. Pérez).

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$t'_{\pm} \equiv t' \pm \delta'$ and $\Delta t_3^{\pm} \equiv \Delta t_3 \pm \delta_3$, where $\pm$ refers to the $\hat{x} \pm \hat{y}$ direction.

For the two-particle case, analytical solutions can be found [8] by means of s-, p- and d-symmetry two-particle wavefunctions and the respective binding energies (Δ_2) are determined by

$$(UV + 4U\Delta t_3 - 16\Delta t^2)(I_0 I_2 - I_1^2) - UI_0 - 8\Delta t I_1 - (V + 4\Delta t_3)I_2 + 1 = 0$$
$$1 - (V - 4\delta_3)I_2 = 0,$$

and

$$1 - (V - 4\Delta t_3)I_2 = 0,$$

where

$$I_n = -\frac{1}{4\pi^2}\int\int_{1BZ} \frac{f^n(k_x, k_y)}{\Delta_2 + 2\varepsilon\left(\vec{k}\right) + 2|E_0|}\,\mathrm{d}k_x \mathrm{d}k_y$$

being

$$\varepsilon\left(\vec{k}\right) = 2t\left[\cos(k_x a) + \cos\left(k_y a\right)\right] + 2t'_{+}\cos\left(k_x a + k_y a\right) + 2t'_{-}\cos(k_x a - k_y a)$$

the dispersion relation, $|E_0|$ the lower one-particle band edge, and $f(k_x, k_y) = \cos(k_x a) + \cos\left(k_y a\right)$, $\cos(k_x a) - \cos\left(k_y a\right)$ and $\sin(k_x a) + \sin\left(k_y a\right)$ for s-, p- and d-channel, respectively. Insets (a) and (b) of Fig. 1, respectively show Δ_2 versus t' for two holes and for two electrons with s (circles), p (triangles) and d (squares) symmetries, using $V = 0$, $\Delta t = 0.5t$, $\Delta t_3 = 0.15t$, $\delta' = 0$, $\delta_3 = 0.1t$, $U = 0$ for electrons and $U = 3t$ for holes. Notice that the maxima of Δ_2 are located at $-t' = -0.6t$ for holes and $-t' = 0.5t$ for electrons, independently of the pairing symmetry, since when $-t' = 0.5t$ the van Hove singularities collapse into the lower band edge and when $-t' = 0.6t$ the bandwidth for holes tends to zero with the chosen parameters.

To analyze the superconducting states we apply a normal Hartree–Fock decoupling of the interaction terms in Eq. (1) [5] and then, within the BCS formalism, we obtain two coupled integral equations, which determine the critical temperature (T_c) and the chemical potential [9]. The results obtained by using the same parameters as in the two-particle analysis are shown in Fig. 1 for the electron density $n = 0.2$ (solid symbols) and $n = 1.8$ (open symbols). Observe that for $n = 0.2$ the maxima of T_c corresponding to the three superconducting symmetries are located at $-t' = 0.4t$, because the mean-field hopping parameters [9] are $t_{MF} = -t + n\Delta t = -0.9t$ and $t'_{MF} = -t + 2n\Delta t_3 = 0.46t$ for $-t' = 0.4t$ and then $-t'_{MF} \cong 0.51 t_{MF}$ close to the two-electron case. On the other hand, for $n = 1.8$ the first-neighbor mean-field hopping parameter is $t_{MF} = -0.1t$ and using the two-hole results, $-t'_{MF} = -0.6 t_{MF} = 0.06t$, we obtain $-t' = t'_{MF} - 2n\Delta t_3 = -0.6t$, which is the expected location of maximum T_c. However, observe that the calculated maximum-T_c locations for s- and d-channels are $-t' = -0.32t$ and $-t' = -0.91t$, respectively. Furthermore, there is no solution for p-channel T_c within the BCS formalism.

In summary, we have presented a comparative analysis of the s-, p- and d-symmetry pairing and superconducting states. For the low-density regime, the finite-density results can be inferred from the two-electron analysis, where the single-particle van Hove singularity determines the location of maximum T_c. However, for high band fillings, the results of superconducting states, depending strongly on the pairing symmetry, differ from the two-hole analysis revealing a complex picture where the van Hove singularity seems to not be the dominant factor.

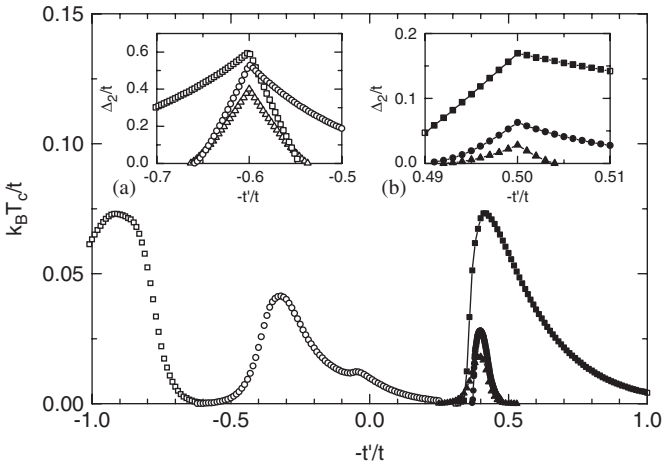

Fig. 1. Critical temperature (T_c) versus second-neighbor hopping parameter (t') for $n = 0.2$ (solid) and $n = 1.8$ (open) with s- (circles), p- (triangles) and d- (squares) symmetries. Insets: binding energy (Δ_2) versus t' for (a) two holes and (b) two electrons.

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