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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

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

and the p-wave superconducting gap is given by $\Delta_{\mathbf{k}} = \Delta_p[\sin(k_x a) \pm \sin(k_y a)]$. It is worth mentioning that for the case of $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$ 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

$$1 = -\frac{(V \mp 4\delta_3)}{N_S} \sum_{\mathbf{k}} (\sin^2 ak_x \pm \sin ak_x \sin ak_y) \times \frac{1}{E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T}\right), \quad (17)$$

where $\delta_3 = (\Delta t_3^+ - \Delta t_3^-)/2$. Notice that, for given n and T, Eqs. (16) and (18) have to be solved simultaneously for μ and Δ_p. In particular, the critical temperature T_c is determined by $\Delta_p(T_c) = 0$. For the case of triplets with $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$ and $q = 0$, the terms U and Δt in Eq. (7) are even functions in the k' space and $\Delta_{\mathbf{k}} = \Delta_p[\sin(k_x a) \pm \sin(k_y a)]$ is odd, and then the sum over the first Brillouin zone of the product of them is zero. Furthermore, the terms V and $\Delta t_3^{\pm}$ reduce to those of $W_{kk'0}$, except for a factor of 2. However, due to the sum over the spin index σ 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]

$$W_T = \langle H_2 \rangle = \frac{1}{2} \int\int_{BZ} (W_{\mathbf{k},\mathbf{k}'} - W_{\mathbf{k},-\mathbf{k}'}) u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} dk_x dk_y dk'_x dk'_y \quad (18)$$

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

$$u_{\mathbf{k}} = \left(\frac{1}{2} - \frac{\varepsilon(\mathbf{k}) - \mu}{2E_{\mathbf{k}}}\right)^{1/2} \quad (19)$$

$$v_{\mathbf{k}} = \left(\frac{1}{2} + \frac{\varepsilon(\mathbf{k}) - \mu}{2E_{\mathbf{k}}}\right)^{1/2}. \quad (20)$$

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

$$W_T = \frac{V}{16\pi^4} \iint_{|BZ} dk_x dk_y dk'_x dk'_y [\sin(k_x a)\sin(k'_x a) + \sin(k_y a)\sin(k'_y a)] \times \left[1 - \frac{(\varepsilon(\mathbf{k}) - \mu)^2}{E_{\mathbf{k}}^2}\right]^{1/2} \left[1 - \frac{(\varepsilon(\mathbf{k}') - \mu)^2}{E_{\mathbf{k}'}^2}\right]^{1/2} - \frac{\delta_3}{4\pi^4} \times \iint_{|BZ} dk_x dk_y dk'_x dk'_y [\sin(k_x a)\sin(k'_y a) + \sin(k'_x a)\sin(k_y a)] \times \left[1 - \frac{(\varepsilon(\mathbf{k}) - \mu)^2}{E_{\mathbf{k}}^2}\right]^{1/2} \left[1 - \frac{(\varepsilon(\mathbf{k}') - \mu)^2}{E_{\mathbf{k}'}^2}\right]^{1/2}. \quad (21)$$

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

3. The results

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

$$\frac{\Delta_p}{\delta_3} = 2\sqrt{2n}\left(1 - \frac{9n}{4}\right), \quad (22)$$

$$\frac{k_B T_c}{\delta_3} = \frac{(1-n)}{\tanh^{-1}(1-n)}, \quad (23)$$

In Fig. 1(a) and (b), numerical results of Δ_p/δ_3 and T_c/δ_3 versus n are, respectively, shown for arbitrary δ_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 Δ_p/δ_3 and T_c/δ_3 are functions of n only.

Fig. 2(a)–(c) show T_c, Δ_p and W_T,, respectively, for $V = \Delta_t = \delta = 0$, $t_0 = 0.4$, $t'_0 = -0.12$ eV, $\delta = 0.15$ eV and $\Delta t_3 =$ 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 $n_{op} \approx 0.52$, 0.55, and 0.61 for $T_c(n)$; $n_{op} \approx 0.528$, 0.592 and 0.64, for $\Delta_p(n)$; and $n_{op} \approx 0.524$, 0.592 and 0.64 for $W_T(n)$, respectively. Notice that for the three systems shown, the optimal doping for Δ_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 (μ) when T changes from T_c to 0 K. However, the optimal electron density for W_T is essentially the same as Δ_p. Moreover, for

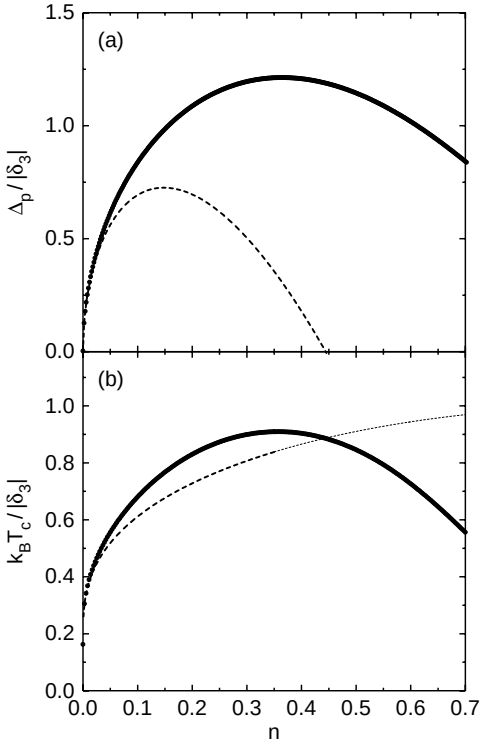

Fig. 1. Numerical results (solid lines) of p-channel (a) superconducting gap (Δ_p) and (b) critical temperature (Δ_c) versus the electron concentration (n), for arbitrary δ_3 and U, and the other are taken parameters equal to zero, in comparison with the analytical solutions (dashed lines) valid for $n \to 0$.

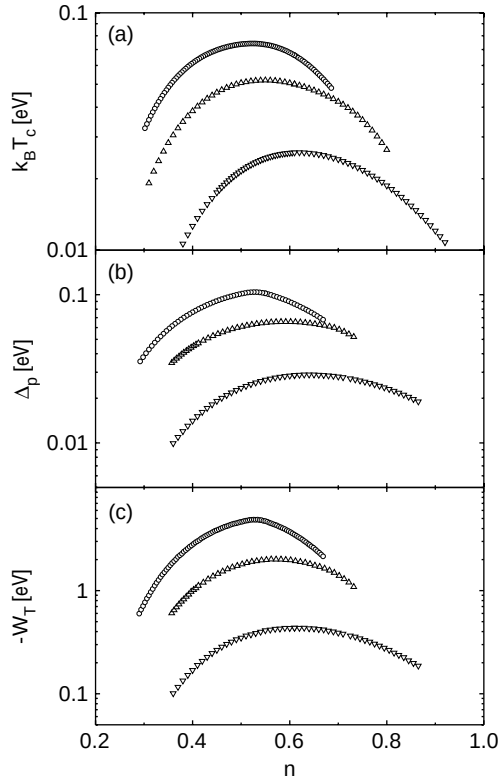

Fig. 2. (a) Critical temperature (T_c), (b) superconducting gap (Δ_p) and (c) potential energy of the system (W_T) versus electron density (n) for $V=\Delta t=\delta=0$, $t_0=0.4$, $t_0'=-0.12$, $\Delta t_3=0.3$ eV (circles), 0.2 eV (up triangles), 0 (down triangles), with $\delta_3=0.15$ eV and arbitrary U.

fixed $t_0>0$ and $t_0'<0$, n_{op} shifts to higher densities when Δt_3 or δ_3 diminish as shown in Fig. 3, where T_c is plotted as a function of n, for $V=\Delta_t=\Delta t_3=\delta=0$, $t_0=0.4$ 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 Δ_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 Δt, n_{op} shifts towards 1, and T_c and Δ_p decrease but if Δt or δ_3 increase, n_{op} moves towards 0 and T_c and Δ_p increase.

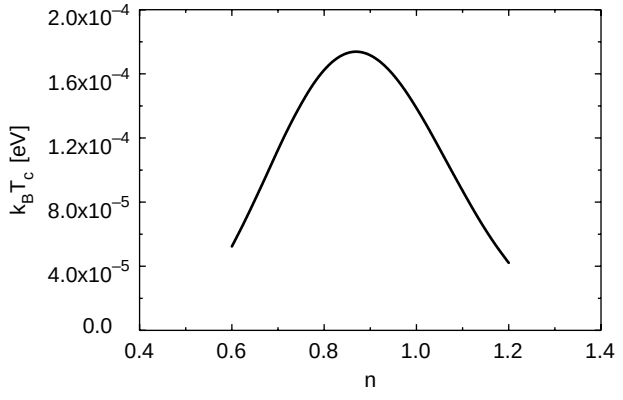

Fig. 3. Critical temperature (T_c) versus electron density (n) for $V=\Delta t=\Delta t_3=\delta=0$, $t_0=0.4$, $t_0'=-0.12$, $\delta_3=0.06$ eV and arbitrary U.

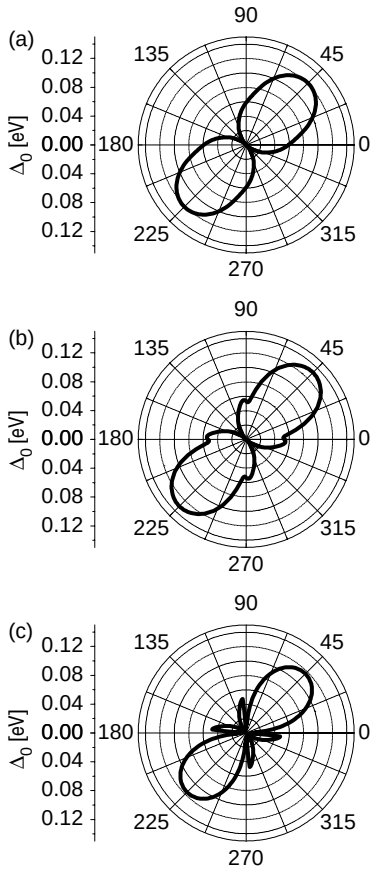

Fig. 4. Single-particle excitation energy gap (Δ_0) as a function of the polar angle for $V=\Delta t=\delta=0$, $t_0=0.4$, $t_0'=-0.12$, $\Delta t_3=0.2$, $\delta_3=0.15$ eV, arbitrary U and electron densities (a) $n=0.5$, (b) $n=0.6$, and (c) $n=0.7$.

However, for $t_0<0$ the effect is inverse for Δt and Δt_3, respectively, the diminished of δ_3 act always with a decreasing for T_c and Δ_p and n_{op} shifting to 1.

In Fig. 4(a)–(c), the angular dependence of the single-particle excitation gap [$\Delta_0(\theta)$] is shown for a system with $V=\Delta t=\delta=0$, $t_0=0.4$, $t_0'=-0.12$ eV, $\Delta t_3=0.2$ eV, $\delta_3=0.15$ 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 Δ_0 is defined as the minimum value of E_k given by Eq. (17), with $\Delta_{\mathbf{k}}=\Delta_p[\sin(k_x a)+\sin(k_y a)]$, and we have measured the energy from the (π,π) point since the minimum is located there. Notice that Δ_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 $\Delta t_3^{\pm}$ in the formation of a p-wave superconducting state. The results also show that the optimal carrier concentration n_{op} for Δ_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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