Optimal doping for d-wave superconducting ground states within the generalized Hubbard model

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Received 16 November 2017; accepted 31 January 2018

A single-band generalized Hubbard model that describes two-dimensional superconductivity with d-wave symmetry on a square lattice within the BCS formalism is considered. For a set of Hamiltonian parameters and varying the ratio between nearest-neighbor and next-nearest neighbor hoppings (t'/t); an optimal electron density (n_{op}) can be found for each t'/t value, where the temperature is maximum (T_{c-max}) . After calculating the superconducting gap at T=0 K and the corresponding ground state energy (E_g) for all the carrier concentrations, a ground state energy minimum (E_{g-min}) is found close to half filling. Since T_{c-max} is the highest critical temperature for a given ratio t'/t, the minimum of all the T_{c-max} values defines a supreme for this set of temperatures, named as $T_{c-max-sup}$. The corresponding optimal doping for $T_{c-max-sup}$ will be called n_{op-sup} , and the results show that E_{g-min} is located at n_{op-sup} . The Fermi surface (FS) is analyzed for carrier concentrations close to n_{op-sup} and it is suggested that the location for over (OD) and under (UD) doping regimes $(n_{OD} > n_{op-sup} > n_{UD})$ could define a pseudogap zone for high critical temperature superconductors.

Keywords: Theories and models of superconducting state; pairing symmetries (other than s-wave); pseudogap regime.

PACS: 74.20.-z; 74.20.Rp; 74.72.Kf

1. Introduction

Anisotropic superconductivity has been subject of study since the discovery of high critical temperature superconductors (HTSC) in 1986 by Bednorz and Müller. d-wave symmetry appears in phase sensitive experiments [1] for several hole- and electron-doped cuprates. Three-band Hubbard models have been proposed to describe the dynamics of the carriers on the CuO_2 planes [2] and the electronic states close to the Fermi energy (E_F) can be reasonably well described by a single-band tight-binding model on a square lattice with second neighbor hoppings [3]. In this work, a generalized Hubbard model that describes d-wave superconductivity on a square lattice within the BCS formalism is considered [4,5]. This model contains nearest-neighbor (Δt) and next-nearestneighbor (Δt_3) correlated hoppings, in addition to on-site (U) and inter-site (V) coulombic repulsions. The mean-field electronic dispersion relation (ε_{MF}) in the studied square lattice includes mean-field single-particle hoppings that are functions of the electron density (n). To clarify the importance of these mean-field hoppings, a systematic study of the superconducting critical temperature (T_c) versus n was performed for a set of Hamiltonian parameters with fixed Δt and Δt_3 . It is important to mention that U does not affect the shape of ε_{MF} , since it only modifies the electron self-energy (E_{MF}) and shifts the superconducting chemical potential (μ) without changing the superconducting critical temperature. Therefore U can be taken equal to zero. On the other hand,

as shown below, to obtain a solution for the superconducting gap equation [Eq. (12)], $(V-4\Delta t_3)$ should to be negative and therefore the condition $V < 4\Delta t_3$ must be satisfied. In order to keep a minimum set of parameters but keeping the d-wave symmetry that arises from Δt_3 , V will be set to zero too. In this work, we determine the optimal electron density (n_{op}) and the corresponding ground state energy for each value of the ratio between next- and next-nearest-neighbor hoppings (t'/t). Since a supreme is the least upper bound of a set of high bound values, we expect that the supreme of T_{c-max} corresponds to that with minimal energy at T=0 K. This scenario has been verified numerically for two different sets of Hamiltonian parameters that can be applied to superconducting systems.

2. The model

We consider a single-band Hubbard model in a square lattice with first- (Δt) and second-neighbor (Δt_3) correlated hoppings, in addition to on site (U) and first-neighbor (V) Coulombic repulsions. The corresponding Hamiltonian (\hat{H}) is [6]:

$$\hat{H} = H_t + H_{t'} + H_U + H_V + H_{\Delta t} + H_{\Delta t_3} \qquad (1)$$

with

$$H_t = t \sum_{\langle i,j \rangle,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} \tag{2}$$

$$H_{t'} = t' \sum_{\ll i, j \gg, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma}$$
(3)

$$H_U = U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{4}$$

$$H_V = \frac{V}{2} \sum_{\langle i,j \rangle} n_i n_j \tag{5}$$

$$H_{\Delta t} = \Delta t \sum_{\langle i,j \rangle,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} (n_{i,-\sigma} + n_{j,-\sigma})$$
(6)

$$H_{\Delta t_3} = \Delta t_3 \sum c_{i\sigma}^{\dagger} c_{j\sigma} n_l \tag{7}$$

where $n_i = n_{i,\uparrow} + n_{i,\downarrow}$, $n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}$, and $c_{i,\sigma}^{\dagger} (c_{i,\sigma})$, is the creation (annihilation) operator with spin $\sigma = \downarrow$ or \uparrow at site i. < i, j > and $\ll i, j \gg$ denote nearest-neighbour and next-nearest neighbour sites, respectively.

The expressions for model parameters, in terms of the Wannier functions $[\varphi(r - R_i)]$, centred at the lattice site R_i , are given in the Table I.

After a Fourier transformation $c_{k,\sigma}^{\dagger} = 1/N_s \sum_j \exp(i\mathbf{k} \cdot \mathbf{R}_j) c_{j,\sigma}^{\dagger}$, Eq. (1) becomes:

$$\hat{H} = \sum_{k,\sigma} \varepsilon(\mathbf{k}) c^{\dagger}_{k,\sigma} c_{k,\sigma} + \frac{1}{N_S} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\sigma} V_{\mathbf{k},\mathbf{k}',\mathbf{q}} c^{\dagger}_{\mathbf{k}+\mathbf{q},\uparrow} c^{\dagger}_{-\mathbf{k}+\mathbf{q},\downarrow} c_{-\mathbf{k}'+\mathbf{q},\downarrow} c_{\mathbf{k}'+\mathbf{q},\uparrow}$$
(8)

where $\varepsilon(\mathbf{k})$ is the dispersion relation and N_s is the total number of lattice sites. The interaction potential $(V_{\mathbf{k},\mathbf{k}',\mathbf{q}})$ considers only Cooper pairs with antiparallel spins and it can be written as:

$$V_{\mathbf{k},\mathbf{k}',\mathbf{q}} = U + V\beta(\mathbf{k} - \mathbf{k}') + \Delta t[\beta(\mathbf{k} + \mathbf{q}) + \beta(-\mathbf{k} + \mathbf{q}) + \beta(\mathbf{k}' + \mathbf{q}) + \beta(-\mathbf{k}' + \mathbf{q})] + \Delta t_3[\gamma(\mathbf{k} + \mathbf{q}, \mathbf{k}' + \mathbf{q}) + \gamma(-\mathbf{k} + \mathbf{q}, -\mathbf{k}' + \mathbf{q})]$$
(9)

with

$$\beta(\mathbf{k}) = 2[\cos(k_x a) + \cos(k_y a)] \tag{10}$$

$$\gamma(\mathbf{k} \cdot \mathbf{k}') = 4\cos(k_x a)\cos(k'_y a) + 4\cos(k_x a)\cos(k_y a) \quad (11)$$

where *a* is the lattice parameter. The chemical potential (μ) and superconducting gap $[\Delta(\mathbf{k})]$ can be obtained from the mean-field BCS coupled equations for d-wave superconductors [7]:

$$1 = -\frac{(V - 4\Delta t_3)a^2}{4\pi^2} \iint_{1Bz} \left\{ \frac{[\cos(k_x a - \cos(k_y a)]^2}{2E(\mathbf{k})} \times \tanh\left(\frac{E(\mathbf{k})}{2k_BT}\right) \right\} dk_x dk_y$$
(12)

$$n - 1 = -\frac{a^2}{4\pi^2} \iint_{1Bz} \frac{\varepsilon(\mathbf{k}) - \mu}{E(\mathbf{k})}$$
$$\times \tanh\left(\frac{E(\mathbf{k})}{2k_BT}\right) dk_x dk_y \tag{13}$$

where 1BZ refers to the first Brillouin zone, defined as $\left[\begin{array}{c} \frac{-\pi}{a}, \frac{\pi}{a} \end{array}\right] \otimes \left[\begin{array}{c} \frac{-\pi}{a}, \frac{\pi}{a} \end{array}\right]$ the quasi-particle energy [E(k)] is given by:

$$E(\mathbf{k}) = \sqrt{(\varepsilon_{MF} - \mu)^2 + \Delta^2(\mathbf{k})}$$
(14)

and the mean field dispersion relation is

$$\varepsilon_{MF}(\mathbf{k}) = E_{MF} + t_{MF}[\cos(k_x a) + \cos(k_y a)] + 4t'_{MF}[\cos(k_x a)\cos(k_y a)]$$
(15)

with

$$E_{MF} = \left(\frac{U}{2} + 4V\right)n\tag{16}$$

$$t'_{MF} = t' + 2n\Delta t_3 \tag{17}$$

$$t_{MF} = t + n\Delta t \tag{18}$$

where n is the electron density.

The d-wave symmetry superconducting gap is given by [7]:

$$\Delta(\mathbf{k}) = \Delta_d[\cos(k_x a) - \cos(k_y a)] \tag{19}$$

where Δ_d is the gap amplitude. The critical temperature can be determined from Eq. (12) by considering that $\Delta_d(T = T_c) = 0$. On the other hand, the ground state energy (E_g) per site can be obtained from the following equation [8]:

$$E_g = \frac{1}{N_s} \sum_{\mathbf{k}} [\varepsilon_{MF}(\mathbf{k}) - E(\mathbf{k})] + \frac{\Delta_d^2}{4\Delta t_3 - V} + (n-1)\mu - \left(\frac{U}{4} + 2V\right)n^2.$$
(20)

3. Results

We fixed $\Delta t_3 = 0.05$ eV as in Ref. 4, and then we consider two cases: $\Delta t = 0.1$ eV, which gives $T_{\text{c-max-sup}} \approx 40$ K; and $\Delta t = 0.5$ eV which gives $T_{\text{c-max-sup}} \approx 100$ K. The first case can be applied to $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) [9], while the second one to $\text{Bi}_2\text{Sr}_2\text{Ca}_{m-1}$ Cu_m O_{4+2m+ δ} (BSCO), where m is the number of superconductors planes, m = 2,3 for $T_{\text{c-max}} = 85, 110$ K, respectively [10]. Figure 1(a) shows the



FIGURE 1. (a) The maximum critical temperature $(T_{\text{c-max}})$ versus the optimal electronic density (n_{op}) and the ratio -t'/t for U = V = 0, $\Delta t = 0.1$ eV, and $\Delta t_3 = 0.05$ eV. (b) $T_{\text{c-max}}$ versus chemical potential (μ_{op}) at the optimal electron density for the same parameters as in (a).

maximum critical temperature (T_{c-max}) versus the electronic density (n) and the ratio -t'/t for $\Delta t = 0.1$ eV. Around half filling, at $n_{\text{op-sup}} = 0.975$ and (-t')/t = -0.07, the supreme value of T_c is $T_{c-\text{max-sup}} = 37$ K. Notice that for n_{op} close to the band filling extremes, 0 and 2, a higher T_{c-max} is found. Likewise, Fig. 1(b) shows $T_{c-\text{max}}$ versus the superconducting chemical potential (μ_{op}) at the optimal doping or optimal electronic density (n_{op}) for the same parameters as in Fig. 1(a). Moreover, Fig. 2 shows the Fermi surface (FS) for the model parameters leading to $T_{c-\text{max-sup}} = 37$ K. Notice that the FS is electron-like and similar to the FS of a square lattice with first-neighbor hopping only at half-filling.

The superconducting properties, such as the superconducting gap amplitude (Δ_d), the Fermi energy (E_F), *i.e.*, the chemical potential at T = 0 K, and the condensation energy (E_{cond}), for electron densities close to $n_{\text{op-sup}} = 0.975$, are summarized in Table II. Observe that E_{cond} attains a minimum value at $n_{\text{op-sup}} = 0.975$. Figure 3 shows the ground state energy versus both t'/t and the optimal electronic density (n_{op}). Notice the match of the minimum energy $E_{g-\min}$



FIGURE 2. Fermi surface for the same parameters as in Fig. 1 and -t'/t = -0.07, $n_{op-sup} = 0.975$ and $E_{F-sup} = -0.1101$ eV.



FIGURE 3. Ground state energy (E_g) versus -t'/t and n_{op} for $\Delta t = 0.1$ eV and $\Delta t_3 = 0.05$ eV.

at $n_{\text{op-sup}} = 0.975$ for -t'/t = -0.07. The location of the minimum energy close to the half filled band agrees with the experimental results reported in Ref. 11. Moreover, it is worth mentioning that a ratio of t'/t = 0.1 has been estimated for the LSCO systems [12] which is very close to the value of 0.07 obtained at the optimal doping.

Figure 3 shows the ground state energy versus both t'/tand the optimal electronic density $(n_{\rm op})$. Notice the match of the minimum energy $E_{\rm g-min}$ at $n_{\rm op-sup}$ = 0.975 for -t'/t = -0.07. The location of the minimum energy close to the half filled band agrees with the experimental results reported in Ref. 11. Moreover, it is worth mentioning that a ratio of t'/t = 0.1 has been estimated for the LSCO systems [12] which is very close to the value of 0.07 obtained at the optimal doping.



FIGURE 4. a) Maximum critical temperature (T_c) versus the opimal electron density (n) and -t'/t for U = V = 0, $\Delta t = 0.5|t|$, $\Delta t_3 = 0.05|t|$. b) T_{c-max} versus t'/t and the optimal chemical potential (μ_{op}) , at the optimal electron density for the same set of parameters as in Fig. 4(a).

We also analyzed the case with $\Delta t = 0.5 \text{ eV}$ which leads to a $T_{\text{c-max-sup}}$ close to 100 K. Figure 4(a) shows T_c versus t'/t and n. Notice that the minimum of $T_{\text{c-max}}$ corresponds to -t'/t = 0.06 and $n_{op} = 0.805$, hence $T_{\text{c-max-sup}} = 99.8$ K. The projection on the plane $n_{op} - t'/t$ (solid circles) shows an inflection point for n_{op} close to half filling. Figure 4(b)



FIGURE 5. Fermi surface for -t'/t = 0.06, $\Delta t = 0.5$ eV, and $n_{op-sup} = 0.805$.

depicts $T_{\text{c-max}}$ versus both t'/t and the optimal chemical potential (μ_{op}) where an almost linear dependence of μ_{op} with respect to $t'/t \in [0.4, -0.2]$ is observed. Moreover, for carrier densities close to full band filling, the band width is reduced to [-2.0,0.6] eV and the critical temperature is enhanced. Moreover, it has been verified that for $-t'/t \rightarrow$ -0.45, there is no Fermi surface. In order to understand this, we recall that the mean-field single-electron band width is proportional to the single-electron mean-field hopping parameters (t_{MF}, t'_{MF}) given by Eqs. (17) and (18). For certain values of electron density (n) and correlated hoppings $(\Delta t, \Delta t_3)$, the effective or mean-field hopping parameters are almost zero and also the corresponding effective band width. When this occurs, the superconducting chemical potential $\mu_{\rm op}$ lies outside the single-electron band, and then there is no single-electron energy that satisfies $\varepsilon_{MF}(\mathbf{k}) = \mu_{op}$. For the parameters used in this work, this band-width shrinking occurs for $-t'/t \in [-0.2, -0.45]$, where we also found that μ_{op} is the same for different t'/t ratios. This regime could be related to the pseudogap one, which is characterized by the disappearance of the Fermi surface and a suppression of the excited states above the superconducting critical temperature T_c and below a characteristic temperature T^* , for a given in-

TABLE I. Expressions for the Hubbard model parameters.

Single-particle parameters						
$t_{i,j} = \int d^3 \mathbf{r} \varphi^*(\mathbf{r} - \mathbf{R}_j) \bigg - \frac{\hbar^2 \nabla^2}{2m} + u(\mathbf{r}) \bigg \varphi(\mathbf{r} - \mathbf{R}_j); u(\mathbf{r})$ is the lattice periodic potential						
$t = t_{i,j}$ with $< i, j >$						
$t'=t_{i,j} ext{ with } \ll i,j \gg$						
Electron-electron interaction parameters						
$U_{ij}^{kl} = \int d^3r d^3r' \varphi * (\mathbf{r} - \mathbf{R}_j) \varphi * (\mathbf{r}' - \mathbf{R}_j) v(\mathbf{r} - \mathbf{r}') \varphi(\mathbf{r} - \mathbf{R}_k) \varphi(\mathbf{r}' - \mathbf{R}_l);$						
$v(\mathbf{r}-\mathbf{r}')$ is the interaction potential between two electrons in the lattice						
$U = U_{ii}^{ii}; \Delta t = U_{ii}^{ij} \text{ with } < i, j >; \Delta t_3 = U_{il}^{lj} \text{ with } < i, l >, < j, l > \text{ and } \ll i, j \gg$						

TABLE II. Superconducting physical properties close to $T_{\text{c-max-sup}}$ for $\Delta t = 0.1$ eV and $\Delta t_3 = 0.05$ eV.							
-t'/t	n	$T_c(\mathbf{K})$	E_g (eV)	$\Delta_d (\mathrm{eV})$	$E_{\rm cond}~({\rm eV})$	E_F (eV)	
-0.02	0.933750	37.37	-1.4567774678	0.0029534054	0.0000076362	-0.2935801622	
-0.07	0.975	37.00	-1.4612415658	0.0029192932	0.0000074563	-0.1101008940	
-0.10	1.0	37.13	-1.4590325950	0.0031720718	0.0000075504	0.0000008715	
TABLE III. Superconducting physical properties close to $T_{\text{c-max-sup}}$ for $\Delta t = 0.5$ eV and $\Delta t_3 = 0.05$ eV.							
-t'/t	$n_{ m op}$	$T_{\text{c-max}}(\mathbf{K})$	E_g (eV)	$\Delta_d (\mathrm{eV})$	$E_{\rm cond}~({\rm eV})$	E_F (eV)	
0.04	0.825	100.27	-0.8952952	0.00869208	0.000075024	-0.487767611	
0.06	0.805	99.8	-0.8963881	0.00863401	0.000070351	-0.555325242	
0.07	0.790	101.27	-0.8973170	0.00865858	0.000073722	-0.592148720	

terval of electron density [11]. The origin of this pseudogap phase is not yet understood and it could be due to the formation of another electronic phase competing with the superconducting one.





FIGURE 6. (a). Ground state (E_g) as a function of -t'/t and optimal electron density (n_{op}) . (b). Ground state energy (E_g) as a function of electron density (n) for -t'/t = 0.06. (c). Condensation energy (E_{con}) as a function of electron density (n) for -t'/t = 0.06 with $\Delta t = 0.5$ eV (squares), and -t'/t = -0.07 with $\Delta t = 0.1$ eV (circles).

Figure 5 shows the FS for -t'/t = 0.06, $n_{\text{op-sup}} = 0.805$, and $\Delta t = 0.5$ eV. Notice that the FS is hole-like in contrast with that shown in Fig. 2, corresponding to -t'/t = 0.06, $n_{\text{op-sup}} = 0.975$ and $\Delta t = 0.1$ eV, which is electron-like.

In contrast with previous studies where the first-neighbor correlated hopping (Δt) only leads to *s**-wave superconductivity [13], in our case, d-wave superconductivity is driven by the second-neighbor correlated hopping (Δt_3) and the value of t'/t strongly affects the superconducting properties. Moreover, the more appropriate t'/t ratio will be that which minimizes the ground state energy for a given set of other model parameters.

Figure 6(a) shows the ground state energy (E_g) versus both t'/t and n_{op} . Likewise, Fig. 6(b) shows E_g versus n for -t'/t = 0.06. Notice the linear dependence of $E_g(n)$ satisfying the condition $E_{g-UD} > E_{g-OP} > E_{g-OD}$, where UD, OP and OD denotes underdoped, optimal doped and



FIGURE 7. The single excitation energy gap (Δ_0) as a function of polar angle $\varphi = \tan^{-1}(k_y/k_x)$ for $\Delta t = 0.1$ eV (light gray) and $\Delta t = 0.5$ eV (dark gray).

overdoped regimes, respectively. This inequality indicates that the underdoped regime is not the most stable, since its energy is higher than the optimal doped one. Moreover, if t'/t is fixed, the largest condensation energy $(E_{\rm con})$, defined as the difference between the ground state energies E_g at $T = T_c$ and T=0 K, is achieved at $n_{\rm op}$, in agreement with experimental results [14]. Figure 6(c) shows $E_{\rm con}(n)$ for both cases, -t'/t = 0.06 with $\Delta t = 0.5$ eV (squares), and -t'/t = -0.07 with $\Delta t = 0.1$ eV (circles).

In practice, as occurs in LSCO and BSCO systems, the electronic doping n can be modified by atomic substitution, which in turn changes the value of t'/t due to the variations in atomic sizes and the corresponding modification of the lattice parameter. It is important to mention that, for d-wave superconductors, U only shifts the mean-field self-energy, E_{MF} (Eq. (16)) whereas a positive V could affect the superconducting state by diminishing the effect of Δt_3 . In fact, the latter interaction parameter is the more important one for d-wave superconductivity, although all of them are present in transition metals with narrow bands [15].

On the other hand, the superconducting properties obtained for $\Delta t = 0.5$ eV and $\Delta t_3 = 0.05$ eV are summarized in Table III. Observe that the minimum energy, $E_{\text{g-min}} = -0.89731704$ eV, occurs at $n_{op} = 0.790$ with $T_{\text{c-max}} = 101.27$ K, *i.e.*, as one could expect, the maximum T_c is attained for the most stable superconducting system. It is important to mention that the chemical potential (μ) is a function of temperature, therefore, for a fixed set of model parameters, they are somewhat different at T = 0K and $T = T_c$. For this case, $\Delta t = 0.5$ eV, which leads to a larger T_c , this difference is also larger and then there is a slight discrepancy between the location of $E_{\text{g-min}}$ and $T_{\text{c-max-sup}} = 99.8$ K.

Figure 7 shows the single-excitation energy gap (Δ_0) , defined as the minimum value of $E(\mathbf{k})$ along the $\varphi = \tan^{-1}(k_y/k_x)$ direction, for the parameter values where the supreme value of T_c is reached with $\Delta t = 0.1$ eV (light gray line) and $\Delta t = 0.5$ eV (dark gray line). For the latter case, notice the sharp feature at the antinodal points 0° , 90° , etc., or at the corresponding points $(\pi, 0), (0, \pi)$, etc., of the first Brillouin zone which could be detected by ARPES technique [16].

4. Discussion

A discussion has already been done along the paper, however, it is important to emphasize that it is possible to define a supreme value for the set of maximum critical temperatures which occurs at the minimum of the ground state energy. The results presented in this work give an alternative way to look for the appropriate set of Hamiltonian parameters to fit the experimental data by studying the supreme value of T_{c-max} as a function of t'/t. From this point of view, the mean field treatment can be considered as a first good approximation to describe the superconductivity for a great variety of superconductors reported in the literature.

5. Conclusions

In summary, we have studied the d-wave superconducting ground state as a function of the ratio t'/t within the generalized Hubbard model, where a second neighbor correlatedhopping term is included. Within the BCS formalism, the superconducting properties are calculated by solving two coupled integral equations (12) and (13), where the integrals involved can be efficiently calculated by isolating the region around the Fermi surface. The ground state energy (E_q) was obtained for all the optimal electron concentrations where T_c is maximum, for both $\Delta t = 0.1$ eV and $\Delta t = 0.5$ eV, with $\Delta t_3 = 0.05$ eV. For the second case, the critical temperature is considerably enhanced and there is a doping regime where the single-electron band width is reduced and the superconducting chemical potential lies out of this band. In this case, the Fermi surface disappears, opening the question about the pseudogap regime experimentally found for superconductors with carrier concentrations close to half-filling. It is suggested that this pseudogap could be found for $n_{op} > n_{op-sup}$. It is worth mentioning that the difference of 0.4 eV between the two values of Δt studied, leads to a critical temperature enhancement of 60 K for d-wave superconductors, even if the d-wave superconductivity is originated from the Δt_3 interaction. This effect is lower than that found for s*-wave superconductors, where only Δt is considered [13]. The results reported in this work suggest a possible semi-analytical approach to Eqs. (12) and (13), where the length and shape of the FS should be considered. Since the computing time needed to obtain $n_{\text{op-sup}}$ is large, it is necessary a complementary numerical method to fit the set of Hamiltonian parameters with a real superconductor system, and this will be the subject of future works. Finally, references [4,5] consider other approaches to fit the model parameters from experimental results, but now it is also suggested to consider that superconductivity occurs at some optimal doping with maximum critical temperature and minimum ground state energy within the parameters space.

Acknowledgments

This work has been supported by UNAM-UNACAR exchange project and DGAPA-UNAM-PAPIIT IN10717. Computations were performed at Miztli of DGTIC-UNAM (Project LANCAD-UNAM-DGTIC-180).

- 1. C.C. Tsuei and J.R. Kirtley, Rev. Mod. Phys. 72 (2000) 969.
- 2. H.B. Schüttler and A.J. Fedro, Phys. Rev. B 45 (1992) 7588.
- 3. I.I. Mazin and D.J. Singh, Phys. Rev. Lett. 79 (1997) 733.
- 4. J.S. Millán, L.A. Pérez, C. Wang, Physica C 471 (2011) 735.
- 5. C. Galván, L.A. Pérez, C. Wang, Phys. Lett. A 376 (2012) 1380.
- L.A. Pérez, J.S. Millán, C. Wang, *Int. J. Mod. Phys. B* 24 (2010) 5229.
- 7. L.A. Pérez, C. Wang, Solid State Commun. 121 (2002) 669.
- J.S. Millán, L.A. Pérez, E. Shelomov, C. Wang, *Physica C* 460-462 (2007) 1051.
- 9. T. Matsuzaki, N. Momono, M. Oda, M. Ido, J. Phys. Soc. Jpn. **73** (2004) 2232.

- 10. J. Tarascon et al., Phys. Rev. B 38 (1988) 8885.
- 11. Masatoshi Imada, Atsushi Fujimori, and Yoshinori Tokura, *Rev. Mod. Phys.* **70** (1998) 1039.
- 12. E. Pavarini, I. Dasgupta, T. Saha-Dasgupta, O. Jepsen, O.K. Andersen, *Phys. Rev. Lett.* **87** (2001) 047003.
- 13. J.E. Hirsch and F. Marsiglio, Phys. Rev. B 39 (1989) 11515.
- T. Matsuzaki, M. Ido, N. Momono, M. Oda, *Physica C* 217 (2003) 388-389.
- 15. J. Hubbard, Proc. Roy. Soc. London A 276 (1963) 238.
- 16. A. Damascelli, Z. Hussain, Z-X. Shen, *Rev. Mod. Phys.* **75** (2003) 473.