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BCS-Hubbard model applied to anisotropic superconductors

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ABSTRACT

Based on the BCS formalism, we study the critical temperature (T_c) as a function of electron density (n) in a square lattice by means of a generalized Hubbard model, in which first (Δt) and second neighbors (Δt_3) correlated-hopping interactions are included in addition to the repulsive Coulomb ones. We compare the theoretical T_c vs. n relationship with experimental data of cuprate superconductors $BiSr_{2-x}La_xCuO_{6+\delta}$ (BSCO) and $La_{2-x}Sr_xCuO_4$, (LSCO). The theory agrees very well with BSCO data even though the complicated association between Sr concentration (x) and hole doping (p). For the LSCO system, it is observed that in the underdoped regime, the T_c vs. n behavior can be associated to different systems with small variations of t'. For the overdoped regime, a more complicated dependence $n = 1 - p/2$ fits better than $n = 1 - p$. On the other hand, it is proposed that the second neighbor hopping ratio (t'/t) should be replaced by the effective mean field hopping ratio t'_{MF}/t_{MF}, which can be very sensitive to small changes of t' due to the doping.

1. Introduction

The study of correlated electron models that could lead to anisotropic superconductivity has been highly motivated by the observation of *d*-symmetry gaps in hole-doped cuprate superconductors [1]. There is a general consensus that in these materials the Cooper pairs are hole singlets, which are mainly restricted to move on the CuO_2 planes [2,3]. Three-band Hubbard models have been proposed to describe the hole dynamics on these planes [4]. These models can be reduced into single-band ones [5] and the electronic states close to the Fermi energy could be reasonably well described by a square-lattice single-band tight binding model with a next-nearest-neighbor hopping [6,7]. Lately, we have found that the second-neighbor correlated-hopping interaction (Δt_3) is essential in the $d_{x^2-y^2}$ wave superconductivity, despite its relative small magnitude in comparison with other interaction terms [8].

2. The model

In this work, we analyze the critical temperature of *d-wave* superconducting ground states within a square lattice containing nearest (t) and next-nearest neighbor (t') hoppings, correlated-hopping interactions between first (Δt) and second (Δt_3) neighbors, along with on-site (U) and nearest-neighbor (V) Coulomb interactions. This Hamiltonian can be written as

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

where $c^+_{i\sigma})(c_{i\sigma})$ is the creation (annihilation) operator with spin $\sigma = \downarrow$ or $\uparrow$ at site i, $n_{i,\sigma} = c^+_{i\sigma}c_{i\sigma}$, $n_i = n_{i,\uparrow} + n_{i,\downarrow}$, $\langle i,j\rangle$ and $\ll i,j\gg$ denote respectively nearest-neighbor and next-nearest-neighbor sites. This model can lead to *s*- and *d*-wave superconducting ground states without negative U and V [8]. Let us consider a square lattice with lattice parameter a, performing a Fourier transform, this Hamiltonian in the momentum space becomes

$$\widehat{H} = \sum_{\mathbf{k},\sigma}\varepsilon_0(\mathbf{k})c^+_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma} + \frac{1}{N_s}\sum_{\mathbf{k},\mathbf{k}'}V_{\mathbf{k},\mathbf{k}',\mathbf{q}}c^+_{\mathbf{k}+\mathbf{q},\uparrow}c^+_{-\mathbf{k}'+\mathbf{q},\downarrow}c_{-\mathbf{k}'+\mathbf{q},\downarrow}c_{\mathbf{k}+\mathbf{q},\uparrow} + \frac{1}{N_s}\sum_{\mathbf{k},\mathbf{k}',\sigma}W_{\mathbf{k},\mathbf{k}',\mathbf{q}}c^+_{\mathbf{k}+\mathbf{q},\sigma}c^+_{-\mathbf{k}'+\mathbf{q},\sigma}c_{-\mathbf{k}'+\mathbf{q},\sigma}c_{\mathbf{k}+\mathbf{q},\sigma}, \quad (2)$$

where N_s is the total number of sites,

$$\varepsilon_0(\mathbf{k}) = 2t[\cos(k_x a) + \cos(k_y a)] + 4t'\cos(k_x a)\cos(k_y a), \quad (3)$$

$$V_{\mathbf{k},\mathbf{k}',\mathbf{q}} = U + V\beta(\mathbf{k}-\mathbf{k}') + 2\Delta t_3\gamma(\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}) + \Delta t[\beta(\mathbf{k}+\mathbf{q}) + \beta(-\mathbf{k}+\mathbf{q}) + \beta(\mathbf{k}'+\mathbf{q}) + \beta(-\mathbf{k}'+\mathbf{q})], \quad (4)$$

and

$$W_{\mathbf{k},\mathbf{k}',\mathbf{q}} = \frac{V}{2}\beta(\mathbf{k}-\mathbf{k}') + \Delta t_3[\gamma(\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}) + \gamma(-\mathbf{k}+\mathbf{q},-\mathbf{k}'+\mathbf{q})] + 2\Delta t_3\gamma(\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}), \quad (5)$$

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being

$$\beta(\mathbf{k}) = 2[\cos(k_x a) + \cos(k_y a)], \tag{6}$$

$$\gamma(\mathbf{k}, \mathbf{k}') = 4\cos(k_x a)\cos(k'_y a) + 4\cos(k'_x a)\cos(k_y a), \tag{7}$$

and $2\mathbf{q}$ is the wave vector of the pair center of mass. After a standard Hartree–Fock decoupling of the interaction terms in Eq. (2), the reduced Hamiltonian for singlet pairing with $\mathbf{q} = \mathbf{0}$ can be written as:

$$\widehat{H} = \sum_{\mathbf{k},\sigma} \varepsilon(\mathbf{k}) c^+_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{1}{N_s} \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}',\mathbf{0}} c^+_{\mathbf{k},\uparrow} c^+_{-\mathbf{k}',\downarrow} c_{-\mathbf{k}',\downarrow} c_{\mathbf{k},\uparrow}, \tag{8}$$

where the mean-field dispersion relation is given by

$$\varepsilon(\mathbf{k}) = \varepsilon_{MF} + 2t_{MF}[\cos(k_x a) + \cos(k_y a)] + 4t'_{MF}\cos(k_x a) \times \cos(k_y a), \tag{9}$$

where $\varepsilon_{MF} = (\frac{U}{2} + 4V)n$ is the mean-field self-energy, $t_{MF} = t + n\Delta t$, and $t'_{MF} = t' + 2n\Delta t_3$ are the first and second neighbor mean field hoppings, respectively.

Applying the BCS formalism [9] to Eq. (2), we obtain the following two coupled integral equations [8], which determine the d-wave superconducting gap (Δ_d) and the chemical potential (μ) for a given temperature (T) and electron density (n),

$$1 = -\frac{(V - 4\Delta t_3)}{N_s} \sum_{\mathbf{k}} \frac{[\cos(k_x a) - \cos(k_y a)]^2}{2E(\mathbf{k})} \tanh\left(\frac{E(\mathbf{k})}{2k_B T}\right) \tag{10}$$

and

$$n - 1 = -\frac{1}{N_s} \sum_{\mathbf{k}'} \frac{\varepsilon(\mathbf{k}') - \mu}{E(\mathbf{k}')} \tanh\left(\frac{E(\mathbf{k}')}{2k_B T}\right), \tag{11}$$

where the single excitation energy is given by

$$E(\mathbf{k}) = \sqrt{(\varepsilon(\mathbf{k}) - \mu)^2 + \Delta^2(\mathbf{k})}, \tag{12}$$

being

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

In particular, the critical temperature (T_c) is determined by $\Delta_d(T_c) = 0$.

3. Results

In Fig. 1, the critical temperature is shown for systems with $t = -1$, any U, $V = 0$, $\Delta t = 0.1|t|$, $\Delta t_3 = 0.05|t|$, $t' = 0.10|t|$ (gray line), $t' = 0.09|t|$ (black line) $t' = 0.08|t|$ (light gray line), in comparison with experimental data for BSCO (solid squares) extracted from Ref. [10], and assuming a mean contribution of $p = 0.002758$ for each experimental point starting from $p = 0.11$, i.e., $n = 1 - [0.11 + 0.002758(i - 1)]$, $i = 1, \ldots, 25$. The mean-field hopping ratio (t'_{MF}/t_{MF}) for these systems are shown in Table 1, and is worth to consider the corresponding hopping ratio of 0.3 for BSCO [11].

For the LSCO system, the comparison was made with a similar set of parameters of BSCO but with small variation of t' in order to shift the optimum values of n more close to half filling ($n = 1$). These results are shown in Fig. 2, for a set of parameters with $t = -1$, any U, $V = 0$, $\Delta t = 0.1|t|$, $\Delta t_3 = 0.05|t|$, $t' = 0.08|t|$ (black line) and $t' = 0.01|t|$ (gray line), in comparison with experimental data for LSCO (solid circles) extracted from Ref. [12], where it has been assumed a contribution of $n = 1 - p$, with $p = x$. Fig. 3 shows the comparison for a system with $t' = 0.01|t|$ (gray line) and $t' = -0.04|t|$ (light gray line), and LSCO from [12] but assuming the rule $n = 1 - p$ and the hole doping (p) obeying $p = x/2$ (open circles).

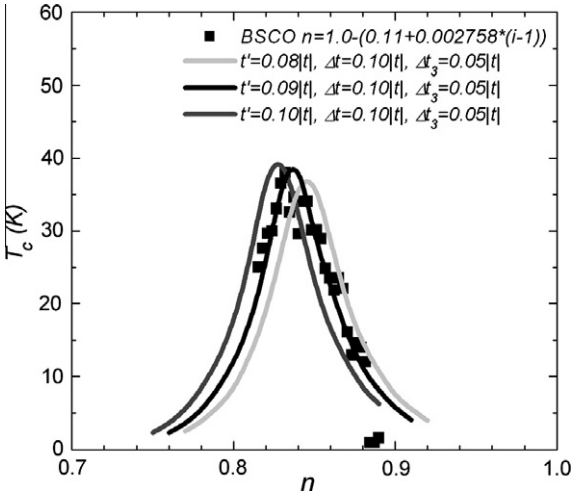

Fig. 1. Critical temperature (T_c) as a function of electronic density (n) for systems with $t = -1$, any U, $V = 0$, $\Delta t = 0.1|t|$, $\Delta t_3 = 0.05|t|$, $t' = 0.10|t|$ (gray line), $t' = 0.09|t|$ (black line) $t' = 0.08|t|$ (light gray line), in comparison with experimental data for BSCO (solid squares) extracted from reference [10] and assuming a mean contribution of $p = 0.002758$ for each experimental value of x starting from $p = 0.11$.

Table 1
t'_{MF}/t_{MF} ratio for the systems of Fig. 1.

$t'/\|t\|$	n_{op}	$\Delta t_3/\|t\|$	$t_{MF}/\|t\|$	$t'_{MF}/\|t\|$	t'_{MF}/t_{MF}
0.10	0.83	0.05	−0.917	0.183	−0.199
0.09	0.84	0.05	−0.916	0.174	−0.189
0.08	0.85	0.05	−0.915	0.165	−0.180

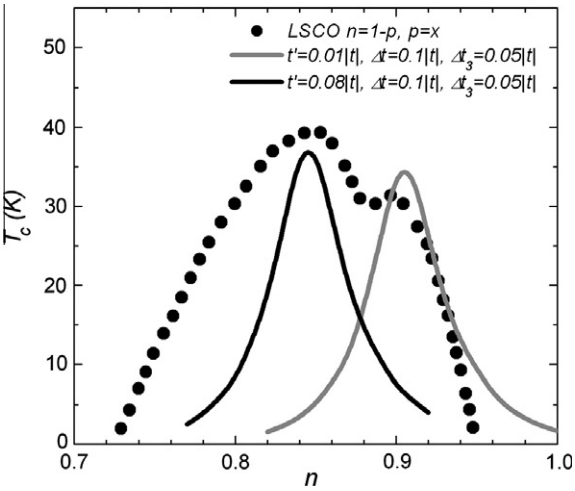

Fig. 2. Critical temperature (T_c) as a function of electronic density (n) for systems with $t = -1$, any U, $V = 0$, $\Delta t = 0.1|t|$, $\Delta t_3 = 0.05|t|$, $t' = 0.08|t|$ (black line) and $t' = 0.01|t|$ (gray line), in comparison with experimental data for LSCO (solid circles) extracted from Ref. [12], where it has been assumed a contribution of $n = 1 - p$, with $p = x$.

The corresponding mean-field ratios for these systems are summarized in Table 2.

It is worth to observe that the mean-field hopping ratio of 0.1 estimated for LSCO [11] is closer for the maximum of the experimental curve located at $n = 0.90$, which corresponds to the system with $t' = 0.01|t|$ leading to $t'_{MF} = 0.1|t|$. For a better adjustment of the critical temperature with the experiment, it would be necessary some small variations of Δt and Δt_3.

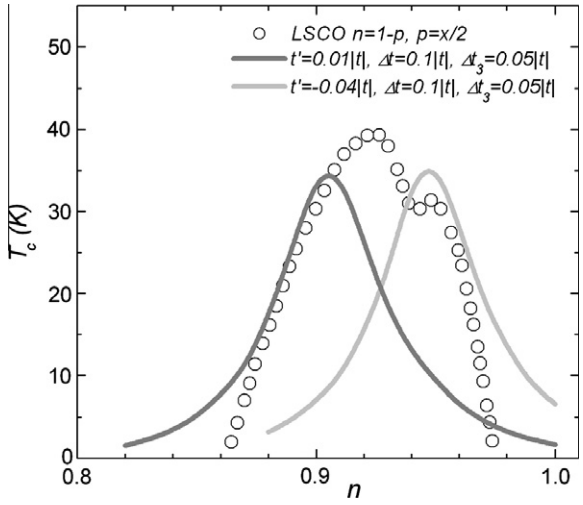

Fig. 3. A comparison for systems with $t = -1$, any U, $V = 0$, $\Delta t = 0.1|t|$, $\Delta t_3 = 0.05|t|$, $t' = 0.01|t|$ (gray line) and $t' = -0.04|t|$ (light gray line), and LSCO data from [12] and assuming the rule $n = 1 - p$ but with the hole doping (p) obeying $p = x/2$ (open circles).

Table 2
t'_{MF}/t_{MF} ratio for the systems of Figs. 2 and 3.

$t'/\|t\|$	n_{op}	$\Delta t_3/\|t\|$	$t_{MF}/\|t\|$	$t'_{MF}/\|t\|$	t'_{MF}/t_{MF}
0.08	0.85	0.05	−0.915	0.165	−0.18
0.01	0.90	0.05	−0.910	0.100	−0.109
−0.04	0.95	0.05	−0.905	0.055	−0.06

4. Conclusions

In summary, we have presented a single-band generalized Hubbard model on a square lattice, which leads to two coupled integral equations within the BCS formalism. The results reveal the key participation of Δt_3 in the appearance of d-wave superconductivity, in spite of its small strength in comparison with other terms of the model. It would be worth mentioning that the thermodynamic properties of d-wave superconducting ground states are independent of U. Hence, the use of BCS mean-field approach is justified, since the other interaction terms in the Hamiltonian (1) are generally small in comparison with the single-particle bandwidth. The critical temperature always shows an optimal value of n where T_c is maximum, and an appropriate set of parameters can be found in order to make a good comparison with the experimental results for BSCO and LSCO compounds. Moreover, the results suggest a nontrivial hole-doping dependence with x concentration. It is worth to mention that different sets of parameters can give the same critical temperature, therefore it is necessary to determine with more precision which t' and correlated hopping parameters Δt and Δt_3 correspond to each compound.

Acknowledgments

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