Journal of Physics and Chemistry of Solids 69 (2008) 3369–3371

Contents lists available at ScienceDirect

Journal of Physics and Chemistry of Solids

journal homepage: www.elsevier.com/locate/jpcs

Analysis of the BCS equations for anisotropic superconductivity

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ARTICLE INFO

Keywords:
A. Superconductors
D. Superconductivity
D. Thermodynamic properties

ABSTRACT

Anisotropic superconducting states have been studied within a generalized Hubbard model and the BCS formalism, which leads to two coupled integral equations that determine the chemical potential and the superconducting gap. In this work, these equations are analyzed. Their integrand functions have sharp walls at the Fermi surface, which mainly determine the integrals. Furthermore, the chemical potential obtained from these equations is close to that from the mean-field density of states (DOS) and quite different to that from non-interacting DOS. Finally, the calculated condensation energy as a function of doping is compared with experimental data obtained from $La_{2-x}Sr_xCuO_4$ and $Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{7-\delta}$.

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 relatively small magnitude in comparison with other interaction terms [8]. In this article, we report the critical temperature, chemical potential, superconducting gap and condensation energy of *d*-wave superconducting ground states by means of a generalized single-band Hubbard model [8] 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 for holes can be written as:

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

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 $\langle\langle i,j\rangle\rangle$ denote, respectively, nearest-neighbor and next-nearest-neighbor sites. This Hamiltonian for holes can be written in the momentum space as:

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

where N_s is the total number of sites,

$$\varepsilon_0(\mathbf{k}) = 2t[\cos(k_x a)+\cos(k_y a)] + 4t'\cos(k_x a)\cos(k_y a),$$
$$V_{\mathbf{k},\mathbf{k}'\mathbf{q}} = U + V\beta(\mathbf{k}-\mathbf{k}') + 2\Delta t_3\gamma(\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}) + \Delta t[\beta(\mathbf{k}+\mathbf{q})+\beta(-\mathbf{k}+\mathbf{q})+\beta(\mathbf{k}'+\mathbf{q}) + \beta(-\mathbf{k}'+\mathbf{q})],$$

and

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

being

$$\beta(\mathbf{k}) = 2[\cos(k_x a)+\cos(k_y a)],$$
$$\gamma(\mathbf{k},\mathbf{k}') = 4\cos(k_x a)\cos(k'_y a) + 4\cos(k'_x a)\cos(k_y a),$$

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 $\mathbf{q}=0$ can be written as:

$$\hat{H} = \sum_{\mathbf{k},\sigma}\varepsilon(\mathbf{k})c^+_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma} + \frac{1}{N_s}\sum_{\mathbf{k},\mathbf{k}'}V_{\mathbf{k},\mathbf{k}',0}c^+_{\mathbf{k},\uparrow}c^+_{-\mathbf{k}',\downarrow}c_{-\mathbf{k}',\downarrow}c_{\mathbf{k},\uparrow}, \quad (3)$$

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doi:10.1016/j.jpcs.2008.06.104

and the mean-field dispersion relation is given by

$$\varepsilon(\mathbf{k}) = \left(\frac{U}{2} + 4V\right)n + 2(t + n\Delta t)[\cos(k_x a) + \cos(k_y a)] + 4(t' + 2n\Delta t_3)\cos(k_x a)\cos(k_y a). \quad (4)$$

Applying the BCS formalism [9] to Eq. (3), 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 hole density (n):

$$1 = -\frac{(V - 4\Delta t_3)}{N_s}\sum_{\mathbf{k}}\frac{[\cos(k_x a) - \cos(k_y a)]^2}{2E(\mathbf{k})}\tanh\left(\frac{E(\mathbf{k})}{2k_B T}\right), \quad (5)$$

$$n - 1 = -\frac{1}{N_s}\sum_{\mathbf{k}}\frac{\varepsilon(\mathbf{k}) - \mu}{E(\mathbf{k})}\tanh\left(\frac{E(\mathbf{k})}{2k_B T}\right), \quad (6)$$

where the single excitation energy is given by

$$E(\mathbf{k}) = \sqrt{(\varepsilon(\mathbf{k}) - \mu)^2 + \Delta^2(\mathbf{k})} \quad (7)$$

being

$$\Delta(\mathbf{k}) = \Delta_d[\cos(k_x a) - \cos(k_y a)]. \quad (8)$$

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

The main difficulty to solve Eqs. (5) and (6) comes from the numerical evaluation of the corresponding integrals. For example, in the case of Eq. (2), the integrand function is given by

$$F(k_x, k_y) = \frac{[\cos(k_x a) - \cos(k_y a)]^2}{|\varepsilon(k_x, k_y) - \mu|}\tanh\left(\frac{|\varepsilon(k_x, k_y) - \mu|}{2k_B T_c}\right) \quad (9)$$

at $T = T_c$. The contour plot of $F(k_x,k_y)$ is shown in Fig. 1 for $U = 6|t|$, $V = 0$, $t' = 0.43|t|$, $\Delta t = 0.5|t|$, $\Delta t_3 = 0.1|t|$, $n = 0.3$, $k_B T_c = 0.024|t|$, and $\mu = -0.711|t|$. Notice that the main contribution to the integral comes from the sharp *wall* located at the Fermi surface defined by $\varepsilon(\mathbf{k}) = \mu$. Then, the superconducting ground-state properties are mainly determined by the Fermi surface. This fact is in accordance to the BCS theory [9]. Furthermore, the integrals can be efficiently calculated by dividing the Brillouin zone into three regions. One corresponds to an area of a certain width around the Fermi surface comprising the high values of the integrand (illustrated by the clear region in Fig. 1), and the other two of them correspond to the inside and outside sections. It is worth mentioning that the integrands in Eqs. (5) and (6) do not diverge, since $\tanh(x)/x \to 1$ as $x \to 0$.

In Fig. 2(a) the chemical potential (μ), Fig. 2(b) the critical temperature (T_c), and Fig. 2(c) the superconducting gap at $T = 0$ (Δ_d) are shown as functions of the hole density (n) for $t' = 0.43|t|$, $V = 0$, $\Delta t = 0.5|t|$, $\Delta t_3 = 0.1|t|$, and arbitrary U, obtained by using the mean-field density of states (DOS) (open squares), the single-particle DOS (open circles), and by solving the coupled Eqs. (5) and (6) (solid squares). In all the calculations it is considered that $t = -1$. Notice that μ, T_c, and Δ_d obtained from the coupled Eqs. (5) and (6) are very close to those from the mean-field DOS and quite different to solutions obtained from the non-interacting DOS. This fact allows reducing significantly the computing time by calculating the chemical potential from the mean-field DOS and inserting it in Eq. (2), i.e., it is only necessary to solve one equation instead of two coupled integral ones. In addition, observe that both the maxima of $T_c(n)$ and $\Delta_d(n)$ are located at low hole concentrations close to the experimental results for high-T_c superconductors [10].

In this work, we also calculate the condensation energy per site (W_c) of the d-wave superconducting ground state, which is defined as the difference between the energy per site in the normal state at T_c (W_n), and the superconducting energy per site at $T = 0$ (W_s), i.e., $W_c = W_n - W_s$. This quantity can be determined experimentally from electronic specific heat measurements [11,12]. In the generalized Hubbard model, the energy per site of the d-channel superconducting ground state (W_s), at $T = 0$, is

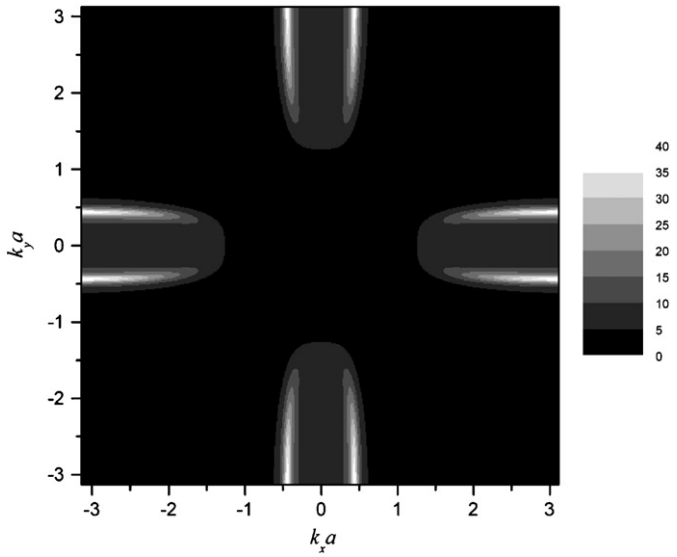

Fig. 1. Contour plot of $F(k_x,k_y)$ on the first Brillouin zone for a system with $U = 6|t|$, $V = 0$, $t' = 0.43|t|$, $\Delta t = 0.5|t|$, $\Delta t_3 = 0.1|t|$, $n = 0.3$, $k_B T_c = 0.024|t|$, and $\mu = -0.711|t|$.

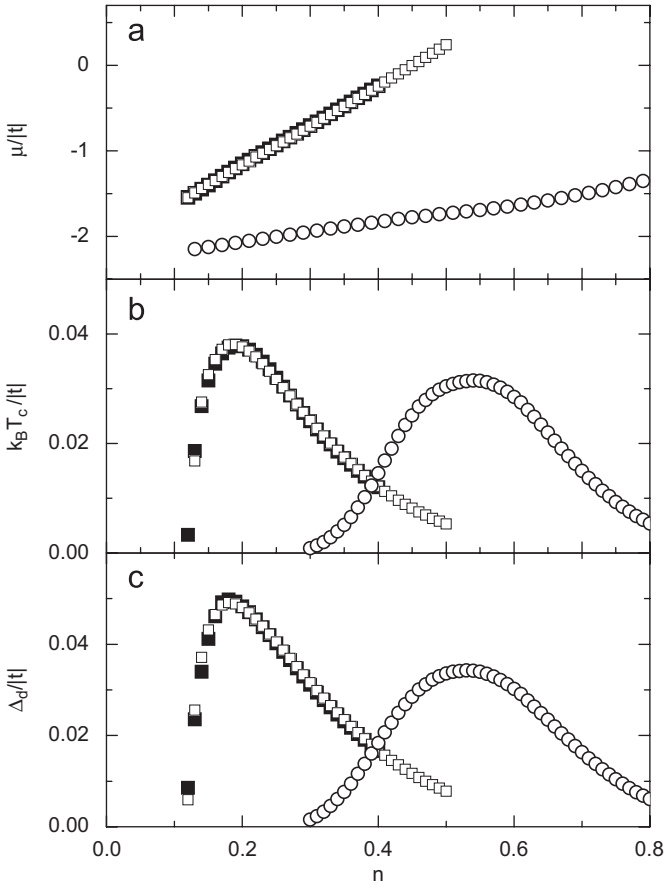

Fig. 2. (a) Chemical potential (μ), (b) critical temperature (T_c), and (c) d-wave superconducting gap (Δ_d) as functions of the hole density (n) obtained from two equations (solid squares), mean-field DOS (open squares), and one-particle DOS (open circles) for $t' = 0.43|t|$, $V = 0$, $\Delta t = 0.5|t|$, $\Delta t_3 = 0.1|t|$, and arbitrary U.

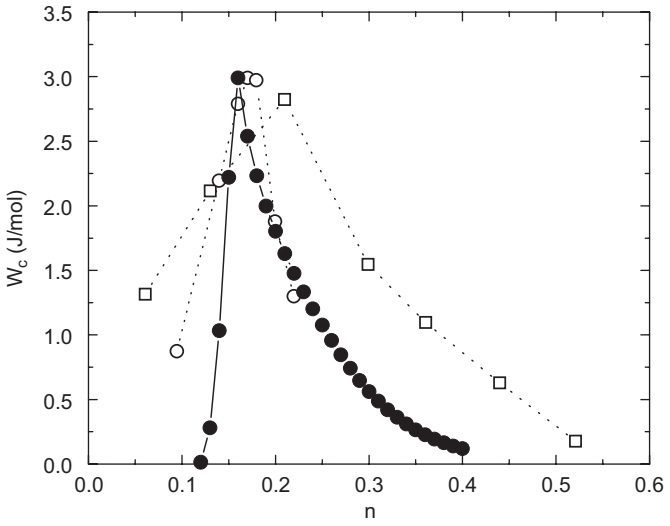

Fig. 3. Condensation energy per site (W_c) as a function of the hole density (n) for the same system in Fig. 2 (solid circles), compared with the experimental data obtained from $La_{2-x}Sr_xCuO_4$ [11] (open circles) and $Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{7-\delta}$ [12] (open squares), assuming that $x=\delta=n$.

given by

$$W_s=\frac{1}{N_s}\sum_{\mathbf{k}}[\varepsilon(\mathbf{k})-E(\mathbf{k})]+\frac{\Delta_d^2}{4\Delta t_3-V}+(n-1)\mu-\left(\frac{U}{4}+2V\right)n^2, \tag{10}$$

where Δ_d and μ are obtained from Eqs. (5) and (6). Likewise, W_n is obtained from Eq. (10) by taking $\Delta_d=0$ together with the appropriate μ.

In Fig. 3, the calculated W_c as a function of the doping for $t'=0.43|t|$, $V=0$, $\Delta t=0.5|t|$, $\Delta t_3=0.1|t|$, and arbitrary U (solid circles), is shown in comparison with the experimental data obtained from $La_{2-x}Sr_xCuO_4$ [11] (open circles) and $Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{7-\delta}$ [12] (open squares). Notice that the theoretical W_c has the same behavior as the experimental results. A more detailed comparison between the theory and the experimental data requires the knowledge of the relationship between the hole density (n) and the doping (x or δ) in the corresponding material.

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. These integrals can be efficiently calculated by isolating the region around the Fermi surface. Moreover, we have shown that the superconducting chemical potential can be safely approximated by that obtained from the mean-field DOS and then the computing time to calculate T_c and Δ_d can be significantly reduced, since it is only necessary to self-consistently solve a single equation. 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 all the Coulomb interaction terms in the model are small in comparison with the single-particle bandwidth. The critical temperature and the d-wave superconducting gap show non-monotonic behaviors as a function of the hole concentration and the maximum T_c is obtained at a hole concentration close to the experimental results. Finally, the theoretical condensation energy as a function of the doping presents a good agreement with the experimental data.

Acknowledgments

This work has been partially supported by UNAM-IN113008, UNAM-IN114008, CONACyT-58938, and the UNAM-UNACAR exchange project. Computations have been performed at Bakliz and KanBalam of DGSCA, UNAM.

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