Superconductivity in a strongly correlated electron system: A theoretical study

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In this work we study the superconductivity within an attractive two-dimensional one-band Hubbard model. We consider a *d*-wave superconducting gap and a Hubbard-I approximation to describe the strongly correlated superconducting regime. We use the Green's function method to obtain the order parameter Δ and the superconducting critical temperature T_c. The results show that for fixed values of the superconducting attractive potential $U(U<0)$, the gap increases for low temperatures but diminishes abruptly as the temperature increases. The effect of pressure is discussed, varying the next-nearest-neighbor hopping t_2, yielding a change in T_c, and also in Δ_0, and a tendency to suppress the superconductivity. © *2009 American Institute of Physics*. [DOI: 10.1063/1.3063667]

I. INTRODUCTION

It is known that some high temperature superconducting (HTSC) materials, such as cuprates, as well as superconducting heavy fermions, show strong electronic correlations.[1] In spite of the large use of the Bardeen–Cooper–Schrieffer (BCS) first order mean field approach to study the behavior of these materials, it is more appropriate to use a more suitable approximation to treat the strong coupling regime. Therefore, we apply here a Hubbard-I approximation[2] to obtain the zero temperature superconducting gap Δ_0 and the superconducting critical temperature T_c in a two-dimensional Hubbard model for different values of densities of charge carriers $\langle n\rangle$. Besides the calculation of Δ_0 and T_c, we have studied the effect of t_2, the next-nearest-neighbor hopping integral, on T_c observing that when t_2 increases, T_c and Δ_0 tend to be suppressed. This is because the pressure effect on the cuprates can be attributed to the variation in t_2 and hence to the variation in the lattice parameter. The effect of t_2 on T_c has been studied by different groups[3,4] for some HTSC materials. Pavarini *et al.*[3] reported a correlation between the experimental maximum superconducting temperature ($T_c^{\max}$) and the value of t_2 evaluated from band structure calculations in different cuprates, but, in most of the cases, the mechanism which may govern the relationship between T_c and t_2 in these materials is not well understood. It should be noticed that both t (the nearest neighbor) and t_2 are affected by external pressure P.[5] The effect of P on t has almost the same behavior as in t_2, in what concerns the variation in lattice parameter of the material,[5] and hence on T_c. Therefore, since we have adopted throughout this work $t(P=0)$ as the energy unity, we expect that the variation in t_2 with P gives a very fair approximation of the effect of P on T_c. In our calculations we fixed $U=-8.0t(t>0)$, a parameter suitable to describe a strong coupling regime.

II. THEORY

In order to study the dynamics of the charge carriers with correlations and the basic attractive interaction, we consider a two-dimensional one-band Hubbard Hamiltonian,

$$H=\sum_{\langle\langle ij\rangle\rangle\sigma} t_{ij}^{d} d_{i\sigma}^{\dagger} d_{j\sigma} + U\sum_{\langle ij\rangle\sigma} n_{i,\sigma} n_{j,-\sigma}, \tag{1}$$

where $d_{i\sigma}^{\dagger}(d_{i\sigma})$ is the fermionic creation (annihilation) operator at site $\mathbf{r}_i$ for the d band and spin $\sigma=\{\uparrow\downarrow\}$. $n_{i\sigma}=d_{i\sigma}^{\dagger}d_{i\sigma}$ is the density operator and t_{ij}^{d} is the hopping integral between sites i and j nearest neighbors and next-nearest neighbors for the d electrons. $U(U<0)$ is the attractive potential between the d electrons, which can result from the elimination of the electron-phonon coupling through a canonical transformation or, as suggested by Hirsch and Scalapino,[6] it may be provided by the competition between on-site and nearest-neighbor site Coulomb interactions for some range of parameters. The dispersion relation is given by

$$\epsilon_{d\mathbf{k}}=-2t[\cos(k_x)+\cos(k_y)]+4t_2\cos(k_x)\cos(k_y)+\epsilon_0, \tag{2}$$

where ϵ_0 is an adjustable constant and it is fixed so that the convergence in each different density is attained. To obtain the superconductor order parameter Δ_0, we calculate the equations of motion of the propagators $\langle\langle d_{i\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$, $\langle\langle d_{i,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$,[7] and the equations of motion for the new generated Green's functions $\langle\langle n_{j,-\sigma}d_{i\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$ and $\langle\langle n_{j\sigma}d_{i,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}$, following the Hubbard-I approach[2] and a higher order mean field treatment,

$$2U\sum_{jp}\langle\langle n_{p,-\sigma}n_{j,-\sigma}d_{i\sigma};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}\approx\tilde{U}\sum_{j}\langle\langle n_{j,-\sigma}d_{i\sigma};d_{l\sigma}\rangle\rangle_{\omega} + 2\langle n\rangle\sum_{j}\Delta_{ij}\langle\langle d_{j,-\sigma}^{\dagger};d_{l\sigma}^{\dagger}\rangle\rangle_{\omega}, \tag{3}$$

where $\tilde{U}=2U\langle n\rangle$ and $\Delta_{mn}=U\langle d_{m,\sigma}^{\dagger}d_{n,-\sigma}^{\dagger}\rangle$ is the superconduct-

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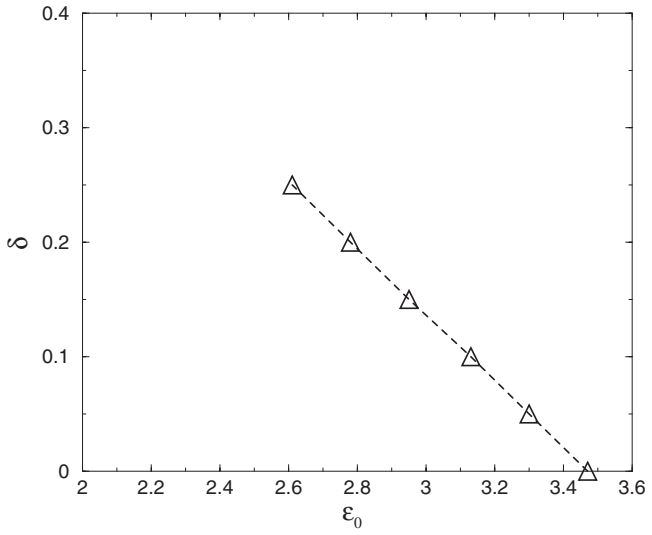

FIG. 1. The dependence of the doping $\delta=1-\langle n\rangle$ on ϵ_0 (see text).

ing order parameter. We stress that the mean field adopted in Eq. (3) is different from the BCS approach since the decoupling is made in a further step of the Green's function. In the momentum space, and considering a d-wave gap symmetry, the order parameter is given by[5] $\Delta_{\mathbf{k}}=2\Delta|\cos(k_x)-\cos(k_y)|$.

From the above relations one obtains the self-consistent gap equation

$$\Delta=-\frac{1}{N_s}\sum_k \frac{2\Delta\gamma_{\mathbf{k}}U}{E_{1\mathbf{k}}^2-E_{2\mathbf{k}}^2}[E_{1\mathbf{k}}\tanh(\beta E_{1\mathbf{k}}/2) - E_{2\mathbf{k}}\tanh(\beta E_{2\mathbf{k}}/2)], \tag{4}$$

where N_s is the number of sites in the lattice, $\gamma_{\mathbf{k}}=|\cos(k_x)-\cos(k_y)|$ for the d-wave symmetry, and $U<0$. Also,

$$E_{1,2\mathbf{k}}=\sqrt{\frac{\zeta_{\mathbf{k}}}{2}\pm\frac{\sqrt{\zeta_{\mathbf{k}}^2-16\tilde{U}^2\Delta_{\mathbf{k}}^2}}{2}}, \tag{5}$$

with $\zeta_{\mathbf{k}}=\tilde{U}^2+\epsilon_{d\mathbf{k}}^2+2\tilde{U}\epsilon_{d\mathbf{k}}$. We hope that our non-BCS approach is good enough to describe some features of the HTSC cuprates.

III. NUMERICAL RESULTS AND CONCLUSIONS

In Fig. 1 we show the dependence of the doping $\delta=1-\langle n\rangle$ on ϵ_0, for $\epsilon_0=-\tilde{U}/4.60$. This value of ϵ_0 gave the expected convergence for each different density $\langle n\rangle$. As expected, δ versus ϵ_0 is monotonically decreasing. A similar result was obtained by Civelli[8] with a cluster extension of dynamical mean field theory. He obtained the dependence of δ on the chemical potential μ and, in the same way, δ decreases with μ. Also, in both works, the range of values of ϵ_0 and μ became near. In Fig. 2 we exhibit the Fermi surface for three different $\langle n\rangle$ values: 0.90 ($\epsilon_0=3.1304$), 0.85 ($\epsilon_0=2.9565$), and 0.70 ($\epsilon_0=2.4$), which are quite similar to some angle resolved photoemission spectroscopy (ARPES) cuprate data.[9]

In Fig. 3 we exhibit the temperature dependence of the gap for two different values of $\langle n\rangle$, in the strong coupling regime, $U=-8t$. We observe that for small temperatures, the

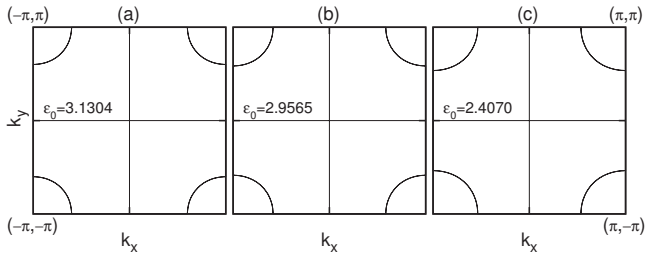

FIG. 2. The Fermi surface for three different densities: (a) $\langle n\rangle=0.90$, (b) $\langle n\rangle=0.85$, and (c) $\langle n\rangle=0.70$.

gap increases slightly, whereas when the temperature increases approaching T_c, the gap decreases abruptly, for all values of $\langle n\rangle$. This behavior is quite different from BCS calculations,[10] where the gap remains almost constant in the whole range of temperature, decaying abruptly when approaching T_c. Hence, we conclude that this is a direct consequence of the Hubbard-I approach, i.e., strong attractive coupling regime. Also, a similar behavior for the gap curve was obtained recently by Aryanpour *et al.*[11] using a Hubbard model, within a Monte Carlo (MC) mean field. Figures 4(a) and 4(b) show the t_2-dependence of Δ_0 and T_c for different $\langle n\rangle$. In all the cases, Δ_0 and T_c decrease when t_2 increases. From Fig. 4(b) one can see that the curve is more inclined for higher values of $\langle n\rangle$, which shows that T_c is more affected by the change in t_2 in this range of $\langle n\rangle$, i.e., when the limit of one electron per site is achieved ($\langle n\rangle=1.0$). When $\langle n\rangle \leq 0.90$, T_c is not so affected by a change in t_2, i.e., the compound is not so dependent on external pressure, similar to the BCS behavior. Also, Khatami *et al.*[12] worked on the same problem. In their work they considered a positive U two-dimensional Hubbard model with a Holstein term and a dynamical cluster approximation with a quantum MC cluster to develop the Hamiltonian. For $\langle n\rangle=0.95$ they have obtained a small increase in T_c when t_2 increases, and for $\langle n\rangle=0.85$, their results indicate an almost constant T_c for increasing t_2.

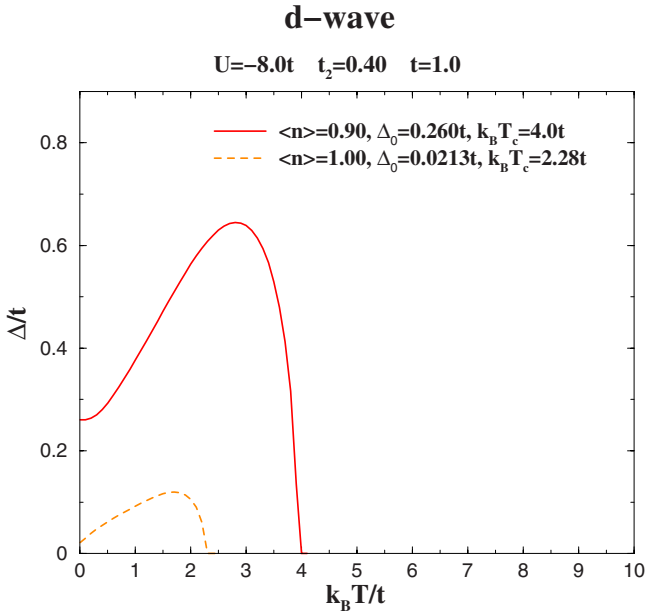

FIG. 3. (Color online) The temperature dependence of the gap.

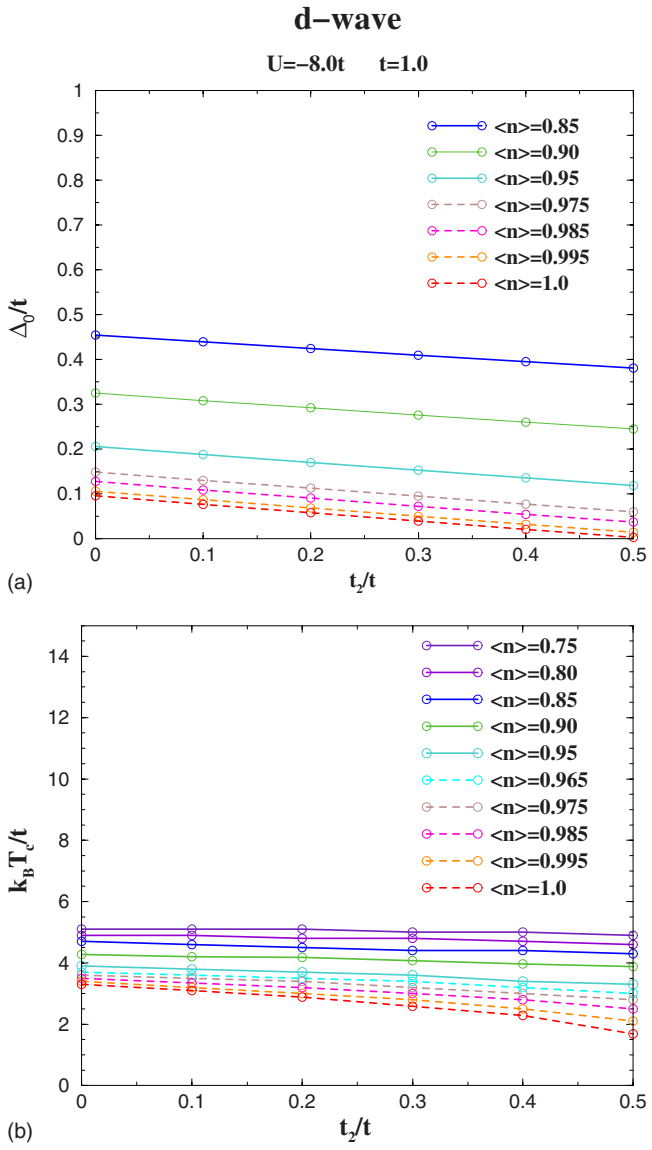

FIG. 4. (Color online) t_2-dependence of Δ_0 and T_c for different values of density $\langle n \rangle$.

In Fig. 5 it is shown the t_2-dependence of $\xi = 2\Delta_0/k_B T_c$. One can see that as t_2 increases, ξ decreases. For higher densities, the curve is more inclined, and ξ is more sensitive to a change in t_2.

Our results indicate that the increase in the hopping t_2 tends to suppress T_c and Δ_0 for both higher and lower values of the density $\langle n \rangle$. Since the lower densities are less affected by a change in t_2, we conclude that they are not so dependent on external pressure since external pressure affects t_2.[5]

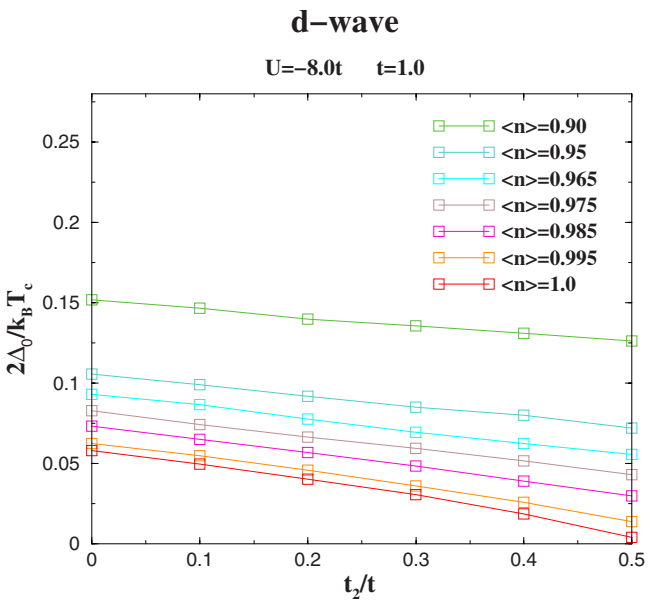

FIG. 5. (Color online) The t_2-dependence of $\xi = 2\Delta_0/k_B T_c$.

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