BCS to Bose-Einstein crossover phase diagram at zero temperature for a $d_{x^2-y^2}$ order parameter superconductor: Dependence on the tight-binding structure

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We study the effect of the next-nearest-neighbor (NNN) hopping matrix element t' on the zero-temperature ($T=0$ K) crossover phase diagram, namely, from the BCS limit to the Bose-Einstein regime, for a model which presents a $d_{x^2-y^2}$ superconductor order parameter symmetry. This theoretical generalization is required by angle-resolved photoemission spectroscopy experiments. Our NNN hopping is characterized by the parameter $\alpha \equiv t'/t \neq 0$, where t is the nearest neighbor hopping matrix element. For $\alpha \geqslant 0$, there is a crossover of BCS binding energy type as described [B. C. den Hertog, Phys. Rev. B **60**, 559 (1999)] by keeping the density fixed. However, for $\alpha < 0$, the system is always in the Bose-Einstein regime for $n \leqslant n_c \approx 0.12$. We conclude that the presence of the NNN hopping matrix element drastically influences the crossover diagram for a $d_{x^2-y^2}$ superconductor.

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I. INTRODUCTION

The existence of a crossover from BCS superconductivy to a *Bose-Einstein* condensation (BEC) has been extensively discussed in recent years. These ideas come from the pioneering works of Eagles,[2] Leggett,[3] and Nozières and Schmitt-Rink.[4] However, the latest interest in the crossover problem is due to its possible application to the understanding of the rich phase diagram of high-temperature superconductors (HTSC's).[5,6] However, the mechanism of high-temperature superconductivity in the cuprates remains a puzzle.[7] Many cuprates with CuO_2 layers have been synthesized and all exhibit a phase diagram with T_c going through a maximum as a function of doping. The prevaling explanation is that at low doping, superconductivity is destroyed with rising temperature by the loss of phase coherence, and at high doping it is destroyed by pair breaking.[8]

Many theories are based on the Hubbard model with one Cu $d_{x^2-y^2}$-like orbital per CuO_2 unit. With t, t', t'', ... denoting the hopping integrals on the square lattice, the electron part of the Hamiltonian is

$$\varepsilon(\vec{k}) = -2t[\cos(k_x)+\cos(k_y)] - 4t'\cos(k_x)\cos(k_y) - 2t''[\cos(2k_x)+\cos(2k_y)] + \cdots, \quad (1)$$

in the $\vec{k}$ representation and setting the lattice constant $a=1$. Usually, only t and t' are taken as nonzero.[9] Guided by Fermi-surface (FS) shapes, it is customary to use $t'/t \approx 0.1$ for doped La_2CuO_4, $YBa_2Cu_3O_7$, and $Bi_2Sr_2CaCu_2O_8$. In our work we also consider the effect of $t'<0$, as well.

We have a large body of experimental data suggesting that pairing in the superconducting cuprates (HTSC's) is predominantly $d_{x^2-y^2}$ in character.[10,11] In consequence, we need a clear understanding of the properties of the BCS-BEC crossover phase diagram when the order parameter symmetry is of $d_{x^2-y^2}$ type.

Here we consider the BCS-BEC crossover at $T=0$ K as function of both coupling strength $(V/4t)$ and carrier density (n), where V is the absolute value of the BCS pairing potential and t is the value of the nearest neighbor (NN) hopping matrix element. We focus on a two-dimensional (2D) toy model which has $d_{x^2-y^2}$ pairing symmetry.

To extend the work of den Hertog[1] we take a free tight-binding structure given by

$$\varepsilon(\vec{k}) = -2t[\cos(k_x)+\cos(k_y)] - 4\alpha t\cos(k_x)\cos(k_y), \quad (2)$$

where $\alpha \equiv t'/t$ is the adimensional next-nearest-neighbor NNN hopping matrix element. In this paper we study the BCS-BEC crossover when $\alpha \neq 0$. Here t' is the NNN hopping matrix element. For $\alpha=0$ we indeed reproduce den Hertog's results.[1] The solutions for $\alpha>0$ and $\alpha<0$ show different behaviors as shown in Fig. 2 for $\alpha=0.1$ and Fig. 4 for $\alpha=-0.1$ (see Sec. III). That the parameter α (or t') is needed in the free band structure has been justified by angle-resolved photoemission spectroscopy (ARPES) as discussed by Pavarini *et al.*[9]

We mention the work of Kuboki,[12] where he studies the effect of band structure on the symmetry of superconducting states. According to this work, states with different symmetries can be stabilized within the same type of attractive interaction. We leave for the future such studies, namely, studying different symmetries due to a change of the band structure or the shape of the Fermi surface. We mention that evidence for nodes in the gap equations for non-HTSC materials have been measured by Bonalde *et al.*[13] They have used penetration depth measurements in Sr_2RuO_4, which is an unconventional superconductor. An unconventional superconductor is that which, in the superconducting phase, breaks both the U(1) and G symmetries. G is the point symmetry group. For inhomogeneous superconductors, G includes the translational group as well.[14] Also, time reversal

symmetry (TRS) could be broken[15] as it is the case of Sr_2RuO_4.[13] This has been verified experimentally by means of spin-polarized resonance (μSR).[16]

Another aspect which is worth pursuing is the study of size shrinking for increasing density in the BCS-BEC crossover. Andrenacci, Pieri, and Strinati[17] have studied this problem for a continuous model in the strong-coupling regime. Of course, finite-tempeature studies are called for, especially those related to the calculation of T_c. Here T_c is the starting point to evaluate the isotope effect exponent.[18]

Our approach here, based on a BCS treatment, is a restricted one since as was discussed by Brovetto *et al.*[19] the BCS electron pairing mechanism is not the only one in unconventional superconductors.[14] For example, there is another known electronic pairing, Lewis's pairing, which is due to two electrons paired in neighboring lattice layers with equal momenta. However, once we have an interacting Hamiltonian, we can proceed along the lines of Ref. 19 using a Bogoliubov-Valatin transformation[20,21] to produce a set of noninteracting quasiparticles for which appears an energy gap $\Delta(\theta)$ in the quasiparticle spectrum, as occurs with Cooper's pairs. So our treatment may also be applicable to Lewis's pairs.[19]

This paper is organized as follows. In Sec. II we present the toy model and the equations to be solved using the BCS mean-field approach to superconductivity. In Sec. III we present our results for $\alpha=0.1$ and $\alpha=-0.1$, while discussing the crossover problem and its dependence on the sign of α. In Sec. IV we present our conclusions and extensions of our work.

II. TOY MODEL

We use an effective Hamiltonian in the BCS sense which describes a two-particle interaction in real space and in the Cooper channel:[22]

$$H=\sum_{i,j,\sigma} t_{i,j}(c^{\dagger}_{i,\sigma}c_{j,\sigma}+\text{H.c.})-\mu\sum_{i,\sigma} n_{i,\sigma} - V\sum_{\langle i,j\rangle} c^{\dagger}_{i,\uparrow}c^{\dagger}_{j,\downarrow}c_{j,\downarrow}c_{i,\uparrow}, \tag{3}$$

where $t_{i,j}=-t$ for NN and $t_{i,j}=-t'$ for NNN hopping. In what follows we adopt the notation $t'\equiv\alpha t$.

By expressing the superconducting gap in terms of its various symmetry components[22] and introducing the BCS variational wave function $|\Psi\rangle=\Pi_{\vec{k}}(u_{\vec{k}}+v_{\vec{k}}c^{\dagger}_{\vec{k},\uparrow}c^{\dagger}_{-\vec{k},\downarrow})|0\rangle$, with $|0\rangle$ the normal state Fermi sea, the $T=0$ K order parameter equation in the $d_{x^2-y^2}$ symmetry channel is expressed by

$$1=\frac{1}{2N}\sum_{\vec{k}}\frac{V[\cos(k_x)-\cos(k_y)]^2}{\{[\epsilon(\vec{k})-\mu]^2+\Delta^2[\cos(k_x)-\cos(k_y)]^2\}^{1/2}}, \tag{4}$$

where $\epsilon(\vec{k})$ is given by Eq. (2). The amplitude of the *d*-wave order parameter is represented by Δ. Here N is the number of lattice points in a square lattice. In Eq. (4) the summation in $\vec{k}$ is taken on the whole Brillouin zone; i.e., the pairing potential is constant on the whole Brillouin zone. Let us point out that a shell potential developed by Quintanilla and Georfy[23] contains a *d*-wave component as well.

Eagles[2] in his pioneering work pointed out that any deviation from weak coupling requires a self-consistent solution of both order parameter and density equations, since the chemical potentials in the normal and superconducting phases are no longer equal. Thus, the density equation for μ and the particle density n is given by

$$n=1-\frac{1}{N}\sum_{\vec{k}}\frac{(\epsilon(\vec{k})-\mu)}{\{[\epsilon(\vec{k})-\mu]^2+\Delta^2[\cos(k_x)-\cos(k_y)]^2\}^{1/2}}. \tag{5}$$

We solved Eqs. (4) and (5) self-consistently at a given n by numerical summation. Here we have assumed pairing over the entire Brillouin zone (BZ) as done by den Hertog.[1] This allows us to couple the gap and carrier density equations, self-consistently. In Sec. III we present some numerical results which convey the role played by α on the crossover phase diagram.

III. SOME NUMERICAL RESULTS ON THE CROSSOVER PROBLEM

A. Results for $\alpha>0$: namely, $\alpha=0.1$

In Fig. 1 we present $\mu/4t$ vs $V/4t$ for fixed densities. We have done the calculations for $n=0.1$ (diamonds), 0.3 (squares), 0.5 (triangles), and 0.875 (circles). From these results we observe that, for small values of carrier concentrations n, the chemical potential has a strong variation with the strength of the attractive interaction, $V/4t$. However, for large values of n, the chemical potential $\mu/4t$ practically remains unchanged as a function of $V/4t$. In consequence, for large values of the carrier concentration the system always remains in the BCS limit; i.e., the chemical potential stays inside the free tight-binding band. This figure will help to evaluate the crossover between the BCS and BEC regions. The horizontal line at $\mu/4t=-1-\alpha$ represents the bottom of the free tight-binding band. For weak coupling, it is well knows that $\mu/4t$ in the superconductor is given, roughly speaking, by the Fermi energy in the normal phase and this is clearly seen in Fig. 1. However, at large doping, μ is almost constant in marked contrast with low-density results. The low density regime shows a rapid deviation from weak coupling as $V/4t$ is increased.

In the inset of Fig. 1 we present results for $\Delta/4t$ vs $V/4t$ for fixed values of n. This figure will allow us to determine the crossover between the normal and BCS regions. This crossover region is technically evaluated by requiring that $\Delta\equiv 0$ in the figure of Δ vs $V/4t$. In other words, the BCS region begins with the onset of a finite order parameter (OP), which is a manifestation of the superconducting state. As is seen, an increase of the carrier density favors the emergency of a $d_{x^2-y^2}$ paired ground state; namely, a higher carrier density requires smaller values of $V/4t$ to get BCS paired states.

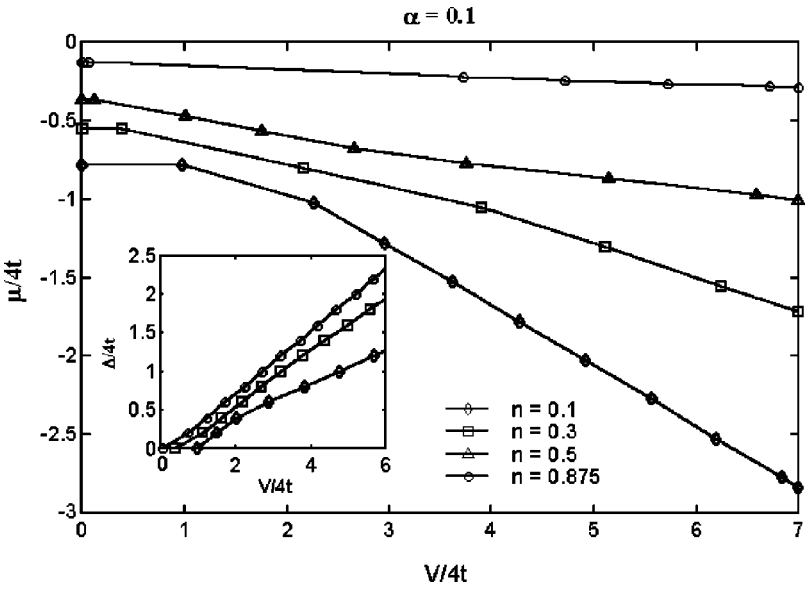

FIG. 1. $\mu/4t$ vs $V/4t$, for $\alpha=0.1$, for different values of n (see text). In the inset we show $\Delta/4t$ vs $V/4t$, for the same parameters (see text for more details).

In Fig. 2 we have a phase diagram, namely, n vs $V/4t$, which has been constructed from Fig. 1, as previously explained. The left (or first) curve is obtained with the onset of the superconducting OP, i.e., for $\Delta=0$. To the left of this curve we have a metal in the normal phase. To the right of this curve we have the BCS regime ($\Delta\neq0$). Now, the second (or right) curve corresponds to the begining of the Bose-Einstein condensation regime, which is defined here as the point where the chemical potential $\mu/4t$ just jumps out below the bottom of the free tight-binding band. Operationally, this curve is obtained by requiring $\mu=-1-\alpha$. This criterium is equivalent to the known definition of the BEC criterium, $\mu\leqslant0$, for an ideal boson gas.[24] From our Fig. 2 we see that bosonic degrees of freedom can only emerge in the dilute regime. For large densities the system behaves more likely a weak-coupling superconductor with a value of μ comparable to that of the normal phase, i.e., $\mu\approx$const.

B. Results for $\alpha<0$: namely, $\alpha=-0.1$

In Fig. 3 we present $\mu/4t$ vs $V/4t$. All that we have said for the case of $\alpha=0.1$ is valid for the case of $\alpha=-0.1$. However, we recall that for the case of an *s*-wave OP superconductor, there is superconductivity for any value of V, namely, $V_{min}=0$. In the inset of Fig. 3 we present Δ vs $V/4t$, for fixed values of n.

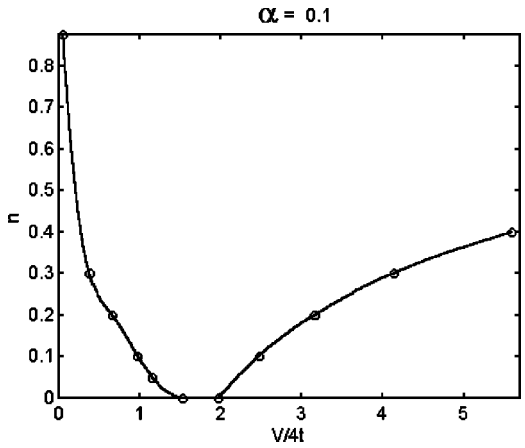

FIG. 2. Phase diagram, i.e., n vs $V/4t$, for $\alpha=0.1$, for different values of n (see text).

In Fig. 4 we present the phase diagram, namely, n vs $V/4t$, following the same criteria as discussed in Fig. 2. From Fig. 4 we observe that our system is always in the BEC regime for $n\leqslant n_c\approx0.12$ if we adopt that the BEC condition is equivalent to $\varepsilon_{min}/4t<-1-\alpha$. Furthermore, we observe that the normal region is located in this region. We conclude that (1) either there is a coexistence region where both BEC and normal conditions are satisfied or (2) that the BEC condition has to be elaborated further. For the case of coexisting phases, we need to go into energy considerations to find the true ground state of the system. All these new features are in striking difference with respect to the $\alpha=0$ (Ref. 1) and $\alpha>0$ cases.

IV. CONCLUSIONS, DISCUSSION, AND OUTLOOK

From our previous results (Sec. III) we conclude that the BCS-BEC crossover phase diagram depends critically on the sign of the NNN hopping matrix element. In fact, for $\alpha>0$, we find that for any fixed value of the carrier density n there is a crossover from the BCS regime (weak coupling) to the BEC regime with bosonic degrees of freedom (strong attraction). In this sense, we find that these results ($\alpha>0$) are similar to the case of $\alpha=0$.[1]

We find that below a critical density ($\alpha<0$) the system is always in the BEC limit. This condition is completely different for the case of $\alpha>0$, indicating that new features appear due to the presence of next-nearest-neighbor hopping matrix elements in the band structure. These features need to be further explored in the sense of finding a working criterium to define the BCS-BEC crossover precisely.

We also find that for $\alpha<0$ and for $n>n_c$, the crossover BCS-BEC happens for smaller values of $V/4t$. For $\alpha<0$,

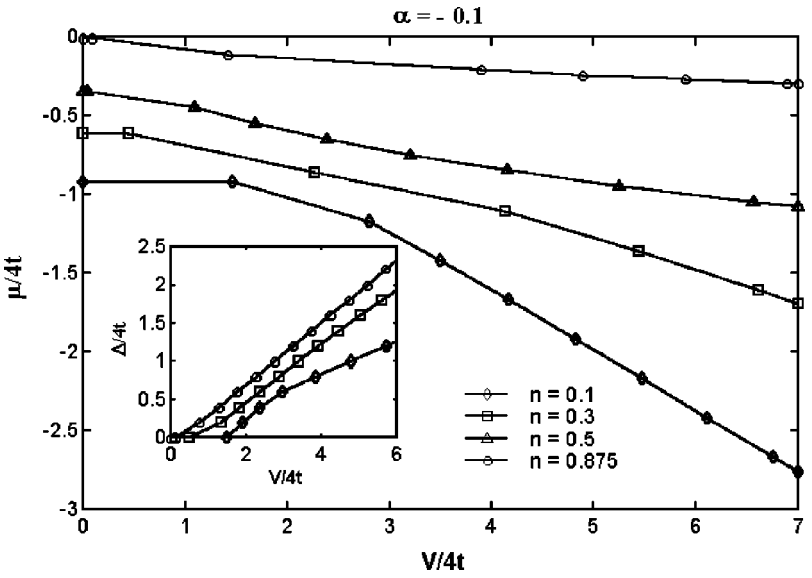

FIG. 3. $\mu/4t$ vs $V/4t$, for $\alpha=-0.1$, for different values of n (see text). In the inset we show $\Delta/4t$ vs $V/4t$, for the same parameters (see text for more details).

$\mu/4t$ vs $V/4t$ has numerical solutions for a minimum value value of n. However, for $n \leqslant n_c$, we are in the BEC limit, because the chemical potential is below the bottom of the band, i.e., $\mu<-1-\alpha$. These considerations do not apply for the case of $\alpha>0$; i.e., there is no critical value of n.

We can go further and say that with doping the hopping amplitude can change sign.[25] This dependence makes the crossover problem a very interesting one. Recently, Quintanilla *et al.*[26] have studied the crossover in the context of free fermions interacting with a nonretarded effective pair potential that is attractive at a well-defined distance r_0: the δ-shell potential. However, they have not considered the normal-BCS line ($\Delta \equiv 0$).

We would like to say again that the summation performed in Eq. (4) corresponds to the whole Fermi sea. However, in their original formulation, the BCS gap equation is given by

$$1=\frac{1}{2N}\sum_{\vec{k}}\frac{Vg(\vec{k})[\cos(k_x)-\cos(k_y)]^2}{\{[\epsilon(\vec{k})-\mu]^2+\Delta^2[\cos(k_x)-\cos(k_y)]^2\}^{1/2}}, \tag{6}$$

where $g(\vec{k})=1$, if $|\epsilon(\vec{k})-\mu| \leqslant \omega_D$, and zero otherwise, with ω_D being the Debye energy. Work is in progress to calculate the phase diagram under the influence of the Debye energy using the two self-consistent equations: namely, Eqs. (5) and (6). We comment that the presence of the Debye cutoff ω_D is needed to evaluate the isotope effect as has been done recently by de Mello and Rodríguez-Núñez.[18]

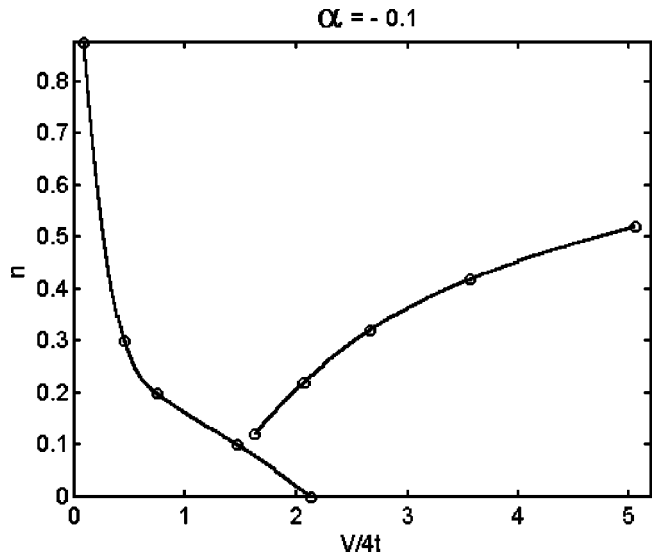

FIG. 4. Phase diagram, i.e., n vs $V/4t$, for $\alpha=-0.1$, for different values of n (see text).

We caution the reader that the present model is very naive if we want to apply it directly to HTSC materials, which, obviously, have a complex primitive cell. In addition, in the toy model, when we use the criterion that $\mu=-1-\alpha$, the chemical potential pulls out from the bottom of the free tight-binding band. According to this the Fermi surface is not well defined. This is the reason to keep the chemical potential inside the free tight-binding band. For example, the fermion-boson model of superconductivity[27] considers a coupled system of fermions, with a well-defined Fermi surface and bosons which are responsible for producing superconductivity. However, this fermion-boson model of superconductivity has been recently challenged by Alexandrov and Edwards,[28] who consider that the relevant mechanism of superconductivity is bipolaronic pairing.

We have studied the phase diagram n vs $V/4t$ using the BCS approach. However, we know that a mean-field treatment is valid for small values of $V/4t$. When we reach intermediate to strong values of $V/4t$, namely, for $V/4t \geqslant 1$, we must take into consideration superconducting fluctuations as done many years ago by Schmid.[29]

It is well established now that the characteristic which makes the cuprate superconductors unique is their non-Fermi-liquid behavior and Coulomb effects in the underdoped regime, as discussed by Rice.[30] Such effects have not been considered in this work, but they can be easily included.[31–33]

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