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The BCS–BE crossover phase diagram at T = 0 K for a d-wave superconductor: the importance of the Debye frequency and the tight binding band structure

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Abstract

We consider the phase diagram of the BCS (Bardeen-Cooper-Schrieffer)-BE (Bose-Einstein) crossover in the ground state (T = 0 K) of a $d_{x^2-y^2}$ -wave superconductor, with a nearest neighbour tight binding structure, when we take into account the Debye (phononic) frequency around the chemical potential, μ . This approach is a continuation of the work of den Hertog (1999 Phys. Rev. B 60 559) and that of Soares et al (2002 Phys. Rev. B 65 174506). The latter authors considered the influence of the second-nearest neighbours, but neither set of authors took into account the effect of the Debye frequency, $\omega_{\rm D}$, or the influence of the next nearest neighbour matrix hopping element. We have found the following results: (1) there is **not** a metallic phase—that is, $\Delta/4t \rightarrow 0$ when $V/4t \rightarrow 0$, $\forall \omega_D/4t$, $\forall \alpha' \in (-1/2, +1/2)$, and $\forall n$, where n is the carrier density per site, V is the attractive interaction, t is the nearest neighbour hopping integral, and α' is the next nearest neighbour hopping ratio; (2) the BCS–BE crossover line is strongly affected by the presence of $\omega_D/4t$ and that of α' —actually, the values of V/4t needed to achieve the Bose–Einstein regime become extremely large for small values of $\omega_D/4t$; and (3) both $\Delta/4t$ and $\mu/4t$ strongly depend on the values of $\omega_D/4t$ and α' . The results (1) are in agreement with the ones found by Perali et al (2003 Phys. Rev. B 68 066501 (Preprint condmat/0211132)) and Rodríguez-Núñez et al (2003 Phys. Rev. B 68 066502), and in disagreement with those of den Hertog and Soares et al.

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1. Introduction

The existence of a crossover from BCS (Bardeen–Cooper–Schrieffer) superconductivity to a Bose–Einstein (BE) condensation regime was found in the pioneering work of Eagles [1], Leggett [2], and Nozières and Schmitt-Rink [3] (for s-wave superconductivity). The importance of this crossover arises from the belief that the high temperature superconductors (HTSC) [4] are in the intermediate coupling regime, that is, $V/4t \approx$ O(1) [5, 6], where perturbation theory is not applicable.

In the following we will study the BCS–BE crossover considering a tight binding structure given by

$$\varepsilon(k) \equiv -2t[\cos(k_x) + \cos(k_y)] + 4t'\cos(k_x)\cos(k_y) \tag{1}$$

which is obtained by Fourier analysing the kinetic part of the model Hamiltonian presented in equation (2). *t* is the value of the nearest neighbour hopping integral and *t'* is the next nearest neighbour hopping integral. In spite of the fact that this tight binding structure is too simple to explain the experimental data (mainly from ARPES (angle-resolved photoemission spectroscopy) experiments [7]), our main concern here is studying the effect of the Debye frequency, $\omega_D/4t$, on the BCS–BE crossover phase diagram at T = 0 K for a $d_{x^2-y^2}$ -wave superconductor. We will consider positive and negatives values of $t' \equiv \alpha' t$, namely, $|t'| \leq 0.5t$ or $|\alpha'| \leq 0.5$. It is possible to go from positive to negative values of α' by doping [12], assuming that the nnn hopping (overlap of nnn orbitals) depends on the doping. For the Bi₂Sr₂CaCu₂O_{8+ δ} compound, $\alpha' = 0.096/0.5908 \approx 0.162$ [8].

We point out that the BE–BCS crossover has also been observed in fermionic atom pairs. For example, Regal *et al* [9] have observed condensation of fermionic atom pairs in the BE–BCS crossover regime. A trapped gas of fermionic ⁴⁰K atoms is evaporatively cooled to quantum degeneracy and then a magnetic field Feshbach resonance is used to control the atom–atom interactions. The tuning of the atom–atom interaction allows one to control the BE–BCS crossover. Furthermore, a Bose–Einstein condensation of molecules has recently been observed [10]. This BE–BCS crossover has been studied theoretically in several papers [11].

This paper is organized as follows. In section 2, we present the system model and the equations to be solved using the mean field approach to superconductivity. In section 3 we present our results for different values of $\omega_D/4t$. In section 4 we present our discussion of the results, conclusions, and an outlook.

2. The system model and self-consistent equations

We use an effective Hamiltonian, in the BCS sense, which describes a two-particle interaction in real space and in the Cooper channel [13]:

$$H = \sum_{i,j,\sigma} t_{i,j} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{H.c.}) - \mu \sum_{i,\sigma} n_{i,\sigma} - V \sum_{\langle i,j \rangle} c_{i,\uparrow}^{\dagger} c_{j,\downarrow}^{\dagger} c_{j,\downarrow} c_{i,\uparrow}$$
(2)

where $t_{i,j} = -t$ for nearest neighbours (nn), $t_{i,j} = t' \equiv \alpha' t$ for next nearest neighbours (nnn), and $t_{i,j} = 0$ otherwise, μ is the chemical potential, H.c. means Hermitian conjugate, and V is the absolute value of the attractive interaction. From now on, our energy scale is taken to be 4t. $\langle i, j \rangle$ stands for nearest neighbour sites. The $d_{x^2-y^2}$ -wave symmetry has also been obtained by Quintanilla *et al* [14] using an attractive Dirac delta function (shell model). In a more recent paper, Quintanilla and Györffy [15] have discussed the stability of a superconductor with a combined symmetry, namely, s- and d-wave symmetry. As we will explore additionally the effect of the band structure, we refer the reader to the paper of Kuboki [16] where he discusses the stability of several superconducting symmetries due to specific values of t and t'. However, in the present paper we consider only the case of d-wave symmetry. Let us mention that our Hamiltonian of equation (2) is described in fermionic variables. As we will find the crossover line where the BCS region touches the BE region (the bosonic region of the phase diagram), our Hamiltonian is not suitable for studying that bosonic region.

Following the notation given in [17, 18], we solve for Δ_0 and μ the following set of self-consistent equations:

$$1 = \frac{V}{2N} \sum_{\vec{k}} \frac{\chi(\vec{k})\varphi^{2}(\vec{k})}{\sqrt{[\varepsilon(\vec{k}) - \mu]^{2} + \Delta_{0}^{2}\varphi^{2}(\vec{k})}}$$

$$n = 1 - \frac{1}{N} \sum_{\vec{k}} \frac{\varepsilon(\vec{k}) - \mu}{\sqrt{[\varepsilon(\vec{k}) - \mu]^{2} + \Delta_{0}^{2}\varphi^{2}(\vec{k})}}$$
(3)

where $\chi(\vec{k}) = 1$ for $|\varepsilon(\vec{k}) - \mu| \leq \omega_D$, and $\chi(\vec{k}) = 0$ for $|\varepsilon(\vec{k}) - \mu| > \omega_D$. ω_D is the Debye frequency; $\varphi(\vec{k})$ and $\varepsilon(\vec{k})$ give the tight binding structure (see equation (1)). The difference of this work and [17, 18] lies in the presence of the factor $\chi(\vec{k})$, which restricts our summation to the neighbourhood of the chemical potential. In equations (3), $N = N_x \times N_y$ is the number of lattice points. In section 3 we present the numerical results.

3. Numerical results for the interaction potential and the tight binding structure chosen

The numerical results were obtained by solving the continuous version of equations (3) which, in a fixed-point iteration form, are given by

$$\begin{split} \Delta_0^{i+1} &= \Delta_0^i \frac{V}{2\pi^2} \int \int d\vec{k} \, \chi(\vec{k}) \, \varphi^2(\vec{k}) \, F^i(\vec{k}) \\ \mu^{i+1} &= \frac{n-1+\frac{1}{\pi^2} \int \int d\vec{k} \, \varepsilon(\vec{k}) \, F^i(\vec{k})}{G^i} \\ G^i &= \frac{1}{\pi^2} \int \int d\vec{k} \, F^i(\vec{k}) \\ F^i(\vec{k}) &= \frac{1}{\sqrt{[\varepsilon(\vec{k}) - \mu^i]^2 + (\Delta_0^i)^2 \varphi^2(\vec{k})}} \\ i &= 0, 1, 2, \dots \end{split}$$

where the initial values Δ_0^0 and μ^0 where obtained by applying a steepest descent technique [34] to the first two equations above. The fixed-point iteration was then performed up to a relative tolerance of 10^{-4} , where the integrals were calculated numerically by means of Gauss–Kronrod rules [35] with a relative tolerance of 10^{-5} .

In the present work we have taken a d-wave superconducting order parameter due to the fact that experimental data [19, 20] on the high temperature cuprates points to this symmetry. The order parameter, with $d_{x^2-y^2}$ symmetry, which is used in equations (3), is given by [21, 22]⁴

$$\Delta_0(\vec{k}) = \Delta_0 \varphi(\vec{k}). \tag{4}$$

Numerical results are presented in figure 1. We observe that:

- (1) $\Delta/4t$ strongly depends on the value of $\omega_D/4t$ —thus, we find that $\Delta/4t$ increases with the value of $\omega_D/4t$ for fixed values of *n* and *V*/4*t*;
- ⁴ This order parameter symmetry has four nodes along the diagonal of the Brillouin zone.



Figure 1. The upper panel shows the superconducting order parameter $\Delta/4t$ versus V/4t for $\omega_D/4t = 0.5$, $\alpha' = -0.10$, and different carrier densities $n = 0.05, 0.1, 0.15, 0.20, 0.30, \dots, 0.90$ —the lowest curve corresponding to n = 0.05 and the uppermost curve to n = 0.90. The lower panel shows the corresponding μ versus V/4t plane. The dotted horizontal line at $\mu/4t = -1 + \alpha' = -0.9$ shows the criterion used to determine the BCS–BE crossover.

(2) the value of the superconducting order parameter goes to zero for small values of the attractive potential—that is, $\Delta/4t \rightarrow 0$ as $V/4t \rightarrow 0$.

This result is at odds with the results presented in [17, 18]. The reason for this discrepancy is explained by our choice of a continuous approach to equations (3) which is, in fact, equivalent to a dramatic increase in the number of lattice points.

These results imply that we do not observe a metallic phase as was previously claimed by the authors of [17, 18]. To be sure that we do not have a metallic region, that is, that $\Delta_0/4t \rightarrow 0$ exponentially for $V/4t \rightarrow 0$, a more detailed version of figure 1 (not shown here) has been analysed and it certainly shows that there is an exponential behaviour of $\Delta_0/4t$ towards zero for small values of V/4t, and no traces of a metallic behaviour or an insulating phase are observed. This result disagrees with those of [17, 18]. However, Perali *et al* have



Figure 2. The upper panel presents the crossover phase diagram for $\omega_D/4t = 0.50$, for several values of α' : 0.0, 0.1, 0.2, 0.3, 0.4, 0.5. The lower panel shows the $\Delta_0/4t$ versus V/4t plane for the corresponding condition for μ , namely, $\mu/4t = -1 + \alpha'$. In both panels the lowest curve corresponds to $\alpha' = 0.0$, the next curve to $\alpha' = 0.1$, and so on.

resolved this point in [23], where they have used a discrete approach with $N_x = N_y = 1024$, i.e., they did not find a metallic phase. See also [24].

In figure 2 we show the crossover phase diagram for $\omega_D/4t = 0.5$ and several values of α' . On each of these crossover curves we have $\mu/4t = -1 + \alpha'$. In consequence, we have a single line of points (n, V/4t) which separates the BCS phase from the BE phase. This line is known as the crossover line, since to the left of each of these curves we have Cooper pairs whose two electrons are well separated in real space (the BCS region), while to the right of this curve we have pairs of two electrons which are on top of each other (the BE region). The approach that we have followed (superconductivity λla BCS) is valid to the left of this crossover line. To the right of this line we have to use a bosonic description for our system.

In figures 3–5 we present the *n* versus V/4t phase diagrams for $\omega_D/4t = 0.5$ and $\alpha' = +0.2$, 0.0, and -0.2, respectively. The insets in these figures present the corresponding phase diagrams for $\omega_D/4t = 0.4$, 0.5, and 0.6. In figure 3 the range of the attractive interaction is restricted to $V/4t \in (0.0, 15.0)$. It is clear in this figure that for increasing values of $\omega_D/4t$, smaller values of V/4t are necessary to obtain the line of crossover from the BCS region (to the left of the line) to the BE region (to the right of the line). In figure 4 ($\alpha' = 0.0$) the range of



Figure 3. We present the crossover BCS–BE phase diagrams for $\omega_D/4t = 0.5$ and $\alpha' = +0.2$ where both the fermionic region (BCS) and the bosonic region (BE, i.e., $\mu/4t < -1.0 + \alpha'$) are shown. The inset shows the crossover lines for three different Debye frequencies $\omega_D/4t = 0.4$, 0.5, and 0.6.



Figure 4. The same as figure 3, but for $\alpha' = 0.0$.

attractive interaction is (17.0, 42.0) and a comparison between this figure and figure 3 shows that for decreasing values of α' the crossover point for a given value of *n* moves to higher values of V/4t. Furthermore, in figure 5, where $\alpha' = -0.2$, the interval for attractive interaction is 40 < V/4t < 120 since the crossover line is now located at much higher values of V/4t.

4. Discussion, conclusions, and outlook

We have calculated the superconducting order parameter, $\Delta/4t$, and $\mu/4t$ as functions of V/4t, considering the influence of the Debye frequency, $\omega_D/4t$. From figures 1–3 we conclude that $\omega_D/4t$ plays an important role in the fixing of the absolute values of the superconducting order parameter and the chemical potential.



Figure 5. The same as figure 3, but for $\alpha' = -0.2$.

We recall that in order to reach the BCS \rightarrow BE crossover the following condition has to be fulfilled: $\mu/4t = -1 + \alpha'$ for a given α' . Again, for $V/4t \rightarrow 0$ we have an exponential behaviour, namely, $\Delta_0/4t \propto \exp(-4at/V)$, where *a* is a numerical factor $a \approx O(1)$, as has been proved analytically by Perali *et al* [23].

In figures 3–5 we present the crossover BCS–BE phase diagrams for $\omega_D/4t = 0.5$ and $\alpha' = 0.2, 0.0, -0.20$, respectively. The BCS (fermionic) and BE (bosonic) regions are shown. The insets in these figures show the crossover lines for different Debye frequencies $\omega_D/4t = 0.4, 0.0, \text{ and } 0.6$. From these figures we observe that, for a given carrier density n, the crossover point moves to the right (i.e., to higher values of V/4t) when the value of α' is decreased. For instance, for $\alpha' = -0.20$, we see that the crossover line is only reached at very high values of V/4t. In addition, from the inset of each of these figures, we note that smaller values of $\omega_D/4t$ also demand higher values of V/4t to reach the crossover line in these phase diagrams where $\mu = -1 + \alpha'$. We point out that in figure 5 the range of values of V/4t is between 40 and 120. Even though these values of V/4t are beyond the plausible values for the cuprates or other materials of interest, we present this figure to clearly show that for $\alpha' < 0$ the crossover line can only be obtained at very large values of V/4t.

To our belief, previous authors [17, 18, 23] have not considered the influence of $\omega_D/4t$ because its presence demands really strong values of the attractive potential to obtain the BCS– BE crossover. As it is known that the BCS approximation works for $V/4t \approx O(1)$, when large values of V/4t are considered the effect of pairing fluctuations has to be taken into account, as it was many years ago by Schmid [25]. That the Debye energy cut-off, ω_D , moves the crossover line to the right is due to the feature that for $\omega_D/4t \neq \infty$ fewer \vec{k} -states are available. This is equivalent to saying that larger values of V/4t are needed to reach the bosonic regime, namely, where the two electrons of the Cooper pair sit on top of each other.

Throughout this work the condition $\mu/4t = -1.0 + \alpha'$ has been used as the criterion for the BCS–BE crossover line. However, very recently, Alexandrov [27] has put forward an alternative condition for reaching the crossover. It is given by $E_F \approx \pi \Delta$, where Δ is the binding energy and E_F is the Fermi energy. According to this criterion the pairing is individual in many high temperature cuprate superconductors. Also, we mention Kopeć [28], who has studied the crossover from a superconducting phase to a regime where the amplitude of the order parameter controls T_c . He establishes a self-consistent theory (involving both fermionic and bosonic



Figure 6. We present the crossover phase diagram for $\alpha' = 0.0$. The solid curves are for Alexandrov's condition, $\mu/t = -4 + 4\alpha' + \pi \Delta_0/t$, with $\omega_D/t = \infty$. The dashed curves represent the BCS–BE crossover phase diagrams with $\alpha' = 0$ and $\omega_D/t = \infty$ and 4.0. The upper dashed curve corresponds to $\omega_D/t = \infty$.

degrees of freedom), and calculates the superconducting phase coherence $T_c = T_c(|U|)$, where |U| is the absolute value of the attractive Hubbard model in three dimensions. According to his results [28], $T_c = T_c(|U|)$ exhibits a maximum where the behaviour crosses over from BCS to BE condensation. He examines a pseudo-gap in the normal state which emerges as a precursor of superconductivity at T_g due to the state with bound pairs but without long range coherence. We say that this precursor scenario is at odds with experimental results on the cuprate superconductors given by Tallon and Loram [29], where the pseudo-gap persists down to zero temperature and is independent from superconductivity.

In figure 6 we present the phase diagram (*n* versus V/t, upper figure) according to the condition given by Alexandrov [27], namely, $\mu/t = -4 + 4\alpha' + \pi \Delta_0/t$ (solid curve), and the BCS–BE crossover phase diagram according to the condition $\mu/t = -4 + 4\alpha'$ (used in the text). We quickly see that to obtain the BCS–BE crossover phase diagram we need higher values of V/t. For the lower curve (on the right axis) we can read off the value of Δ_0/t . It is the presence of the additional contribution $\pi \Delta_0/t$ which moves the phase diagram of Alexandrov to small values of V/t. We should mention that we have used the following approximation: $\Delta_0 \approx$ binding energy of two electrons bound by an attractive interaction.

We would like to study the effect of a phenomenological pseudo-gap on the crossover phase diagram, which was considered in another context in [30, 31]. In this case, the normal

state one-particle self-energy, in terms of the free one-particle Green function, is given by

$$\Sigma(\vec{k},\omega) = -E_g^2(\vec{k})G_0(\vec{k},-\omega)$$
(5)

where $E_g(\vec{k})$ is the value of the phenomenological pseudo-gap. We recall that the normal state one-particle Green function and the self-energy are related by [26]

$$G(\vec{k},\omega) = \frac{1}{[\omega + \mu - \varepsilon(\vec{k}) - \Sigma(\vec{k},\omega)]}.$$
(6)

In short, we conclude the following:

- The values of $\Delta_0/4t$ strongly depend on the chosen values of $\omega_D/4t$. For example, small values of $\omega_D/4t$ decrease the value of $\Delta_0/4t$, or require larger values of V/4t to produce the same values of $\Delta_0/4t$.
- The values of $\Delta_0/4t$ strongly depend on the chosen values of α' . For example, $\forall \alpha' \in (-1/2, +1/2)$ studied, increasing the values of α' increases the values of $\Delta_0/4t$.
- There is not a metallic phase, i.e., we have found that $\Delta/4t \rightarrow 0$ exponentially for $V/4t \rightarrow 0, \forall n, \forall \alpha', \text{ and } \forall \omega_D/4t$.
- The crossover BCS–BE line, namely (n, V/4t) for fixed values of n, moves towards larger values of V/4t for small values of $\omega_D/4t$ as well as for decreasing values of α' .
- The pure BE limit is reached at large values of ω_D/t , namely, $\omega_D/t \ge 8.0$. This is equivalent to taking $\chi(\vec{k}) \equiv 1, \forall \vec{k}$.

Finally, we recognize that the present model is too simple to be applicable to the high temperature cuprate superconductors, since we should include self-energy effects, such as the pseudo-gap discussed previously. Moreover, Andrenacci *et al* [32] have studied the evolution from BCS superconductivity to Bose–Einstein condensation using the current correlation function for a three-dimensional system of fermions embedded in a homogeneous background and mutually interacting via an attractive short range potential, below the superconducting critical temperature. They have used diagrammatic techniques in the broken phase. Work along these lines is in progress [33], taking into account the effect of a phenomenological pseudo-gap on the crossover phase diagram. One of the relevant conclusions reached with this phenomenological model of the pseudo-gap is that a metallic line and an insulating phase are present, which were not present in previous papers [2, 23, 24].

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