# Ground-state properties of the BCS–Bose Einstein crossover in a $d_{x^2-y^2}$-wave superconductor

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We examine the ground-state properties of the crossover between BCS superconductivity and Bose Einstein condensation within a model that exhibits $d_{x^2-y^2}$ pairing symmetry. We compare results for zero temperature with known features of *s*-wave systems and show that bosonic degrees of freedom are likely to emerge only in the dilute limit. We relate the change in properties of the ground state as a function of density to the effect of the exclusion principle and show that the one-particle distribution function undergoes a significant change when bosonic behavior appears. [S0163-1829(99)00822-X]

## I. INTRODUCTION

The existence of a crossover from BCS superconductivity to Bose Einstein (BE) condensation of preformed pairs has received increasing attention in the literature over the last few years. Originally discussed by Eagles[1] within the context of pairing in thin-film semiconductors, and considerably expanded upon by the works of Leggett[2] and Nozières and Schmitt-Rink,[3] the latest resurgence in interest has been due to its possible application to the understanding of the phase diagram of high-temperature cuprate superconductors.[4]

In particular, the appearance of a pseudogap in both charge and spin excitations of the normal state[5–9] has led to a number of suggestions that pairing correlations well above $T_c$ may occur in these systems. Whether these correlations are in the bosonic form of pre-formed pairs,[10,11] or pair resonances originating from the intermediate regime of a BCS-BE crossover,[12,13] or simply from classical phase fluctuations[14] is still however a controversial issue.

Furthermore, now that there is a large body of evidence to suggest that pairing in the cuprates is predominantly $d_{x^2-y^2}$ in character,[15–17] there is a clear need to understand the properties of the BCS-BE crossover within the context of this type of pairing symmetry. Although there have been some attempts to discuss the effect of $d_{x^2-y^2}$ pairing on pseudogap formation above $T_c$ in the cuprates,[18] there has been little discussion on the systematic ground-state properties of the BCS-BE crossover in the $d_{x^2-y^2}$ channel. This is an important issue, since pairs with this symmetry cannot contract to pointlike bosons and so accordingly one expects that there will be severe consequences for the properties of the ground state of this type of system. This is of direct importance in terms of the validity of the crossover scenario for the cuprates, while also being of general interest in understanding macroscopic pairing in higher angular momentum channels.

In this paper, we consider the BCS-BE crossover at zero temperature as a function of both coupling strength and carrier density, within a two-dimensional toy model that has a $d_{x^2-y^2}$ pairing instability. The study at zero temperature is well controlled by use of the BCS variational wave function (which contains the BE limit[2]) and allows us to establish at the two-body level the qualitative ground-state properties of the system upon which future studies may be based. In particular, we show that the ground-state properties of the system are severely modified from the *s*-wave picture, where a smooth crossover exists for all densities.[3,4] For the $d_{x^2-y^2}$ case the effect of the exclusion principle as the density of carriers is increased results in a suppression of the emergence of bosonic degrees of freedom for moderately large densities and strong coupling, where the system instead remains fermionic (BCS-like). We find that only in the dilute limit is a crossover possible, and that when this occurs the single-particle distribution particle undergoes a radical redistribution. We summarize most of our results in Fig. 1, which shows when bosonic degrees of freedom can emerge as a function of both density and coupling strength.

## II. TOY MODEL

We introduce as our toy model a ''reduced'' Hamiltonian in the BCS sense that describes an effective two-particle in-

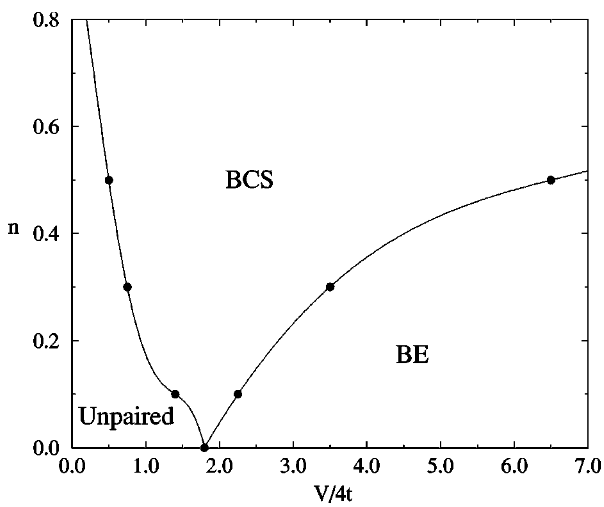


FIG. 1. The crossover between fermionic and bosonic degrees of freedom as a function of carrier density and coupling strength (as defined in text). The left boundary is determined by the onset of a finite gap amplitude, and the right boundary by when the chemical potential falls below the band minimum. The solid lines are a guide for the eye only.

 

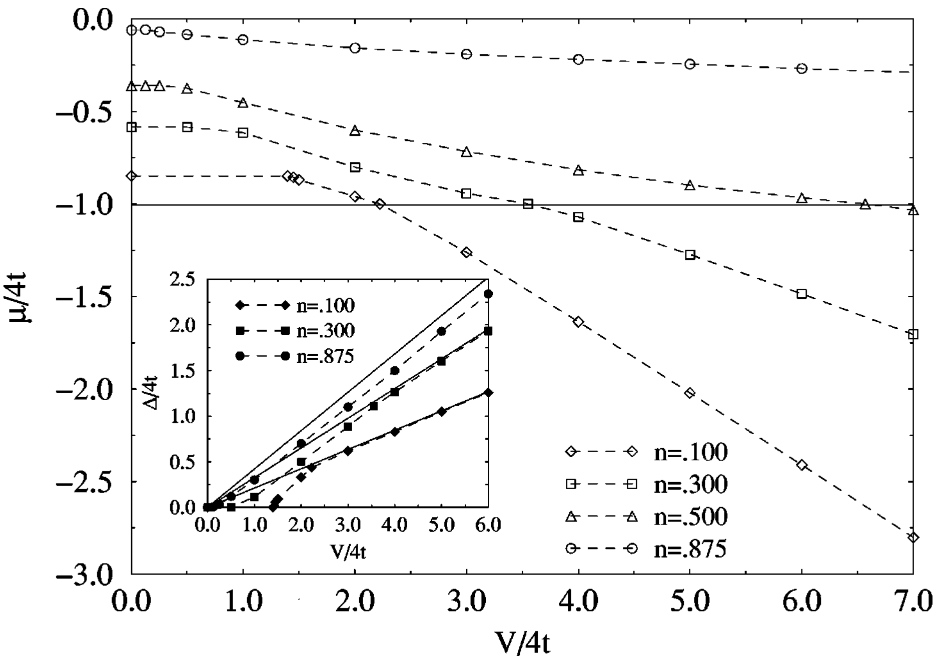


FIG. 2. The dependence of $\mu$ on coupling strength for various densities. Inset: The gap $\Delta$ as a function of coupling strength (dashed lines and data points). The solid lines are the asymptotic behavior derived in the text.

teraction in real space and in the singlet pairing channel.[19] Specifically, it is

$$H=\sum_{\langle ij\rangle\sigma} -t(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})-\mu^{*}\sum_{i\sigma} n_{i\sigma}+W\sum_{i} c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}c_{i\downarrow}c_{i\uparrow} -V\sum_{\langle ij\rangle} c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}c_{j\downarrow}c_{i\uparrow}, \quad (1)$$

where first and second terms describe nearest-neighbor hopping on a two-dimensional square lattice with chemical potential $\mu^{*}$, and the third and fourth terms describe an effective two-body pairing interaction in real space. In particular, the third term represents the repulsive part of the effective interaction while the last term provides an attractive interaction for nearest-neighbor particles.[20]

By expressing the superconducting gap in terms of its various symmetry components and introducing the BCS variational wave function $|\Psi\rangle=\Pi_{\mathbf{k}}(u_{\mathbf{k}}+v_{\mathbf{k}}c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger})|0\rangle$, the zero-temperature gap equation in the $d_{x^2-y^2}$ channel is given by

$$1=\frac{1}{2M}\sum_{\mathbf{k}}\frac{V(\cos k_x-\cos k_y)^2}{\{[\xi(\mathbf{k})-\mu]^2+\Delta^2(\cos k_x-\cos k_y)^2\}^{1/2}}, \quad (2)$$

where $\xi(\mathbf{k})=-2t\eta_k$ is the nearest-neighbor tight-binding energy dispersion, the geometric factor $\eta_{\mathbf{k}}=\cos k_x+\cos k_y$, and the effective chemical potential $\mu=\mu^{*}-n(W/2-2V)$. The amplitude of the $d$-wave gap is denoted by $\Delta$.

As Eagles first pointed out,[1] any deviation from weak coupling requires a self-consistent solution of both gap and number equations, since the BCS approximation of the chemical potential, being equal to its value in the normal state, can no longer be reasonably justified. Specifically, the number equation for the chemical potential $\mu$, which defines the particle density $n=N/M$, is

$$n-1=\frac{1}{M}\sum_{\mathbf{k}}\frac{-[\xi(\mathbf{k})-\mu]}{\{[\xi(\mathbf{k})-\mu]^2+\Delta^2(\cos k_x-\cos k_y)^2\}^{1/2}}. \quad (3)$$

We have solved Eqs. (2) and (3) self-consistently at a given density by numerical integration. In this theory, pairing takes place over the entire Brillouin zone (BZ). The zone edge acts as a natural boundary or momentum cutoff that avoids the renormalization methods used to remove ultraviolet divergences in continuum model treatments of strong coupling within the BCS framework.[21]

## III. CROSSOVER AND ANALYSIS

The inset of Fig. 2 shows the gap parameter $\Delta$ for densities ranging from the dilute limit to the almost half-filled case. Taking the onset of a finite gap parameter as the signal for the manifestation of the superconducting state, an increase in the particle density clearly favors the emergence of a $d_{x^2-y^2}$ paired ground state. On the other hand, as the system becomes more dilute, there is a need for stronger coupling to induce pairing.

In the dilute limit (of relevance to the underdoped cuprates, where the density of carriers is proportional to the doped hole concentration $x$), the occurrence of $d_{x^2-y^2}$ bound states for the two-particle problem on an empty lattice is for our system, equivalent to that problem for the $t$-$J$ model. Kagan and Rice[22] have shown that a $d_{x^2-y^2}$ bound state will not occur unless the coupling $J$ (equivalent to $V$ in our case) is greater than $V_c/4t\sim1.8$. Also, Randeria *et al.*[23] have shown that in two dimensions, a necessary and sufficient condition for a dilute many-body $s$-wave Cooper instability to occur is that an $s$-wave bound state exists for the corresponding two-body problem on the empty lattice. Importantly, in the context of $d_{x^2-y^2}$ symmetry, they have also shown that such a condition does not exist for higher angular momentum pairing.

In our study, we find that the onset of pairing occurs for progressively weaker coupling as the density is increased, contrary to an $s$-wave system. In the $d_{x^2-y^2}$ channel at a coupling strength less than $V_c/4t$, the dilute system gains more kinetic energy compared to pairing energy and thus has a total condensation energy that is positive, whereas for the more dense system the kinetic energy of the carriers is on average less effected and a pairing instability occurs. This steady evolution from the extreme dilute limit where pairing does not occur until $V/4t \geq 1.8$, to the near half-filled case where superconductivity can manifest itself at a much weaker coupling than that required for a two-body bound state, is indicated by the boundary on the left in Fig. 1. The $n=0$ point corresponds to the critical coupling strength $V_c$ discussed above and calculated initially by Kagan and Rice.[22]

In Fig. 2 we show $\mu$ as found in conjunction with the solutions for the gap $\Delta$ at various densities and as a function of the coupling strength. The horizontal line at $\mu/4t=-1.0$ represents the bottom of the tight-binding band. For weak coupling, it is well known that $\mu$ in the superconducting phase is given roughly by the Fermi energy of the normal state and this can be seen in the figure. However, at large doping, $\mu$ shows little deviation from its normal state value over a large variation in the the coupling strength. This is to be contrasted with the low-density results, which show a relatively rapid deviation from weak-coupling behavior as $V$ is increased.

In general, bosonic degrees of freedom can be expected to emerge once the chemical potential of the many-body ground state slips below the band minimum in a tight-binding system, or below zero in a continuum model. For an $s$-wave system, Nozières and Schmitt-Rink[3] were able to show that a crossover from fermionic superconductivity to bosonic degrees of freedom can occur for all densities as the coupling strength is increased. For the $d$-wave system considered here, this is not the case. Bosonic degrees of freedom can only emerge in the dilute regime, while for large densities, the system behaves more like a weak-coupling superconductor with a value of the chemical potential comparable to that of the normal state. These results are expressed by the boundary on the right in Fig. 1. Given that the BCS wave function only takes two-body correlations into account, we expect that the suppression of bosonic degrees of freedom would be increased in a more sophisticated treatment that would include a repulsive interaction between fermion pairs.[24]

Further insight into this feature of a $d$-wave system can be gained by examining the limit of infinite coupling strength. In the case $V\rightarrow\infty$, the kinetic term (and thus any Fermi surface geometry) becomes negligible and the asymptotic behavior of the gap and chemical potential can be shown from Eqs. (2) and (3) to have the form $\Delta\rightarrow\gamma V/2$ and $\mu\rightarrow\gamma V(n-1)/2\alpha$, implying that in the infinite coupling limit, $\mu/\Delta\rightarrow(n-1)/\alpha$. Here the parameter $\alpha$ is given by the solution to

$$\alpha=\frac{1}{M}\sum_{\mathbf{k}}\frac{1}{\{(\cos k_x-\cos k_y)^2+([n-1]/\alpha)^2\}^{1/2}}, \quad (4)$$

while $\gamma$ is defined by

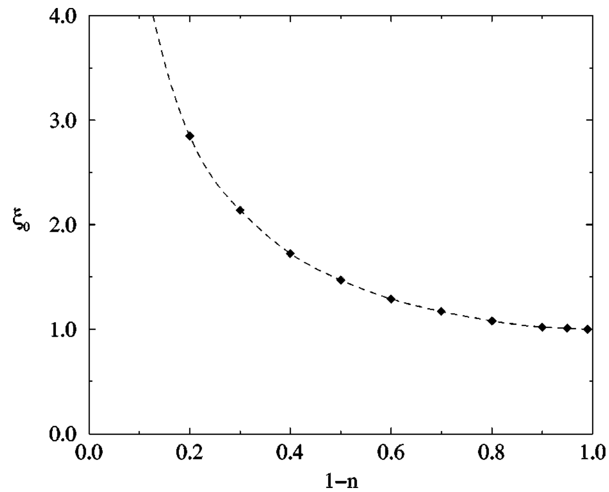


FIG. 3. The coherence length in the strong-coupling limit as a function of density. The lattice spacing has been set to unity.

$$\gamma=\frac{1}{M}\sum_{\mathbf{k}}\frac{(\cos k_x-\cos k_y)^2}{\{(\cos k_x-\cos k_y)^2+([n-1]/\alpha)^2\}^{1/2}}. \quad (5)$$

We have indicated the asymptotic behavior of $\Delta$ at various densities in the inset of Fig. 2 by the solid lines. As one increases the density, the convergence to the asymptotic behavior is poor for large densities, indicating that the $\mu$ is still of the order of the band energy. In the strong-coupling regime, if true bosonic characteristics emerge then one expects that $\mu$ should simply reduce to the binding energy per particle for the "diatomic" electron molecule. It can readily be shown that only in the dilute limit does the ratio $\gamma/\alpha$ approach unity. This indeed leads to the result $\mu=-V/2$, exactly one half of the binding energy for the two-body problem in the strong-coupling limit.[25] On the other hand, at half filling $(n=1)$ $\mu$ clearly remains zero even in the limit of infinite coupling. Remarkably, the ground state remains a fermionic superconductor for all coupling strengths and has characteristics equivalent to a weak-coupling BCS system. For densities in between these two limits, an increase in coupling will eventually reduce the chemical potential below the bottom of the band; however, it will always be somewhat greater than the binding energy per particle of the two-body case.

This general dependence on the density for the BCS-BE crossover in $d$-wave systems can be viewed as a manifestation of the effect of the exclusion principle. Due to the symmetry of the pairs, they cannot contract in real space to point bosons, but must always retain a finite spatial extent. As the density increases, the overlap of the pair wave functions exerts its influence through the exclusion principle contributing a positive energy to the system. At half filling, this overlap prevents the system from crossing over to a system displaying bosonic qualities even in the infinite coupling limit.

This interpretation can be further supported by a calculation of the average pair coherence length. We can define this length $\xi_0$ through the expectation value of the quantity $\xi_0^2=\langle F_{\mathbf{k}}|-\nabla_{\mathbf{k}}^2|F_{\mathbf{k}}\rangle/\langle F_{\mathbf{k}}|F_{\mathbf{k}}\rangle$ where $F_{\mathbf{k}}=u_{\mathbf{k}}^*v_{\mathbf{k}}$ plays the role of the pair wave function.[26]

In Fig. 3 we show the behavior of $\xi_0$ in the infinite coupling limit as a function of density. It is clear that a shrinking

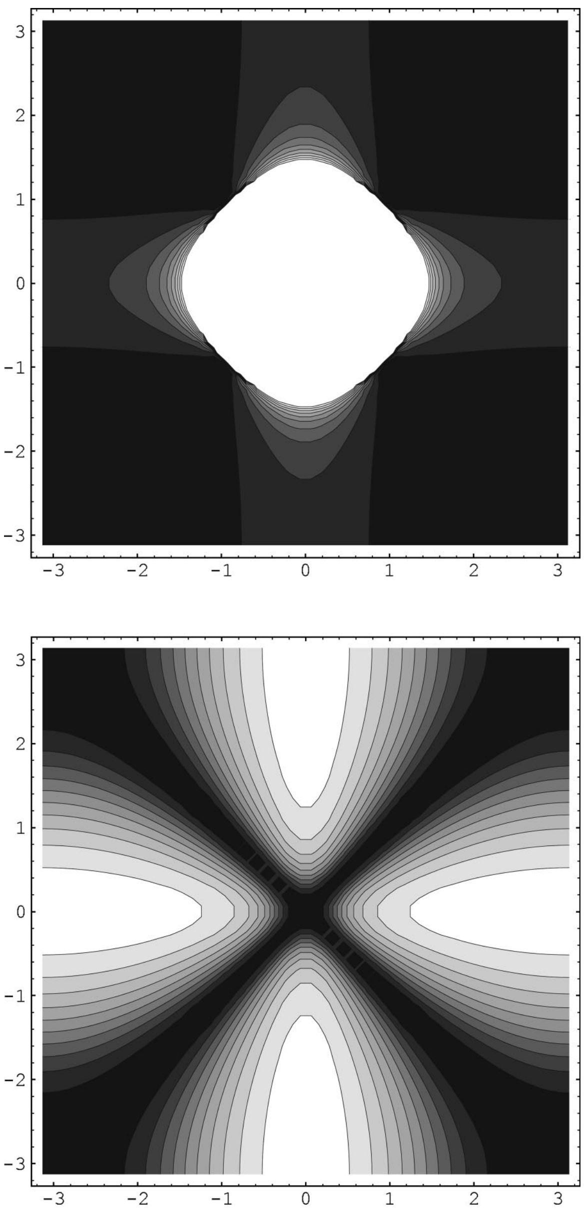

FIG. 4. Contour plots within the first BZ of $n_{\mathbf{k}\sigma}$ for $V/4t=1$ (top) and $V/4t=4$ (bottom) and $n=0.3$. The brighter the region the larger the value of $n_{\mathbf{k}\sigma}$.

of the pair size in real space to a compactified boson spread out over nearest-neighbor sites can only occur in the dilute limit, where the exclusion principle becomes irrelevant. For higher density, the overlap of the pair wave functions has the effect of increasing the correlation between particles, which then increases the average pair size in order that the total energy of the system can be minimized.

Lastly, we examine the single-particle distribution function $n_{\mathbf{k}\sigma}$ as a function of the coupling strength. We find that in weak coupling, the system behaves as a typical BCS system, with $n_{\mathbf{k}\sigma}$ resembling a step function up to a point close to the normal-state Fermi surface, whereupon it becomes smeared over a small region about $\mu=E_F$. The degree of smearing increases with the coupling until the chemical potential drops below the bottom of the band. At this point, the behavior of the single-particle distribution function radically changes.

In Fig. 4, we compare contour plots of $n_{\mathbf{k}\sigma}$ for $n=0.3$ throughout the BZ for the weak coupling case $V/4t=1$, where $\mu$ is well approximated by its normal-state value, and the stronger coupling case $V/4t=4$, where the chemical potential falls just below the bottom of the band.

In the weak-coupling case, the Fermi surface of a tight-binding band with a small density per unit volume can be clearly seen by the bright region in the middle of the plot. On the other hand, when $\mu$ drops below the bottom of the band and bosonic degrees of freedom emerge, $n_{\mathbf{k}\sigma}$ undergoes a redistribution within the BZ. For $V/4t=4$, the probability for occupation of highest-momentum states is now found in the regions around $(\pm\pi,0)$ and $(0,\pm\pi)$. For $d_{x^2-y^2}$ pairing, this change in behavior of the single-particle distribution function $n_{\mathbf{k}\sigma}$ as the chemical potential falls below the minimum of the tight-binding band is an interesting feature. For $s$-wave systems, $n_{\mathbf{k}\sigma}$ becomes a constant for strong coupling, representing the Fourier transform of a point internal wave function. Accordingly, we can interpret the new structure for $n_{\mathbf{k}\sigma}$ as the $d$-wave version of a local pair.

One may speculate what the effect of this new structure for $n_{\mathbf{k}\sigma}$ may be at finite temperatures. Above $T_c$, if a pseudogap in the normal-state excitation spectrum can arise from pairing fluctuations in the crossover regime,[13] then one would expect these fluctuations to occur predominantly in the region of the BZ, which has the largest probability of occupation by pairs. On the one hand, it is interesting to note from the bottom plot in Fig. 4 that these regions correspond to the angular dependence of the pseudogap in the underdoped cuprates.[8,9] However, it is still unknown whether these materials correspond to such a regime.

## IV. SUMMARY

In summary, we find that for $d_{x^2-y^2}$ pairing, only in the dilute limit is it likely that a BCS-BE crossover can occur, while it is possible at any density for $s$-wave systems. If bosonic behavior does emerge, the $d_{x^2-y^2}$ symmetry causes the single-particle distribution function to undergo a radical redistribution.

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