

A BCS–Bose-Einstein Crossover Theory and its Application to the Cuprates

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Abstract. We use a “pairing fluctuation” approach to address the behavior of T_c and pseudogap in d -wave superconductors. This theory yields a BCS–Bose-Einstein crossover description of the superconducting transition, which reduces to BCS in the weak coupling (small g) limit and to a Bose-Einstein description at large g . We investigate the effects of quasi-two dimensionality, lattice bandstructure and d -wave symmetry, and obtain a cuprate phase diagram, in quantitative agreement with experiment.

INTRODUCTION

BCS–Bose-Einstein condensation (BEC) crossover theories have been applied to the high T_c problem since the discovery of cuprate superconductors in 1986 [1]. Interest in these theories is based on the fact that these materials have short coherence lengths. Moreover, as a function of doping the system evolves smoothly from BCS-like behavior in the overdoped regime to the underdoped regime, where BCS theory manifestly fails as a consequence of an excitation gap at T_c [2]. Uemura’s plot [3] has also been used to suggest that the cuprates are intermediate between BCS and BEC systems. However, the application of crossover theories to the cuprates is made complex by the high anisotropy, lattice periodicity and d -wave pairing symmetry of these materials. Here we investigate these effects on the BCS-BEC crossover, and address pseudogap phenomena in cuprate superconductors.

THEORETICAL FORMALISM

Our system is composed of fermions with dispersion $\epsilon_{\mathbf{k}}$ in the presence of an effective pairing interaction $V_{\mathbf{k},\mathbf{k}'} = g\varphi_{\mathbf{k}}\varphi_{\mathbf{k}'}$, where the coupling strength $g < 0$. In a jellium gas, $\epsilon_{\mathbf{k}} = k^2/2m$ and the symmetry factor $\varphi_{\mathbf{k}} = (1 + (k/k_0)^2)^{-1/2}$; On a lattice, $\epsilon_{\mathbf{k}} = \sum_i^d 2t_i(1 - \cos k_i) - \mu$, and $\varphi_{\mathbf{k}} = 1$ (s -wave) or $\varphi_{\mathbf{k}} = \cos k_x - \cos k_y$ (d -wave). In quasi-2d cases, the hopping integrals satisfy $t_{\perp} \equiv t_z \ll t_{\parallel} \equiv t_x = t_y$.

At small g , the system is fermionic, and undergoes a BCS superconducting transition at T_c . At large g , composite bosons form above T_c , and the system undergoes

BEC at T_c . The effective *pair* chemical potential is identically zero for $T \leq T_c$. In the intermediate regime, both single fermions and (metastable) pairs exist above T_c and similarly, below T_c , the excitations consist of quasiparticles and finite momentum pair excitations (i.e., pairons). These new excitations, not present in BCS theory, are responsible for the pseudogap.

We first calculate T_c following the T-matrix approach, of Kadanoff and Martin [4]. We have for the self-energy $\Sigma(K) = G_0^{-1}(K) - G^{-1}(K) = \sum_Q t(Q) G_0(Q - K) \varphi_{\mathbf{k}-\mathbf{q}/2}^2$, and T-matrix $t(Q) = [g^{-1} + \sum_K G(K) G_0(Q - K) \varphi_{\mathbf{k}-\mathbf{q}/2}^2]^{-1}$, where $G_0(K)/G(K)$ are the bare/full Green's functions in the four-vector notation, $K \equiv (\mathbf{k}, i\omega)$, etc. At T_c , finite \mathbf{q} pairs are long lived for small \mathbf{q} , and the T-matrix can be approximated by $t_{\mathbf{q},\Omega} \approx a_0^{-1}/(\Omega - \Omega_{\mathbf{q}})$, with pair dispersion $\Omega_{\mathbf{q}} \approx \sum_i q_i^2/2M_i^*$. a_0 can be obtained by expanding $t^{-1}(Q)$.

The BEC condition requires the effective *pair* chemical potential $-\Omega_{\mathbf{q}=0} = 0$. This is equivalent to the superconducting instability condition $t^{-1}(0) = 0$ from the fermionic perspective. Because of the divergence of $t(Q)$ at $Q = 0$, $\Sigma(K) \approx G_0(-K) \varphi_{\mathbf{k}}^2 \sum_Q t(Q) \equiv -G_0(-K) \Delta_{pg}^2 \varphi_{\mathbf{k}}^2$, where $\Delta_{pg}^2 \equiv -\sum_Q t(Q)$ defines the pseudogap. Including the particle number equation, we obtain

$$\text{BEC condition} \quad 1 + g \sum_{\mathbf{k}} \frac{1 - 2f(E_{\mathbf{k}})}{2E_{\mathbf{k}}} \varphi_{\mathbf{k}}^2 = 0, \quad (1)$$

$$\text{Number equation} \quad \sum_{\mathbf{k}} [1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} + 2\frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} f(E_{\mathbf{k}})] = n, \quad (2)$$

$$\text{Pseudogap Equation} \quad \Delta_{pg}^2 \approx \frac{1}{a_0} \sum_{\mathbf{q}} b(\Omega_{\mathbf{q}}). \quad (3)$$

where $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}} + \Delta^2 \varphi_{\mathbf{k}}^2}$, $a_0 = \frac{1}{2\Delta^2} \sum_{\mathbf{k}} \left[[1 - 2f(\epsilon_{\mathbf{k}})] - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} [1 - 2f(E_{\mathbf{k}})] \right]$, $\Delta = \Delta_{pg}$ at T_c , and $f(x)/b(x)$ is the Fermi/Bose function.

Below T_c , the superconducting order parameter Δ_{sc} adds to the excitation gap $\Delta = \sqrt{|\Delta_{sc}|^2 + \Delta_{pg}^2}$. As can be easily seen from Eq. (3), at $T = 0$, Δ_{pg} vanishes, and we recover Leggett's ground state [5].

NUMERICAL RESULTS

Figure 1 shows typical T_c behavior obtained by solving Eqs. (1)-(3), as a function of g at low densities. While at small g , T_c follows the BCS functional form, as g increases, μ decreases and simultaneously Δ_{pg} increases. The system becomes bosonic as μ becomes negative. At large g , T_c approaches the BEC temperature ($T_c \approx 0.218E_F$) in the jellium case or vanishes asymptotically in the lattice case. The effective pair mass M^* increases with g in the presence of the lattice. In both cases, the figure shows $T_c \propto 1/M^*$ for large g , characteristic of BEC.

By contrast, at high densities, T_c decreases to zero at finite g reflecting the behavior of M^* . The pairs become too heavy to move and Bose condense.

Figure 2(a) plots T_c , μ , and Δ_{pg} for *d*-wave superconductors on a quasi-2d lattice

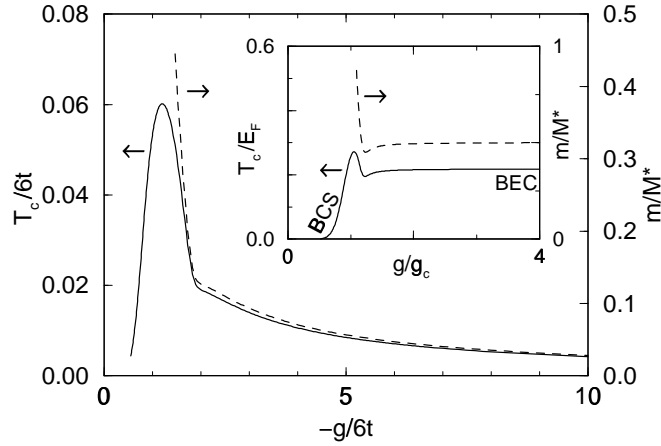


FIGURE 1. BCS-BEC crossover of T_c (solid lines) on a 3d lattice (main figure, $n = 0.1$) and in a 3d jellium gas (inset, $k_0 = 4k_F$) with an s -wave pairing symmetry in the low density or short range interaction case. Also plotted are the inverse effective pair mass m/M^* (dashed lines).

for densities relevant to the cuprates. T_c vanishes at a nearly universal value of g , well before the bosonic regime is reached; μ is still close to E_F . This is attributable to the finite pair size due to the d -wave symmetry. It indicates that there is no bosonic (or preformed pair) regime in d -wave superconductors.

Figure 2(b) shows the effect of mass anisotropy on T_c on a quasi-2d lattice. As $t_\perp/t_\parallel \rightarrow 0$, the system changes from 3d to 2d, and T_c is suppressed logarithmically to zero. In this way, pseudogap effects are enhanced by the low dimensionality.

To address the cuprates, we include Mott-insulator effect behavior near half filling. This leads to a renormalization of the in-plane hopping integral t_0 to $t_\parallel(x) \approx t_0(1 - n) = t_0x$. For lack of further information we assume g is x independent and calculate T_c , T^* , $\Delta(0)$, and $\Delta(T_c)$ as a function of x , as shown

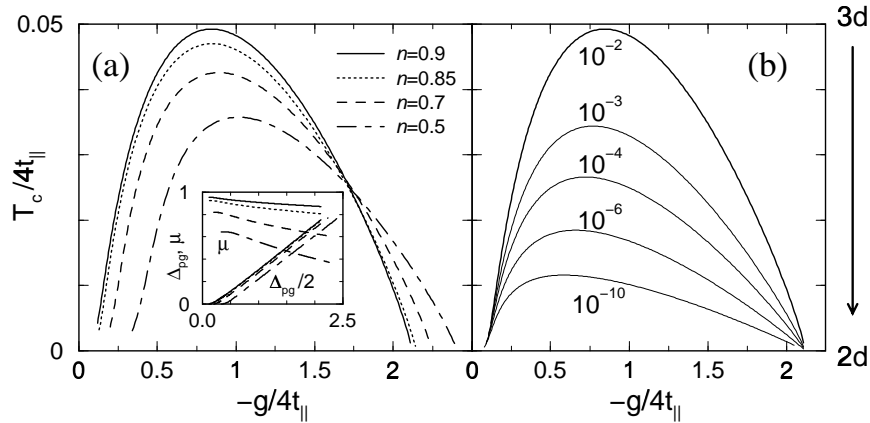


FIGURE 2. (a) T_c (main figure) and μ and Δ_{pg} (inset) as a function of coupling g on a quasi-2d lattice ($t_\perp/t_\parallel = 0.01$) with a d -wave pairing symmetry. (b) Effects on T_c of the mass anisotropy ($n = 0.9$). t_\perp/t_\parallel is labeled on the T_c curves.

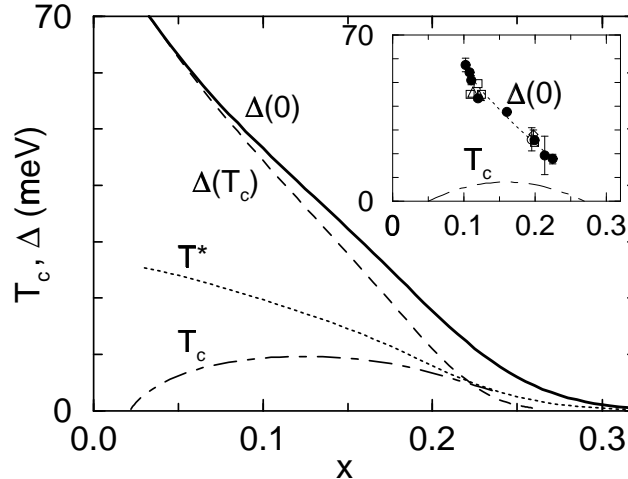


FIGURE 3. Calculated cuprate phase diagram for $t_{\perp}/t_{\parallel} = 0.01$. The gaps plotted here are the magnitude at $(\pi, 0)$, twice those in Eqs. (1-3). Experimental data from ref. [6] are plotted (inset).

in Fig. 3. T^* is estimated from the mean-field solution of Eqs. (1-2). To optimize agreement between the theoretical and measured phase diagram, we choose $-g/4t_0 = 0.045$. Taking $t_0 = 0.6$ eV (consistent with photoemission data) yields quite good agreement with experiment.

CONCLUSIONS

In constructing a BCS-BEC crossover theory, we find it necessary to include finite momentum pair excitations. These pair excitations lead to the pseudogap effects, which are enhanced by low dimensionality. When lattice effects and d -wave symmetry are included, T_c will vanish well before the bosonic regime is reached. A phase diagram is obtained, in quantitative agreement with cuprate experiments.

ACKNOWLEDGMENTS

This work was supported by the National Science Foundation under grant DMR No. 91-20000 through the Science and Technology Center for Superconductivity.

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