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

Qijin Chen, Ioan Kosztin, Boldizsár Jankó, and K. Levin

James Franck Institute, University of Chicago, 5640 South Ellis Avenue, Chicago, IL 60637

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 $\epsilon_k$ in the presence of an effective pairing interaction $V_{kk'} = g \varphi_k \varphi_{k'}$, where the coupling strength $g < 0$. In a jellium gas, $\epsilon_k = k^2/2m$ and the symmetry factor $\varphi_k = (1 + (k/k_0)^2)^{-1/2}$; On a lattice, $\epsilon_k = \sum_i 2t_i (1 - \cos k_i) - \mu$, and $\varphi_k = 1$ ($s$-wave) or $\varphi_k = \cos k_x - \cos k_y$ ($d$-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 $\Sigma(K) = G_0^{-1}(K) - G^{-1}(K) = \sum Q t(Q) G_0(Q - K) \varphi_{k-q/2}^2$, and T-matrix $t(Q) = [g^{-1} + \sum K G(K) G_0(Q - K) \varphi_{k-q/2}^2]^{-1}$, where $G_0(K)/G(K)$ are the bare/full Green’s functions in the four-vector notation, $K \equiv (k, i\omega)$, etc. At $T_c$, finite $q$ pairs are long lived for small $q$, and the T-matrix can be approximated by $t_{q,\Omega} \approx a_0^{-1}/(\Omega - \Omega_q)$, with pair dispersion $\Omega_q \approx \sum q_i^2/2M^*_i$. $a_0$ can be obtained by expanding $t^{-1}(Q)$.

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

\begin{align*}
\text{BEC condition} & \quad 1 + g \sum_k \frac{1 - 2f(E_k)}{2E_k} \varphi_k^2 = 0, \quad (1) \\
\text{Number equation} & \quad \sum_k [1 - \frac{\epsilon_k}{E_k} + 2 \frac{\epsilon_k}{E_k} f(E_k)] = n, \quad (2) \\
\text{Pseudogap Equation} & \quad \Delta^2_{pg} \approx \frac{1}{a_0} \sum_q b(\Omega_q), \quad (3)
\end{align*}

where $E_k = \sqrt{\epsilon_k + \Delta^2 \varphi_k^2}$, $a_0 = \frac{1}{2\pi^2} \sum_k \left[1 - 2f(\epsilon_k) + \frac{2\epsilon_k}{E_k} \left[1 - 2f(E_k)\right]\right]$, $\Delta = \Delta_{pg}$ at $T_c$, and $f(x)/b(x)$ is the Fermi/Bose function.

Below $T_c$, the superconducting order parameter $\Delta_{sc}$ adds to the excitation gap $\Delta = \sqrt{|\Delta_{sc}|^2 + \Delta^2_{pg}}$. As can be easily seen from Eq. (3), at $T = 0$, $\Delta_{pg}$ 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, $\mu$ decreases and simultaneously $\Delta_{pg}$ increases. The system becomes bosonic as $\mu$ 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 $T_c$, $\mu$, and $\Delta_{pg}$ for $d$-wave superconductors on a quasi-2d lattice.
for densities relevant to the cuprates. $T_c$ vanishes at a nearly universal value of $g$, well before the bosonic regime is reached; $\mu$ 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 $t_{\perp}/t_{\parallel} \to 0$, 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 $t_{\parallel}(x) \approx t_0(1-n) = t_0 x$. 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 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).

**Figure 2.** (a) $T_c$ (main figure) and $\mu$ and $\Delta_{p\parallel}$ (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 $t_{\perp}/t_{||} = 0.01$. 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.

REFERENCES