Within the pseudogap regime of the cuprates, it has been widely argued that the excitations of the superconducting state are either fermionic [1] or bosonic [2] in character. In this paper we discuss a third scenario [associated with the BCS to Bose-Einstein condensation (BEC) crossover approach], in which the excitations contain a mix of bosonic and fermionic properties [3].

The BCS-BEC crossover scheme has been viewed as relevant to the cuprates and other “exotic” [4,5] superconductors where their short coherence lengths, ξ, naturally lead to a breakdown of strict BCS theory. The BCS-BEC scenario [3,6–9] owes its origin to Eagles [10] and Leggett [11] who proposed a ground state wave function that describes the continuous evolution between a BCS problem. For brevity, we use a four-momentum notation: $K = (k, i\omega)$, $\Sigma_K = T \Sigma_{K,\omega}$, etc. We also suppress $\varphi_k$ until the final equations.

BCS theory involves the pair susceptibility $\chi(Q) = \Sigma_K G(K)G_0(Q - K)$, where the Green’s function $G$ satisfies $G^{-1} = G_0^{-1} + \Sigma$, with order parameter $\Delta_{sc}$ and $\Sigma(K) = -\Delta_{sc}^2 G_0(-K)$. In this notation, the gap equation is

$$1 + g\chi(0) = 0, \quad T \leq T_c. \quad (1)$$

At $Q = 0$, the summand in $\chi$ is the Gor’kov “F” function (up to a multiplicative factor $\Delta_{sc}$) and this serves to highlight the central role played in BCS theory by the more general quantity $G(K)G_0(Q - K)$. Note that (for $Q \neq 0$) $\chi(Q)$ is distinct from the pair susceptibility of the collective phase mode which enters as $\Sigma_K[G(K)[G(Q - K) + G(-Q - K)] + 2F(K)F(Q - K)]$ [12,15]. Here, each Gor’kov $F$ function introduces one $GG_0$, so that the collective mode propagator depends on effectively higher order Green’s functions than does the gap equation.

The observations in italics were first made in Ref. [13] where it was noted that the BCS gap equation could be rederived by truncating the equations of motion so that only the one $(G)$ and two particle $(T)$ propagators appeared. Here, $G$ depends on $\Sigma$ which in turn depends on $T$. In general, $T$ has two additive contributions [14], from the condensate (sc) and the noncondensed (pg) pairs. Similarly, the associated self-energy [13] $\Sigma(K) = \Sigma_{sc} + \Sigma_{pg}T(Q)G_0(Q - K)$ can be decomposed into $\Sigma_{sc}(K) + \Sigma_{pg}(K)$. The two contributions in $\Sigma$ come, respectively, from $T_{sc}(Q) = -\Delta_{sc}^2 \delta(Q)/T$, and from the $Q \neq 0$ pairs, with $T_{pg}(Q) = g/[1 + g\chi(Q)]$. In this notation, the leading order mean field theory $\Sigma = \Sigma_{sc} = -\Delta_{sc}^2 G_0(-K)$ which, from Eq. (1), yields the usual BCS gap equation.

More generally, at larger $g$, the above equations hold but we now include feedback into Eq. (1) from the finite momentum pairs, via $\Sigma_{pg}(K) = \sum_{Q} T_{pg}(Q)G_0(Q - K) = G_0(-K)\Sigma_{pg}T_{pg}(Q) \equiv -\Delta_{pg}^2 G_0(-K)$, which defines a pseudogap parameter, $\Delta_{pg}$. This last approximation is valid only because [through Eq. (1)] $T_{pg}$ diverges as $Q \rightarrow 0$. In this way, $\Sigma_{pg}(K)$ has a BCS-like form, as
does the total self-energy $\Sigma(K) = -\Delta^2 G_0(-K)$, where
$\Delta^2 = \Delta_{sc}^2 + \Delta_{pg}^2$. Thus, in the present approach, the
energy gap for single electron excitations reflects the presence
of both finite center-of-mass momentum pairs as well as the condensate. While the structure of the gap equation
will be seen to be formally identical to that in BCS theory,
the vanishing of the excitation gap, $\Delta$, takes place at a
higher temperature than that at which the order parameter,
$\Delta_{sc}$, vanishes. The latter defines $T_c$.

If we now expand $\mathcal{T}^{-1}_{pg}(q, \Omega) = a_1 \Omega^2 + a_0 \Omega +
\tau_0 - B q^2 + i \Gamma_q$, we see that the chemical potential of
the pairs $\mu_{pair}$ is proportional to $\tau_0$ and, via Eq. (1),
precisely zero at and below $T_c$. This provides an inter-
pretation along the lines of ideal Bose gas condensation.
(Here, also, at small $q$, $\Gamma_q' \rightarrow 0$.) As $g$ increases, the
term $a_0 \Omega$ in $\mathcal{T}^{-1}_{pg}$ becomes progressively dominant with
respect to $a_1 \Omega^2$. For the physically relevant regime of moderate $g$, we have found, after detailed numerical
calculations, that $a_1$ may be safely neglected. At weak
coupling, there is no loss of generality in approximating $\mathcal{T}_{pg}$ in this more particle-hole asymmetric way, since its
contribution is negligible. In this way, we can write
\[ \mathcal{T}^{-1}_{pg}(q, \Omega) = a_0(\Omega - \Omega_{sc} + \mu_{pair} + i \Gamma_q). \]  
(2)

For small $g$ and in three dimensions (3D), the poles of $\mathcal{T}_{pg}$
(at $T = 0$) occur at $\Omega = \sqrt{3} e q$, where $e$ is the usual phase
mode velocity. At moderate $g$, where the pairs become
increasingly more relevant, and for quasi-2D dispersion
$\epsilon_k$, $\Omega_{pg} = q^2 / 2 M^2 + q^2 / 2 M^2_{sc}$. Here we find that the
ratio $M^2 / M^2_{sc} \propto (t_1 / t_0)^2$, where $t_0$ and $t_1$ are the in-
and out-of-plane hopping integrals, respectively. Numerical
calculations show that the masses, as well as the residue
$a_0$, are roughly $T$ independent constants at low $T$ [17]. In
the BEC regime at low density and with $s$-wave pairing in
a 3D continuous model, $M^* = 2 M_0$ for all $T \leq T_c$, [16],
as found previously [7]. The examples in this paper, which
apply to the fermionic regime, correspond to somewhat
smaller $M^*_0$.

It is important to note that in strictly 2D the logarithmic
divergence on the right-hand side of the pseudogap equa-
tion (3) (which is essentially a boson number equation) im-
plies $T_c = 0$, as in an ideal Bose gas. For large anisotropy,
or small $t_1$, $T_c \propto -1 / \ln(t_1 / t_0)$, which vanishes logarith-
ically [16]. Finally, since both $a_0$ and the effective pair
mass (tensor) $M^*$ are constants at low $T$, Eq. (3) implies
$\Delta_{pg}^2(T) = \Delta^2(T) - \Delta_{sc}^2(T) \propto T^{3/2}$. Moreover, because $\Delta$
depends on $T$ only exponentially, $\Delta_{sc}^2(T) = \Delta^2(0) - AT^{3/2}$ at low $T$, where $A$ is $T$ independent.

We now calculate physical quantities such as the mag-
netic penetration depth ($\lambda$) and related superfluid density
($n_s$), the Knight shift ($K_s$), and the NMR relaxation rate
($R_\perp$) using techniques similar to those used to study flu-
tuation effects in normal metal superconductors [18]. Here
the usual (lowest order) Maki-Thompson and Aslamazov-
Larkin diagrams are extended to be compatible with $\Sigma$ and
$\mathcal{T}$ by applying the generalized Ward identity to incor-
porate the pairon vertex correction [12,18]. Finally, the spe-
cific heat $C_v$ can be computed following a similar analysis as
for the paramagnon problem [19].

While in the BCS limit the expressions for $\lambda$ (or $n_s$), $K_s$, and
$R_\perp$ contain only the total gap $\Delta$, here, they, in principle,
depend on both the quasiparticle (via $\Delta^2$) and the pairon
(via $\Delta_{pg}^2$) contributions [12,14]. This decomposition leads
to a form of “three fluid” model (including the condensate,
fermionic quasiparticles, and bosonic pairons). In the same
way, $C_v$ can also be decomposed into a sum of two contrib-
utions corresponding to an ideal Bose gas of pairons, with
dispersion $\Omega_{pg}$ and an ideal Fermi gas of quasiparticles,
with dispersion $E_k$. The pairon contributions to $n_s$ enter
as follows [3,14]: the general expression is identical to its
BCS counterpart, but with the overall multiplicative fac-
tor of $\Delta^2$ replaced by $\Delta_{sc}^2 = \Delta^2 - \Delta_{pg}^2$. By contrast, for spin-singlet pairing, there is no explicit pairon contribution
to $K_s$ and $R_\perp$, and the corresponding expressions reflect
the generalized excitation gap $\Delta$, as might have been ex-
pected physically. The single most important conclusion of
this analysis is that the presence of low lying pair ex-
citations will introduce new low temperature power law
dependences with ideal Bose gas character into physical

As a consequence, we have
\[ \Delta_{pg}^2 = - \sum_q T_{pg}(Q) = \frac{1}{a_0} \sum_{q \neq 0} b(\Omega_q). \]  
(3)

We now rewrite Eq. (1), along with the fermion number
constraint, as
\[ 1 + g \sum_k \left[ 2 f(E_k) - \frac{\epsilon_k}{E_k} \right] \varphi_k^2 = 0, \]  
(4)
\[ \sum_k \left[ 1 - \frac{\epsilon_k}{E_k} + \frac{2 \epsilon_k}{E_k} f(E_k) \right] = n. \]  
(5)

Here, $f(x)$ and $b(x)$ are the Fermi and Bose functions and
$E_k = \sqrt{\epsilon_k^2 + \Delta^2 \varphi_k^2}$ is the quasiparticle dispersion.
Equations (3)–(5) are consistent with BCS theory at small$g$, and with the ground state $\Psi_0$ at all $g$; in both cases the
right-hand side of Eq. (3) is zero. The simplest physical
interpretation of the present decoupling scheme is that it
goes beyond the standard BCS mean field treatment of the
single particles (which also acquire a self-energy from the
finite $q$ pairs) but it treats the pairs at a self consistent,
mean field level.

The dispersion $\Omega_q = q^2 B / a_0$, as well as the coefficient
$a_0$, are determined by a Taylor expansion of $\mathcal{T}_{pg}^{-1}$ [16]:
\[ \mathcal{T}_{pg}^{-1}(q, \Omega) = g^{-1} + \sum_k \left[ 1 - \frac{f(E_k)}{E_k} - \frac{\epsilon_k}{E_k} \right] \varphi_k^2 \]  
(6)

\[ \mathcal{T}_{pg}^{-1}(q, \Omega) = \frac{\Omega - \Omega_{sc} + \mu_{pair} + i \Gamma_q}{E_k - \epsilon_k - \Omega - \Omega_{pq}}. \]  
(2)
quantities. Below, we explore these power laws in the context of highly anisotropic 3D, i.e., quasi-2D systems.

Figures 1(a) and 1(b) present a comparison between an s-wave short ξ pseudogap (PG) superconductor and an s- and d-wave BCS system. It should be noted that the short ξ superconductors are still far from the BEC limit. For the parameters illustrated by the figures, μ deviates from \(E_F\) by roughly 3%. Here, and throughout this paper, we take \(t_\perp/t_\parallel = 0.01\). The main body of Fig. 1(a) indicates that the Knight shift (and NMR relaxation rate, not shown) at \(T_c\) are substantially reduced relative to their high \(T\) asymptotes, i.e., \(K_n\), as is illustrated by the solid line (for the PG s wave). Because pairon effects are not explicit, the low \(T\) behavior is exponentially activated as for the BCS s-wave case, but here the ratio \(\Delta(0)/T_c\) is significantly enhanced over the BCS value. Overall, the behavior of \(R_s\) will yield rather similar plots; however, the s-wave BCS limit exhibits the well-known Hebel-Slichter peak, which is absent below \(T_c\), for the other two cases.

In the inset of Fig. 1(a), we plot the behavior of the low \(T\) specific heat “coefficient,” \(\gamma(T) = C_v/T\), for the same parameters as above. In the short ξ, quasi-2D case, slightly above \(T = 0\), \(\gamma(T)\) will appear to be a constant \(\gamma(T) = \gamma^*\), although it vanishes strictly at \(T = 0\) as \(T^{1/2}\). This intrinsic \(\gamma^*\) effect, which may have been seen in both organic and cuprate (layered) superconductors [20], has, in the past, been related to extrinsic effects. Figure 1(b) plots the normalized superfluid density \(n_s\), or \(\lambda^{-2}\), vs \(T/T_c\), which for the PG (s-wave) case exhibits a \(T^{3/2}\) dependence. Here, \(\lambda\) (unlike \(C_v\)) is not particularly sensitive to the mass anisotropy ratio, and the boson power law dependence is more 3D.

In order to address d-wave effects in short ξ superconductors, we turn to the cuprates. Note, the dimensionless coupling is \(g/t_\parallel\). To be consistent with the observed metal-insulator transition at half filling \((x = 0)\), we introduce a hole concentration \(x\) dependent renormalization of the in-plane hopping integral \(t_\parallel(x) = t_0 x\) deriving from Coulomb correlations, and presume, in the absence of any more detailed information about the pairing mechanism, that \(g\) is \(x\) independent. Our quasi-2D band structure is taken from the literature [21]; the one free parameter \(-g/4t_\parallel\) is chosen (= 0.045) to optimize agreement with the energy scales in the cuprate phase diagram. This calculated phase diagram [3], deduced from Eqs. (3)–(5), can be shown to yield reasonable agreement with experimental data. Two important points should be stressed: (i) The chemical potential \(\mu/E_F\) differs from unity by at most a few percent over the entire range of \(x\). (ii) While the band mass increases with underdoping due to Coulomb effects, the thermodynamically measured mass, obtained from, for instance, the Knight shift \(K_s(T_c)\) (or specific heat \(C_v/T\) at \(T_c\)), decreases with under doping, as a consequence of the opening of the pseudogap [see Fig. 2(c)].

Figures 2(a) and 2(b) illustrate the predicted behavior of the Knight shift for the cuprates as a function of \(x\) and \(T\). Because it depends only on \((d\text{-wave nodal})\) quasiparticle excitations, \(K_s\) exhibits a scaling with \(T/\Delta(0)\) which is illustrated in Fig. 2(b) via plots of \(K_s\) (normalized to its high \(T\) asymptote \(K_s\)) for the entire range of \(x\), and for temperatures below each respective \(T_c(x)\). An alternate scaling form is shown in Fig. 2(a) where we plot \(K_s\) normalized to \(T_c\) as a function of \(T/T_c\) for various \(x\) (with \(x\) increasing from top to bottom). The near-collapse of the different \(x\) dependent curves is similar to that found in the experimental data [22] shown in the inset. The normalization factor \(K_s(T_c)\) for this figure [which varies as the band mass multiplied by \(T_c/\Delta(0)\)] is plotted as a function of \(x\) in Fig. 2(c). Also plotted here are our specific heat \((C_v/T)\) predictions for the pairon contribution to \(\gamma^*\) as compared with the usual \(d\text{-wave} quasiparticle term [20] \(\alpha T_c\) as a function of \(x\). The pairon term becomes increasingly more important with underdoping.
In Fig. 3 we present a-axis penetration depth data, \( \Delta \lambda(T) \), in a nominally clean optimally doped \( \text{YBa}_2\text{Cu}_3\text{O}_{7-\delta} \) (YBCO) single crystal, from Ref. [23], along with \( d \)-wave fits to our BCS-BEC theory and to a straight line associated with a BCS superconductor. Because these two fitted curves are essentially indistinguishable, in the lower inset we plot the slopes \( d\Delta/dT \) where the difference between the two sets of curves is more apparent. Here it is shown that the low temperature downturn of the derivative, seen to a greater or lesser extent in all \( \Delta \lambda(T) \) measurements, fits our predicted \( T^{1/2} + \text{const} \) dependence rather well. This downturn has been frequently associated with impurity effects, which yield a linear in \( T \) slope for \( \Delta \lambda \) at very low \( T \), and, in this case, provide a poorer fit. While these cuprate experiments were performed on a nearly optimal sample, the same analysis of an underdoped material yielded similarly good agreement, but with a \( T^{3/2} \) coefficient about a factor of 2 larger. Future more precise and systematic low \( T \) experiments on additional underdoped samples are needed. Plotted in the upper inset are data [24] on the organic superconductor \( \kappa-(\text{ET})_2\text{Cu}[\text{N}(_2\text{CN})_2]\text{Br} \) (BEDT, \( T_c \approx 11 \text{ K} \)) which fit a pure \( T^{3/2} \) power law over a wide temperature regime; in contrast to the cuprates, there is no leading order linear term. At present, there seems to be no other explanation (besides the pairon mechanism presented here) for this unusual power law at the lowest temperatures.

In summary, within a BCS-BEC crossover theory (based on the Leggett ground state), we find that new low \( T \) power laws associated with a quasi-ideal gas of bosonic pair excitations appear in the thermodynamic and transport properties, which may be generally relevant to short \( \xi \) superconductors.

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[17] At low \( T \), we find that the leading order corrections are \( \Delta M_{\text{pair}} \approx T^2 \) for \( s \)-wave and \( \Delta M_{\text{pair}} \approx T^4 \) for \( d \)-wave; \( \Delta a_0 \approx T^2 \) in both cases. These correction terms are all very small.
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