



Short Coherence Length Superconductivity: A Generalization of BCS Theory for the Underdoped Cuprates

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On the basis of the observed short coherence lengths in the cuprates we argue that a BCS–Bose-Einstein condensation (BEC) crossover approach is an appropriate starting point for correcting the mean field approach of BCS and, thereby, for addressing pseudogap phenomena in these materials. Our version of the BCS-BEC approach is based on a particular Green's function decoupling scheme which should be differentiated from others in the literature, and which yields (i) the Leggett crossover ground state (for all coupling constants g , at $T = 0$) and (ii) BCS theory (for all $T \leq T_c$ over a range of small g). In this paper we provide a simple physical picture of the pseudogap phase above and below T_c , and review the quantitative and qualitative implications of this theory, which, for the most part have been published in a series of recent papers.

1. Introduction and Formalism

While two main alternatives have been suggested for addressing the cuprate pseudogap (the phase fluctuation approach[1] and the “nodal” d -wave quasiparticle picture[2]), this paper presents a third alternative which is based on the presumption that one should investigate small excursions from BCS without abandoning it altogether. This philosophy rests on the observation that (i) ξ is short so that the mean field theoretic approach of BCS should not be expected to be correct in detail and (ii) on Uemura's observation[3] that the cuprate superconductors belong to a large class of “exotic” materials. While the possible role of stripes, spin-charge separation and d -wave pairing has received much attention in the cuprate literature, here we argue that Uemura's famous plot suggests that one formulate a theory of superconductivity around a more universal approach without invoking specific materials-dependent features.

In this paper we present an extension of BCS theory, capable of describing short ξ superconductors, which is intermediate between a BCS and Bose-Einstein condensation (BEC) picture (the “BCS–BEC crossover scenario”). At the heart of our approach is the distinction between the fermionic excitation gap Δ and superconducting order parameter Δ_{sc} which distinction holds for $T \neq 0$, both above and below T_c . The difference parameter (or pseudogap energy scale) $\Delta_{pg}^2 = \Delta^2 - \Delta_{sc}^2$ can be associated with low energy, weakly damped, pair excitations of finite momentum.

It is essential to note that our generalization of BCS theory is based on the *particular* ground state of the crossover problem[4]: the Leggett state ($|\Psi_{\mathbf{k}} = \Pi_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}}c_{\mathbf{k}}^{\dagger}c_{-\mathbf{k}}^{\dagger})|0\rangle$), which has a BCS-like character but should be thought of as applicable to arbitrary values of the attractive coupling constant g . Here $u_{\mathbf{k}}, v_{\mathbf{k}}$ are given by the usual BCS-like expressions in terms of the fermionic dispersion $E_{\mathbf{k}}$. The variational conditions which ensue from Leggett's calculations are the same as those written below in Eqs. (1) and (2), for $T = 0$. We have shown, based on the work of Kadanoff and Martin[5] (KM), that these self consistent equations can be derived from a Green's function decoupling scheme. We stress here the three important but subtle observations of KM: (i) to obtain BCS-like theories, it is sufficient to truncate the system of equations so that only one and two particle propagators enter and (ii) the correlation functions associated with this KM scheme – at the level of the gap equations and thermodynamics – are *not* the same correlation functions which enter into the electro-dynamical response. (iii) The pair susceptibility χ which appears in the T-matrix, or pair propagator $\mathcal{T} = g/(1 + g\chi)$, is of the form $\chi = GG_0$; this differs from other T-matrix schemes (where, frequently, $\chi = GG$), but is required to obtain the BCS-like gap equations and their thermodynamics[5]. It should also be noted that this ground state has 100% condensation for all g , unlike that of the non-ideal Bose gas.

Without any detailed calculations, we can anticipate the form of the generalized BCS theory, which

applies below T_c [6]. As expected by a natural extension of the Leggett ground state variational conditions (and, as is consistent with BCS theory) we have

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

$$\sum_{\mathbf{k}} \left[1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} + \frac{2\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} f(E_{\mathbf{k}}) \right] = n \quad (2)$$

Here $\epsilon_{\mathbf{k}}$ is the bare fermion dispersion, measured from the chemical potential μ , $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2 \varphi_{\mathbf{k}}^2}$ is the quasi-particle dispersion and $\varphi_{\mathbf{k}}$ represents the symmetry of the pairing state. The new physics of the pseudogap phase is embodied in a third equation which represents the difference of the two energy gap parameters in terms of the number of excited pairs (with Bose distribution $b(\Omega_{\mathbf{q}})$), as

$$\Delta^2 - \Delta_{sc}^2 = \Delta_{pg}^2 = a_0 \sum_{\mathbf{q}} b(\Omega_{\mathbf{q}}), \quad (3)$$

where the coefficient of proportionality, a_0 , and the pair excitation energy, $\Omega_{\mathbf{q}}$, can both be determined from the above microscopic theory. These calculations[6,7] indicate that (at small, but non-zero (q, Ω)) the pair propagator can be approximated by

$$\mathcal{T} \approx a_0 / [\Omega - \Omega_{\mathbf{q}} + \mu_{pair} + i\Gamma_{\mathbf{q}}] \quad (4)$$

for the purposes of calculating the self energy Σ of the fermions (which self energy enters into the resulting gap equations and thermodynamics). One can interpret this theoretical approach as follows. Here we go beyond BCS to include self energy Σ effects associated with the incoherent, finite \mathbf{q} pair excitations. *Whereas, BCS is a mean field treatment of the particles, the present approach should be thought of as a mean field treatment of the pairs.* This represents the next level in a hierarchy of (superconducting) mean field theories, which hierarchy is similar to that encountered in magnetic problems. This mean field approximation of the pairs is associated with the truncation of the equations of motion, so that pair-pair interactions are not directly present. Residual inter-boson interactions arise only indirectly via the self energy of the fermions. As a consequence, both above and below T_c , the pair dispersion is quadratic $\Omega_{\mathbf{q}} = q^2/M_{pair}$, as in a quasi-ideal Bose gas. In this way, as in the KM paper, the pair correlation function is to be distinguished from that associated with the collective modes of the order parameter[8].

2. Results

The results summarized here represent those deduced from solving the coupled equations[5] for the pair propagator \mathcal{T} and its single particle analogue (G), along with the fermionic number constraint.

Pseudogap onset: In our earliest work[9] we found that the temperature T^* at which the Fermi liquid state first breaks down corresponds to the onset of a splitting of the single peaked (broadened Fermi liquid-like) electronic spectral function into two peaks separated by a (pseudo)gap. This pseudogap state is characterized by the presence of metastable pairs or “resonances” which effectively reduce the single particle density of states. Near, but above T_c , the latter takes the form of a broadened BCS-like structure. Moreover, between T_c and T^* , the wave-vector dependence of Σ (and of the pseudogap) departs from that of a strict $\varphi_{\mathbf{k}}$ symmetry[7]. Note, also, that in the present approach we always have $T^* \geq T_c$.

Superconducting transition: As the temperature decreases from T^* , the density of meta-stable pairs with momentum q continues to increase, until at $T = T_c$, a macroscopic fraction with $\mathbf{q} = 0$ undergoes Bose condensation. At this temperature, the pair propagator or T-matrix diverges as expected from the Thouless criterion, so that both μ_{pair} and $\Gamma_{\mathbf{q}=0}$ vanish. Moreover, near T_c , the inverse lifetime of the $\mathbf{q} \neq 0$ pairs, as well as that associated with fermion states γ becomes very small[7]. This is an important set of observations. Once the vicinity of T_c is reached, the interaction between the long wavelength (soft) bosons and the (gapped) fermions becomes weak. This same behavior continues to hold below T_c so that to leading order, lifetime effects can be dropped in Eqs. (1)-(3).

The dependence of T_c on g which results from Eqs (1)-(3) is highly non-monotonic, even for the s -wave case[7]. At low g , the curve for T_c vs g follows the BCS result until Δ_{pg} becomes sufficiently large; then T_c decreases, with g , thereby reflecting the difficulty of forming a superconducting state in the presence of a fermionic gap. Once μ becomes negative, T_c then increases with increasing g approaching a (mass) renormalized, but otherwise ideal BEC limit. For the d -wave case, the situation is even more complex[10]. As a result of the extended size of the d -wave pairs, the effects of the Pauli principle repulsion are more extreme, and T_c vanishes well before the

system reaches the $\mu < 0$ limit (except in the limit of unphysically small densities). In strictly 2d, we find T_c is always zero.

Behavior of the superconducting gap equations: Equations (1)-(3) were solved to yield the results plotted in Figure 1, for the case of weak, moderate and large g . Also indicated is a “cartoon” characterizing the excitations of the condensate at each value of g . Above T_c , where the computations are more complicated we used a simple extrapolation procedure[8] to facilitate the numerics. As can be seen from the Figure and from Eq. (3), as the number of excited pair states increases, so does the difference between the fermionic excitation gap and the order parameter. These figures represent a natural generalization of BCS theory.

Thermodynamical consequences; mostly C_v : The pair excitations shown schematically in Figure 1 necessarily lead to corrections to the quasiparticle-derived thermodynamics of BCS theory, via new low T power laws. Indeed, it would be difficult to imagine how fermionic quasiparticles could be relevant to the thermodynamics of the BEC limit. That these excited pair states have a nearly ideal Bose gas character is a consequence of the BCS-like, Leggett ground state; they arise from a mean field treatment of the pair propagator. One might imagine an improved approach to the strong coupling limit (which includes direct pair-pair interactions) would lead to results which are more analogous to those of the non-ideal Bose gas. It should, however, be noted that the cuprates are in the clear fermionic regime where μ is essentially E_F , as is consistent with our calculations[10,11]. Moreover, for the d -wave case, our analysis shows that the BEC limit is virtually inaccessible, and concerns about inaccuracies of the KM approach, in this limit, appear to be less relevant. What is most important is to properly capture the physics of the BCS regime, so that small excursions from it can be considered in a controlled manner. As a result of these pair excitations, in a quasi-2d system such as the cuprates we find[12] $C_v = \alpha T^2 + \gamma^* T$. At this time, a low T , linear specific heat contribution is well documented in the cuprates, although it is not known whether it is intrinsic or extrinsic. Elsewhere in this journal[13], we compare our quantitative calculations for C_v with experiment.

We have not yet completed a full calculation of the

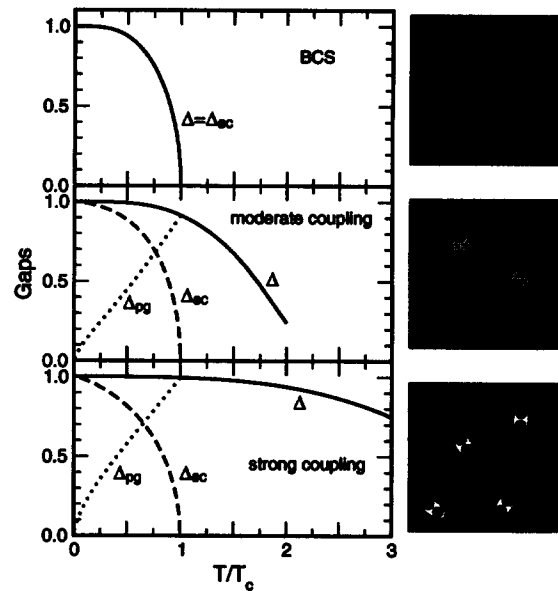


Figure 1. Temperature dependence of the gaps. Pair excitations become progressively more important with increasing coupling strength.

thermodynamical properties such as C_v from above to below T_c . Nevertheless, it can be anticipated on physical grounds that C_v/T starts to decrease once T^* is reached and that the overall behavior of that contribution to C_v which is associated with the fermionic degrees of freedom, is rather similar to that of a much-broadened BCS theory above T_c . The density of states is depleted precisely at E_F , once the temperature passes below T_c . This long range order-induced depletion, is, thereby, reflected in thermodynamical properties, such as C_v jumps which become progressively weaker the stronger the coupling g .

Behavior of the penetration depth: We find[11, 12], that the penetration depth at low T , behaves as $\lambda = \lambda_0 + AT + BT^{3/2}$. Here the second and third terms represent respectively the fermionic quasiparticle and the bosonic contributions. This additional $T^{3/2}$ bosonic contribution may be difficult to distinguish from the “dirty” d -wave T^2 term, which was previously invoked in fits to the data, at the lowest T . A quantitative discussion of this term is given elsewhere in this journal[13], along with comparisons to the data. [The hole concentration (x) dependence must be also addressed, as will be summarized be-

low]. It should be stressed that this bosonic term is responsible for the quasi-universal scaling of the penetration depth[11], which we have reported. Indeed, our calculations indicate that there are systematic deviations from perfect scaling, and the general trends for these deviations appear to have been observed by the Cambridge group[18].

The present approach should be contrasted with the “*d*-wave nodal quasiparticle” picture (in its Fermi liquid rendition[14]) where Landau parameters F_{1s} are thought to be important below T_c . In the present context, these F_{1s} effects are not as primary as is incorporating the new (non Fermi-liquid) physics of the pseudogap state. Ultimately Landau effects can be added here, as elsewhere, for detailed fits to data.

Phase Diagram: In order to incorporate the Mott insulator constraint, the band-width or alternatively n/m^* must be fit to the x -dependence of the zero temperature penetration depth[11]. In the absence of any detailed information about the source of the pairing attraction g (which presumably derives from Coulomb interactions[15] in some direct or indirect form, in the *d*-wave channel), we assume that g is x -independent and fit its ratio to the “bare bandwidth” via one adjustable parameter, which is chosen to optimize agreement with the entire phase diagram[10,11]. With this transcription, one can see that the ratio of g to the effective Fermi energy must increase as the insulator is approached, so that the bosonic degrees of freedom become more evident with underdoping. This prescription provides a quite good fit to T^* , T_c , $\Delta(0)$ over the entire range of x . It also can be used as a “tool” for addressing the x and T dependence of a wide collection of experimental data, including the critical current I_c , Knight shift and NMR relaxation rate[12]. All of these can be written in terms of the contributions from “three fluids”: the condensate (via Δ_{sc}), the fermionic excitations (via Δ), and the pair excitations (via Ω_q , or Δ_{pg}).

Neutron scattering and relation to condensation energy: Elsewhere[16], and in this journal[17] we have shown that the incommensurate and commensurate peaks in the neutron cross section can be interpreted as reflecting the *d*-wave superconducting gap. Moreover, above T_c , the pseudogap will lead to a residue of these peaks, albeit broadened. Within the present picture the neutron resonance (commensurate structure) and the behavior of the specific heat with its

discontinuity at and around T_c are both consequences of the same underlying pseudogap physics, but *not* directly of each other. Moreover, in contrast to BCS theory, where one can extrapolate the zero field normal state to estimate the condensation energy, here we find that because of the non-Fermi liquid nature of the normal state (and its instability at T_c) such extrapolations are problematical. This (along with other features, such as coherent and incoherent contributions to ARPES and tunneling, and general finite magnetic field effects on the pseudogap) will be discussed in more detail in future work.

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