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Abstract. The presence of a normal state spectral (pseudo) gap at the superconducting transition temperature in the underdoped cuprates has important implications for the associated superconducting phase. We argue that this normal state pseudogap derives from pairing fluctuations, which necessarily persist below T_c and which have important implications on the superconducting state. Our Greens function approach, based on the equation of motion method, can be viewed as a a natural extension of BCS theory for sufficiently strong pairing interaction, suggested by the short coherence length of the cuprates. In addition to the usual fermionic excitations, there are also incoherent (but not pre-formed) pairs of finite center of mass momentum which must be self consistently incorporated in computing T_c and other superconducting properties, such as the superfluid density and the Josephson critical current. Finally, we discuss some of the experimental implications of our theory for the cuprates.

INTRODUCTION

ARPES experiments [1] on the cuprates underline the important point that in these exotic materials, the excitation gap Δ and the order parameter Δ_{sc} must be distinct. The former is finite above T_c, where the latter is zero. This situation, which is to be distinguished from that of BCS theory, leads us to define a new parameter

$$\Delta_{pg}^2 = \Delta^2 - \Delta_{sc}^2 \qquad (1)$$

which can be calculated quantitatively and plays a central role in this paper.

In what follows we show that Δ_{pg} (i) is most naturally incorporated into extensions of BCS theory which are based on the BCS-Bose Einstein (BEC) crossover scenario [2], (ii) corresponds to a new degree of freedom, with associated dynamics, which we call the "pairon", (iii) is responsible for important corrections to the results of BCS theory in physical properties such as the penetration depth λ and in ratios such as $\Delta(0)/T_c$.

The BCS-BEC crossover theory was first formulated by Leggett [2] as a description of the ground state of a superconductor. As a function of variable coupling constant g it was demonstrated that the $T = 0$ state could be continuously deformed between the two limiting cases. For intermediate coupling (corresponding to the pseudogap phase of the cuprates), the excitations of this ground state are expected to be a
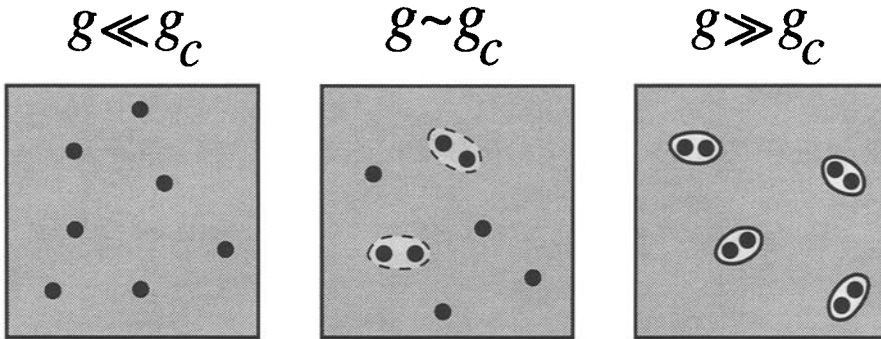
$$g \ll g_c \qquad g \sim g_c \qquad g \gg g_c$$

FIGURE 1. BCS-BEC crossover scenario below T_c. The gray background denotes the condensate of Cooper pairs. The pseudogap phase ($g \sim g_c$) is intermediate between the BCS ($g \ll g_c$) and BEC ($g \gg g_c$) limits.

combination of those of the BCS limit (which have fermionic character) and those of the BEC case (which correspond to bosons, or pairs of fermions). This situation is indicated schematically in Fig. 1. The finite center of mass momentum pair excitations are the pairons characterized by Δ_{pg}.

Before introducing the mathematical formalism, several important points should be stressed. Equation (1) is of interest only in the case of intermediate coupling: in the BCS case the right hand side is trivially zero, and in the BEC limit this equation is of little relevance, since fermionic excitations (and the related energy scale Δ) are not considered. Pairons are associated with the amplitude, not phase degrees of freedom. Their energy dispersion Ω_q will be seen to be *quadratic* and not linear in q as in the phase collective modes. (In this sense, the calculations are similar to those used to obtain the $q^2 \xi^2$ contributions to the Landau-Ginzburg free energy). Pairons are gapless. This is in contrast to the normal state resonant pairs [3] which retain a gap. This gaplessness, shown from Eq. (3a) below, is associated with the continuity in the fluctuation spectrum of the excitation gap around its q = 0 value. A gap in the pairon spectrum would require that the system be rigid with respect to deviations of the excitation gap Δ from the order parameter Δ_{sc}. While different from collective modes (which relate to correlation functions involving Δ_{sc}), pairons play an important role in obtaining the correct collective mode spectrum of the superconducting state (discussed elsewhere), as well as through the generalized Ward identity, arriving at a consistent treatment of the superfluid density.

MATHEMATICAL FORMALISM

As a simple model for the cuprate band structure, we consider a tight-binding, anisotropic dispersion $\epsilon_k = 2t_\parallel(2 - \cos k_x - \cos k_y) + 2t_\perp(1 - \cos k_\perp) - \mu$, where $t_\parallel$ ($t_\perp$) is the hopping integral for the in-plane (out-of-plane) motion and $t_\perp \ll t_\parallel$. We assume that the fermions interact via an effective pairing interaction with d-wave symmetry $V_{k,k'} = -|g|\varphi_k\varphi_{k'}$ so that $\varphi_k = \frac{1}{2}(\cos k_x - \cos k_y)$. The present approach is built

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on previous work [3–6] based on the equation of motion method for Greens functions, first introduced by Kadanoff and Martin [7], and subsequently extended by Patton [8].

The "pairing approximation" of Refs. [7,8] leads to

$$\Sigma(K) = \sum_Q t(Q)\, G_o(Q - K)\, \varphi^2_{\mathbf{k}-\mathbf{q}/2} \,, \tag{2a}$$

$$g = [1 + g\chi(Q)]t(Q)\,, \tag{2b}$$

where $\Sigma(K)$ is the self-energy, and $\chi(Q) = \sum_K G(K)\, G_o(Q - K)\varphi^2_{\mathbf{k}-\mathbf{q}/2}$ is the pair susceptibility. Equations (2), along with the number equation $n = 2\sum_K G(K)$, self-consistently determine both the Green's function $G(K)$ and the pair propagator, i.e., T-matrix $t(Q)$. We use a four-vector notation, e.g., $K \equiv (\mathbf{k}; i\omega)$, $\sum_K \equiv T\sum_{i\omega,\mathbf{k}}$ and $G_o(K) = (i\omega - \epsilon_{\mathbf{k}})^{-1}$.

We write the T-matrix and self-energy below T_c as $t(Q) = t_{sc}(Q) + t_{pg}(Q)$, and $\Sigma(K) = \Sigma_{sc}(K) + \Sigma_{pg}(K)$. The condensate contribution assumes the familiar BCS form $t_{sc}(Q) = -\delta(Q)\Delta^2_{sc}/T$, where Δ_{sc} is the superconducting gap parameter (and can be chosen to be real) and $\Sigma_{sc}(K) = \Delta^2_{sc}\,\varphi^2_{\mathbf{k}}/(i\omega + \epsilon_{\mathbf{k}})$. Inserting the above forms for the T-matrix into Eq. (2b), one obtains the excitation gap equation $1 + g\chi(0) = 0$, as well as (for any non-zero Q), $t_{pg}(Q) = g/(1 + g\chi(Q))$. Note that because of the gap equation, $t_{pg}(Q)$ is highly peaked about the origin, with a divergence at $Q = 0$. As a consequence, in evaluating the associated contribution to the self-energy, the main contribution to the Q sum comes from this small Q divergent region so that $\Sigma_{pg}(K) \approx -G_o(-K)\Delta^2_{pg}\varphi^2_{\mathbf{k}}$, where we have defined the pseudogap parameter

$$\Delta^2_{pg} \equiv -\sum_Q t_{pg}(Q) = -\sum_Q \frac{g}{1 + g\chi(Q)} \,. \tag{3a}$$

Thus, both Σ_{pg} and the total self-energy Σ can be well approximated by a BCS-like form, i.e., $\Sigma(K) \approx \Delta^2\,\varphi^2_{\mathbf{k}}/(i\omega + \epsilon_{-\mathbf{k}})$, where $\Delta \equiv \sqrt{\Delta^2_{sc} + \Delta^2_{pg}}$ is the magnitude of the total excitation gap, with the $\mathbf{k}$ dependence given by the d-wave function $\varphi_{\mathbf{k}}$. Within the above approximations, the gap and number equations reduce to

$$1 + g\sum_{\mathbf{k}} \frac{1 - 2f(E_{\mathbf{k}})}{2E_{\mathbf{k}}}\, \varphi^2_{\mathbf{k}} = 0 \,, \tag{3b}$$

$$\sum_{\mathbf{k}} \left[1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} + \frac{2\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\, f(E_{\mathbf{k}})\right] = n \,, \tag{3c}$$

where the quasiparticle energy dispersion $E_{\mathbf{k}} = (\epsilon^2_{\mathbf{k}} + \Delta^2\varphi^2_{\mathbf{k}})^{1/2}$ contains the full excitation gap Δ.

The set of equations (3) can be used to determine the superconducting transition temperature T_c (where $\Delta_{sc} = 0$), and the temperature dependence of the various gap parameters. Equation (3a) contains the physics of the pair excitations, or pseudogap. The remaining two Eqs. (3b) - (3c) are analogous to their BCS counterparts but with a finite (as a result of non-zero Δ_{pg}) excitation gap at T_c. In a similar fashion, this formalism can be used to deduce other measurable quantities [6], such as the penetration depth and critical current. Here the generalized Ward identity plays a profoundly important role.
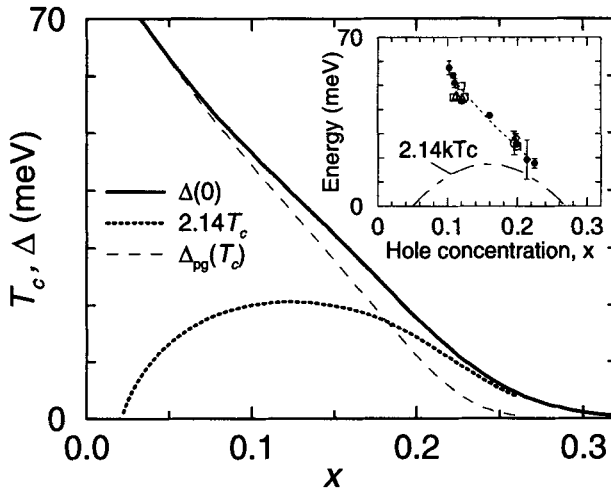
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FIGURE 2. The cuprate phase diagram. Plotted are T_c, $\Delta(0)$, and $\Delta(T_c)$, as a function of hole doping x. Experimental data from ref. [11] are shown in the inset. The gaps plotted are the magnitude at $(\pi,0)$.

APPLICATION TO THE CUPRATES

The remainder of this paper is directed towards understanding three experimental characteristics of the cuprates: the phase diagram, the superfluid density and the Josephson critical current.

In order to generate physically realistic values of the various energy scales, we make two assumptions: (1) We take g as doping-independent (which is not unreasonable in the absence of any more detailed information about the pairing mechanism) and (2) incorporate the effect of the Mott transition at half filling, by introducing an x-dependence into the in-plane hopping matrix elements $t_\parallel$, as would be expected in the limit of strong on-site Coulomb interactions in a Hubbard model [9]. Thus the hopping matrix element is renormalized as $t_\parallel(x) \approx t_0(1-n) = t_0 x$, where t_0 is the matrix element in the absence of Coulomb effects. This x dependent energy scale is consistent with the requirement that the plasma frequency vanish at $x = 0$. These assumptions leave us with one free parameter $-g/4t_0$, for which we assign the value 0.15 to optimize the overall fit of the phase diagram to experiment. We take $t_\perp/t_\parallel \approx 0.01$, and $t_0 \approx 0.6$ eV, which is reasonably consistent with experimentally based estimates [10].

The results for T_c, obtained from Eqs. (3), as a function of x are plotted in Fig. 2. Also indicated is the corresponding zero temperature excitation gap $\Delta(0)$ as well as the pseudogap Δ_{pg} at T_c. These three quantities provide us, for use in subsequent calculations, with energy scales which are in reasonable agreement with the data of Ref. [11], shown in the inset. The relative size of $\Delta_{pg}(T_c)$, compared to $\Delta(0)$, increases with decreasing x. In the highly overdoped limit this ratio approaches zero, and the BCS limit is recovered. Moreover, while not shown here, our calculations indicate that the excitation gap Δ is, generally, finite at T_c, the superconducting gap Δ_{sc} is established at and below T_c, while the pseudogap Δ_{pg} decreases to zero as T is reduced from T_c to 0. This last observation
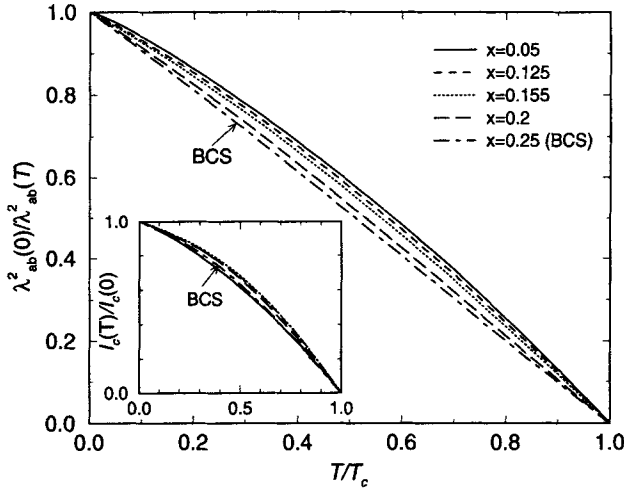
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FIGURE 3. Normalized in-plane superfluid density (main figure) and the c-axis Josephson critical current (inset) as a function of T/T_c for various doping concentrations x.

is consistent with general expectations for $\Delta_{pg}^2 \approx \langle |\Delta|^2 \rangle - |\Delta_{sc}|^2$.

It is important to stress, that our subsequent results for the superfluid density and Josephson current, need not be viewed as contingent on the detailed x-dependence used to derive the phase diagram. One can approach the calculations of these quantities by taking $T_c(x)$ and the various gap parameters (shown in the inset) as phenomenological inputs, within the context of the present formalism.

The superfluid density (normalized to its $T = 0$ value) is plotted in Fig. 3 as a function of T/T_c for several representative values of x, ranging from the highly over- to highly underdoped regimes. These plots clearly indicate a "quasi-universal" behavior with respect to x: $\rho_s(T)/\rho_s(0)$ vs. T/T_c depends only slightly on x. Moreover, the shape of these curves follows closely that of the weak-coupling BCS theory. The, albeit, small variation with x is systematic, with the lowest value of x corresponding to the top curve. Recent experiments provide some preliminary evidence for this universal behavior [12,13]. However, a firm confirmation requires further experiments on a wider range of hole concentrations, from extreme under- to overdoped samples. This universal behavior, which has been discussed elsewhere [6], is associated with pairon effects.

Similar quasi-universal behavior is also predicted for the normalized c-axis Josephson critical current $I_c(T)/I_c(0)$, as shown in the inset of Fig. 3. This behavior is in contrast to the strongly x dependent quasiparticle tunneling characteristics which can be inferred from the temperature dependent excitation gap. At this time, there do not appear to be detailed studies of $I_c(T)$ as a function of x. In future experiments the quasiparticle tunneling characteristics should be simultaneously measured, along with $I_c(T)$, so that direct comparison can be made to the excitation gap, and the predictions can be tested.

Physically, this universality is associated with two compensating contributions, arising from the quasiparticle and pair excitations. In the overdoped regime the former dominate,

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whereas in the underdoped regime the latter are more important. One can thus infer that the destruction of the superconducting state comes predominantly from pair excitations at low x, and quasiparticle excitations at high x.

CONCLUSIONS

In summary, in this paper we have proposed a scenario for the superconducting state of the cuprates. This state evolves continuously with hole doping x, exhibiting unusual features at low x (associated with a large excitation gap at T_c) and manifesting the more conventional features of BCS theory at high x. In this scenario the pseudogap state is associated with pair excitations, which act in concert with the usual quasiparticles. Despite the fact that the underdoped cuprates exhibit features inconsistent with BCS theory ($T_c/\Delta(0)$ is strongly x dependent and Δ is finite at and above T_c) we deduce an interesting quasi-universality of the normalized ρ_s and I_c as a function of T/T_c. In these plots the over- and under-doped systems essentially appear indistinguishable. Current experiments lend support to this universality in ρ_s, although a wider range of hole concentrations will need to be addressed, along with future systematic measurements of I_c.

ACKNOWLEDGMENTS

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