Coulomb correlations and pseudogap effects in a preformed pair model for the cuprates

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We extend previous work on preformed pair models of superconductivity to incorporate Coulomb correlation effects. For neutral systems, these models have provided a useful scheme which interpolates between BCS and Bose-Einstein condensation with increasing coupling and thereby describes some aspects of pseudogap phenomena. However, charge fluctuations (via the plasmon, ω_p) significantly modify the collective modes and therefore the interpolation behavior. We discuss the resulting behavior of the pseudogap and thermodynamic quantities such as T_c, χ, and C_v as a function of ω_p. [S0163-1829(96)50846-5]

The role of the pseudogap[1] in the high-T_c cuprates is emerging as an important indicator of the nature of the superconductivity as well as the normal state. There are two widely discussed but competing explanations for pseudogap effects but no clear and decisive experiments to support one scenario over the other. Early observations associated the pseudogap with magnetic pairing[2] above T_c (often called the ''spin gap''). It is now clear, however, that some form of normal-state pairing is seen in photoemission as well as charge transport data. Moreover, at least in the photoemission data the pseudogap appears to have the d-wave symmetry[1] of the ordered state and this leads naturally to the association of this ''gap'' with precursor superconductivity.[3–5] This second scenario is further supported by the observation of low dimensionality and short coherence lengths in high-T_c superconductors, which suggests important deviations from ideal mean field or BCS transitions. Indeed, the approach of the present paper assumes the precursor superconductivity scenario, in large part because it is important to establish, at least as a base line, the extent to which such superconducting ''fluctuation'' effects may be responsible for pseudogap behavior.

Among those models which subscribe to a precursor superconductivity scenario there are additionally two rather distinct viewpoints. Emery and Kivelson[5] have argued that the pseudogap state of the cuprates is similar to that observed in granular films where phase coherence is not fully established, although large regions of the material have a well established superconducting amplitude. Because it is small, in some sense, in the cuprates their approach focuses on n/m^* or alternatively on the plasma frequency ω_p as the key ''phase stiffness'' parameter. Alternatively, others[3,4,6,7] have focused on the observed small size of the superconducting correlation length ξ to argue for important corrections to BCS theory associated with preformed or nearly formed pairs[8] which exist well above T_c and therefore give rise to significant pseudogap effects. The present paper is based on the viewpoint that in the cuprates the characteristic parameter of the charge degrees of freedom, n/m^* or equivalently ω_p, should be treated on a relatively equal footing with the correlation length, ξ.

To study the role of Coulomb interactions on pseudogap phenomena, we adopt a natural microscopic framework which incoporates charge fluctuations into theories which treat the crossover from BCS pairing to Bose-Einstein condensation (BEC) of preformed pairs.[9] In neutral systems, this crossover has been studied by a variety of investigators.[3,4,6] Numerical simulation studies,[7] which have been performed in the context of attractive Hubbard models, include, in principle, all diagrammatic contributions. On the other hand, analytical work has mostly been confined to the T-matrix approximation. The issue of nonconserving and conserving T-matrix schemes has been widely discussed in the literature[6] in the context of the BCS-BEC crossover problem. In the original work of Nozières and Schmitt-Rink a nonconserving approach was used. Recent work[6] on neutral systems has extended this scheme using a T-matrix approximation which satisfies global conservation laws and in the process introduces renormalized Green's functions into the generalized susceptibilities. In the charged system, as a consequence of gauge invariance, the analogue renormalized susceptibilities must then appear in the particle-hole channel. As has been known for some time,[10] however, the collective mode spectrum is then treated incorrectly at this level of approximation and a more sophisticated scheme is needed. In order to avoid this complexity and to develop an intuitive understanding of the effects of charge, however, we restrict the analysis, in this paper, to the more familiar scheme introduced by Nozières and Schmitt-Rink and defer consideration of a fully conserving formalism. We note, however, that our formulation will be locally conserving and in the case of charged systems this approximation does not yield qualitatively different physics from that expected using a globally conserving approach. Furthermore, it is our contention that mode-mode coupling effects will ultimately lead to important insights which we will discuss in a future paper.

The Hamiltonian under consideration contains an attractive interaction $V_{\mathbf{k},\mathbf{k}'}$, parametrized by a coupling constant g, as well as long-range Coulomb terms. For definiteness we take the same separable pairing potential, $V_{\mathbf{k},\mathbf{k}'}=gv_{\mathbf{k}}v_{\mathbf{k}'}$ where $v_{\mathbf{k}}=(1+k^2/k_0^2)^{-1/2}$, as was used initially by Nozières and Schmitt-Rink. Within this model, the pairing energy scale (or ''Debye frequency'') is the Fermi energy. We assume a three-dimensional free electron model for the electrons and defer discussion of anisotropy effects until later in the text. It is assumed that in the cuprates there is sufficient interlayer hopping so that a strictly two-dimensional model and its associated Kosterlitz-Thouless transition is not the

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appropriate starting point. We generalize the path integral formulation of Ref. 4, replacing the usual fermionic fields by Nambu spinors, $\psi_{\mathbf{k}}^{\dagger}=(c_{\mathbf{k}\uparrow}^{\dagger},c_{-\mathbf{k}\downarrow})$, and decoupling in four real fields given by $\eta_i=\psi^{\dagger}\tau_i\psi$ ($\tau_i, i=0,\ldots,3$, are the identity and three Pauli matrices). The interaction in the off-diagonal channels ($i=1,2$) is the pairing interaction while the Coulomb term appears in the diagonal channels ($i=0,3$). Finally, the field η_0 may be eliminated by a suitable gauge transformation and the thermodynamic potential Ω is computed for the remaining degrees of freedom at the Gaussian approximation level,

$$\Omega=\Omega_0+\frac{T}{2}\sum_{\mathbf{q},\nu_m}\ln\det(\Gamma^{-1}_{\mathbf{q},\nu_m})-\frac{n_f}{2}\sum_{\mathbf{q}} V_{\mathbf{q}}^{(3)},$$

$$\Gamma_{\mathbf{q},\nu}^{(i,j)-1}=\delta_{i,j}-TV_{\mathbf{q}}^{(i)}\sum_{\mathbf{k},\omega_l}\mathrm{tr}(\tau_i\mathcal{G}_{\mathbf{k}+\mathbf{q}/2,\omega_l}\tau_j\mathcal{G}_{\mathbf{k}-\mathbf{q}/2,\omega_l-\nu_m})\times v_{\mathbf{k}}^{(i)}v_{\mathbf{k}}^{(j)}.$$

Here Ω_0 is the usual contribution from noninteracting fermions and n_f denotes the corresponding number density of free fermions. In the interaction $V_{\mathbf{q}}^{(i)}=g, v_{\mathbf{k}}^{(i)}=v_{\mathbf{k}}$ for $i=1,2$, and $V_{\mathbf{q}}^{(3)}=4\pi e^2/\kappa q^2, v_{\mathbf{k}}^{(3)}=1$. Finally, $\mathcal{G}_{\mathbf{q},\omega}$ is the single-particle Green's function in Nambu space and T is the temperature, while ν_m and ω_l are the even and odd Matsubara frequencies, respectively. Above T_c the fluctuation propagator Γ is diagonal; thus all three channels (the particle-particle, particle-hole, and uncorrelated fermions) contribute additively to Ω as well as to the various derived thermodynamic quantities which we calculate below.

In the present formalism,[4] the transition temperature is obtained from the BCS gap equation with a self-consistently determined chemical potential, μ, obtained from the condition $n_{\mathrm{tot}}=-\partial\Omega/\partial\mu$. The resulting coupled equations are solved numerically for μ and T_c. In the limit of arbitrarily large g the effects of the Coulomb interaction drop out, since mode-mode coupling is neglected at the Gaussian level, so that T_c is given by the ideal BEC temperature. At small g, the collective mode contribution to μ becomes arbitrarily small and the BCS limit is approached, albeit with a Coulomb renormalized chemical potential.[11] When the superconducting coupling constant g vanishes, the above form for Ω reflects the plasmon contribution and reduces to that of the usual Coulomb gas.[11] The Gaussian approximation to Ω gives a random-phase-approximation-like treatment of the collective modes and so provides a reasonable scheme for interpolating between these two limits. It should be noted, however, that Coulomb pseudopotential effects (which would act to renormalize g) are, for simplicity, not included in our calculations. Here we focus principally on the effects introduced by the long-range Coulomb interaction [which enters via the parameter $\omega_p^2=4\pi ne^2/(m^*\kappa)$].

To illustrate the effects of charge fluctuations we plot, in Fig. 1(a), T_c as a function of g/g_c for various values of the plasma frequency. The dotted line represents the BCS result (for the neutral system) and the solid line is the corresponding (neutral) transition temperature which includes Gaussian fluctuations. The remaining curves from left to right demonstrate the effects of increasingly large ω_p. For the purposes of focusing on charging effects only we fix E_F and k_F/k_0; in this way all the Gaussian derived curves have the same high g asymptote. Moreover, with these assumptions the neutral system reference curve is unchanged as ω_p is varied. Two effects of Coulomb interactions can be observed in Fig. 1(a): (i) T_c decreases with increasing ω_p, and (ii) the nonmonotonic behavior as a function of g found for the neutral case (which is believed to be unphysical)[6] progressively disappears with increasing ω_p.

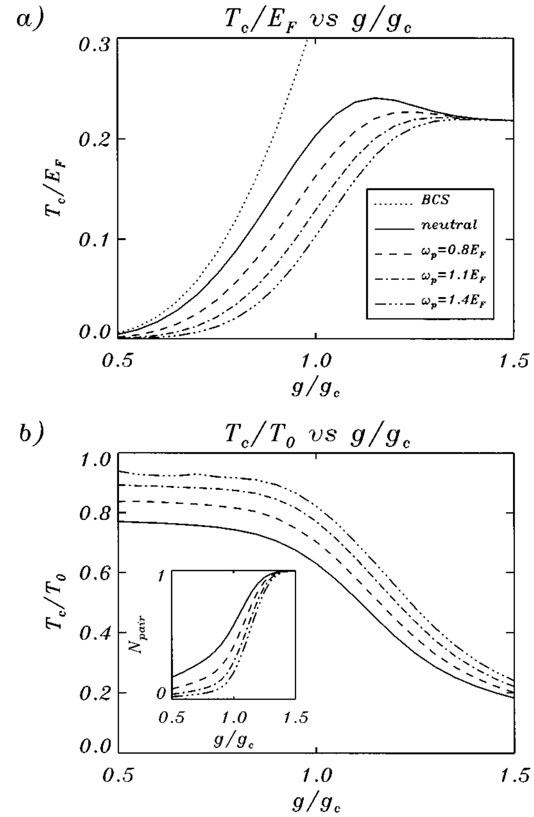

FIG. 1. (a) The variation of T_c as a function of coupling constant in the BCS and Gaussian approximation theories for neutral and charged systems with increasing plasma frequencies. (b) T_c normalized by the Coulomb mean-field result (see text) T_0 for the same plasma frequencies as in (a). The inset in (b) plots the number of paired electrons vs g/g_c for the same parameter set.

The first observation, which is perhaps the more important, is a consequence of the fact that an attraction due to Coulomb interactions in the particle-hole channel reduces the effectiveness of the attraction in the pairing channel. We illustrate this first point more directly in the inset of Fig. 1(b), which plots the number of superconducting pairs as a function of increasing ω_p. This effect may seem counter to the expectation that systems with larger ω_p will have reduced T_c suppression (i.e., larger T_c) due to phase fluctuations. However, when the appropriate reference temperature is used, Coulomb interactions are found to lead to better agreement with mean-field theory; in this sense superconducting fluctuations are, indeed, suppressed by Coulomb interactions. We plot in the main portion of Fig. 1(b) the ratio of T_c to the critical temperature T_0 obtained by neglecting pair fluctuations (but including Coulomb effects) for the same range of plasma frequencies as in Fig. 1(a). As can be seen, the larger the plasma frequency, the higher the ratio

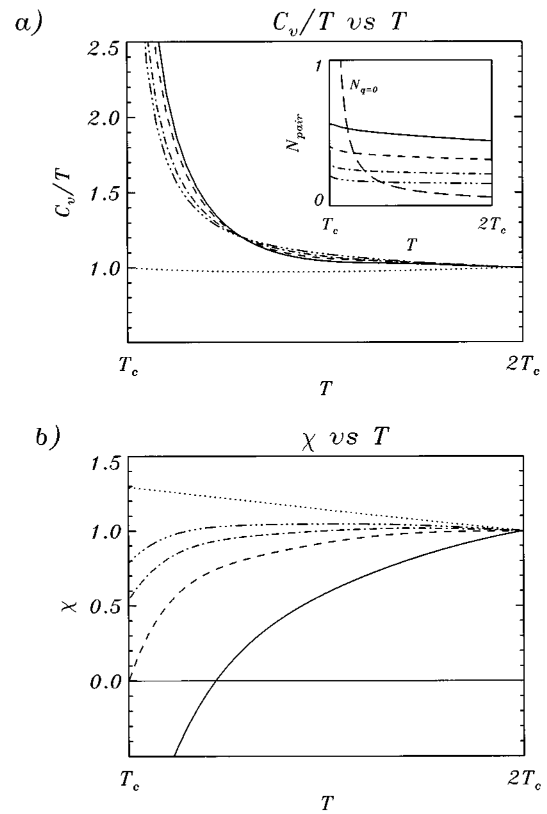

FIG. 2. Temperature-dependent specific heat (a) and spin susceptibility (b) for the same parameters as in Fig. 1. The dotted lines are the BCS results (with slightly temperature-dependent chemical potential). The inset in (a) plots the total number of pairs vs T, along with the number at $q=0$.

T_c/T_0 and thus the better the agreement with a mean-field treatment of the pairing channel.

A more convenient way of illustrating fluctuation effects and the associated role of the plasma frequency, however, is to study thermodynamic properties directly. Here pseudogap effects enter as precursor superconducting contributions in, for example, the specific heat and spin susceptibility. As in Fig. 1(b), these fluctuation effects are expected to weaken as the plasma frequency increases and mean-field behavior is restored. We plot C_v and χ in Fig. 2 for the same parameter set as in Fig. 1, with g/g_c set equal to unity. This choice of coupling strength is consistent with the observation of relatively short coherence lengths in the cuprates and with the claim that high-T_c compounds lie close to the bound-state limit.[8] Here the dotted lines again represent the BCS value (with a properly T-dependent μ). As is appropriate[12] for Gaussian fluctuation theories, the specific heat varies as $(T-T_c)^{-1/2}$. Comparison with the neutral (solid) reference curve shows that the effects of variable ω_p are not as evident in the specific heat as in the spin susceptibility. Similarly, deviations from mean-field behavior appear at higher temperatures in χ than in C_v.

It is worth noting that in the present formulation there is no well defined ''onset temperature'' for the appearance of a pseudogap, as might exist if a sharp phase transition occurred at some temperature T^* above T_c. Moreover, in discussing the onset of fluctuations, it should be stressed that their appearance is unrelated to the temperature dependence of the total number of fluctuations or preformed pairs. As shown in the inset of Fig. 2(a), for fixed ω_p, the total number of pairs is relatively constant up to temperatures many times higher than T_c; however, their distribution shifts to lower momenta as T_c is approached and long-range coherence is established. Detailed calculations indicate that varying ω_p does not alter the critical behavior in the pairing channel as T_c is approached; the narrowing of the pseudogap region with increasing ω_p is a result of the smaller relative contribution that pairing fluctuations make to the thermodynamics as Coulomb correlations become more dominant. Finally, it should also be noted that the neutral system yields unphysical thermodynamic behavior at smaller coupling constants than when Coulomb effects are included. This is illustrated by the negative values of χ indicated in the figure. Such unphysical behavior has been shown to result from the nonconserving nature of the approximations used.[13]

While the above figures were designed to illustrate the effect of Coulomb correlations, they do not fully represent the physical system in which variations in the plasma frequency are necessarily associated with changes in the electronic energy scale. In reality both ω_p and $E_F=k_F^2/2m^*$ depend on similar combinations of the carrier density n and effective mass m^*. As the insulator is approached ω_p decreases as $\omega_p^2 \approx x$ (where x denotes the number of doped holes); however, whether one assumes a Fermi-liquid $(n\approx 1+x)$ or non-Fermi-liquid $(n\approx x)$ approach to the insulator, it follows necessarily that the electronic energy scale E_F must also vanish as the hole concentration x approaches 0. In scenarios based on electronic pairing mechanisms, therefore, it is difficult to escape the conclusion that the onset temperature for coherent superconducting fluctuations, T^*, should also become small as the insulator is approached. Our numerical calculations of C_v and χ exhibit this effect, principally because ours is a single energy scale theory: both T^* and T_c derive from the same pairing mechanism. This behavior is in contrast to experiment[1] where even in highly underdoped systems T^* is of the order of 100 K or more. Large T^* seems to be most naturally associated with a high-energy scale in the insulating parent compound, such as a magnetic energy.[2] However, in such a scenario it then becomes problematic to understand how the other important energy scale[8] ω_p enters to determine T_c. We speculate that a crossover from three- to two-dimensionality may play some role in lowering T_c at low doping concentrations where enhanced (quasi-two-dimensional) critical fluctuation effects are most apparent.[14]

In Fig. 3, we explore these issues within the context of our model. We consider three situations in which the Gaussian derived T_c is plotted as a function of ω_p (which may be directly related to hole concentration x) to arrive at a form of ''phase diagram.'' The solid line corresponds to the case in which the characteristic energy for pairing (called ''E_F'') is held fixed, and as observed in Fig. 1(a), T_c monotonically decreases. This should be contrasted with the situation in which E_F is allowed to vary self-consistently (dotted line) in accord with the measured ω_p. Here for definiteness, we assume a Luttinger volume Fermi surface. The latter case yields[8] $T_c\approx\omega_p$; however, T_c is suppressed at low doping

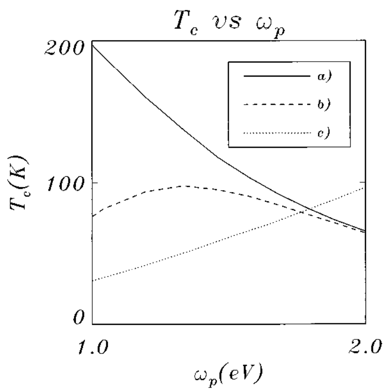

FIG. 3. Variation of T_c with ω_p (in units of eV, where optimal doping corresponds to $\omega_p \approx 1.2$ eV) with E_F held fixed [curves (a) and (b)] as well as using self-consistently determined E_F [curve (c)]. Curve (b) corresponds to $2+\epsilon$ dimensions with $\epsilon=0$ when $\omega_p=0$ and growing linearly to $\epsilon=1$ near optimal. See text for details.

primarily as a result of the lowering of the electronic energy scale, E_F, rather than from increased phase fluctuations. Neither of the above cases is entirely satisfactory for understanding the larger pseudogap regime at low doping. We address this issue phenomenologically by introducing the effects of a dimensionality crossover for fixed pairing energy scale E_F and calculating T_c for a system in $2+\epsilon$ dimensions (dashed curve) where ϵ varies smoothly from zero when $\omega_p \approx 0$ (at half filling) to one when $\omega_p \approx 1.2$ eV (corresponding to optimal doping) and then remains constant.[15] Here T_c is suppressed at low doping, as a consequence of two-dimensional fluctuation effects. Moreover, one can associate T^* with the solid curve, which exhibits the observed experimental trends. Thus the low doping regime is characterized by a large pseudogap. On the other hand, at higher doping or ω_p, both T_c and T^* converge and the pseudogap region vanishes. Whether or not this phenomenology is appropriate, the above discussion underlines the importance of multiple energy scales (ω_p, as distinct from the pairing energy scale) and the possible role of a dimensionality crossover[14] in understanding pseudogap behavior.

In summary, we have presented a preformed pair model in which the effects of Coulomb correlations are clearly seen to suppress superconducting fluctuations (above T_c) and thereby tune pseudogap behavior in the calculated specific heat and spin susceptibility. Moreover, these two thermodynamic variables, as a function of T, are found to be reasonably consistent with experiment. However, it should be stressed that within our microscopic model, the effects of Coulomb correlations enter in a rather different way than has been assumed in previous phenomenological schemes.[5,16] Our approach focuses more directly on correlated pairs rather than superconducting grains; therefore, phase and amplitude fluctuations appear on a relatively equivalent basis. As a consequence, introducing Coulomb interactions into the preformed pair formalism leads to a narrowing of the pseudogap region by providing a competing attraction in the particle-hole channel and thus reducing the effectiveness of superconducting pairing.

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