The pseudogap in underdoped high $T_c$ superconductors in the framework of the Boson Fermion model

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The question of whether the pseudogap in high $T_c$ cuprates is related to superconducting precursor effects or to the existence of extrinsic bosonic massive excitations is investigated on the basis of the Boson-Fermion model. The characteristic three peak structure of the electronic spectral function and the temperature dependent Fermi vector derived here are signatures for a two component scenario which can be tested by ARPES and BIS experiments.

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The recent direct experimental verifications \cite{1,2} of a pseudogap in the density of states of the electrons in the metallic layers of the cuprate high temperature superconductors in the underdoped regime is presently considered to be one of the key elements to guide us in unravelling the underlying mechanism for superconductivity in these materials.

The most immediate temptation to explain the pseudogap which opens at a certain temperature \( T^* \), sometimes well above the superconducting transition temperature, is to consider it as a consequence of superconducting phase fluctuations corresponding to a finite and relatively long lived amplitude of the order parameter above \( T_c \). Support in favor of such a scenario comes from the fact that the symmetry of the pseudogap is the same as that of the true gap and that the materials are quasi 2D structures, for which Cooper pairs are expected to exist in form of propagating states above \( T_c \) \cite{3}. It is in this context that many theoretical papers base their study on the intricate interplay between electronic quasi-particles and their bosonic resonant states.

Scenarios for the pseudogap based on systems with attractive interaction between the electrons exhibit such a precursor pseudogap in the cross-over regime between BCS an a superfluid state of preformed tightly bound electron pairs. Quite generally and independent of any particular scenario \( T_c \) is then determined by a temperature \( T_{MF} \) characterizing the onset of phase fluctuations of the order parameter, while the meanfield critical temperature \( T_{MF} \) describes the formation of pairs. This leads to a suppression of intensity of low lying single particle excitations and thus to the appearance of a pseudogap \( g \). Specific scenarios attempting to describe such behavior are based on generic models for superconductivity with some effective attractive interaction \( g \) and on the negative U Hubbard problem \[8,9\].

Contrary to such scenarios implicating a direct precursor effect, others have been proposed where the pseudogap is induced by antiferromagnetic spin fluctuations rather than pair fluctuations. For single component systems such scenarios are based on strong repulsive interactions between the electrons. The pseudogap is then related to a SDW and/or Hubbard pseudogap close to a corresponding transition \[10,11\]. More precisely, the pseudogap features in the charge sector are derived from the pseudogap features of bosonic resonant states in the spin sector \[12\]. A somewhat different scenario for the pseudogap is presented for the RVB physics, according to which chargeless spinons pair up at \( T^* \) and holons condense at \( T_c \) \cite{13}. Similar in spirit are the \( SU(2) \) symmetry meanfield studies of slave boson approaches in strongly correlated systems \[14\], which relate the pseudogap to the transition between small and large Fermi surfaces. Van Hove singularities also may play a role and were shown to stabilize d wave RVB states with pseudogaps near those singularities \[17\].

Apart from those single component scenarios, scenarios involving two component systems have been proposed. Experiments on the optical conductivity have for a long time suggested that in high \( T_c \) cuprates two types of carriers may be at stake, almost localized ones and itinerant ones \[18\]. Recent experiments on the specific heat are in support of such a hypothesis \[19\] and chemical analysis \[20\] favors the picture of metallic layers imbedded in highly polarizable dielectrics which could be the seat of localized polaron or bi-polarons. These results clearly point in the direction of two component scenarios such as described by the generic Boson-Fermion (B-F) model introduced by us along time ago \[21\]. On the basis of this model we have initially shown the opening of a pseudogap in the density of states of the Fermionic subsystem setting in below a certain temperature \( T^* \), the breakdown of Fermi liquid properties \[22,23\] and the manifestations of that in the thermodynamic, magnetic and transport properties \[24,25\]. A scenario related to
that has been proposed on the basis of stripes in the metallic layers, where 1D spin stripes alternate with 1D metallic stripes \[26\]. The spin stripes produce bosonic entities in form of tightly bound spin singlets which are exchanged by pair hopping processes with electron pairs in the neighboring metallic stripes.

The purpose of this communication is to elucidate the nature of the pseudogap as given in the scenario of the Boson-Fermion model. Is it due essentially to a precursor effect in low dimensional systems \[27\] or is related to a two particle resonant state triggered by the existence of extrinsic (in contrast to intrinsic in single component systems) bosonic modes such as localized bi-polarons which form part of the charge carriers of the system? For this purpose we shall try to interpret our previous numerical calculations \[22,23\] in terms of an approximative analytic approach. This will permit us to intuitively understand the three peak structure for the spectral properties of the electronic subsystem, the reasons for the breakdown of Fermi liquid properties and indicate to what extent the opening of the pseudogap is related to a precursor to superconductivity. Moreover we shall show that for this model the Fermi vector will change as a function of temperature. This should in principle be measureable and thus help to clarify whether high \( T_c \) superconductors are one or two component systems.
II. AN ANALYTIC APPROACH TO UNDERSTAND THE PSEUDOGAP

The B-F model describes a system of localized Bosons hybridized with conduction electrons. The Bosons can be thought of as bipolarons (localized electron pairs with opposite spin) mainly located in the dielectric layers surrounding the \(CuO_x\) planes which contain the Fermions (conduction electrons) \[28\]. The corresponding Hamiltonian for this model is given by

\[
H = (zt - \mu) \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{(i \neq j),\sigma} c_{i\sigma}^\dagger c_{j\sigma} + (\Delta_B - 2\mu) \times \sum_i b_i^\dagger b_i + v \sum_i [b_i^\dagger c_{i\uparrow} c_{i\downarrow} + c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger b_i]
\]  

(1)

where \(c_{i\sigma}^\dagger\) refers to the Fermion operators of the itinerant electrons and \(b_i^\dagger\) to the Boson operators. The spin indices are given by \(\sigma\), the bare hopping integral for the electrons is given by \(t\), the Boson energy level by \(\Delta_B\) and the Boson-Fermion pair exchange coupling constant by \(v\). \(i\) denotes some effective site involving adjacent molecular clusters of the metallic and dielectric planes, which, as far as the metallic planes are concerned, should involve a unit of two neighboring \(CuO_x\) clusters and as far as the dielectric planes are concerned could be thought of two adjacent apex oxygens together with their nearby dopant atoms. Such pairs of electrons, corresponding to the term \(c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger\) in the metallic layers should be considered as intersite rather than onsite pairs. Correlation effects which are certainly important are totally neglected here, because we want to focus on physics introduced by pair hopping between the metallic and the dielectric layers. Since we are dealing here with a two-component system we have to impose a common chemical potential \(\mu\) in order to guarantee charge conservation.

We have previously evaluated the Fermion spectral functions and the density of states for this model for a one and respectively two dimensional bare (i.e., in the absence of Boson Fermion hybridization, \(v = 0\)) density of states using a selfconsistent lowest order fully conserving diagramatic procedure \[22,23\]. In the present work we focus on the normal state temperature variation of the spectral function for the Fermions at wave vector \(k_F\) as well as on the imaginary part of the self energy as a function of frequency. Since we are only interested here in qualitative features such as the temperature variation of the pseudogap, we carry out our study for the case of a 1D bare density of states, knowing from past experience \[22,23\] that the dimensionality only quantitavely influences the pseudogap features in this model. We therefore adopt the same procedure as outlined in ref \[22\] but with a much denser mesh of 1000 \(k\) vectors in the Brillouin zone. This is required in order to track the temperature effects on the spectral function and to determine \(k_F\) as a function of temperature, given the fact that for our two component system the number of Fermions and Bosons is not conserved separately.

Before reporting on these numerical results, let us consider some basic features of the B-F model from which the underlying physics can be understood. The self energies for the Fermions \(\Sigma_F(k, i\omega_n)\) and Bosons \(\Sigma_B(q, i\omega_m)\) within lowest order perturbation theory are given by

\[
\Sigma_F(k, i\omega_n) = \frac{v^2}{N} \sum_q \frac{n_F(\varepsilon_{-k+q}) - n_B(\varepsilon_{-k+q})}{i\omega_n - E_0 + \varepsilon_{-k+q}} \quad (2)
\]

\[
\Sigma_B(q, i\omega_m) = \frac{v^2}{N} \sum_k \frac{1 - n_F(\varepsilon_{-k+q}) - n_F(\varepsilon_{k})}{i\omega_m - \varepsilon_{-k+q} - \varepsilon_k} \quad (3)
\]

where \(n_{F,B}(...)\) denote the Fermi and respectively Bose distribution function. \(\varepsilon_k \equiv t(z - \sum_\delta \text{exp}(i\mathbf{k}\delta) - \mu)\) is the free Fermion dispersion with \(\delta\) being the vectors linking nearest neighbour sites, \(E_0 \equiv \Delta_B - \Delta_F\) and \(N\) is the number of \(k\) vectors in the Brillouin zone. Considering the problem of the B-F model within the framework of a selfconsistent RPA scheme requires to look for distribution functions \(n_k^F\) and \(n_k^B\) which replace \(n_F(\varepsilon_k)\) and \(n_B(\varepsilon_k)\) in Eqs.(2,3) and which have to be determined selfconsistently via the equations

\[
n_k^F = \frac{1}{2} + \frac{1}{\beta} \sum_{i\omega_n} G_F(k, i\omega_n) \quad n_k^B = -\frac{1}{2} - \frac{1}{\beta} \sum_{i\omega_m} G_B(q, i\omega_m) \quad (4)
\]

with the Fermi and Bose Green’s functions given by

\[
G_F(k, i\omega_n) = [i\omega_n - \varepsilon_k - \Sigma_F(k, i\omega_n)]^{-1}, \quad (5)
\]

\[
G_B(q, i\omega_m) = [i\omega_m - E_0 - \Sigma_B(q, i\omega_m)]^{-1} \quad (6)
\]
Contrary to the conserving diagramatic approach to this problem which we have solved previously \[22,23\], we are unable to find numerically stable solutions for the set of equations corresponding to the above set of selfconsistent RPA equations Eqs.(2-6) in 2D as well as in 3D. That is a first indication that the Fermi liquid properties in the B-F model are destroyed.

Let us next attempt to understand this behaviour by closer examining those expressions for the self energies. Considering to begin with the situation of \(E_0 \gg k_B T\) for which we obtain

\[
\Sigma_F(i\omega_n) = \frac{v^2}{N} \sum_{\mathbf{q}} \frac{n_F(\varepsilon_{\mathbf{q}})}{i\omega_n - E_0 + \varepsilon_{\mathbf{q}}}
\]

which is independent on the wavevector. Introducing the imaginary part of this contribution to the retarded self energy i.e., \(\Gamma(\omega) = -2i m \Sigma_F(\omega)\) we find

\[
\Gamma(\omega) = 2\pi v^2 \frac{1}{N} \sum_{\mathbf{q}} n_F(\varepsilon_{\mathbf{q}}) \delta(\omega - E_0 + \varepsilon_{\mathbf{q}})
= 2\pi v^2 n_F(E_0 - \omega) \rho_0(E_0 + \mu - \omega)
\]

where we have taken the limit \(i\omega_n \to \omega + i0\). Let us now consider for simplicity a constant model density of states such as \(\rho_0(\omega) = 1/2zt\) for \(-zt \leq \omega \leq +zt\). Upon Hilbert transforming the expression for \(\Gamma(\omega)\) we obtain for the corresponing real part of the Fermion self energy

\[
R(\omega) = \frac{v^2}{2zt} \ln \left| \frac{\omega - E_0}{\omega - E_0 - \mu} \right|
\]

The excitation spectrum for the Fermions is then determined by the poles of the Fermion Green’s function:

\[
G_F(\mathbf{k}, \omega_k) = \left[ \omega_k - \varepsilon_k - R(\omega_k) + i \frac{\omega - \omega_k}{2} \Gamma(\omega_k) \right]^{-1}
\]

where \(\omega_k\) denote the complex solutions which determine the real and imaginary part of the energy spectrum. As can be seen from the graphical procedure for determining the poles of this Green’s function, see Fig.1, we generally expect three poles to occur. The lowest energy real pole corresponds to the bonding state, the highest energy real pole to the anti-bonding state and the complex pole in the intermediary energy range to the non-bonding state. Given the fact that \(E_0 > 0\), since the chemical potential always must lie below the Bosonic level, the distribution function \(n_k\) for the Fermions is enterly described by the lowest energy solution of Eq.(10) and for which \(\Gamma(\omega_k) \equiv 0\). We thus obtain:

\[
n_k = \int_{-\infty}^{\infty} d\omega \delta(\omega - \varepsilon_k - R(\omega)) n_F(\omega)
\equiv Z_k n_F(\omega_k) = Z_k
\]

with \(Z_k \equiv [1 - dR/d\omega|_{\omega_k}]^{-1}\) representing the spectral weight of the lowest energy pole \(\omega_k \leq 0\) of the Fermion Green’s function i.e., \(G_F(\mathbf{k}, \omega) = Z_k/(\omega - \omega_k + i0)\). The standard way of determining the Fermi wavevector for Fermi liquids is to use the relation for the Fermion distribution function derived from Eq.(10), together with the condition \(\omega_k \leq 0\) which leads to \(\varepsilon_{k_F} + R(0) = 0\). The relations describing the quasi-particle properties at the Fermi surface are then given by:

\[
\varepsilon_{k_F} = \frac{v^2}{2zt} \ln \left| \frac{E_0 + \mu}{E_0} \right|
\]

\[
\frac{dR}{d\omega} \bigg|_0 = -\frac{v^2}{2zt} \left( \frac{1}{E_0} - \frac{1}{E_0 + \mu} \right)
\]

\[
n_{k_F} = \left[ 1 + \frac{v^2}{2zt} \left( \frac{1}{E_0} - \frac{1}{E_0 + \mu} \right) \right]^{-1}
\]

The B-F model thus predicts two well separated peaks at the Fermi wave vector whose energies are given by \(\omega \simeq 0\) and \(\omega \simeq E_0 + \mu + \mu \frac{E_0 - \mu}{E_0} \exp(-(E_0 + \mu)/v^2)\).

From the above Eqs. (11,12) we notice that although in general the Fermionic distribution function has a discontinuity at \(\mathbf{k}_F\), this discontinuity disappears in the limit \(E_0 \Rightarrow 0\) (which corresponds to the limit \(T \Rightarrow T_c(\equiv 0\) in our
case of a 1D bare density of states) and for which \( \varepsilon_{kF} \Rightarrow \infty \) and \( n_{kF} \Rightarrow 0 \). The physical reasons for this breakdown of Fermi liquid properties becomes obvious by inspection of the contribution proportional to \( n_B(E_0) \) in the self energy and which for \( E_0 \ll k_B T \) becomes singular. Let us for that purpose suppose that the Bosons have acquired some itinerancy i.e., \( E_q = E_0 + (\hbar q)^2/2m_B \) where \( m_B \) denotes some Boson mass \([30]\). In the limit \( E_0 \Rightarrow 0 \) the term proportional to \( n_B(E_q) \) becomes singular for \( q \Rightarrow 0 \). Putting \( n_B(E_q) = n_B(E_q) + \delta_q,0(Nn_0 - n_B(E_q)) \) leads to

\[
\Sigma(k, \omega) \simeq v^2 \frac{n_0}{\omega + \varepsilon_k + \eta}
\]

and ultimately to a contribution to the Fermion Green’s function, given by

\[
G_F(k, \omega) = \frac{\omega + \varepsilon_k}{\omega^2 - \varepsilon_k^2 - v^2 n_0}
\]

This is precisely the BCS Green’s function with its two poles \( \omega_k = \pm \gamma_k = \pm \sqrt{\varepsilon_k^2 + v^2 n_0} \) showing its gap in the excitation spectrum given by \( \sqrt{v^2 n_0} \) and a Fermion distribution function \( n_k = \frac{1}{2} [1 - \varepsilon_k/\gamma_k] \) which has no longer a discontinuity at \( k = k_F \).

### III. SPECTROSCOPIC SIGNATURES OF A TWO-COMPONENT SCENARIO

After these phase space considerations for the spectral properties of the B-F model, let us now come to the numerical solution of this problem. Following the procedure discussed previously \([22]\) we derive the Fermionic spectral function

\[
A(k, \omega) = -2 Im G(k, \omega + i0)
\]

at \( k_F \). There is no unambiguous way of determining \( k_F \) for an interacting system at finite temperatures. We follow here the method spectroscopists use, namely to determine \( k_F \) as that vector for which the distribution function

\[
n_F^F = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(k, \omega)n_F(\omega)
\]

has an inversion in slope. As in our previous calculations we use here as representative parameters \( v = 0.1 \) and \( \Delta_B = 0.4 \) in units of the band width \( 8t \) and a total density of charge carriers \( n = 2n_F + 2n_B = 1 \). The number of Fermions per spin is given by \( n_F = \sum_{k<k_F} n_F^F \). The values of \( k_F \) determined in this way are given as a function of temperature in Table I, where we compare them with values derived by other criteria such as \( n_{k_F}^F = 0.5 \) and using the Luttinger sum rule \( \sum n_{k<k_F} = 1 = Nn_F \).

In Fig.2 we illustrate \( A(k_F, \omega) \) for a set of temperatures from which we can see the evolution of the peak structure of this spectral function at the Fermi level. We also observe that the lowest energy peak, corresponding to the bonding single particle state shifts to energies below the Fermi energy (equal to zero in our notation) while the non-bonding single particle state shifts to energies above the Fermi level, thus indicating the opening of a pseudogap as the temperature is reduced. These findings are in qualitative agreement with the recent experiments of ARPES on the underdoped high \( T_c \) materials \([12]\).

Our theoretical predictions of the evolution of the three pole structure of the Fermionic spectral function should be a testing ground for

(i) the two component scenario of high \( T_c \) superconductivity

(ii) the pre-existence of bound electron pairs which would be at the origine for the deviations from Fermi liquid properties and responsible for the opening of the pseudogap.

ARPES and BIS experiments should be able to see those features, inspite of the relatively poor resolution available for these type of experiments at present.

The existence of the three peaks in the spectral function can be inferred from the solution of the B-F model in the atomic limit for which they are given by \( \varepsilon_{\pm} = (E_0 + E_0/2) \pm \gamma \) for the lowest energy bonding and highest energy anti-bonding two particle states respectively and by \( \varepsilon_0 \) for the intermediary non-bonding single particle state. It should be noticed that those expressions for the two particle poles with \( \gamma = \sqrt{(E_0 - E_0/2)^2 + v^2} \) correspond to those in the Green’s function given by Eq.(14).

The deviations from Landau Fermi liquid behaviour are contained in the frequency dependence of the Fermionic self energy. We trace the real and imaginary part of this function for different temperatures in Fig.(3). As we can see and as we have pointed out previously, this function does not go to zero at the Fermi level when the temperature decreases, as would be expected to happen for a standard Fermi liquid. We also notice from Fig.(3) that the real
part of the Fermionic self energy is indeed very similar to the model self energy discussed above and which led to the form given by Eq.(9). This guarantees that the essential physics of the normal state properties of the B-F model, as discussed above in terms of the model density of states, is basically correct and should be rather insensitive to dimensionality.

Our work totally neglects correlation effects as well as such important questions as the symmetry of the pseudogap and the incoherent background, seen in ARPES and associated with this pseudogap in certain direction [12]. Such questions are presently being considered by us and will make the topic of some future publication.

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[29] As we have shown in our previous work ref( [22,23]), as well as in some forthcoming publication of the B-F model in infinite dimension, the dimensionality of the bare density of states does not influence the qualitative features of our results.
[30] As shown in our fully conserving treatment of the B-F model, refs. [22,23] the intrinsically localized Bosons acquire itinerancy upon lowering the temperature.
**Fig.1** Plot of the real and imaginary part of the Fermion self energy for the constant model density of states and the graphic solution of the poles for the Fermion Green’s function.

**Fig.2** The temperature dependence of the Fermion spectral function $A(k_F, \omega)$ at the Fermi vector showing the opening of the pseudogap and the evolution of a three-pole structure as the temperature is decreased (a). The temperature evolution of the photo emission spectrum intensity (b). $T = 0.007$ solid line, $T = 0.01$ dashed line and $T = 0.02$ dotted line.

**Fig.3** The temperature dependence of the imaginary part (a) and the real part (b) of the Fermion self energy at the Fermi vector, $T = 0.007$ solid line, $T = 0.01$ dashed line and $T = 0.02$ dotted line.
TABLE I. The temperature dependence of $n_F$ and $k_F$ in units of $\pi/1001$. We compare $k_F$ as determined by $d^2 n_k/dk^2 = 0$ (a) with $k_F$ as determined by $n_{k_F} = 1/2$ (b) and with $k_F$ determined by the Luttinger sum rule $\sum_{k \leq k_F} 1 = N n_F$ (c).

| $T$  | $n_F$ | $k_F(a)$ | $k_F(b)$ | $k_F(c)$ |
|------|-------|----------|----------|----------|
| 0.020| 0.276 | 145      | 143      | 138      |
| 0.015| 0.230 | 147      | 147      | 146      |
| 0.010| 0.283 | 150      | 148      | 142      |
| 0.007| 0.284 | 151      | 149      | 142      |
| 0.006| 0.285 | 152      | 150      | 143      |
\[ \omega - \varepsilon_k \]

\[ u \]

\[ \Gamma \]

\[ R \]
Figure (a) shows the spectral function, while Figure (b) displays the PES intensity as a function of energy.
(a) Energy, Imaginary Part

(b) Energy, Real Part