

## Metal-Insulator Crossover in the Boson-Fermion Model in Infinite Dimensions

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The boson-fermion model, describing a mixture of tightly bound electron pairs and quasifree electrons hybridized with each other via a charge exchange term, is studied in the limit of infinite dimensions using the noncrossing approximation within the dynamical mean field theory. It is shown that a metal-insulator crossover, driven by strong pair fluctuations, takes place as the temperature is lowered. It manifests itself in the opening of a pseudogap in the electron density of states, accompanied by a corresponding effect in the optical and the dc conductivity. [S0031-9007(98)07175-0]

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The discovery of high- $T_c$  superconductors (HTS) has led to the questioning of a large number of basic physical concepts. In particular, great attention has been devoted to the conjecture that in the normal state HTS do not behave as standard Fermi liquids [1]. A signature for the possible breakdown of this concept might be the existence of a pseudogap in the normal state which opens up at a temperature  $T^*$  which, depending on doping, can be well above the superconducting transition temperature  $T_c$ . The origin of this pseudogap is presently an issue of controversy. The fact that, upon lowering the temperature, this pseudogap smoothly merges into the superconducting gap in the entire Brillouin zone [2] strongly favors the idea that it is related to strong pair correlations which set in below a certain characteristic temperature  $T^*$  and lead to condensation below  $T_c$ . This does not mean that these pair correlations are due to some superconducting fluctuations but rather that they are a precursor to the superconducting state. They can exist without superconductivity and can in principle be stable all the way down to the lowest temperatures if the superconducting state is inhibited for some reason. If not, they will lead to condensation in some kind of superfluid state. Local probe tunneling spectroscopy inside and outside vortex cores at temperatures below  $T_c$  represents precisely this situation [3]. Such experiments rule out a pseudogap due to superconducting fluctuations and moreover confirm that the normal state pseudogap goes over continuously into a true superconducting gap as one moves across the border of the vortex cores.

We have in the past attempted to understand the physics of HTS in terms of a phenomenological model consisting of two components: localized pairs of electrons (bosons) and quasifree electrons (fermions), hybridized with each other via a charge exchange term. It is understood that the electrons are confined to the  $\text{CuO}_2$  planes while the localized electron pairs are of the form of bipolarons and are confined to the dielectric highly polarizable layers which are sandwiching the  $\text{CuO}_2$  planes [4]. The physics

of this scenario is described by the boson-fermion model (BFM)

$$H = \varepsilon_0 \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + E_0 \sum_i b_i^\dagger b_i + g \sum_i [b_i^\dagger c_{i\downarrow} c_{i\uparrow} + c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger b_i], \quad (1)$$

with  $\varepsilon_0 = D - \mu$  and  $E_0 = \Delta_B - 2\mu$ . Here  $c_{i\sigma}^{(\dagger)}$  denote fermionic operators for electrons with spin  $\sigma$  at some effective sites  $i$  (involving molecular units rather than individual atoms) and  $b_i^{(\dagger)}$  are hard-core bosonic operators describing tightly bound electron pairs. The bare hopping integral for the electrons is given by  $t$ , the bare electronic half bandwidth by  $D$ , the boson energy level by  $\Delta_B$ , and the boson-fermion pair-exchange coupling constant by  $g$ . The chemical potential  $\mu$  is common to fermions and bosons (up to a factor of 2 for the bosons) in order to guarantee charge conservation.

The underlying physics of this model is that the charge exchange term between bosons and free electrons induces local pairing among the latter and thus leads to a depletion of the density of states near the Fermi level which reflects itself in the opening of a pseudogap. Our previous studies of this model on the basis of lowest order self-consistent conserving approximations bore this out [5] and showed how the appearance of such a pseudogap manifests itself in the thermodynamic, transport, and magnetic properties of the system [6]. These studies indicated that  $T^*$  was intimately related to a precursor of a condensation of the intrinsically localized bosons due to some highly nonlinear feedback effect from the itinerant electrons. This finding was verified independently by a method summing up the most diverging diagrams [7]. Our follow-up study of this model in the atomic limit [8] (which excluded from the outset any global superconducting state) gave the first indications that the opening of the pseudogap was related to a metal-insulator crossover rather than

to superconducting pair fluctuations. Both effects, of course, will determine the temperature dependence of the pseudogap, but with different importance depending on the temperature regime. We shall present in this Letter a dynamical mean field study of the BFM in infinite dimensions in which full use is made of those atomic limit results and which permits one to incorporate the itinerancy of the electrons in a controlled fashion. We shall below sketch the main lines of this algorithm and then concentrate on the normal state properties of this model.

In infinite dimensions a many body system can be treated as a purely local system coupled to a "medium" described by a Weiss field, with which it interacts in the form of an impurity Anderson problem [9]. In such a scheme the effective Hamiltonian for the BFM is

$$H = \sum_{\sigma} \varepsilon_0 c_{\sigma}^{\dagger} c_{\sigma} + E_0 b^{\dagger} b + g [c_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger} b + b^{\dagger} c_{\downarrow} c_{\uparrow}] + \sum_{k,\sigma} w_k d_{k,\sigma}^{\dagger} d_{k,\sigma} + \sum_{k,\sigma} v_k [d_{k,\sigma}^{\dagger} c_{\sigma} + c_{\sigma}^{\dagger} d_{k,\sigma}], \quad (2)$$

where  $c_{\sigma}^{(\dagger)}$  and  $b^{(\dagger)}$  denote the original fermion and boson operators at the impurity site, and  $d_{k,\sigma}^{(\dagger)}$  denote the auxiliary fermionic variables of the Weiss field. For these latter the energy spectrum  $w_k$  and their coupling  $v_k$  to the impurity

electrons have to be determined self-consistently. Setting  $H = H_0 + H_I$ , with  $H_I$  denoting the interaction term between the electrons and the auxiliary fermions, we have that  $H_0$  can be written in the form  $H_0 = \sum_{n=1}^8 |n\rangle E_n \langle n| + H_{\text{med}}$ , where  $H_{\text{med}} = \sum_{k,\sigma} w_k d_{k,\sigma}^{\dagger} d_{k,\sigma}$  and

$$\begin{aligned} |1\rangle &= |0\rangle, & E_1 &= 0, \\ |2(3)\rangle &= |\uparrow(\downarrow)\rangle, & E_2 &= E_3 = \varepsilon_0, \\ |4\rangle &= u|\uparrow\downarrow\rangle - v|\bullet\rangle, & E_4 &= \varepsilon_0 + E_0/2 - \gamma, \\ |5\rangle &= v|\uparrow\downarrow\rangle + u|\bullet\rangle, & E_5 &= \varepsilon_0 + E_0/2 + \gamma, \\ |6(7)\rangle &= |\uparrow(\downarrow)\bullet\rangle, & E_6 &= E_7 = \varepsilon_0 + E_0, \\ |8\rangle &= |\uparrow\downarrow\bullet\rangle, & E_8 &= 2\varepsilon_0 + E_0, \end{aligned} \quad (3)$$

are the eigenstates and the eigenvalues of the Hamiltonian (1) in the atomic limit. Here the arrows denote the presence of an electron with spin up or down, and the dot indicates the presence of a boson on the effective impurity site. In Eqs. (3) we have defined  $u^2 = 1/2 - (2\varepsilon_0 - E_0)/(4\gamma)$ ,  $v^2 = 1 - u^2$ , and  $\gamma = \sqrt{(\varepsilon_0 - E_0/2)^2 + g^2}$ .

Introducing the Hubbard operators  $X_{mn} = |m\rangle\langle n|$  we can rewrite the original fermion operators as

$$c_{\sigma} = \sum_{mn} F_{mn}^{\sigma} X_{mn}, \quad c_{\sigma}^{\dagger} = \sum_{mn} F_{nm}^{\sigma} X_{mn}, \quad (4)$$

where

$$\begin{aligned} F_{12}^{\uparrow} &= F_{78}^{\uparrow} = 1, & F_{34}^{\uparrow} &= F_{56}^{\uparrow} = u, & F_{35}^{\uparrow} &= -F_{46}^{\uparrow} = v, \\ F_{13}^{\downarrow} &= -F_{68}^{\downarrow} = 1, & F_{24}^{\downarrow} &= -F_{57}^{\downarrow} = -u, & F_{25}^{\downarrow} &= F_{47}^{\downarrow} = -v. \end{aligned}$$

The interaction Hamiltonian then becomes

$$H_I = \sum_{k\sigma} \sum_{mn} v_k [F_{mn}^{\sigma} d_{k,\sigma}^{\dagger} X_{mn} + F_{nm}^{\sigma} X_{mn} d_{k,\sigma}]. \quad (5)$$

We shall now solve the  $d \rightarrow \infty$  BFM within the so-called noncrossing approximation (NCA) in  $H_I$ . A similar approach was recently used in the dynamical mean field theory (DMFT) context [9] by Lombardo *et al.* for a multiband Hubbard model for perovskites [10] and by Schork and Blawid for the Anderson lattice model with

correlated conduction electrons [11]. For this purpose we introduce the resolvents  $R_{mn}(z)$ , where  $m$  can be different from  $n$ , defined through the Dyson equation

$$R_{mn}(z) = \delta_{mn} R_m^0(z) + \sum_l R_m^0(z) \Sigma_{ml}(z) R_{ln}(z), \quad (6)$$

together with the associated spectral functions given by  $A_{mn}(\omega) = -2 \text{Im} R_{mn}(\omega + i\delta)$ . The free diagonal resolvents in Eq. (6) are  $R_m^0(z) = (z - E_m)^{-1}$  and the self-energies  $\Sigma_{ml}(z)$  are determined self-consistently through the equations

$$\Sigma_{mm'}(z) = \sum_{nn',\sigma} F_{nm}^{\sigma} F_{n'm'}^{\sigma} \int \frac{dx}{2\pi} \Delta(x) n_F(-x) R_{nn'}(z - x) + \sum_{nn',\sigma} F_{mn}^{\sigma} F_{m'n'}^{\sigma} \int \frac{dx}{2\pi} \Delta(x) n_F(x) R_{nn'}(z + x) \quad (7)$$

with the use of the Weiss field spectral function

$$\Delta(\omega) = 2\pi \sum_k v_k^2 \delta(\omega - w_k). \quad (8)$$

Within the NCA the local fermion Green's function

$$G_F(z) = \sum_{mn} \sum_{m'n'} F_{mn}^{\sigma} F_{n'm'}^{\sigma} \langle\langle X_{mn}; X_{m'n'} \rangle\rangle_z \quad (9)$$

is expressed in terms of the resolvents according to the relations

$$\langle\langle X_{mn}; X_{m'n'} \rangle\rangle_z = \frac{1}{Z_{\text{loc}}} \int \frac{dx}{2\pi} e^{-\beta x} [A_{m'm}(x) R_{nn'}(x + z) + \xi A_{nn'}(x) R_{m'm}(x - z)], \quad (10)$$

where

$$Z_{\text{loc}} = \sum_{mm'} \int dx e^{-\beta x} A_{mm'}(x) \quad (11)$$

and  $\xi = -1$  for fermions and  $+1$  for bosons. The above set of self-consistent equations is evaluated for a Bethe lattice with a semicircular density of states  $D(\varepsilon)$  of width  $2D = 4t$ . In this case the DMFT self-consistency condition takes the simple form  $\Delta(\omega) = t^2 A_F(\omega)$  [9], where  $A_F(\omega) = -2 \text{Im} G_F(\omega + i\delta)$  is the fermionic spectral function. We should stress that our approach represents a generalization of the NCA (originally devised for the single-impurity Anderson model [12]), suited for models with a total number of particles per site greater than one. The original NCA formulation is recovered when all the nondiagonal resolvents are neglected, as was recently done for the multiband correlated electron models studied in Refs. [10,11]. In general, the iterative procedure determining those resolvents will lead to an increasing number of such nondiagonal elements, the relevance of which will depend on the model under consideration. For the problem studied here, the only nonvanishing nondiagonal element is  $R_{45}(= R_{54})$ .

The results presented below have been obtained in the symmetric limit of the model, i.e., for  $\varepsilon_0 = E_0 = 0$  (from now on all energies are in units of  $2D$ ). In this case the chemical potential is fixed in the middle of the electronic band, giving  $n_F = \sum_{\sigma} \langle c_{\sigma}^{\dagger} c_{\sigma} \rangle = 1$  and  $n_B = \langle b^{\dagger} b \rangle = \frac{1}{2}$ . We furthermore choose  $g = 0.2$  such that the characteristic temperature of the opening of the pseudogap lies in the regime of a few hundred degrees K. From the behavior of the density of states  $A_F(\omega)$ , plotted in Fig. 1 for various temperatures  $T$ , we can see that the pseudogap opens up below a characteristic temperature  $T^* \approx 0.15$  and gradually deepens as  $T$  is reduced. This value of  $T^*$

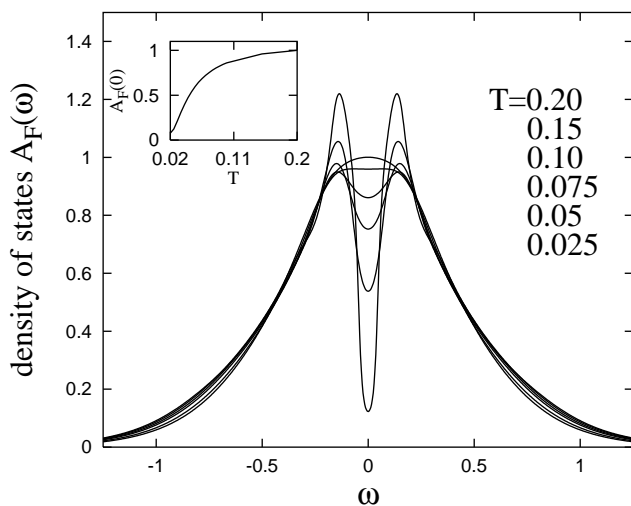


FIG. 1. Fermion DOS for several temperatures  $T$  (all energies in units of  $2D$ ), the deepest pseudogap corresponding to the lowest  $T$ . The inset shows the DOS at the Fermi energy as a function of  $T$ .

gives a reasonable estimate of the onset of the pseudogap regime, provided that the fermions are assumed to be quasiparticles with a strongly renormalized bandwidth. We also notice that temperatures lower than those reported in the figure are not considered here, since they do not lead to reliable convergency rates. This is probably a sign of the failure of the NCA at low temperatures.

The behavior of the pseudogap is best studied in terms of the fermionic self-energy  $\Sigma_F(z)$  or its imaginary part  $\Gamma(\omega) = -2 \text{Im} \Sigma_F(z = \omega + i\delta)$ .  $\Sigma_F(z)$  is introduced by expressing the local Green's function in the form  $G_F(z) = [z - \varepsilon_0 - \Sigma^W(z) - \Sigma_F(z)]^{-1}$ , where the Weiss self-energy  $\Sigma^W(z)$  is determined from  $\Delta(\omega) = -2 \text{Im} \Sigma^W(\omega + i\delta)$  or, alternatively, using the self-consistency condition  $\Sigma^W(z) = t^2 G_F(z)$ . For an ordinary Fermi liquid, one expects that  $\Gamma(\omega) \sim \omega^2$  such that the lifetime of the quasiparticles at the Fermi energy  $\tau_F = 1/\Gamma(0)$  becomes infinite. In Fig. 2a, we plot  $\Gamma(\omega)$  for the same parameters as in Fig. 1 and observe that the pseudogap is linked to a strong resonant scattering of the quasiparticles with the bosons at the Fermi energy. As one lowers the temperature, the lifetime at the Fermi energy tends to zero and a metal-insulator crossover takes place. The form of  $\Sigma_F$  clearly shows that our system does not correspond to a Fermi liquid, as we can see from an inspection of the poles of the lattice Green's function  $G_F(z, \omega) = [z - \varepsilon_k - \Sigma_F(z)]^{-1}$  ( $\varepsilon_k$  denoting the bare electronic dispersion). At high temperatures,  $T \gg T^*$ , we see from Fig. 2b that the straight line representing the inverse of the free-particle Green's function at  $k = k_F$  (with  $\varepsilon_{k_F} = 0$ ) cuts  $\text{Re} \Sigma_F(\omega)$  only at the Fermi energy  $\omega = 0$ . Considering, however, that  $\Gamma(\omega)$  develops a minimum at  $\omega = 0$  which tends to a constant as  $T$  is increased, we still cannot attribute this feature to a normal Fermi liquid behavior. Upon lowering the temperature, we observe an inversion of slope which results in a cut occurring at three distinct frequencies, with the solution

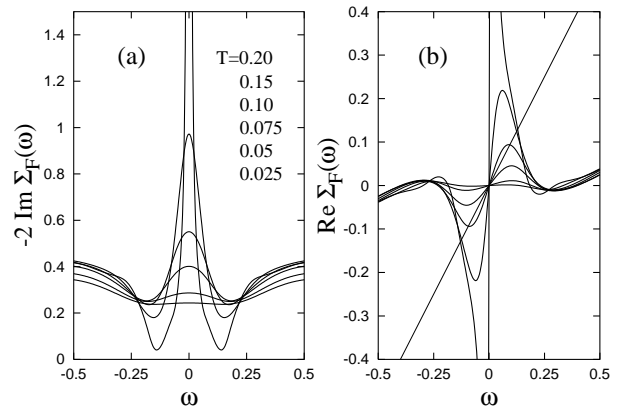


FIG. 2. Frequency dependence of the imaginary (a) and the real (b) part of the fermion self-energy for several temperatures  $T$  (same units as in Fig. 1). The lowest  $T$  corresponds to the highest value of  $\text{Im} \Sigma_F(0)$  and the steepest slope of  $\text{Re} \Sigma_F(0)$ , respectively.

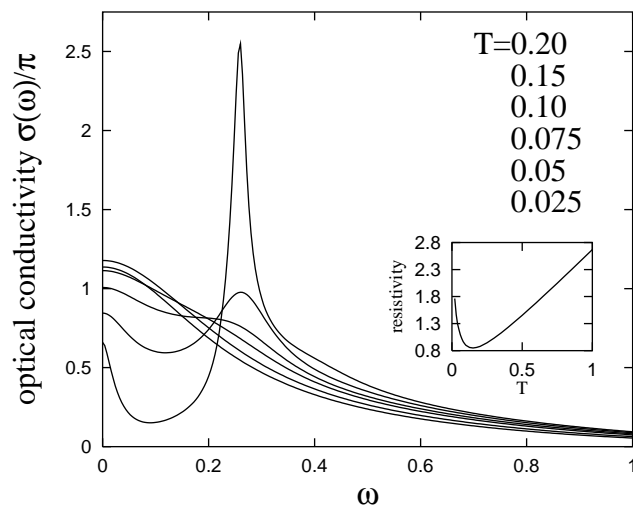


FIG. 3. Fermion optical conductivity for several temperatures  $T$ , the lowest  $T$  corresponding to the highest value of  $\sigma(\omega)$  at high frequencies (same units as in Fig. 1). The inset illustrates the dc resistivity  $[\sigma(0)/\pi]^{-1}$  as a function of  $T$ .

at  $\omega = 0$  being now accompanied by a large imaginary part of  $\Sigma_F$ . The pseudogap is thus a consequence of a spectral weight transfer from the Fermi energy away to the wings in the density of states associated with bonding and antibonding two-particle states [8]. This is very similar to what has been obtained for the 2D Hubbard model at half filling [13], where a pseudogap develops due to antiferromagnetic correlations. The results presented here are also in line with the precursor pairing correlation ideas developed by Randeria [14].

The present study does not contain any superconducting fluctuations and hence excludes the possibility of a transition to a superconducting state. The opening of the pseudogap is hence entirely related to a crossover from a metalliclike state at high temperatures to an insulating one at lower temperatures. We now show that this behavior is also manifest in the real part of the optical conductivity which in the limit  $d \rightarrow \infty$  takes the form [9]

$$\sigma(\omega) = \pi \int d\varepsilon D(\varepsilon) \int d\omega' A_F(\varepsilon, \omega') A_F(\varepsilon, \omega + \omega') \times \frac{1}{\omega} [n_F(\omega') - n_F(\omega + \omega')]. \quad (12)$$

Here the sum over momenta in the spectral function  $A_F(\varepsilon_k, \omega)$  of the lattice Green's function has been expressed as an energy integration over  $D(\varepsilon)$ . From the results presented in Fig. 3, we notice that the opening and gradual deepening of the pseudogap, as the temperature is reduced, is associated with a changeover in the dc resistivity  $\sigma(0)^{-1}$  from a linear in  $T$  decrease to an upturn (see the inset). We stress that the linear behavior does not arise from the temperature dependence of the single-particle lifetime  $\Gamma(0)^{-1}$ , which for  $T \gg T^*$  becomes independent on  $T$ , but is exclusively due to an intrinsic non-Fermi liquid behavior even above  $T^*$ . This is also manifest in the

fact that the fermion density of states (DOS) never recovers the unperturbed semicircular shape, however high  $T$  is. As far as the frequency dependence of  $\sigma(\omega)$  is concerned, we observe below  $T^*$  a well defined isosbestic point around which the spectral weight is shifted from low to higher frequencies and at which the various curves for the optical conductivity, corresponding to different  $T$ , cross. This behavior, recently confirmed by optical measurements [15], is in line with our previous results [6] on the optical conductivity in the 1D and 2D BFM.

In conclusion, we have reported in this Letter on a metal-insulator crossover described by the BFM for HTS, driven by strong pair fluctuations and leading up to the opening of a pseudogap in the density of states. The results obtained are similar to those for strongly correlated systems where the pseudogap is due to antiferromagnetic correlations. In order to decide which of the mechanisms is relevant for HTS, a detailed knowledge is required of the  $k$  dependence of this pseudogap in the Brillouin zone, together with the temperature behavior of the incoherent part of the single-particle spectrum. A study for the latter, on the basis of a generalized BFM in the atomic limit, associates it with phonon shakeoff effects, when the bosons are considered as bipolarons [16]. Whatever the mechanism of pairing might be, the present study of the BFM clearly suggests a normal state pseudogap due to uncorrelated pair fluctuations which, upon approaching  $T_c$  from above, will tend to correlate and lead to a true superconducting gap.

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- [1] See, for instance, P.W. Anderson, *The Theory of Superconductivity in the High- $T_c$  Cuprates* (Princeton University Press, Princeton, NJ, 1997).
  - [2] H. Ding *et al.*, Phys. Rev. Lett. **78**, 2628 (1997).
  - [3] Ch. Renner *et al.*, Phys. Rev. Lett. **80**, 3606 (1998).
  - [4] J. Röhler *et al.*, in *High- $T_c$  Superconductivity 1996: Ten years after the discovery*, edited by E. Kaldis *et al.* (Kluwer Academic Publishers, Dordrecht, 1997), p. 469.
  - [5] J. Ranninger, J.-M. Robin, and M. Eschrig, Phys. Rev. Lett. **74**, 4027 (1995); J. Ranninger and J.-M. Robin, Solid State Commun. **98**, 559 (1996).
  - [6] J. Ranninger and J.-M. Robin, Phys. Rev. B **53**, R11961 (1996).
  - [7] H.-C. Ren, Physica C (Amsterdam) (to be published).
  - [8] T. Domanski, J. Ranninger, and J.-M. Robin, Solid State Commun. **105**, 473 (1998).
  - [9] See, for instance, A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
  - [10] P. Lombardo *et al.*, Phys. Rev. B **54**, 5317 (1996).
  - [11] T. Schork and S. Blawid, Phys. Rev. B **56**, 6559 (1997).
  - [12] N.E. Bickers, Rev. Mod. Phys. **59**, 845 (1987).
  - [13] Bumsoo Kyung, e-print cond-mat/9802113.
  - [14] M. Randeria, e-print cond-mat/9710223.
  - [15] T. Timusk (private communication).
  - [16] J. Ranninger and A. Romano, Phys. Rev. Lett. **80**, 5643 (1998).