Manifestations of the pseudogap in the BOSON-FERMION model for Bose-Einstein condensation driven Superconductivity

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Abstract

The normal state behaviour of the density of states of the electrons described by the BOSON - FERMION model for Bose-Einstein condensation driven superconductivity is characterized by the appearance of a pseudogap which develops into a true gap upon lowering the temperature and the superconducting critical temperature is approached. The consequences of this on the temperature dependence of the specific heat, the NMR relaxation rate and the optical conductivity is examined.

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The opening of a pseudogap in the density of states (DOS) of the electrons in the normal state of high $T_c$ superconductors (HTcSC) is one of the characteristic features of these materials [1]. One possible interpretation involves spin fluctuations as the underlying mechanism. This pseudogap is then called the spingap, the discussion of which has given rise to intense work based on the $t - J$ model or the nearly antiferromagnetic Fermi liquid. In this Letter, we want to address an alternative mechanism for this pseudogap in terms of superconducting fluctuations. The existence of such a pseudogap together with the experimental indications that possibly two types of charge carriers (fairly localized ones and itinerant ones) are involved in the high $T_c$ phenomenon [2] supports a scenario of a mixture of intrinsically localized Bosons (tightly bound electron pairs) and itinerant electrons (Fermions). This situation can be described in its simplest form by the so called BOSON - FERMION (BM) model which was first introduced in connection with the many polaron problem in the cross-over regime between adiabatic and non-adiabatic behaviour. In such a scenario [3] bipolarons (Bosons) are envisaged to coexist with quasifree electrons (Fermions) and an exchange coupling between the Bosons and the Fermions is assumed by which Bosons can decay into pairs of itinerant Fermions and vice versa. The physically interesting regime of parameters of this model is that where the superconducting state below a certain critical temperature $T_c$ is controlled by a condensation of the Bosons [4] and thus can in principle lead to rather high values of $T_c$. This happens when the Boson level lies close to the Fermi level of the Fermionic subsystem. Assuming the exchange coupling to be local, we have shown [4] how, upon lowering the temperature, a pseudogap in the DOS of the Fermions gradually opens up - ultimately developing into a true gap below $T_c$. The opening of such a pseudogap is driven by the onset of itinerancy of the intrinsically bare localized Bosons due to a precursor effect of their superfluidity which implies a concomitant onset of strong local pairing of the itinerant Fermions. The increased correlations of the Fermions into Fermion-pairs results in a DOS for single particle excitations which, close to the Fermi level, is drastically diminished and thus leads to the appearance of a pseudogap and single particle excitations which show strong deviations from Fermi liquid behaviour [5]. The underlying BF model on which this behaviour has been studied so far is given by the following Hamiltonian

$$H = (zt - \mu) \sum_{i,\sigma} c_{i\sigma}^+ c_{i\sigma} - t \sum_{<i,j>,\sigma} c_{i\sigma}^+ c_{j\sigma} + (\Delta_B - 2\mu) \sum_i b_i^+ b_i$$
\[ + v \sum_i \left[ b_i^+ c_{i\uparrow} c_{i\uparrow} + c_{i\uparrow}^+ c_{i\downarrow}^+ b_i \right] \]  

(1)

where \( c_{i,\sigma}^{(+)} \) and \( b_i^{(+)} \) refer to the Fermion and Boson annihilation (creation) operators at site \( i \) and \( \sigma \) denotes the spin quantum number. \( t \) represents the bare hopping integral for tight binding electrons, \( \Delta_B \) the energy level for the bare localized Bosons and \( v \) the local Boson-Fermion pair exchange. The chemical potential \( \mu \) is taken to be common to both the Bosons and Fermions such as to ensure charge conservation during the Boson-Fermion exchange.

We have previously evaluated the single particle Boson and Fermion spectral properties for a 1D system within the lowest order fully selfconsistent conserving approximation \[6\] and have shown explicitly the opening of the pseudogap and the destruction of Fermi liquid properties \[5\]. In order to ascertain that these features were indeed unrelated to any physics of one dimensional systems we further considered the case of a 2D square lattice \[7\] and obtained results which are qualitatively analogous the the 1D case thus confirming that the pseudogap in the DOS of the Fermions is an intrinsic feature of the BF model.

It is the purpose of this Letter to demonstrate how this opening of the pseudogap in the DOS of the Fermions and the destruction of the Fermi liquid properties show up in physically accessible thermodynamic (specific heat, compressibility), magnetic (NMR relaxation rate, spin susceptibility) and transport (optical conductivity) properties. We shall use the same approximative scheme as that which served us for the evaluation of the single particle properties previously \[5,7\] and which is based on a fully selfconsistent lowest order evaluation of the thermodynamic potential, given by the closed loop diagram illustrated in Fig.1 and presenting a functional of the full one particle Fermion et Boson Green’s functions. Within such a scheme the one and two particle Green’s functions are derived from this closed loop diagram by standard functional derivatives with respect to an external space-time varying field \[8\] which for our approximation gives rise to the following expressions for the Boson and Fermion selfenergies:

\[
\Sigma_F(k, \omega_n) = -\frac{v^2}{N} \sum_{q, \omega_m} G_F(q - k, \omega_m - \omega_n) G_B(q, \omega_m)
\]

\[
\Sigma_B(q, \omega_m) = \frac{v^2}{N} \sum_{k, \omega_n} G_F(q - k, \omega_m - \omega_n) G_F(k, \omega_n)
\]  

(2)
where $G_B(q, \omega_m) = [i\omega_m - E_0 - \Sigma_B(q, \omega_m)]^{-1}$ and $G_F(k, \omega_n) = [i\omega_n - \epsilon_k - \Sigma_F(k, \omega_n)]^{-1}$ represent the fully selfconsistently determined Fermion and Boson one particle Green’s functions. The selfconsistent set of Eqs.(2) are solved numerically for a square lattice with sizes up to $41 \times 41$ and for a set of Matsubara frequencies $\omega_n$ with $n$ up to 100. This turns out to be enough to cover a wide enough temperature regime in order to track the evolution of the pseudogap in the DOS and its repercussions on the physical quantities which we want to discuss here. For computational reasons we work as usual with the difference between the total Green’s function and its zero order approximation; i.e for $v = 0 \ [8]$. In order to treat the physically most interesting situation of the BF model (where the superconducting phase is essentially due to a Bose condensation of the Bosons) we choose the model parameters such that the Bosonic level lies well inside the Fermion band and the number of Bosons per site $n_B = \sum_i \langle b_i^\dagger b_i \rangle$ is comparable to the number of Fermions per site $n_F = \sum_{i,\sigma} \langle c_i^\dagger c_i \rangle$. For that purpose we choose as representative parameters for our numerical work: $\Delta_B = 0.4$, $v = 0.1$ in units of the bandwidth $8t$ and $n_{tot} = 2n_B + n_F = 1$ per site.

The properties of the one particle spectral functions for the Bosons and Fermions have adequately been dealt with previously and we refer the reader to refs[5,7]. We hence shall not discuss them here in any further detail but rather concentrate on the evaluation of the specific heat, the NMR relaxation rate and the optical conductivity and show to what extent they are influenced by the opening of the pseudogap in the DOS and the breakdown of Fermi liquid properties of the Fermions. We evaluate for that purpose the total free energy $F = E - \mu N_{tot} - TS$ where the inner energy $E = \langle H_0 \rangle + \langle vH_1 \rangle + \mu N_{tot}$ is separated into a component of the uncoupled BF system and into that of Boson-Fermion exchange coupling. $N_{tot} = n_{tot} N$ where $N$ is the total number of sites in the system. The expression for the exchange coupling contribution to $F$ can be obtained directly by evaluating the closed loop diagram (Fig.1) which yields

$$\langle vH_1 \rangle = -\frac{2}{\beta} \sum_{q,\omega_m} \Sigma_B(q, \omega_m) G_B(q, \omega_m)$$

(3)

Inserting the solutions of Eq.2 into the above expression we evaluate $F$ using

$$F = F_0 + \int_0^\beta \frac{d\lambda}{\lambda} \langle \lambda H_1 \rangle$$

(4)

where $F_0$ is the free energy of the non-interacting system, and consecutively derive the
specific heat at constant volume $C_V = (dE/dT)$ and the entropy $S = (E - \mu N_{tot} - F)/T$ \[9\]. As can be seen from the temperature dependence of the DOS of the Fermions at the Fermi level $N(0)$ (see Fig. 2), a pseudogap starts opening up below a certain characteristic temperature $T^*$ which for our choice of parameters is around 0.015. $T^*$ shows up noticeably in the temperature behaviour of $C_V$ where it corresponds to a net upturn of $C_V$ which, with lowering the temperature below $T^*$, increases as $\ln T$. This behaviour can be traced back to the onset of a precursor to superfluidity of the Bosons which acquire coherency i.e. quasi free particle like behaviour with an effective mass which diminishes as the superconducting state is approached \[10\]. $T^*$ is equally visible in the temperature behaviour of the entropy $S$ which at this temperature shows a noticeable deviation from linearity which is observed for higher temperatures and is due to effectively free Fermions. Both the inverse Boson mass and the compressibility show a monotonic increases with decreasing temperature with a cross-over to a much steeper rise below $T^*$. The lowest temperature results for the specific heat, as well as for the Boson correlation function show a critical behaviour with a finite value of $T_C$. We identify this transition, as it should be, as a Kosterlitz-Thouless transition \[10\], since one expects a Bose-Einstein condensation for a 2D system \[11\].

The onset of a pseudogap and a concomitant coherence of the Bosons is also visible in the magnetic response of the system measured by the magnetic susceptibility

$$\chi(q,\omega) = \frac{1}{2\pi i\hbar} \int d\tau e^{i\omega \tau} \Theta(\tau) \langle [S^-(q,\tau), S^+(q,0)] \rangle \tag{5}$$

where $S^+(q,\tau) = c^+_q(\tau)c_q(\tau)$ and $S^-(q,\tau) = (S^+(q,\tau))\dagger$. Due to the Boson-Fermion exchange coupling local magnetic correlations are induced among the bare uncorrelated electrons arising from the singlet character of the Bosons. The onset of the long range superfluid coherence of the Bosons leads to an onset of long range magnetic correlations which can be seen in the static homogeneous susceptibility $S_O = \frac{1}{2\pi} \chi(0,0)$ and the NMR relaxation rate $\frac{1}{T_1} = \frac{k_B T}{2\pi} \sum_q \chi''(q,\omega)/\omega$ where $\chi''(q,\omega) = Im\chi(q,\omega)$. Evaluating the expression Eq.(4) to within lowest order i.e., neglecting vertex corrections but fully taking into account the selfconsistent expressions for the Fermion one particle Green’s function we obtain the results for $(T_1 T)^{-1}$ as a function of temperature as illustrated in Fig.(3). We again notice a drastic changeover of a fairly well represented temperature independent Koringa behaviour for $T > T^*$ to a rapid drop of $1/(T_1 T)$ below $T^*$. Nevertheless even for $T > T^*$
the usual Korringa ratio \((T_1 T)^{-1}/S_0^2\) does turn out not to be temperature independent as it should be expected for free uncorrelated Fermions. On the contrary \((T_1 T)^{-1}/S_0\) is fairly temperature independent for \(T > T^*\) as can be seen from Fig.(3) and tracks the temperature behaviour of \(N(0)\).

As the last manifestation of the pseudogap in the DOS of the Fermions we want to discuss here the optical conductivity which is defined by

\[
\sigma^{\alpha\beta}(\omega) = \text{Im} \frac{1}{i\hbar \omega} \int \frac{d\tau}{2\pi} e^{i\hbar \omega \tau} \Theta(\tau) \langle j^{\alpha}(\tau) j^{\beta}(0) \rangle
\]

where the \(\alpha\)'s component of the total current is given by \(j^{\alpha}(\tau) = i e \sum_{i,\delta} \delta^{\alpha}_{i,\delta} c_{i+\delta \sigma}^{+} (\tau) c_{i\sigma}(\tau)\). \(e\) denotes the charge of the Fermions and \(\delta^{\alpha}\) the \(\alpha\)'s component of the lattice vectors linking nearest neighbor sites. Evaluating the isotropic optical conductivity \(\sigma(\omega) = \frac{1}{3} \sum_{\alpha} \sigma^{\alpha\alpha}(\omega)\) within the lowest order approximation (neglecting vertex corrections but fully taking into account the selfconsistently determined Fermion one particle Green'functions) we obtain the optical conductivity as a function of frequency which for different temperatures is plotted in Fig.(4). In the inset of Fig.(4) we plot the dc conductivity for different temperatures and notice that upon decreasing the temperature one passes at \(T^*\) from a metallic like behaviour to one which has activated semiconducting like behaviour as a result of the opening of the pseudogap below \(T^*\). These features are also present in the optical conductivity which for temperatures below \(T^*\) shows a shift of the oscillator strength from the frequency regime \(\omega \leq \omega^* \simeq 2T^*\) to \(\omega \geq \omega^*\) for \(T \leq T^*\), while for \(T \geq T^*\) a similar shift is observed in the opposite direction. The emptying out of the spectral weight of \(\sigma(\omega)\) for \(\omega \leq \omega^*\) which would show up as a dip in the optical conductivity can only be approached without being reached because of computational difficulties in reaching sufficiently low temperatures.

These manifestations of the pseudogap of the DOS of the Fermions and in particular those seen in the magnetic [12] and transport [13] response functions are very reminiscent of what is observed in the normal state of underdoped \(HTeSC\). Such features have been previously attempted to be interpreted in the framework of the negative \(U\) Hubbard model [14,15]. While both models lead to pseudogaps in the one particle spectrum and give similar results as far as the magnetic response is concerned, the physics of those two models is nevertheless quite different. In the \(U < 0\) Hubbard model electron pair states exist as "fluctuating states" with very short life times for long wavelength excitations and the Fermilquid properties of
the one particle excitations are conserved [15]. The increase in the value of $T_c$, obtained in the intermediary coupling regime, is then due to a strengthening of the Cooperpair correlations rather than to a Bose condensation of electron pairs. In the BF model on the contrary electron pairs with total momentum close to zero are longlived, condense upon lowering the temperature and give rise to deviations from Landau Fermi liquid properties. Those effects on the thermodynamic and transport properties have been studied here and should be noticeably different from those obtained on the basis of the $U < 0$ Hubbard model.
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FIGURES

FIG. 1. Diagram for thermodynamic potential. Solid lines denote the propagators for renormalized Fermion Green’s functions and the wavy line for the fully renormalized Boson Green’s function.

FIG. 2. Specific heat $C_V$, entropy $S$ and density of states at the Fermi level $N(0)$ as a function of temperature. Entropy and specific heat are normalized to their values at $T = 0.1$ and the density of states is normalized to it’s value at $T = 0.02$.

FIG. 3. NMR relaxation rate $1/T_1 T$ and the ratio $1/T_1 T S_0$ (in arbitrary units) as a function of temperature.

FIG. 4. Optical conductivity (in arbitrary units) $\sigma(\omega)$ as a function of frequency (in units of the bandwidth $8t$). Also shown in the inset is the value at $\omega = 0$ as a function of temperature.