The Spin Gap in the Context of the Boson-Fermion Model for High $T_c$ Superconductivity

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Abstract

The issue of the spin gap in the magnetic susceptibility $\chi''(q, \omega)$ in high $T_c$ superconductors is discussed within a scenario of a mixture of localized tightly bound electron pairs in singlet states (bi-polarons) and itinerant electrons. Due to a local exchange between the two species of charge carriers, antiferromagnetic correlations are induced amongst the itinerant electrons in the vicinity of the sites containing the bound electron pairs. As the temperature is lowered these exchange processes become spatially correlated leading to a spin wave-like spectrum in the subsystem of the itinerant electrons. The onset of such coherence is accompanied by the opening of a pseudo gap in the density of states of the electron subsystem whose temperature dependence is reflected in that of $\chi''(q, \omega)$ near $q = (\pi, \pi)$ where a “spin gap” is observed by inelastic neutron scattering and NMR.

keywords: Pseudo gap, Magnetic susceptibility, Neutron scattering.

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The thermodynamic, magnetic and transport properties in underdoped samples of high $T_c$ superconductors (HT$_c$SC) show noticeable deviations from the usual Fermi liquid properties \cite{1} in the normal state phase above the superconducting transition temperature $T_c$ and below a characteristic temperature $T^*$. We have recently suggested \cite{2} that these effects might be due to the opening of a pseudo gap in the density of states (DOS) of the electrons. Numerous experimental studies have led to the conclusion that possibly two types of charge carriers, almost localized ones and itinerant electrons, are involved in those materials \cite{3}, which can be phrased in terms of a simple model where free fermions on a lattice coexist with tightly bound localized electron pairs (such as bi-polarons) —the Boson-Fermion model. As we have shown previously \cite{4, 5}, such tightly bound localized electron pairs acquire itinerancy due to a precursor effect towards superconductivity, as the temperature is lowered and $T_c$ is approached. Such a scenario can potentially lead to very high values of $T_c$ since the superconductivity state is controlled by the Bose-Einstein condensation of the tightly bound electron pairs \cite{6, 7}. The itinerancy of tightly bound electron pairs is achieved by resonating exchange processes between them and pairs of itinerant electrons and leads to the opening of a pseudo gap in the DOS in the subsystem of the itinerant electrons which, close to the Fermi energy, show strong deviations from Fermi liquid behaviour. The signature of this pseudo gap on the specific heat, the optical conductivity and the NMR relaxation rate have been recently studied by us in details \cite{2}. A further eminent effect in the temperature interval $[T_c, T^*]$ involves the magnetic correlations in the electronic subsystem which is the topic of this short note. One of the puzzling features of high $T_c$ compounds which has received considerable attention from experimental as well as theoretical studies is related to the so-called “spin gap” observed in the magnetic susceptibility $\chi''(\mathbf{q}, \omega)$ for the antiferromagnetic wave vector $\mathbf{q} = [\pi, \pi]$ in the metallic CuO$_2$ planes of these materials. Inelastic neutron scattering studies show a gap in the spin wave excitation spectrum at a frequency $E_G$ which opens up as soon as these materials are doped from the insulating into the metallic regime and increases in size upon further doping, until the optimally doped regime is reached \cite{8}. As a function of temperature this “spin gap” is characterized by a transferral of spectral weight from frequencies above $E_G$ to below as the temperature increases from $T_c$ towards $T^*$ without that $E_G$ would noticeably change. Upon increasing the doping further through the so-called optimally doped into the overdoped situation, these spin gap
features in $\chi''(q, \omega)$ rapidly disappear for very small amounts of additional doping. This indicates that a major part of the magnetic correlations have disappeared \[9\] under the influence of this extra minute doping while $T_c$ is hardly at all affected as compared to its value of the optimally doped case. There is experimental evidence that the “spin gap” given by $E_G$ and the pseudo gap controlled by $T^*$ are essentially unrelated, given their contrasting dependence with doping which varies in opposite directions \[8, 10\]. The present consensus is that the value of $E_G$ is essentially determined by band structure \[11, 12\] while the temperature dependence of the spin gap is controlled by $T^*$ which is largely determined by the onset of superconducting phase coherence \[2, 13\]. The closeness of the numerical values of $E_G$ and $T^*$ in the underdoped case may thus be completely fortuitous. From the theoretical side this problem has received attention primarily from scenarios based on the strong electronic correlations of the CuO$_2$ planes in terms of the Hubbard model \[11\], the $t-J$ model \[12\] and the some heuristic antiferromagnetic 2D-Heisenberg model \[14\]. The scenario based on the 2D correlated electron systems \[11, 12\] leads to a “spin gap” which is of kinematic origin, linked to nesting properties of the free electron dispersion. For a standard electron system having a Fermi surface centered around the $\Gamma$ point of the Brillouin zone, $E_G$ for the antiferromagnetic wave vector turns out to be given by $D - 2\mu$ where $D$ denotes the bandwidth and $\mu$ the chemical potential measured from the bottom of the band. The evolution of the Fermi surface in HT$_c$SC as a function of doping is badly understood. The present experimental situation \[15\] suggests that for underdoped samples it consists of small closed ellipsoid like pockets centered roughly around $\left(\pm\frac{\pi}{2}, \pm\frac{\pi}{2}\right)$ while approaching the optimally doped case it changes into a large Fermi surface, roughly given by that of a nearly half-filled quasi free tight binding model on a square lattice. Presently there is no unanimously accepted theoretical interpretation of this behaviour which is certainly linked to the strong correlations as well as charge transfer processes in the CuO$_2$ layers.

The purpose of the present study is to investigate the influence of the pseudo gap in the DOS of the fermionic subsystem upon the “spin gap” features seen by neutron scattering. We shall do this on the basis of the 2D Boson-Fermion mixture scenario for which the appearance of the pseudo gap and its manifestations in a number of physical quantities has been studied
by us before [2]. The Boson-Fermion model is described by the Hamiltonian
\[
H = (z t - \mu) \sum_{i,\sigma} c^+_i c_{i\sigma} - t \sum_{(i \neq j),\sigma} c^+_i c_{j\sigma} + (\Delta_B - 2\mu) \times \sum_i b^+_i b_i + v \sum_i [b^+_i c_{i\uparrow} c_{i\downarrow} + c^+_i c^+_i b_i]
\] (1)
where \(c^{(+)}_{i\sigma}\) refers to the Fermion operators of the itinerant electrons in the metallic CuO\(_2\) planes and \(b^{(+)}_i\) refers to the Boson operators denoting the localized electron pairs in the dielectric layers separating the metallic planes. \(i\) denotes some effective site involving adjacent molecular clusters of the metallic and dielectric planes [10], 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 \(v\). In order to preserve charge conservation we impose a common chemical potential \(\mu\). We have previously evaluated the Fermion and Boson one particle Green’s function [4, 5] within a fully self-consistent lowest order diagramatic formulation amounting to solve the following set of non-linear equations for the Fermion and Bose single particle Green’s function \(G_F(k, \omega_n)\), \(G_B(q, \omega_m)\) together with their corresponding self-energies \(\Sigma_F(k, \omega_n)\), \(\Sigma_B(q, \omega_m)\):
\[
\begin{align*}
G_F(k, \omega_n) &= \frac{i\omega_n - \epsilon_k - \Sigma_F(k, \omega_n)}{\omega_n}, \\
\Sigma_F(k, \omega_n) &= \frac{1}{\beta} \sum_{q,\omega_m} |G_F(-k + q, \omega_m - \omega_n)|^{-1} \times G_B(q, \omega_m), \\
G_B(q, \omega_m) &= \frac{i\omega_m - E_0 - \Sigma_B(q, \omega_m)}{\omega_m}, \\
\Sigma_B(q, \omega_m) &= -\frac{1}{\beta} \sum_{k,\omega_n} |G_F(-k + q, -\omega_n + \omega_m)|^{-1} \times G_F(k, \omega_n).
\end{align*}
\] (2)
where \(E_0 = \Delta_B - 2\mu\), \(\epsilon_k = t(4 - \sum_\delta e^{i\delta}) - \mu\). \(\beta\) denotes \(1/k_BT\) and \(N\) the total number of sites, while \(k\) and \(q\) refer to the wave vectors and \(\omega_n\) and \(\omega_m\) to the Matsubara frequencies of the Fermions and Bosons respectively.

Using the previously numerically determined one particle Fermion Green’s function we now evaluate the magnetic susceptibility
\[
\chi''(q, \omega) = \mu_B^2 \Im G^R(q, \omega)
\]
\[
G^R(q, t) = -\mu_B^2 \frac{\theta(t)}{i\hbar} \langle [S^-(q, t), S^+(q, 0)] \rangle,
\] (3)
where $G^R(q, \omega)$ denotes the Fourier transform of the retarded two-particle Green’s function and

$$S^+(q, t) = \frac{1}{N} \sum_i e^{iqr_i} S^+_i(t)$$  \hspace{1cm} (4)

with $S^+_i = c^+_{i\uparrow} c_{i\downarrow}$ and $(S^+_i)^+ = S^+_i$. Evaluating $G^R(q, \omega)$ to lowest order (neglecting vertex corrections) we obtain:

$$G^R(q, \omega_m) = -\frac{1}{N \beta} \sum_k \sum_{i\omega_n} G_F(k, i\omega_n) G_F(k + q, i\omega_n + i\omega_m)$$  \hspace{1cm} (5)

which in the absence of Boson-Fermion exchange coupling yields the particularly simple form

$$\chi''(q, \omega) = \frac{\pi \mu D}{2N} \sum_k [f(\epsilon_{k+q}) - f(\epsilon_k)] \delta(\omega + \epsilon_k - \epsilon_{k+q})$$  \hspace{1cm} (6)

which for the antiferromagnetic $q$ vector $q_A = [\pi, \pi]$ and $T \to 0$ reduces to

$$\chi''(q_A, \omega) = \frac{\pi}{2} \rho \left(-\frac{\omega}{2} - \mu + \frac{D}{2}\right) \theta(\omega + 2\mu - D)$$  \hspace{1cm} (7)

where $D = 8t$ and $\rho(\omega) = \frac{1}{N} \sum_k \delta(\omega - \epsilon_k)$ is the DOS of the electrons. From Equ. (7) we notice that the “spin gap” occurs at $\omega = D - 2\mu$ which is the same result as that obtained in ref. and based on a $U > 0$ Hubbard model (notice that in ref. the chemical potential is measured from the center of the band rather than from the bottom as in our case). In our previous study of the interacting problem for a 2D system we have studied the evolution of the pseudo gap in the DOS of the single particle spectrum which occurs for $\omega \simeq 0$ showing an increase of spectral weight for $\omega$ slightly above and below $\omega \simeq 0$ in a region of width $2v$. Hence we expect from Equ. (7) a peak in $\chi''(q_A, \omega)$ slightly above the spin gap which grows as $T$ is diminished, while for higher frequencies $\chi''(q_A, \omega)$ is essentially be given by the free DOS $\rho\left(-\frac{\omega}{2} - \mu + \frac{D}{2}\right)$. In Fig. 1 we present the full numerical study of $\chi''(q_A, \omega)$, given by Equ. (7). We notice that as the temperature is lowered the “spin gap” becomes better and better defined with a slope of $\chi''(q_A, \omega)$ at $\omega = E_G \simeq D - 2\mu$ which steadily increases as one approaches $T^*$ and then rapidly saturates as the temperature is further decreased below $T^*$. This behaviour of $\chi''(q_A, \omega)$ coincides with a Korringa type behaviour of $1/T_1 T$ above $T^*$ and a noticeable
deviation from it below \( T^* \), which previously we have attributed to the opening of the pseudo gap in the DOS of the Fermions \[2\]. The appearance of this pseudo gap has been found to be due to a destruction of well defined quasi particles in the vicinity of the Fermi level and the occurrence of a BCS-like spectrum involving several excitation branches \[5\]. As a consequence, similar to a BCS state, coherence effects play a dominant role as the temperature is decreased below \( T^* \) and influence the magnetic susceptibility via the spectral one particle Fermion Green’s functions entering the expression for \( \chi''(q, \omega) \) in Equ. \[5\].

Our study of \( \chi''(q, \omega) \) in the entire Brillouin zone (Fig. 2) showed that apart from the region around the wave vector \( q_A \) there is another domain in \( q \)-space, corresponding to excitations of frequency \( \sim \mu \), where the magnetic response is strongly influenced by coherence effects. This corresponds to wave vector \( q_B \approx [\pm \pi/4, \pm \pi/4] \) where the onset of coherence effects leads to the appearance of two well defined peaks in \( \chi''(q_B, \omega) \) as compared to the case where Boson-two Fermion exchange processes are absent. This is particularly visible in the spectrum of the 1D Boson-Fermion model where our calculations are of better resolution (see Fig. 3). An experimental verification of this prediction of a strong temperature dependence of \( \chi''(q_B, \omega) \) (apart from that already established for \( \chi''(q_A, \omega) \)) would shine new light on the origin of the peculiar spin dynamics of HTc,SC and in particular the two component scenario for HTc,SC.

The Boson-Fermion model discussed here describes a superconducting state controlled by phase rather than amplitude fluctuations with a mean field gap energy of the fermionic subsystem being much bigger than the energy of the phase fluctuations (see the discussion in ref. 7). Thus the Boson-Fermion model might be a reasonably good realization of the underdoped HT,SC which can be considered as doped insulators and which, because of their low doping, have a very low superfluid density of the fermionic subsystem. In such a case phase fluctuations are expected to be determinant for the value of \( T_c \) and the system’s properties near \( T_c \) are then essentially controlled by phase fluctuations \[13\].

Throughout this work we have assumed the following set of parameters \( v = 0.1, \Delta_B = 0.4 \), and \( n_{\text{tot}} = \sum_{i,\sigma} \langle c_{i\sigma}^+ c_{i\sigma} \rangle + 2 \sum_i \langle b_i^+ b_i \rangle = 1 \). This choice corresponds to a small pocket Fermi surface centered around the \( \Gamma \) point and with a \( k_F \sim \pi/3 \) \[3\]. Certainly in order to obtain a more realistic description of the “spin gap” phenomenon, these parameters not only will have to be
modified, but also the Boson-Fermion model itself (Equ. [1]) would have to be generalized by explicitly distinguishing the fermionic sites from the bosonic ones and including correlations amongst the electrons which can yield the set of pockets of Fermi surfaces in fact observed experimentally. The present work, in complete analogy with previous work on this matter and involving electronic and magnetic correlations [11, 12], cannot therefore be expected to provide reliable values for $E_G$ as measured by neutron scattering. It is however expected to correctly describe the temperature variation of $\chi''(q, \omega)$ controlled by the same characteristic temperature $T^*$ at which the pseudo gap in the DOS of the electrons begins to open up and a superconducting phase coherence sets in above $T_c$.

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Figure Captions

**Figure 1**: $\chi''(q_A, \omega)$ as a function of frequency and for different temperatures (both in units of the bandwidth $D$), the steepest slope at $\omega=D-2\mu \sim 0.6$ corresponding to $T = 0.0085$. In the inset we present for comparison the temperature variation of the pseudo gap in the DOS of the Fermions, the doped pseudo gap corresponding to $T = 0.0085$.

**Figure 2**: $\chi''(q, \omega)$ as a function of $q$ over the entire Brillouin zone $q_x = q_y = [0, \pi]$ and $T = 0.0085D$.

**Figure 3**: $\chi''(q, \omega)$ as a function of frequency for $T = 0.001D$ for the 1D Boson-Fermion model and $q_x = q_y = [0, \pi/2]$. 