Breakdown of Landau Fermi liquid properties in the 2D BOSON-FERMION model

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( November 18, 2021)

Abstract

We study the normal state spectral properties of the fermionic excitations in the Boson-Fermion model. The fermionic single particle excitations show a flattening of the dispersion as the Fermi vector $k_F$ is approached from below, forshadowing a Bogoliubov spectrum of a superconducting ground state. The width of the quasiparticle excitations near $k_F$ increases monotonically as the temperature is lowered. In the fermionic distribution function this temperature dependence is manifest in a strong modification of $n(k)$ in a small region below $k_F$, but a nearly $T$ independent $n(k_F)$.

Keywords: A. high $T_C$ superconductors, D. electronic states, E. electron emission spectroscopy
Intense theoretical work and controversy concerning the foundations for a novel non-Fermi liquid metallic ground state has followed the suggestion [1] that in high $T_c$ superconductors the normal state might not behave as a standard Fermi liquid (FL). In attempting to fit the various anomalous thermodynamic and transport properties of these materials, the concept of a marginal FL was proposed [2] in which the imaginary part of the fermionic self-energy is supposed to vary like $|\omega - \epsilon_p|$ rather than like $(\omega - \epsilon_p)^2$ as in an ordinary FL. Apart from this phenomenological approach to non-FL behavior, it is well established that 1D systems show in fact a branch cut spectrum rather than poles for the single particle Green’s function. For interacting Fermion systems such a non-FL behavior for 1D is however not maintained if one goes to $D > 1$ [3].

Since possibly the non-FL properties of the high $T_c$ materials are a prerequisite for the large values of $T_c$ themselves [4] and also since the concept of a non-FL in itself is of fundamental theoretical importance, it is of great interest to study models which exhibit transitions between FL and non-FL behavior as some parameter of the model is varied.

In anticipation of a breakdown of FL behavior for the Anderson impurities lattice model with finite range interaction, the single impurity problem has been studied [5]. When the repulsive interaction is increased beyond a certain threshold a change-over from FL to non-FL is indeed observed due to the coupling to the ensemble of the orbital channels rather than to only the one which hybridizes with the impurity orbital.

There are so far few attempts to study models in which such effects are active in a cooperative fashion and for $D > 1$. Khodel and Shaginyan [6] have recently proposed that a 3D system with long range Coulomb interaction shows a breakdown of FL behavior with the development of a horizontal inflexion point in the one particle excitation spectrum at the Fermi momentum $k_F$. Such a feature leads to a restructuring of the Fermi filling and hence of the Fermi distribution function at $T = 0$ resulting in a finite slope (rather than a jump) at $k_F$. This phenomenon is very reminiscent of what happens in a BCS superconductor with a Bogoliubov like excitation spectrum. It has since been shown [7], that the Khodel-Shaginyan state is an artifact of the Hartree Fock analysis and that it is indeed unstable towards a superconducting ground state. Nevertheless it was recognized [7] that such inherent features like potentially flat portions of the Hartree Fock excitation spectrum should be very sensitive
when including particle–particle scattering. Quasi particle broadening should then become a dominant feature and possibly lead to results which resemble in nothing an ordinary FL.

On the basis of a detailed analyses of the anomalous lattice properties of high $T_C$ materials we have recently attempted to argue for the applicability of the Boson-Fermion model to high $T_C$ superconductivity [8]. As we shall see in this letter, a detailed analysis of this model shows features which were recognized as potential ingredients for the breakdown of FL behavior [7] in connection with the study of the Khodel-Shaginyan model. The Boson-Fermion model was initially introduced by one of us [9] in order to provide a heuristic description of intermediate coupling electron-phonon systems and to study the resulting superconducting properties. This model was then extensively studied (although in a slightly generalized form) in connection with high $T_C$ superconductors, in the superconducting state [10]. It is therefore compelling to examine its normal state properties and to compare them to the experimentally established anomalous properties – which are the real testing grounds for any theory of high $T_C$ superconductivity.

The Boson-Fermion model describes systems with both localized Bosons with charge $2e$ and itinerant Fermions with charge $e$ on a lattice. An exchange of a Boson with two Fermions with opposite spins is assumed and the conservation of charge requires a common chemical potential for the two species of charge carries. This model exhibits a superconducting ground state with a BCS like gap in the Fermion excitation spectrum [8] and collective excitations of the Bosons. What is new in this model as compared to a standard BCS systems is, that well above $T_C$ a pseudo-gap in the density of states develops which ultimately is expected to open up into a true gap at the critical temperature $T_C$. It is this regime of temperature above $T_C$ which is of interest to us here and where clear non-FL properties manifest themselves.

In this letter we shall study the Boson-Fermion model

$$H = (zt - \mu) \sum_{i,\sigma} c_{i\sigma}^+ c_{i\sigma} - t \sum_{<i\neq j>,\sigma} c_{i\sigma}^+ c_{j\sigma} + (\Delta_B - 2\mu) \sum_i b_i^+ b_i$$

$$+ v \sum_i [b_i^+ c_{i\uparrow} c_{i\downarrow} + c_{i\uparrow}^+ c_{i\downarrow}^+ b_i]$$

(1)

for a square lattice. $t$ denotes the electron hopping integral, $z$ the number of nearest neighbors, $\Delta_B$ the atomic level of the Bosons (bi-polarons) and $v$ the strength of the Boson-Fermion exchange coupling. The commutation relations for the Fermion and Boson operator
are given by \( \{c_{i\sigma}, c_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'} \) and \([b_i, b_j^+]=\delta_{ij}\) respectively. We evaluate the excitation spectrum of the Fermions in the normal state in a fully self consistent way \([11]\) to second order in the exchange interaction. The expressions for the self energies for Fermions and Bosons are:

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

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

This leads to the set of equations for the Fermion and Boson Green’s functions

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

\[
G_B(q, \omega_m) = [i\omega_m - E_0 - \Sigma_B(q, \omega_m)]^{-1}
\]

which are determined selfconsistently, together with the expressions for the self-energies, Equ.(2). \(k\) and \(q\) denote the momenta, \(\omega_n\) and \(\omega_m\) the Matsubara frequencies for Fermions and Bosons respectively and \(N\) the number of sites.

The unperturbed Fermion dispersion including the chemical potential is given by \(\epsilon_k = \xi_k - \mu\), \(\xi_k = t(z - \sum_{\delta} e^{ik\cdot\delta})\), with \(\delta\) denoting the vectors linking nearest neighbor lattice site. The unperturbed Boson energies are given by \(E_0 = \Delta_B - 2\mu\); the factor two in front of the chemical potential taking account that each Boson is constituted of two Fermions.

The self-consistent coupled equations (2, 3) are solved by an iterative procedure in which \(G_F(k, \omega_n)\) and \(G_B(q, \omega_m)\) are evaluated for a set of Matsubara frequencies \(\omega_n = 2\pi k_B T(n+\frac{1}{2})\) for \(-100 < n < +99\) and \(\omega_m = 2\pi k_B Tm\) for \(-100 < m < +100\). As usual we compute the difference between the full and bare Green’s functions, so that only a small number of Matsubara frequencies is necessary. We restrict ourselves in the present study to summing the \(k\) and \(q\) vectors over a two-dimensional Brillouin zone with a set of \(41 \times 41\) equally spaced vectors for the Bosons as well as the Fermions. Convergence of the iterative solutions of these self-consistent equations is obtained relatively fast for temperatures down to \(T = 0.0085\) in units of the Fermionic band width \(8t\). The solutions for the Fermion and Boson Green’s functions in terms of the Matsubara frequencies are then analytically continued to the real
frequencies axis and into the lower half plane using a standard Padé approximants procedure in order to obtain the poles of the retarded Green’s functions and hence the excitation spectra for the Fermions and Bosons.

In Fig. (1) we plot the Fermion spectral function $A_F(k, \omega) = -2Im G_F(k, i\omega_n = \omega + i0^+)$ as a function of Fermion momentum $k$ which clearly shows how the spectral weight is split and redistributed in the region near $k_F$; $k_F$ being defined by $\Sigma_F(k_F, 0) + \epsilon_{k_F} = 0$. This behavior manifests itself in the Fermionic density of states $\rho_F(\omega)$ in form of the appearance of a pseudo-gap which deepens with decreasing temperature (Fig. 1). Throughout the present work we assume as parameters: $\Delta_B = 0.4$ and $v = 0.1$ in terms of the bandwidth. $v$ is chosen in such way that for realistic temperatures (a few hundred degrees Kelvin) we can expect noticeable effects due to the Boson-Fermion exchange coupling. The total average number of particles per site, $n_{tot} = n_F + 2n_B = \frac{1}{N} \sum_{k, \sigma} < c_{k, \sigma}^\dagger c_{k, \sigma} > + \frac{2}{N} \sum_q < b_q^\dagger b_q >$, Bosons and Fermions included, is taken to be unity.

The spectral functions of the Fermionic single particle excitations near $k_F$ have not a simple Lorentzian behavior and are best described by the continued fraction Padé approximants for $G_F(k, \omega)$. For practically all $k$ vectors around $k_F$, one obtains essentially three poles whose spectral weight adds up to essentially unity. These three poles are given by a cosine like dispersion – indicative of the unrenormalized Fermion excitation spectrum $\epsilon_k$ – and two flat dispersionless branches separated by an energy equivalent to $\mu$. Solving the Hamiltonian, Equ.(1) in the atomic limit ($t \to 0$ and $\Delta_B < 0$) we find that for states containing two charge carriers per site there are two distinct eigenstates having energy $\epsilon_\pm = \Delta_B/2 \pm \sqrt{(\Delta_B/2)^2 + v^2 - 2\mu}$, $\epsilon_+ \sim 0$ corresponds to a state where the charge carriers exist predominantly in form of on site bosons – a bonding state –, $\epsilon_- \sim -2\mu \sim |\Delta_B|$ corresponds to a state where the charge carriers exist predominantly in form of two uncorrelated fermions – an antibonding state.

The real ($\omega_k$) and imaginary ($-\gamma_k/2$) part of these poles are presented in Fig.(2.a, b) and the modulus of their residues is given in Fig.(2.c) as a function of Fermion momentum. The residues are in general complex numbers whose imaginary part is biggest for the modes with largest damping $\gamma_k$. Complex residues in general indicate strong interference between poles, meaning that the single particle excitations are no longer described by a
simple pole of the Green’s function as in a classical FL. In the description of deviations from FL properties the frequency dependence of the imaginary part of the Fermion self-energy, \( \Gamma(k, \omega) = -2m \Sigma_F(k, i\omega_n = \omega + i0^+) \), is of capital importance. For a classical FL we have \( \Gamma(k, \omega) \sim aT^2 + b(\omega - \mu)^2 \). In the Boson-Fermion model the deviations from such a FL behavior are significant as can be seen from Fig.(3) where we plot \( \Gamma(k_F, \omega) \) for various temperatures. As in a FL, \( \Gamma(k, \omega) \) turns out to be very weakly dependent on \( k \). \( \Gamma(k_F, \omega) \) at finite temperature has a minimum which occurs for slightly negative frequencies. The reasons for that are at present not understood. As the temperature decreases this minimum shifts towards \( \omega = 0 \) but \( \Gamma(k_F, 0) \sim T^{-\alpha} \) increases with decreasing temperature (with \( \alpha = 0.086 \) for 2D and \( \alpha = 0.60 \) for 1D) which is exactly the opposite of what occurs in a standard FL. All these manifestly non-FL properties of the Boson-Fermion model show up in the Fermion distribution function \( n(k) \) only in a relatively minor fashion. \( n(k) \) turns out to be practically \( T \) independent at \( k_F \), (all lines of \( n(k, T) \) cross within a very small regime around \( k_F \)) but increases substantially with decreasing temperature for \( k \) just below \( k_F \).

The breakdown of FL properties characterized by the disappearance of well defined quasiparticles near the Fermi energy is found to go hand in hand with the appearance of well defined itinerant excitations of the intrinsically (bare) localized Bosons due to a precursor to superfluidity. Such a precursor induced coherence of intrinsically localized Bosons has recently been studied by us \[12\] on the basis of the 1D Boson-Fermion model.

As the temperature is decreased the low \( q \) vector excitations, manifest in the poles of \( G_B(q, \omega) \), acquire the spectrum \( \omega_B^q = \hbar^2 q^2 / 2m_B(T) \) with a temperature dependent mass which decreases upon decreasing the temperature. We estimate the decrease of \( m_B(T) \) to be given by \( m_B = 24.2, 25.7, 51.3 \) and 195.6 for \( T = 0.0085, 0.01, 0.02 \) and 0.05.

The present analysis of the Boson-Fermion model shows that for 1D as well as for 2D the FL properties are totally destroyed. This is due to strong superconducting fluctuations setting in well above \( T_C \) as can be seen from the pair correlation function – essentially determined by the Bose Green’s function \( G_B(q, \omega) \) – which has perfect Lorentzian line shape well above \( T_C \). From the static part of \( G_B(q, \omega) \) we can estimate the coherence length, determined by \( < b_q^+ b_q > \approx a(1 + \xi^2 q^2)^{-1} \) which varies as \( \xi \sim (T - T_C)^{-\nu} \) (with \( \nu \approx 1.25 \) and \( T_C \approx 0 \) for 2D and \( \nu \approx 1.1 \) and \( T_C \approx 0 \) for 1D. The precursor effects of the
onset of joint superfluidity of the Bosons and superconductivity of the Fermions can also be seen in how the Hugenholtz-Pines theorem \( (G_B^{-1}(\mathbf{q} = 0, \omega = 0) = 0 \) at \( T_C \) \) is approached \( i.e. \)
\[ E_0 + \Sigma_B(0, 0) \simeq (T - T_C)^{-\alpha} \] with \( \alpha \simeq 2.7 \) for 2D and \( \alpha \simeq 2.4 \) for 1D. These precursor effects forshadow a Bogoliubov like spectrum in which flat portions of the Fermionic excitations spectrum appear near \( k_F \) which however are heavily overdamped. As a consequence, a pseudo-gap in the Fermion density of states begins to open up well above \( T_C \). It gradually deepens and is expected to become a true gap at \( T_C \). At present our numerical analyses of the normal state does not permit to prove this but our previously mean field results \([13]\) as well as preliminary RPA results for the superconducting state suggest such a behavior.

The fully selfconsistent scheme employed in the present study corresponds to the simplest approximation in such a treatment. We believe nevertheless that the results obtained here should be qualitatively correct since vertex corrections to the selfenergies are of order \( v^4 \) smaller than the selfenergies taken into account here. Moreover the Hugenholtz-Pines theorem in the limit \( T \to T_C \) is fulfilled, satisfying the selfconsistent equation
\[ E_0 - \Sigma_B(\mathbf{q} = 0, \omega = 0) = 0 \] for \( T = T_C = 0 \).

At this points the Boson-Fermion model should be compared with the negative \( U < 0 \) Hubbard model for which a two particle resonant state appears inside the two particle continuum. Contrary to the Boson-Fermion model, these Bosonic states are however heavily overdamped in the \( U < 0 \) Hubbard model \([14]\) and thus are not expected to control the superconducting state via their Bose Einstein condensation. The absence of well defined bosonic excitations does not cause single Fermion excitations to become overdamped and the \( U < 0 \) Hubbard model, in spite of many similarities with the Boson-Fermion model thus remains a standard FL in the intermediate coupling regime \( i.e. \) \( U \simeq 4t \) \([14]\).

Concerning the applicability of the Boson-Fermion model to high \( T_C \) superconductors, it shows at least one predominant feature which a series of experiments suggest; namely the existence of a pseudo gap and non-FL behavior in the normal state. NMR, Knight shift, susceptibility measurements, optical conductivity, specific heat, etc \([15]\) all suggest such a pseudo-gap in the underdoped samples. The behavior of the width of the fermionic spectral function, measured by photo-emission, favors however more the picture of a marginal FL than a completely destroyed one as discussed in this letter. In this connection we should
however remember that the Boson-Fermion model examined here is the prototype of this model which does not take into account any details of the cristallin lattice and electronic structure of real materials. Further work on this matter, also including shortrange spin correlations in the Fermionic subsystem, will eventually elucidate these questions.

ACKNOWLEDGMENTS

We thank K. Matho and T. Kostyrko for valuable conversations.
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FIGURES

FIG. 1. Density of states and the spectral functions of the electrons for a set of $k$ vectors, $k = k_x = k_y = \frac{2\pi}{41} \times [0...11]$. The results for additional equidistant $k$ vectors was obtained by an interpolation of the selfenergy. In the inset we show the deepening of the pseudo-gap, centered at energy 0, as the temperature decreases, for three characteristic temperatures.

FIG. 2. a) The real part of the poles of the Fermion Green’s function $G_F(k, \omega)$ for $k$ vectors along the diagonal of the Brilloin zone $k = k_x = k_y = \frac{2\pi}{41} \times [0...20]$. b) The imaginary part divided by the real part of the poles of $G_F(k, \omega)$. c) The modulus of the residues of the poles of $G_F(k, \omega)$

FIG. 3. The imaginary part of the electron self-energy for $k_x = k_y = k_F$ for various temperatures. $\Gamma(k_F, 0)$ increases with decreasing temperature.