Bogoliubov shadow bands in the normal state of superconducting systems with strong pair fluctuations

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On the basis of a scenario where electron pairing is induced by resonant two-particle scattering (the Boson Fermion model), we show how precursors of the superconducting state - in form of overdamped Bogoliubov modes - emerge in the normal state upon approaching the transition temperature from above. This result is obtained by a renormalization technique based on continuous unitary transformations (the flow equations), projecting out the coherent contributions in the electron spectral function from an incoherent background.

PACS numbers: 03.75.Gg, 03.75.Ss, 67.20.+k, 74.20.Mn

The discovery of high temperature superconductivity (HTS) and the enormous theoretical effort following this discovery has led to reconsider the whole issue of superconductivity and to put it into a more general and broader perspective than that of the familiar BCS scenario. It became clear early on that in these new superconductors one is confronted with a situation between that of classical Cooper pairing (controlled by the amplitude of the order parameter) and that of a superfluid phase of tightly bound electron pairs (controlled by the phase fluctuation). The theoretical issue is to understand the interplay between the two, which amounts to fully taking into account the interaction between single electron states and electron pair fluctuations. A particularly clear presentation of this problematic was given by Tchernyshyov \cite{1}, who introduced an effective amplitude for electron pairs in the normal state by including in the propagator of an electron a process involving the simultaneous propagation of a hole together with a Cooperon. This leads to the emergence of two-electron resonant states (long lived pair fluctuations) inside the Fermi sea, manifest in form of a pseudogap - a precursor of the superconducting gap in the normal state.

The phenomenon of superconducting correlations building up above $T_c$ - the onset temperature of superconductivity - is by no means restricted to the HTS. It is encountered in a great variety of physical systems, where resonance pairing of fermionic quasi particle plays a key role and which can be discussed on the basis of the phenomenological Boson Fermion model (BFM). This model describes the formation of resonance bound Fermion-pairs inside the Fermi sea of uncorrelated Fermions. The resonant bound states are monitored by an exchange interaction with localized Bosons (tightly bound Fermion pairs, the specific origin of which will be of no importance for the present study). Realizations of such physics are be found in: i) electron-phonon coupled systems in the intermediary coupling limit (see for instance ref.\cite{2} for which this BFM was devised initially) describing an exchange interaction between localized bipolarons and itinerant electrons, ii) the positive U Hubbard model\cite{3} describing an exchange interaction between spinon singlets of RVB electron pairs and holons, iii) low density nuclear matter with isospin singlet pairing\cite{4} and iv) the Feshbach resonance in atomic physics\cite{5,6} invoked for tuning a quasi-bound state of atoms through a threshold resulting in a resonance superfluidity in traps\cite{7,8}, and which involves entanglements of atoms in squeezed states\cite{9}.

A salient feature of this BFM is the appearance of a pseudogap in the normal state single Fermion density of states when decreasing the temperature below a certain value $T^*$. Accompanied with this is a qualitative change in the transport: going from single Fermion transport above $T^*$ (describing a relatively good metal) to one involving well defined itinerant bosonic charge carriers (describing a bosonic metal coexisting with a poor fermionic metal\cite{10,11}). Below a certain critical temperature $T_c$, the itinerant Bosons together with finite momentum Cooperons, induced in the fermionic subsystem, end up in a phase correlated superfluid state. One hence should not only expect a pseudogap in the Fermionic density of states as a precursor to the superconducting phase, but also corresponding modifications of the sizable incoherent component of the Fermionic spectral functions, which characterizes the pseudogap phase in the temperature interval [$T_c$, $T^*$], to evolve into damped, but nevertheless clearly discernible, Bogoliubov modes as one approaches $T_c$. The feasibility of such a scenario will be the issue of the present study.

Applying a flow equation renormalization technique to the BFM permits us to construct renormalized Fermionic operators which posses features of potentially containing residues of Bogoliubov type modes in the normal state. The essence of this technique consists in devising an infinite series of continuous unitary transformations\cite{12,13} for the Hamiltonian, such as $H(l) = e^{S(l)} He^{-S(l)}$, where $l$ denotes the continuous flow parameter. Imposing a constraint structure on the renormalized Hamiltonian defines renormalization equations for the parameters of this Hamiltonian which are devised in such a way that the ex-
change interaction between the Bosons and the Fermions is renormalized to zero giving rise to decoupled systems of Bosons and itinerant Fermions, whose parameters however have been rendered interdependent in the course of such a renormalization procedure. In the momentum representation this Hamiltonian consists of two parts $H(l) = H_0(l) + H_{int}(l)$ and has the following structure in the l-th step of this continuous transformation

$$H_0(l) = \sum_{k, \sigma} (\varepsilon_k(l) - \mu) c_{k, \sigma}^\dagger c_{k, \sigma} + \sum_q (E_q(l) - 2\mu) b_q^\dagger b_q + \frac{1}{N} \sum_{k, p, q} U_{k, p, q}(l) c_{k, \uparrow}^\dagger c_{p, \downarrow}^\dagger c_{k, \downarrow} c_{p, \uparrow}$$

$$H_{int}(l) = \frac{1}{\sqrt{N}} \sum_{k, p} v_{k, p}(l) \left( b_{p+k}^\dagger c_{k, \uparrow} c_{p, \uparrow} + \text{h.c.} \right).$$

$c_{k, \sigma}^\dagger$ refer to annihilation (creation) operators for the itinerant Fermions with the energy $\varepsilon_k(l)$ and $b_q^\dagger$ ($b_q$) denote boson operators representing bound Fermion pairs with energy $E_q(l) - 2\mu$. The Boson-Fermion exchange coupling is denoted by $v_{k, p}(l)$ and the interaction between Fermions by $U_{k, p, q}(l)$. For $l = 0$ these parameters reduce to the bare quantities $\varepsilon_k - \mu$, $\Delta B - 2\mu$, $v$ and 0 respectively, which characterize the initial Hamiltonian.

In some recent work we investigated the structure of the final renormalized Hamiltonian. Its resulting energy spectrum and single Fermion density of states showed the opening up of a pseudogap below a certain $T^*$ of the order of $v$. We here shall investigate the spectral function of these Fermions and how it changes as we go from the pseudogap phase $[T_c, T^*]$ into the superconducting one below $T_c$. We propose for that purpose a flow equation for evaluating correlation functions within such a flow equation technique, which closely follows the standard procedure for renormalizing the Hamiltonian, determined by the differential equation:

$$dH(l)/dl = [\eta(l), H(l)],$$

and subject to the initial condition $H(0)$, presenting the original Hamiltonian. A suitably generating operator

$$\eta(l) = -\frac{1}{\sqrt{N}} \sum_{k, p} \alpha_{k, p}(l) \left( b_{p+k}^\dagger c_{k, \uparrow} c_{p, \uparrow} + \text{h.c.} \right)$$

where $\alpha_{k, p}(l) = (\varepsilon_p(l) + \varepsilon_p(l) - E_{k+p}(l)) v_{k, p}(l)$ is chosen in such a way that $\lim_{l \to \infty} H_{int}(l) = 0$. This leads to a set of differential equations (given by eqs. (16-21) in Ref. [14]) which determines the evolution of the $l$ dependent parameters of the Hamiltonian. For consistency reasons, a flow equation procedure for an arbitrary operator $O(l)$ ought to be controlled by a formally equivalent equation of that defining the evolution of the Hamiltonian, i.e., eq. 3 where $H(l)$ is replaced by $O(l)$. This leads to a flow parameter dependent parameterization of the various operators for which we impose (similar to the procedure for deriving a renormalized Hamiltonian) the following constraint structure for the fermion operators:

$$\left( \begin{array}{c} c_{k, \uparrow}(l) \\ c_{k, \downarrow}(l) \end{array} \right) = \left( \begin{array}{cc} \mathcal{P}_k(l) & \mathcal{R}_k(l) \\ -\mathcal{R}_k^*(l) & \mathcal{P}_k(l) \end{array} \right) \left( \begin{array}{c} c_{k, \uparrow}^\dagger(l) \\ c_{k, \downarrow}^\dagger(l) \end{array} \right) + \frac{1}{\sqrt{N}} \sum_{q \neq 0} \left( \begin{array}{c} p_{k, q}(l) \\ r_{k, q}(l) \end{array} \right) \mathcal{P}_k(l) \left( \begin{array}{c} b_q^\dagger c_{k, \uparrow}^{\dagger} \\ -b_q^\dagger c_{k, \downarrow}^{\dagger} \end{array} \right)$$

which generalizes the standard Bogoliubov transformation in two ways: (a) the initial particle and hole operators are transformed into Bogoliubov modes in a continuous way, (b) the correlated motion involving Fermion holes and Cooperons is taken into account via the terms proportional to $p_{k, q}(l)$ and $r_{k, q}(l)$.

These flow dependent parameters are then determined by the following set of differential equations:

$$\frac{d\mathcal{P}_k(l)}{dl} = \sqrt{\alpha_{k, k}^\dagger(l)} \mathcal{R}_k(l)$$

$$\frac{d\mathcal{R}_k(l)}{dl} = -\sqrt{\alpha_{k, k}^\dagger(l)} \mathcal{P}_k(l)$$

$$\frac{dp_{k, q}(l)}{dl} = \alpha_{k, k}^\dagger(l) \mathcal{R}_k(l)$$

$$\frac{dr_{k, q}(l)}{dl} = -\alpha_{k, k}^\dagger(l) \mathcal{P}_k(l)$$

with the initial conditions $\mathcal{P}_k(0) = 1$, $\mathcal{R}_k(0) = 0$, $p_{k, q}(0) = 0$, $r_{k, q}(0) = 0$, $n_{\text{cond}}^B$ denotes the fraction of the condensed bosons and $n_{\text{cond}}^B \equiv \langle b_q^\dagger b_q \rangle = \langle \exp(\tilde{E}_q/k_B T) - 1 \rangle^{-1}$ the distribution of the finite momentum ($q \neq 0$) bosons. This set of equations has to be solved in conjunction with those (eqs 16-21 in ref. 14) determining the evolution of the various parameters entering the Hamiltonian ($\varepsilon_k(l)$, $E_q(l)$ and $U_{k, p, q}(l)$) being linked together via the expression for $\alpha_{k, p}(l)$. The above flow equations satisfy the sum rule

$$1 = |\mathcal{P}_k(l)|^2 + \frac{1}{N} \sum_{q \neq 0} (n_{q}^B + n_{q+k}^F) |p_{k, q}(l)|^2$$

relating the weights of the various coherent and incoherent contributions to the spectral function. With these definitions, the single Fermion spectral function becomes

$$A^F(k, \omega) = |\mathcal{P}_k(\infty)|^2 \delta(\omega - \tilde{\varepsilon}_k) + |\mathcal{R}_k(\infty)|^2 \delta(\omega + \tilde{\varepsilon}_k)$$

$$+ \frac{1}{N} \sum_{q \neq 0} (n_{q}^B + n_{q+k}^F) |p_{k, q}(\infty)|^2 \delta(\omega + \tilde{E}_q - \tilde{\varepsilon}_{q+k})$$

$$+ \frac{1}{N} \sum_{q \neq 0} (n_{q}^B + n_{q-k}^F) |r_{k, q}(\infty)|^2 \delta(\omega - \tilde{E}_q + \tilde{\varepsilon}_{q-k})$$

(11)
which is composed of a coherent part \( A_{coh}^F(k, \omega) \), represented by a \( \delta \)-function like peak, and a remaining incoherent background \( A_{inc}^F(k) \), given by the last two terms in eq. (11). \( \tilde{\varepsilon}_k \) and \( E_\mathbf{q} \) refer to the end results of the renormalization procedure \( (l = \infty) \) for the Fermion and, respectively, Boson spectra. We now analyze the structure of (11) for different characteristic temperature regimes: \( T > T^* \), the pseudogap regime \( [T_s, T^*] \) and the superconducting regime \( T < T_c \).

In the normal phase we have \( n_{cond}^B = 0 \), which implies \( R_k(l) = p_{k, \mathbf{q}}(l) = 0 \) for any \( l \) and hence

\[
\begin{align*}
A_{coh}^F(k, \omega) & = |P_k(\infty)|^2 \delta(\omega - \tilde{\varepsilon}_k) \\
A_{inc}^F(k, \omega) & = \frac{1}{N} \sum_{\mathbf{q} \neq 0} (n_{\mathbf{q}}^B + n_{\mathbf{q}-k}^B) |r_{k, \mathbf{q}}(\infty)|^2 \times \delta(\omega - E_\mathbf{q} + \tilde{\varepsilon}_{\mathbf{q}-k})
\end{align*}
\]

for the coherent and incoherent contributions to the Fermion spectral function. As discussed in ref. [14], for temperatures above a certain \( T^* \) the Fermion dispersion is essentially unrenormalized and given by exclusively \( A_{coh}^F(k, \omega) \) with \( \mathcal{P}_k \simeq 1 \). Below \( T^* \), on the contrary, the Fermion renormalization is becoming increasingly important and gives rise to the opening of a pseudogap in the single particle density of states with a spectral weight becoming smaller than unity and a consequent redistribution of this lacking spectral weight into an incoherent part given by \( A_{inc}^F(k, \omega) \). The fully selfconsistent solutions to this problem by numerical means are presented in Fig. 1. Throughout this work we take as energy unit the Fermion bandwidth \( 2\pi \), \( z \) denoting the coordination number and the initial parameters \( \Delta_B = -0.6 \) and \( \nu = 0.1 \). We, moreover, choose the total particle concentration \( n_{tot} = n^F + 2n^B = 1.0 \). Since we are interested here only in the qualitative aspects of the underlying physics and since the physics in the normal state is controlled by very local correlations and hence little dependent on the dimensionality, we can approximate the various integrals in this temperature regime by their sum over a 1D Brillouin zone with 2000 wavevectors, \( k_n = n \frac{\pi}{a} \) \( (n \leq 1000) \) as long as we don’t get too close to \( T_c \).

In the superconducting phase, from inspection of eq. (11), we notice the appearance of two contributions to the coherent part of the spectral function with spectral weights \( \mathcal{P}_k(\infty)^2 \) and \( R_k(\infty)^2 \), with a total weight \( \mathcal{P}_k(\infty)^2 + R_k(\infty)^2 \) amounting to less than unity because of the sum rule, Eq. (10). Well below \( T_c \), the quasi particle energies are given by \( \tilde{\varepsilon}_k = \text{sgn}(\varepsilon_k - \mu) \sqrt{\varepsilon_k - \mu}^2 + v^2 n_{cond} \) and present the standard Bogoliubov modes which follow from a straightforward well field analysis of this BFM. The characteristic features of the Fermion spectral function in the superconducting phase can be assessed from their zero temperature limit. There, \( n_{\mathbf{q}}^B = 0 \) for any \( \mathbf{q} \neq 0 \) and the

![FIG. 1: The single particle fermion spectral function \( A^F(k, \omega) \) decomposed into its coherent (thick bars whose height indicate the intensity of the delta like contributions) and incoherent (thin lines) components.](image-url)
Fermion distribution function reduces to a step function $n_{k\sigma}^F = \theta(-\tilde{\varepsilon}_k)$. Hence,

$$A_{inc}^F(k,\omega) = \frac{1}{N} \sum_{q\neq 0} \left[ |p_{k,q}(\infty)|^2 \delta(\omega + \tilde{E}_q - \tilde{\varepsilon}_{q-k}) \theta(-\tilde{\varepsilon}_{k-q}) + |r_{k,q}(\infty)|^2 \delta(\omega - \tilde{E}_q + \tilde{\varepsilon}_{q+k}) \theta(-\tilde{\varepsilon}_{q+k}) \right] \quad (14)$$

In the spirit of the qualitative study, presented here, the sum over the wave vectors $q \neq 0$ in this expression for $A_{inc}^F(k,\omega)$ can again be safely approximated by a sum over a 1D Brillouin zone.

In Figs. 1a-1d we illustrate the evolution with temperature $T$ of the coherent (the $\delta$-function like peaks) and the incoherent components (the broad hump like features) of the Fermion spectral function in the relevant wave vector regime around $k_F$ where qualitative changes are manifest. In the high temperature regime ($T > T^*$, Fig. 1a) the single Fermion spectrum is practically unrenormalized, but is constraint to the minimum of a broad “high temperature incoherent contribution” which is visible for energies above as well as below this coherent contribution. As we go, upon lowering $T$, into the pseudogap phase ($T_c < T < T^*$, Figs. 1b, and 1c), an additional “low temperature incoherent component” emerges, having a dispersion opposite to that of the “high temperature incoherent contribution”. That latter remains practically unchanged all the way down in temperature, and right into the superconducting phase. The “low temperature incoherent component”, on the contrary, noticeably narrows upon decreasing $T$, and eventually strongly modifies the behavior of the coherent component, foreshadowing Bogoliubov modes of the superconducting phase. The spectral shape of this low temperature incoherent component” becomes increasingly better defined, as we approach the superconducting phase. Below the pseudogap it shows a dispersion which bends downwards for increasing wavectors above $k_F$. Above the pseudogap this dispersion of the shadow Bogoliubov mode bends upwards for decreasing wavectors below $k_F$. These features are clearly apparent from a comparison of Fig. 1c with Fig. 1d for the superconducting phase at $T = 0$. In Fig. 1d the standard well defined Bogoliubov modes are clearly visible.

In order to highlight this emergence of the Bogoliubov modes out of the incoherent contribution of the Fermion spectral function in the normal state we illustrate in Fig. 2 the Fermion spectral function at $k_F$ for different temperatures. We notice the gradual narrowing of this low temperature incoherent contribution to this spectral function as we approach the superconducting phase upon lowering the temperature, with peak positions practically being independent on temperature.

In conclusion, we have shown that in systems with precursor pairing, such as given by the Boson Fermion scenario, we can expect rather well defined remnants of the Bogoliubov modes in the normal phase in a restricted regime above $T_c$. These modes eventually broaden into intrinsically incoherent contributions of the spectral function as the temperature increases and approaches $T^*$ where resonance pairing of the Fermions ceases. Experimental verification of such shadow Bogoliubov bands in the high HTS would be decisive in determining whether the pseudogap and the superconducting gap in these materials are of common nature or not. In the present calculation we neglected the effect coming from the two-body interaction $U_{k,p,q}(\infty)$ whose magnitude is small and of the order $\propto v^2$. Nevertheless in the pseudogap frequency regime this interaction would lead to a shifting away of the quasiparticle peaks from this frequency region (and hence reinforce the pseudogap features qualitatively) and simultaneously lead to a broadening of the delta peak structure of the coherent contributions of order of the Cooperons bandwidth $\propto v^2$. This will be discussed in detail in some future study.

FIG. 2: Evolution with temperature of the Fermion spectral function $A^F(k_F,\omega)$ at $k_F$ in the vicinity of the Fermi energy. The spectral weights of the $\delta$-function like peaks (corresponding to the coherent components sitting on top of the incoherent ones) are indicated by squares, circles and triangles.

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