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THE PSEUDOGAP PHENOMENON IN HIGH-T_c SUPERCONDUCTORS

J. RANNINGER[a] AND A. ROMANO[b]

[a]Centre de Recherches sur les Très Basses Températures
Laboratoire Associé à l'Université Joseph Fourier
Centre National de la Recherche Scientifique, B.P. 166, 38042, Grenoble Cédex 9, France
[b]Dipartimento di Scienze Fisiche "E.R. Caianiello", Università di Salerno
Unità I.N.F.M. di Salerno, 84081 Baronissi (Salerno), Italy

We review the possible mechanisms leading up to the phenomenon of a pseudogap which characterizes the normal-state properties of high-T_c superconductors. We suggest that this pseudogap is not due to superconducting phase fluctuations and hence is not related to a crossover between a BCS state of Cooper pairs and a Bose–Einstein condensation of local pairs. We rather argue that it is due to uncorrelated pairing which is already manifest in the local electronic structure and accessible by photoemission and tunneling experiments.

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1. Introduction

In absence of any consensus on the microscopic mechanism responsible for superconductivity in the cuprates, it is nevertheless possible to ask certain model--independent questions which can be verified experimentally. Such questions concern in particular the phenomenon of the pseudogap in the normal state, which is seen in angle-resolved photoemission spectroscopy (ARPES) [1] and tunneling measurements [2], and to what extent this gap is induced by superconducting fluctuations and what its remnants are in the superconducting phase. In the so-called underdoped systems where these effects are particularly pronounced, specific heat measurements [3] show a much reduced condensation energy which suggests that the gap in the superconducting state is not solely given by the order parameter but consists as well and predominantly of a practically temperature independent contribution arising from a continuation of the pseudogap from above the critical temperature T_c to below it. These results are corroborated by a comparative study of tunneling and Andreev reflection spectroscopy [4], the first being independent of any condensed state, the second depending on its existence and measuring directly that part of the gap which is determined by the order parameter. These experiments suggest that the pseudogap in the normal state is not due to

superconducting fluctuations and is not a simple continuation of superconducting gap extending into the normal phase. To what extent superconducting fluctuations play a role in the normal phase has been studied on the basis of transient Meissner screening [5] which tests the existence of phase fluctuations on a time scale of the order of the inverse superconducting gap (a few hundred GHz) and over a spatial extent of the order of the coherence length. These experiments show that superconducting phase fluctuations cease to exist at about 20 K above T_c for well underdoped samples and more rapidly as one approaches the optimally doped samples. Hence superconducting phase fluctuations are absent for most of the temperature regime where a pseudogap in the single-particle spectra is observed.

Theoretical phenomenological approaches attempting to describe the pseudogap phenomenon are based on:

i) effective BCS-like Hamiltonians as well as the negative-U Hubbard Hamiltonian [6], which try to study the pseudogap as a crossover feature in an intermediate state between a BCS state and a Bose–Einstein condensation (BEC) of preformed pairs,

ii) the boson–fermion model (BFM) [7] which, contrary to the first scenario describing the pseudogap as being induced by superconducting phase fluctuations, describes it as being due to local electronic structures involving the formation of uncorrelated pairs [8].

In this lecture we trace the pseudogap back to such a local electronic structure and then introduce the itinerancy of the electrons by means of a dynamical mean field study. Superconducting fluctuations will be excluded in such an approach. Hence such a study is limited to a temperature regime above the onset of phase fluctuations which are known to set in relatively close above T_c and require different techniques for their study such as diagrammatic approaches [9] in order to describe them. We shall show how the formation of local electron pairing without coherence is related to the onset of the pseudogap and concomitantly to the upturn of the dc resistivity upon lowering the temperature, signaling the tendency of the system towards an insulating state. In Sec. 2 we shall discuss the motivations behind the boson–fermion scenario and in Sec. 3 we shall indicate the local electronic structure and how it leads up to the pseudogap phenomenon. In Sec. 4 we summarize the physical consequences of this scenario as far as ARPES is concerned.

2. The boson–fermion model

The experimentally established linear relationship between T_c and n_s/m [10] (the latter being determined by the London penetration depth) suggests at first sight the idea of a BEC of preformed electron pairs, in particular since the number of electrons per coherence volume in those materials is very small. Yet it is known experimentally that these systems exhibit a Fermi surface, though with spectral features which are very distinct from those of ordinary Fermi liquids. The theoretical challenge then is to see to what extent we can have such a BEC of preformed pairs in the background of a kind of the Fermi liquid. The BFM might do just that. Let us briefly remind us of the origin of this model.

In the early eighties Alexandrov and Ranninger [11] investigated the possibility of superconductivity in systems with strong electron–phonon coupling. They found that small polarons tend to form bound pairs, the so-called small bipolarons, which have hard-core Bose statistics and hence can in principle condense into a superfluid state, which has been termed bipolaronic superconductivity. At that time it was neither clear from experiments nor from theory whether in principle such bipolarons can exist in form of itinerant states in the normal state, which is a prerequisit for their condensation. It was for this reason that the BFM was suggested by Ranninger, shortly after the publication of the papers on the bipolaronic superconductivity. The idea which led up to this model was to consider a situation of intermediary rather than strong electron–phonon coupling where the energy level of the bipolarons would overlap with the excitation spectrum of itinerant electrons. This is what one intuitively expects for the intermediary coupling case where such bipolaronic states exist for a finite time and then disintegrate into uncorrelated pairs of itinerant electrons, which in turn re-assemble into bipolarons after some time. Such a scenario can be cast into the following model Hamiltonian describing the BFM:

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

where $\varepsilon_0 = D - \mu$ and $E_0 = \Delta_B - 2\mu$ is the energy level of the bipolarons with respect to their chemical potential. $c_{i\sigma}^{(\dagger)}$ denote fermionic operators for the itinerant electrons with spin σ at some effective sites i (involving molecular units rather than individual atoms) and $b_i^{(\dagger)}$ describe tightly bound electron pairs (bipolarons) which have to be treated as hard-core bosons. The bare electronic half-bandwidth is given by D and the boson–fermion pair-exchange coupling constant by g. The chemical potential μ is common to fermions and bosons (up to a factor 2 for the bosons) in order to guarantee charge conservation. In this formulation we neglect the internal phononic degrees of freedom of the hard-core bosons, which is justified as long as we restrict our attention to the low energy features of this model such as the pseudogap. This model exhibits a superconducting ground state [12] which is due to a mutually induced macroscopic coherent quantum state exploiting the itinerancy of the electrons and the bosonic features of the electron pairs. Electron pairing which is induced in the fermionic subsystem via the charge exchange term in the Hamiltonian is however not enough to produce a superconducting state. In order for such a state to materialize, it is necessary that these electron pairs exist as well defined itinerant states. That this in fact happens as the temperature is decreased was first demonstrated on the basis of a fully conserving and self-consistent approach [7]. It showed how the purely diffusive modes at high temperature gradually evolve due to the onset of local phase coherence [9] into well defined propagating modes with a q^2 spectrum and little damping as the temperature is reduced.

3. The origin and nature of the pseudogap

As indicated in the introduction the present experimental situation favors the picture of an opening of the pseudogap being unrelated to the onset of any

superconducting phase correlations. We shall show that the BFM is compatible with such a scenario. Solving the above Hamiltonian in the atomic limit, i.e., setting $t_{ij} = 0$, we have the following set of eigenstates $|n\rangle$ and eigenvalues E_n:

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

The presence on a given site of an electron with spin up or down is denoted by corresponding arrows and the presence of a boson is denoted by a dot. Moreover we have

$$
\begin{aligned}
&u^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_0 - E_0/2}{\gamma}\right), \qquad v^2 = \frac{1}{2}\left(1 + \frac{\varepsilon_0 - E_0/2}{\gamma}\right),\\
&\gamma = \left[(\varepsilon_0 - E_0/2)^2 + g^2\right]^{1/2}, \qquad uv = \frac{g}{2\gamma}. \qquad (3)
\end{aligned}
$$

The local Green function can then be cast into the form [8]

$$
\begin{aligned}
G_{\mathrm{Loc}}(\mathrm{i}\omega_n) &= -\left\langle T\left[c_{j,\uparrow}(\tau)c^{\dagger}_{j,\uparrow}\right]\right\rangle\\
&= \frac{Z_{\mathrm{f}}}{\mathrm{i}\omega_n - \varepsilon_0} + (1 - Z_{\mathrm{f}})\left(\frac{u^2}{\mathrm{i}\omega_n - E_4} + \frac{v^2}{\mathrm{i}\omega_n - E_5}\right). \qquad (4)
\end{aligned}
$$

Here Z_{f}, $(1 - Z_{\mathrm{f}})\mathrm{u}^2$, and $(1 - Z_{\mathrm{f}})v^2$ represent the spectral weights of, respectively, the non-bonding, the bonding, and antibonding two-particle excitations, with Z_{f} given by

$$
Z_{\mathrm{f}} = \frac{1 + \mathrm{e}^{-\beta\varepsilon_0} + \mathrm{e}^{-\beta(\varepsilon_0 + E_0)} + \mathrm{e}^{-\beta(2\varepsilon_0 + E_0)}}{1 + 2\mathrm{e}^{-\beta\varepsilon_0} + 2\mathrm{e}^{-\beta(\varepsilon_0 + E_0)} + \mathrm{e}^{-\beta(2\varepsilon_0 + E_0)} + \mathrm{e}^{-\beta E_4} + \mathrm{e}^{-\beta E_5}}. \qquad (5)
$$

Notice that this form of the Green function is formally equivalent to that of a BCS Green function where g^2 plays the role of the usual gap function. Z_{f} is in general a function which decreases with decreasing temperature, thus indicating a diminishing of the spectral weight of the single-particle excitations in favor of the two-particle ones. This is in full equivalence to the situation of a BCS superconductor below T_{c}. The local Green function contains all the necessary ingredients to describe the opening of the pseudogap in the normal state. In order to describe a situation where these features are maintained when introducing the itinerancy of the electrons, this local electronic structure must serve as a starting point of such a study. If not, as in the case of diagrammatic formulations such as self-consistent

conserving T-matrix approaches to this problem, a pseudogap is obtained only as a consequence of superconducting phase fluctuations and exists only in dimensions less than 3 [13]. In order to ensure the prevailance of the local electronic structure we use a formulation of this problem in terms of local Hubbard operators $X_{mn} = |m\rangle\langle n|$ and then solve the above Hamiltonian in a controlled way. The best way of doing that at the moment is to resort to a dynamical mean field approach based on the use of the so-called non-crossing approximation (NCA) [14]. The detailed description of this approach has been reported previously [15]. Here we simply report the results for such a procedure and discuss it in connection with the physics of the cuprates. For that purpose we choose a set of parameters which comply to the following conditions:

1) at temperatures large compared to the interaction g the number of fermions $n_{\mathrm{F}} = \sum_{i,\sigma}\langle c_{i\sigma}^{\dagger} c_{i\sigma}\rangle$ should lie in the interval [1, 0.75] which covers the typical experimental doping regime;

2) $n = n_{\mathrm{F}} + 2n_{\mathrm{B}}$ ($n_{\mathrm{B}} = \frac{1}{N}\sum_i \langle b_i^{\dagger} b_i\rangle$ denoting the number of bosonic electron pairs) should lie in the interval [1, 2], in order to account for the appearance of a pseudogap phase. For the present analysis we choose $n = 1.5$ as a representative value;

3) T^* — the temperature at which the pseudogap opens — should be of the order of a few hundred degrees K which means $g \approx 0.2$ (all energies being measured in units of the bare electronic band width $2D$).

In the following we discuss the resulting single-particle spectral properties for this model in view of its pseudogap features.

4. The pseudogap features in ARPES

The single-particle spectral function is obtained from the fermionic Green function, which within the dynamical meanfield theory takes the form $G_{\mathrm{F}}(\varepsilon_k, \omega) = [\omega - \varepsilon_k - \Sigma_{\mathrm{F}}(\omega)]^{-1}$. Here the k-independent self-energy $\Sigma_{\mathrm{F}}(z)$ is obtained from the self-consistently determined local Green function

$$G_{\mathrm{F}}(z) = \langle\langle c_{i\sigma}; c_{i\sigma}^{\dagger}\rangle\rangle_z = \left[z - \varepsilon_0 - \Sigma^{\mathrm{W}}(z) - \Sigma_{\mathrm{F}}(z)\right]^{-1}, \tag{6}$$

where $\Sigma^{\mathrm{W}}(z)$ denotes the Weiss self-energy arising from the itinerancy of the electrons [16]. The detailed procedure for that has been given in Ref. [15]. We shall here simply consider the results of such calculations.

As a representative example of the signatures of the pseudogap seen in ARPES we choose $\Delta_{\mathrm{B}} = 1$, which is particularly suited to see how this pseudogap evolves from the local electronic structure. We plot in Fig. 1 the single-particle spectral function for the electrons at the Fermi vector $A_{\mathrm{F}}(\varepsilon_{k_{\mathrm{F}}}, \omega) = -\frac{1}{\pi}\mathrm{Im}G_{\mathrm{F}}(\varepsilon_{k_{\mathrm{F}}}, \omega)$ (ε_k denoting the bare electron dispersion) for a series of temperatures. $\varepsilon_{k_{\mathrm{F}}}$ is usually determined as that energy for which the fermionic distribution function is practically temperature independent. We notice that, in accordance with the temperature evolution of the local non-bonding single-particle states whose intensity diminishes as the temperature is lowered (transferring its spectral weight onto the bonding and antibonding two-particle states), the single-peak structure in Fig. 1 corresponding to the non-bonding states smoothly evolves into two side peaks associated with the bonding and antibonding two-particle states. The usual procedure to determine T^* is to identify the temperature at which the

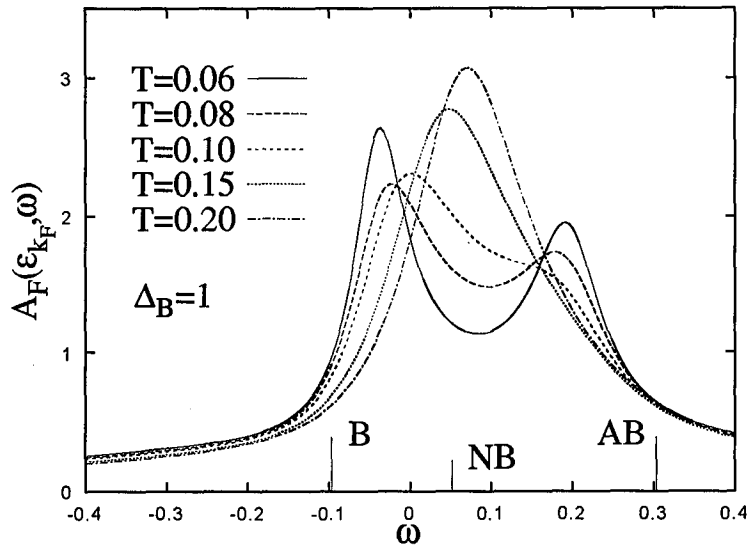

Fig. 1. The temperature dependence of the single-particle spectral function of the electrons at the Fermi surface. We compare the peak structure to that of the local atomic levels of our system where B, NB, and AB refer to the local bonding, non-bonding, and antibonding states. The energies ω are given in units of the total band width $2D$.

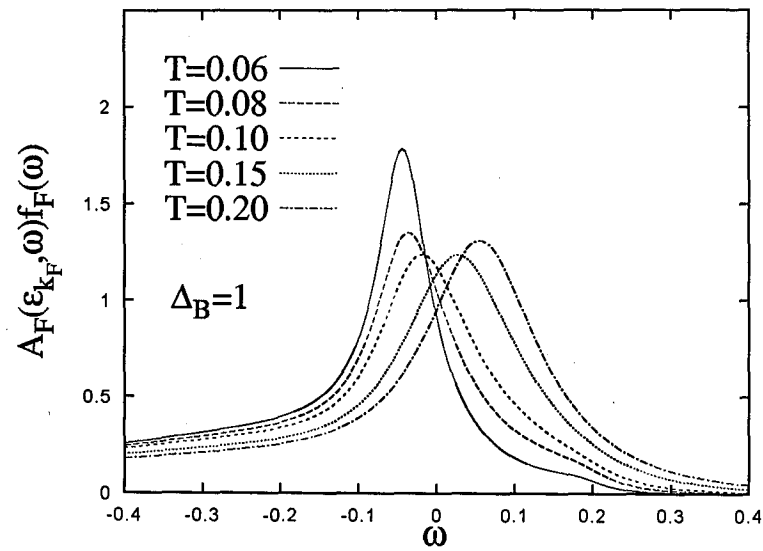

Fig. 2. The temperature dependence of the single particle ARPES intensity for the electrons at the Fermi surface, showing the shift of the leading edge with decreasing temperature. The energies ω are given in units of the total band width $2D$.

midpoint of the leading edge of the ARPES intensity $I(\varepsilon_{k_F},\omega) = A_F(\varepsilon_{k_F},\omega)f(\omega)$ ($f(\omega)$ denoting the Fermi function) goes through the chemical potential. This behavior is seen from Fig. 2 where we plot $I(\varepsilon_{k_F},\omega)$ for the same parameters as those in Fig. 1. As the leading edge of $I(\varepsilon_{k_F},\omega)$ moves towards the left upon decreasing the temperature, the pseudogap opens. This pseudogap in the single-particle spectrum is reflected in the thermodynamic and transport properties. The electrical resistivity shows indications for a tendency towards an insulating state as the temperature decreases in response to the strengthening of the pseudogap feature. Similarly, the Hall coefficient shows a change in sign upon decreasing the temperature changing from electron-like carriers at high temperatures to hole-like ones at low temperatures [17]. Upon approaching the superconducting state these results are however expected to be qualitatively modified and the onset of Cooper-pair fluctuations leads to a Drude type behavior of the conductivity overruling the semiconducting behavior [9]. A full understanding of the pseudogap phase must necessarily involve both effects: the local electronic pair correlations and the superconducting short-range and short-time phase correlations. Such studies are at present in progress.

5. Summary

In this paper we have tried to highlight the intricate nature of the pseudogap phase in the high-temperature superconducting cuprates. The picture which evolves, both experimentally and theoretically, is one where the pseudogap opens due to local pair fluctuations which are unrelated to phase fluctuations. On the basis of this, a BCS–BEC crossover scenario to explain these features seems to be an unlikely explanation. A scenario which can possibly account for at least part of such phenomena is one of a two-component system of localized electron pairs and itinerant electrons interacting with each other via a charge exchange term. This gives us the necessary freedom to separate amplitude from phase fluctuations. This touches on a fundamental problem in solid state physics and amongs others is fully equivalent to that of itinerant magnetism where local magnetic moments form at some temperature, but only order at a temperature below that.

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