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# THE POLARON SCENARIO FOR HIGH-$T_c$ SUPERCONDUCTIVITY

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On the basis of experimental evidence we conclude that high-$T_c$ superconducting materials are composed of two distinct subsystems: one in which electrons are bound together in form of localized pairs of small polarons (bipolarons) and one in which electrons exist as strongly correlated Fermions. Upon doping one passes at a critical doping rate from the insulating parent compounds to metallic compounds. There, a charge transfer mechanism between the two subsystems sets in abruptly by which bipolarons can decay into pairs of electrons and vice versa. Such a picture can be modelled by a mixture of interacting Bosons and Fermions. A superconducting ground state for such a system develops at low temperature which is characterized by the opening of a gap in the single electron spectrum and the appearance of collective Boson excitations with a linear spectrum which is confined to the energy regime of the gap. Above $T_c$, a pseudo-gap remains upon closing the superconducting gap. There are strong indications that the normal state has non Fermi liquid behaviour.

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## 1. Introduction

During several decades before the discovery of the high-$T_c$ superconductors [1], the total absence of any experimental breakthrough to produce superconductors with critical temperatures $T_c$ substantially larger than 20 K has led to consider the subject of superconductivity as a closed field of solid state physics. A summary and final assessment of this field was published in the classical two volumes of Parks "putting the last nail into the coffin of superconductivity" [2].

Only few theoretical groups [3, 4] basing their works on refinements of Eliashberg theory and general considerations of the dielectric properties of materials continued to claim that there were no principle obstacles in achieving relatively high values of $T_c$, in any case much higher than 20 K. When finally such materials were indeed produced, the large majority of theorists (including many new comers) simply ignored these systematic developments in the theory of superconductivity

and based their arguments on the status of BCS theory [5] as it was formulated in 1957, i.e. the weak coupling limit in which $T_c$ is given by

$$T_c = 1.13\omega_0 \exp(-1/\lambda_{\text{eff}}). \tag{1.1}$$

There, the effective electron–phonon coupling constant $\lambda_{\text{eff}}$ is assumed to be much smaller than unity, on the basis of which $T_c$ is not expected to exceed 35–40 K. For most purposes this weak coupling theory worked very well for superconductors before the high-$T_c$ materials became available.

There were of course "outsiders" which did not quite fit into this picture, requiring $\lambda_{\text{eff}}$'s which were not as small as those permitted by the range of validity of the theory (as for example Pb with $\lambda_{\text{eff}} = 1.55$) and isotope effects with negative exponents (PdH). On the whole however the situation was under control and deviations from the weak coupling theory could be handled in the frame of the Eliashberg theory [6].

As far as the high-$T_c$ compounds are concerned, six years after their discovery there is still no consensus either on the underlying mechanism for electron pairing in these systems or about the nature of its superconducting state. It is now experimentally established that the above-mentioned universal relations of weak coupling BCS theory are strongly violated that there is almost no isotope effect, no Hebel–Slichter peak and no peak in the thermal and optical conductivity below $T_c$. These facts together with the values of $T_c$ which largely exceeded the prediction of *weak* coupling BCS theory led the majority of theorists to reject the electron–phonon mechanism for electron pairing and a BCS-type state for superconductivity for explaining high-$T_c$ superconductors (H$T_c$SC).

H$T_c$SC are known to be structurally and chemically extremely complex systems showing strong electron–electron correlations as well as strong electron–lattice interactions. Then it is doubtful that the basic assumptions for the classical BCS–Eliashberg theories might be satisfied for which the adiabatic limit and Fermi liquid behaviour in the normal state are supposed from the outset.

There is now ample experimental evidence leaving no doubt that the superconducting state and the lattice dynamics are strongly correlated in high-$T_c$ materials. It appears that the phonons in these materials play a role which is qualitatively different from those assumed in classical strong coupling theories. The onset of superconductivity seems to freeze the dynamics of the lattice into a coherent state. Ion channeling experiments [7] and resonant neutron scattering [8] show that upon reducing the temperature below $T_c$ the atomic displacements become correlated and the thermal vibrational amplitude of the individual atoms decreases abruptly at $T_c$. EXAFS measurements show strong dynamical fluctuations of certain intramolecular distances in the vicinity of $T_c$ [9, 10]. Such effects can only be understood if the electronic degrees of freedom and the lattice vibrational ones are locked together in some kind of coherent state — a manifestation of which might be the occurrence of small polarons (or bipolarons) which will be discussed below in detail.

These effects which are essentially restricted to specific atomic units with anomalously large and local molecular fluctuations [11] may contain the key to our understanding of the pairing mechanism in high-$T_c$ materials.

This picture of lattice modulated pairing goes beyond the classical Eliashberg theory in which such dynamical local lattice instabilities are not taken into account. Eliashberg theory is restricted to the adiabatic approximation. In systems like $HT_cSC$, the electron motion might be slowed down to such an extent that during the process of transferring in electron from one site to another, the molecular states may change considerably. The empirically suggested negative values of the dielectric constant $\varepsilon(q \sim 1/a,\ \omega = 0)$ [12] may be indications for such dynamical local lattice instabilities leading to polaron formation and as a consequence real space pairing of such polarons. These effects change qualitatively the physics of a BCS state and the conventional concepts of Fermi liquid may need to be modified in order to incorporate strong electron–phonon coupling.

We shall in the following discuss a possible scenario for $HT_cSC$, based on polaronic charge carriers, which leads to a superconducting state which is closer to superfluidity of paired polarons (bipolarons) than to a BCS state.

## 2. Polaron induced pairing

$HT_cSC$ are structurally and chemically complex systems in which one and the same type of electrons participate in the covalent bonding and transport processes. Thus chemical doping requires the binding of extra O atoms in for instance $YBa_2Cu_3O_{6+x}$ for $x \geq 0.5$ which triggers off a dynamical charge transfer between the $CuO_2$ planes and the O(4)–Cu(1)–O(4) chains, a process associated with huge intramolecular distance fluctuations of the O(4)–Cu(1)–O(4) units in the chains (EXAFS). This is an unmistakable signature of the polaronic [9, 10] nature of charge carriers located on the chains in $YBa_2Cu_3O_{6+x}$.

It seems to be a common feature of all the hole doped $HT_cSC$ to be made out of two subsystems, the one accommodates the charge carriers as polarons (or bipolarons) and the second where the same charge carriers are essentially uncoupled to the lattice. The molecular units showing strong electron–lattice coupling are the dumbbell units O(4)–Cu(1)–O(4) in $YBa_2Cu_3O_{6+x}$ and $CuO_5$ units in $La_2Sr_{2-x}CuO_4$ and other Cu based $HT_cSC$ having pyramidal ligand environment. The latter are evident from the corrugate shell structure [10] seen by EXAFS in these materials. In the fullerenes the strong electron lattice coupling involves a tangential deformations of the pentagon units of carbon atoms in each $C_{60}$ molecule. For $BaBi_xPb_{1-x}O_3$ and $Ba_{1-x}K_xBiO_3$ the strong molecular deformation are breathing type motions of the oxygen cubic ligand environment of Bi atoms.

A characteristic feature of small polarons is that they exist preferentially as fairly locally bound pairs spreading over a few atomic distances. From the experimental evidence for such bound polaron pairs in $Ti_4O_7$, $Na_xV_2O_5$ and $WO_{3-x}$ [13] it is clear that the Coulomb repulsion between the electrons must have been overcome by the polaron induced attraction potential $\propto \omega_0\alpha^2$, where $\omega_0$ is the frequency of the local mode and $\alpha$ the dimensionless electron–phonon coupling constant; $\alpha$ being of the same order as $\lambda_{\text{eff}}$ which appears in the theory of superconductivity. Electrons strongly coupled to the lattice deformations lead to local

(in contrast to global) lattice instabilities in form of small polarons

$$\tilde{c}^{+}_{i\sigma} = c^{+}_{i\sigma}|\phi(x - x_0))_i. \tag{2.1}$$

This happens already for $\alpha \geq 1$ as initially shown by us [14]. From Eq. (2.1) we notice that a small polaron is described by a local entity centred at site $i$ and being composed of the charge carrier and a local lattice deformation of amplitude $x_0$ surrounding it. The latter is characterized by a shifted oscillator state $|\phi(x-x_0))_i$. Since polarons preferentially exist as bound pairs, the so-called bipolarons, $\tilde{c}^{+}_{i\uparrow}\tilde{c}^{+}_{i\downarrow}$, for singlet pairs, these pairs can in principle induce superconductivity, in the sense originally envisaged by Schafroth [15] provided these bipolarons exist in form of itinerant states [14]. There is no a priori reason why such a superconducting state in form of a Bose condensation of bipolarons should not be realized.

The simplest model to study small polaron physics is the so-called Holstein molecular crystal model.

$$H = \sum_{(i\neq),\sigma} t c^{+}_{i\sigma} c_{j\sigma} - \lambda \sum_{i,\sigma} n_{i\sigma} x_i + \frac{M}{2}\sum_i (\dot{x}_i^2 + \omega_0^2 x_i^2) + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{2.2}$$

composed of molecular units, with electrons hopping between these units and coupling locally to the intramolecular deformations $x_i$ of those molecular units at sites $i$. $c^{+}_{i\sigma}$ denotes electron (creation) annihilation operator with molecular orbital states, $\sigma$ being their spin and $n_{i\sigma} = c^{+}_{i\sigma} c_{i\sigma}$. In the regime where polarons are expected to form, the coupling term $\lambda \sum_{i,\sigma} n_{i\sigma} x_i$ is is the dominant term in $H$. Eliminating this term by a shift transformation [16]

$$S = \exp \sum_i \frac{\lambda(a_i - a_i^{+})(n_{i\uparrow} + n_{i\downarrow})}{\hbar\omega_0 (2\pi\omega_0/\hbar)^{1/2}}, \tag{2.3}$$

$H$ can be phrased in terms of polaron operators $\tilde{c}_{i\sigma} = S c_{i\sigma} S^{-1}$

$$\begin{aligned}\tilde{H} = &\sum_{(i\neq j),\sigma} t\tilde{c}_{i\sigma} e^{(\varepsilon_p/\hbar\omega_0)[(a_i - a_i^{+}) - (a_j - a_j^{+})]} \tilde{c}_{j\sigma} - \varepsilon_p \sum_{i,\sigma} \tilde{n}_{i\sigma} \\ &+ (U - 2\varepsilon_p) \sum_i \tilde{n}_{i\uparrow}\tilde{n}_{i\downarrow} + \sum_i \frac{M}{2}(\dot{\tilde{x}}_i^2 + \omega_0^2 \tilde{x}_i^2),\end{aligned} \tag{2.4}$$

where $\tilde{x}_i = (a_i + a_i^{+})/\sqrt{2M\omega_0}/\hbar$ are the dynamical displacements of the deformed molecular units. The transformation $S$ is different from that employed in the weak coupling limit where the coupling term $\lambda$ is eliminated to only the lowest order in $\lambda$ giving rise to the well-known phonon mediated electron–electron interaction

$$\lambda^2 \sum_{kk'q} \omega_0 \left[(\varepsilon_k - \varepsilon_{k'})^2 - \omega_0^2\right]^{-1} c^{+}_{k'\uparrow} c^{+}_{k+q\downarrow} c_{k'+q\downarrow} c_{k\sigma} \tag{2.5}$$

acting only in a thin layer of thickness $w_0$ around the Fermi surface such that $\varepsilon_F - \omega_0 < \varepsilon_k, \varepsilon_{k'} < \varepsilon_F + \omega_0$ and $|\varepsilon_k - \varepsilon_{k'}| < \omega_0$.

In the strong coupling limit we notice from Eq. (2.4) that small polarons attract each other locally and essentially in an unretarded fashion.

The existence of such lattice-deformation-induced on-site bipolarons have been established experimentally beyond doubt in amorphous semiconductors [17] for which they were postulated in order to explain the anomalous thermodynamic properties. Intersite or the so-called Heitler–London bipolarons [13] have been

verified in such systems as $Ti_4O_7$, $Na_xV_2O_5$, $WO_{3-x}$. The typical binding energy of such pairs is of the order of a few tenth of an eV.

All these experimentally established forms of bipolarons are of localized nature and exist in thermally activated dynamically disordered form such as in $Ti_{4-x}V_xO_7$ and $WO_{3-x}$.

Hence, the idea that such bipolarons (representing hard core Bosons on a lattice) could become superconducting in form of a Schafroth superconductivity suggests itself in a very natural way. Such a phenomenon is expected to occur for any strong coupling electron–phonon systems [14] provided that bipolarons exist in form of band states. The corresponding superconducting ground state would be described by

$$|\psi\rangle_{BP} = \Pi_i \left(u_i e^{i\varphi/2} + u_i e^{-\varphi/2} \tilde{c}_{i\uparrow}^{+} \tilde{c}_{i\downarrow}^{+}\right)|0\rangle, \tag{2.6}$$

which is the formal equivalent of the BCS wave function but with phase locking of real space rather than $k$-space (Cooper) pairs. The elementary excitations of such a bipolaron condensate are however quite distinct from that of a BCS state. They consist exclusively of phase fluctuations which due to their coupling to density fluctuations give rise to a linear in $q$ spectrum just as in $^4$He(II).

$$\lim_{q\to 0} \omega_q = s|q|, \qquad s = t^* \sqrt{n_0(T)}, \tag{2.7}$$

where $n_0(T)$ is the temperature dependent condensate density and $t^*$ the bipolaron hopping integral. For long range Coulomb interaction between the bipolarons the excitation spectrum is plasmon like

$$\lim_{q\to 0} \omega_q = \frac{4\pi(2e)^2 n_0}{\varepsilon_0 m^{**}}. \tag{2.8}$$

As initially shown by Schafroth [15], both the neutral and the charged Bose gas with long range Coulomb interaction have a Bose condensation temperature given by

$$k_B T_c \approx 3.3\hbar^2 n^{2/3}/m^{**}, \tag{2.9}$$

where $m^{**} = 3/t^{**}a^2$ is the bipolaron mass and $a$ — the lattice constant. It is interesting to speculate that $HT_cSC$ might be a manifestation of such a bipolaronic superconducting state. Their short coherence length of the order of the inter-particle distances — a few Angstroms — is very much in favour of such a picture. Also in favour is the experimentally verified universal linear dependence of $T_c$ on $n/m^{**}(\sim \lambda_H^2)$ [18] ($\lambda_H$ denoting the London penetration depth). Furthermore the specific heat data of a number of Cu based $HT_cSC$ are more akin to a $\lambda$-like transition than to the usual second order transition expected for a BCS system [19]. Taking the experimental data for the electronic part of the specific heat they can be scaled onto that of $^4$He over a wide relative temperature range, i.e. $|(T-T_c)/T| \leq 0.2$. It is remarkable that, on the basis of the specific heat data and the experimentally established $T_c \sim n/m^{**}$ relation, one obtains an extraordinary coherent picture for Schafroth superconductivity predicting the correct order of magnitude of the mass tensor of the bipolarons and their concentration, both of which can be checked by independent experimental techniques.

Yet, this simply picture of a Schafroth Bose condensation of bipolarons may not hold in view of certain by now well-established experiments.

The rapidly increasing improvements of the resolution in photoemission spectroscopy (about 20 meV) permits to plot out a Fermi surface and even the opening up of a gap below $T_c$ in the metallic $HT_cSC$ [20]. In the insulating parent compound the bipolaronic nature of charge carriers located on the O(4)-network has been verified by photoinduced absorption and photomodulation experiments [21] which show bimolecular recombination after photo excitation of such carriers. Comparing the photoinduced modification of certain local modes involving the molecular units housing the polarons (O(4)–Cu(1)–O(4) in $YBa_2Cu_3O_{6+x}$) with modes in the metallic compounds [22] suggests that the bipolaronic state on these units persists upon going from the insulating into the metallic compound upon chemical doping. The absence of the Koringa law above $T_c$ [23] and the absence of any qualitative change of the optical conductivity $\sigma(\omega)$ as a function of temperature for frequencies $\omega$ smaller than or equal to the gap [24] indicates a gap in the single particle spectrum which fades away rather than goes to zero at $T_c$.

## 3. A generic model for high-$T_c$ superconductivity

One might get a hint of the likely mechanisms at play in these $HT_cSC$ when carefully looking at their behaviour upon doping. Let us consider for that purpose the most widely studied compound, i.e. $YBa_2Cu_3O_{6+x}$. The undoped parent compound consists of $CuO_2$ layers sandwiching chains of $O^{--}(4)$–$Cu^{+}(1)$–$O^{--}(4)$ units (Fig. 1). The $CuO_2$ planes form a highly correlated electron system with

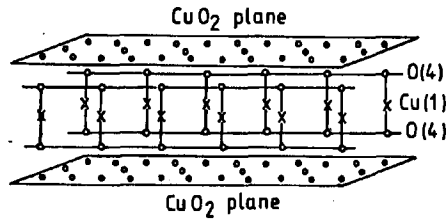


Fig. 1. Schematic plot of the basic building units of $YBa_2Cu_3O_{6+x}$ consisting of $CuO_2$ planes and chains of O(4)–Cu(1)–O(4). The full (open) circles represent Cu(O) atoms in the $CuO_2$ planes.

an insulating antiferromagnetic ground state. As the system is doped by putting oxygens between two adjacent $O^{--}(4)$–$Cu^{+}(1)$–$O^{--}(4)$ units, these oxygens are bound by an ionic bonding whereby $Cu^{+}(1)$ changes into $Cu^{++}(1)$. For low doping with oxygens O(1) the $CuO_2$ planes are thus unaffected as far as their electronic properties are concerned. Beyond a certain critical concentration of dopant oxygens however ($x \sim 0.5$), there are no more any $O^{--}(4)$–$Cu^{+}(1)$–$O^{--}(4)$ units available which could bind those extra oxygens [25]. As experiments show, a reordering of the dopant oxygens occurs which aligns them along chains and concomitantly a charge transfer between the $CuO_2$ planes and the chains containing the O(4)–Cu(1)–O(4)

units sets in. The oxygens begin to be bound covalently, the insulating antiferromagnetic state breaks down and gives way to a superconducting state which sets in abruptly within a small region of dopant concentration.

We can summarize these experimental results by the following physical situation illustrated in Fig. 2.

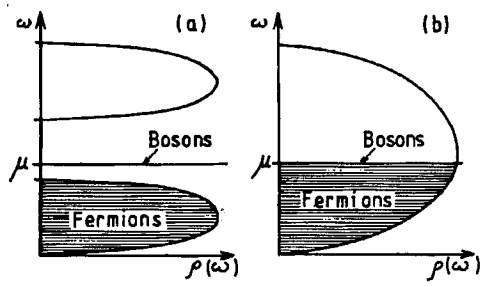


Fig. 2. (a) Schematic plot of the density of states for insulating $HT_cSC$ exhibiting a charge transfer gap inside of which resides localized Bosonic states. (b) The density of states for the metallic $HT_cSC$ with a Bosonic resonance state.

For low doping the system is described by the electronic structure of the $CuO_2$ planes exhibiting a charge transfer gap. Upon doping localized pairs of holes (bipolarons) are created on isolated units containing a dopant O(1) surrounded on either side by a O(4)–Cu(1)–O(4) complex. These states correspond to localized energy levels lying inside the charge transfer gap (Fig. 2a). When this gap breaks down beyond a certain critical doping rate, these states continue to exist as resonant states where bipolarons in the chains of $YBa_2Cu_3O_{6+x}$ are exchanged with pairs of electrons in the $CuO_2$ planes (Fig. 2b). Due to the Bosonic character of the bipolaronic states, the chemical potential of the system is then pinned below the level of these bipolarons.

This picture leads to predictions which in principle can be verified experimentally:

1. Doping in the metallic compounds should primarily change the number of Bosonic degrees of freedom — the resonant bipolaronic states.

2. Those Bosonic states should be seen in the normal state. One of the clearest evidence for them would be the demonstration of the existence of a pseudo-gap near the Fermi level in the electronic structure.

3. Upon decreasing the temperature, below a certain critical value $T_c$, this pseudo-gap should open up into a true gap and a mutually induced superconducting state should appear. In order for this to happen, not only a gap in the electron spectrum has to appear, but at the same time the initially localized bipolarons should become itinerant and finally superfluid.

The simplest generic model for such a picture is the Boson–Fermion mixture which we initially proposed [26] in order to describe the transitory regime between

the adiabatic and non-adiabatic limit of an electron phonon coupled system. In its simplest version this model is described by the Hamiltonian

$$H = \sum_{k\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_q E_q b^+_q b_q + \frac{v}{\sqrt{\Omega}} \sum_{k,q} (c^+_{k+q\uparrow} c^+_{-k\downarrow} b_q + \text{h.c.})$$
$$-\mu \left( \sum_{k\sigma} c^+_{k\sigma} c_{k\sigma} + 2 \sum_q b^+_q b_q \right), \tag{3.1}$$

where $c^{(+)}_{k\sigma}$ represent the electron operators in the itinerant subsystem and $b^{(+)}_q$ the operators for bipolarons in the subsystem in which bipolaron formation takes place. The charge exchange between bipolarons and electron pairs is described by the hybridization term proportional to $v$. The charge conservation is guaranteed by a common chemical potential for the bipolarons and itinerant electrons. The Hamiltonian, Eq. (3.1), is constructed such as to capture the physics depicted in Fig. 2b.

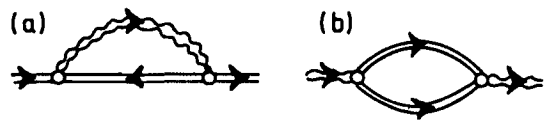


Fig. 3. (a) Fully self-consistent Fermion self-energy. (b) Fully self-consistent Boson self-energy.

Due to the hybridization term the electron (Fermion) and bipolaron (Boson) self-energies describing this process are illustrated in Fig. 3a,b and are given to the lowest order in $v$ by

$$\Sigma_F(k,\omega) = \frac{v^2}{\Omega} \sum_q \frac{n_F(\varepsilon_{k-q}) + n_B(E_q)}{\omega - E_q + \varepsilon_{k-q} + i\eta},$$

$$\Sigma_B(q,\omega) = \frac{v^2}{\Omega} \sum_k \frac{1 - n_F(\varepsilon_k) - n_F(\varepsilon_{k-q})}{\omega - \varepsilon_{k-q} - \varepsilon_k}, \tag{3.2}$$

where $n_F$ and $n_B$ denote the Fermi and respectively Bose distribution function and $\Omega$ — a normalization volume. Both, the electron energies $\varepsilon_k$ and Boson energies $E_q$ are measured with respect to the chemical potential, i.e. $\varepsilon_k = \xi^F_k - \mu$ and $E_q = \Delta + \xi^B_q - 2\mu$. The quantity $\Delta$ denotes the atom level of the bipolarons and $\xi^F_k$ and $\xi^B_q$ the dispersion for electrons and Bosons.

For the physical picture developed above, the Bosons are completely dispersionless. However, from our numerical study (in progress) of the fully self-consistent evaluation of the Boson and Fermion self-energies we know that due to the Boson–Fermion exchange mechanism these Bosons become itinerant although heavily damped modes. For the purpose of the present discussion where we shall extract the essential physics of this model, we shall therefore assume a small but finite dispersion for the Bosons from the outset.

We then obtain for the imaginary part of the electron self-energy

$$\Gamma_F(\omega) \simeq 2\pi v^2 g_F(E_0 + \mu - \omega) n_F(E_0 - \omega), \tag{3.3}$$

which is different from zero only for $E_0 < \omega < E_0 + \mu$. The parameter $g_F(\omega)$ denotes the Fermionic density of states. The real part for $\Sigma_F(k, \omega)$ : $R_F(\omega)$ is obtained by a Hilbert transformation of $\Gamma_F(\omega)$. The renormalised spectrum $\omega_k$ of the electrons is then obtained by the solutions of $(\omega_k - \varepsilon_k - R_F(\omega_k) = 0)$. We notice that as long as $E_0 > 0$ there exists always a $k_F$ such that $\omega_k < 0$ for $k \leq k_F$ and $\omega_k > 0$ for $k > k_F$. This determines the renormalized Fermi vector $k_F$ and leads to a corresponding discontinuity in the Fermi distribution function.

As $E_0$ approaches zero, we reach a situation where $\omega_k$ has exclusively negative values for any wave vector $k$ inside the Brillouin zone. This signals the breakdown of the Fermi liquid picture in the sense that there is no longer a discontinuity in the Fermi distribution function.

$$n_k = \int \frac{d\varepsilon}{2\pi} A_F(k, \varepsilon) n_F(\varepsilon) \tag{3.4}$$

at zero temperature, where $A_F(k, \varepsilon)$ denotes the electron spectral function

$$A_F(k, \omega) = \frac{\Gamma_F(\omega)}{(\omega - \varepsilon_k - R_F(\omega))^2 + \frac{1}{4}\Gamma_F^2(\omega)}. \tag{3.5}$$

At low temperature this breakdown of the Fermi liquid behaviour can be related to an instability towards a superconducting state. For $E_0 = 0$, namely, the Bose distribution function in $\sum_F(k, \omega)$ becomes singular because of Bose condensation. Rewriting $n_B(E_q)$ as

$$n_B(E_q) = n_B(E_q) + \delta_{q0}[n_0 - n_B(E_q)], \tag{3.6}$$

the dominant contribution to $\sum_F(k, \omega)$ for $E_q = E_0 = 0$ becomes

$$\Sigma_F(k, \omega) \sim \frac{n_0 v^2}{\omega + \varepsilon_k + i\eta}. \tag{3.7}$$

This yields the poles of electron Green's function

$$\omega_k = \pm\gamma_k = \pm\sqrt{\varepsilon_k^2 + n_0 v^2} \tag{3.8}$$

and hence an electron distribution function

$$n_k = \frac{1}{2}\left(1 - \frac{\varepsilon_k}{\gamma_k}\right), \tag{3.9}$$

which shows indeed no discontinuity in $\varepsilon_k$ as expected from the above considerations. Thus the system described by the Boson–Fermion mixture is unstable towards a superconducting ground state having BCS character for $T \to 0$. Let us now turn to the properties of the Bosons.

From the previous discussion of the electronic instability we know that this instability occurs for $q = 0$, being related to the condensate of the Bosons. The imaginary part of the Boson self-energy is given by

$$\Gamma_B(\omega) = 2\pi \frac{v^2}{\Omega} \sum_k \operatorname{tgh}\left(\frac{1}{2}\beta\varepsilon_k\right) \delta(\omega - 2\varepsilon_k), \tag{3.10}$$

which for $\omega = 0$ is identical to zero, signaling undamped Boson excitations. In that case the poles of Boson Green's function are given by

$$E_0 = R_B(\omega = 0) = \frac{v^2}{2\Omega} \sum_k \frac{1}{\varepsilon_k} \mathrm{tgh}\left(\frac{1}{2}\beta\varepsilon_k\right), \tag{3.11}$$

where $R_B(\omega)$ denotes the real part of the Boson self-energy. Rewriting the sum in Eq. (3.11) as an integral over the density of states of the unrenormalized electrons $g_F(\varepsilon)$ we obtain

$$E_0 = \frac{v^2}{2} \int \mathrm{d}\varepsilon g_F(\varepsilon) \frac{1}{\varepsilon - \mu} \mathrm{tgh}\, \frac{1}{2}\beta(\varepsilon - \mu). \tag{3.12}$$

For $\varepsilon \to \mu$ the integrand behaves like $g_F(\mu)\frac{1}{2}\beta$ which for $T \to 0$ diverges unless $g_F(\mu)$ has a gap at the Fermi energy, which is indeed the case as we have seen above from the discussion of electron Green's function.

The picture, which then evolves in quite a coherent fashion, is a superconducting ground state with a BCS-like gap in the single electron spectrum, inside of which undamped Bosonic modes exist.

According to the fully self-consistent treatment of the Fermion and Boson self-energies in the normal state our preliminary results suggest the following picture.

In the normal state, Bosons coexist with Fermions. The Bosons are heavily damped and there is a pseudo-gap in the density of states for the Fermions. As $T_c$ is approached from above, this pseudo-gap opens up into a true BCS-like gap. The Bosonic excitations become well-defined and acquire a linear in $q$ dispersion, which is a signature of the superfluid state of the Bosons.

$T_c$ as a function of doping shows a dependence on the total particle density $n = n_F + n_B$, which is closely related to that for a Bose gas with a density $n_B$. This is due to the blocking of the chemical potential just below the Bosonic level. Another consequence of this fact is, as earlier mentioned, the weak dependence of the Fermi surface on the total number of carriers which seems to be actually observed [27]. *The change in the number of carriers essentially results in the change of the number of Bosons.* This may be the reason why so many thermodynamic and electromagnetic properties of $HT_cSC$ can seemingly be understood on the basis of Bosons only [28]. One of the most spectacular manifestations of this is the $\lambda$-like specific heat for $HT_cSC$ which we shall discuss in the next section.

## 4. Specific heat anomaly in $HT_cSC$

To extract the electronic contribution of the specific heat, amounting to about 5% of the total specific heat, is a delicate undertaking and not free from a number of uncontrolable steps. Nevertheless several experimental groups independently find coinciding results [29, 30] which gives us a certain confidence in them.

Moreover the information which we are able to extract from these results [31] fit into a perfectly coherent picture of a Bose condensation and provides us with quantitative values for the concentration and mass of the carriers which can be

determined by independent experimental measurements. Following our work [31] we plot in Fig. 4 the specific heat of $^4$He together with the electronic contribution to the specific heat of $YBa_2Cu_3O_{6+x}$ and $Br_2Sr_2Ca_2Cu_3O_x$ per Boson and per molar volume. The specific heat of $HT_cSC$ is scaled down to that of 4He at a

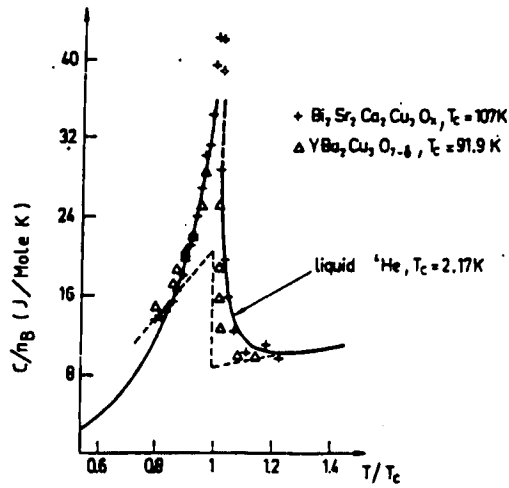


Fig. 4. Comparison (after Ref. [31]) of the $\lambda$-like behaviour of the specific heat of $^4$He (solid line) with that of $Ba_2Sr_2Ca_2Cu_3O_x$ [30] (x) and $YBa_2Cu_3O_{6+x}$ [29, 30] ($\Delta$). $n_B$ denotes the number of "Bosons" per molar unit which for $^4$He is evidentially equal to unity. The dashed line indicates the mean-field BCS-like fit to the specific heat.

single temperature $T/T_c \sim 0.9$. We then find that this scaling factor permits to fit the specific heat of $HT_cSC$ with the $\lambda$-like shape of $^4$He over the entire temperature regime $0 \leq |T - T_c|/T_c \leq 0.2$. This comparison of the specific heat of $HT_cSC$ with that of $^4$He allows us to extract the number of "Bosons" $n_B$ per molar volume $V$ and the corresponding densities $\tilde{n}_B$ in these materials

$$n_B^{123} = 0.3/V^{123}, \qquad \tilde{n}_B^{123} = 1.8 \times 10^{21}/\mathrm{cm}^3,$$

$$n_B^{2223} = 0.06/V^{2223}, \qquad \tilde{n}_B^{2223} = 2.4 \times 10^{20}/\mathrm{cm}^3. \tag{4.1}$$

Using the experimentally established linear relation $T_c \propto n/m$ [18] we then attempt to describe the superconducting critical temperature by the Bose condensation temperature for a quasi 2D system

$$k_B T_0^{2D+\varepsilon} = \frac{\hbar 2\pi n d}{m_{ab} \ln(2k_B T_0 m_c d^2/\hbar^2)}, \tag{4.2}$$

where $m_{ab}$ and $m_c$ denote the Boson masses in the $ab$ plane and along the $c$ axes, respectively. Taking an ad hoc mass ratio of $m_c/m_{ab} \sim 100$, together with the experimentally determined values of $T_0$ and the densities of Bosons determined from our analyses of the specific heat, we can evaluate the masses in the $ab$ plane

$$m_{ab}^{123} = 2.8 m_e, \qquad m_c^{2223} = 3.4 m_e,$$

where $m_e$ denotes the free electron mass. Both the number of effective charge carriers $\tilde{n}_B$ and their mass is in good overall agreement with independent measurements of these quantities. Moreover, assuming the Bosonic charge carriers to determine the London penetration depth $\lambda_{H,c} = \sqrt{m_{ab}c^2/16\pi ne^2}$ we obtain

$$\lambda_{H,c}^{123} = 2500 \text{ Å}, \qquad \lambda_{H,c}^{2223} = 4700 \text{ Å}$$

for the magnetic field aligned along the $c$ axes. Again, these values agree very well with those obtained by direct independent measurements [31].

This fully self-consistent picture of the $\lambda$-like specific heat of $HT_cSC$ gives us confidence that effective Bose particles, such as proposed in the interacting Boson–Fermion model presented here, might well describe the basic physics of $HT_cSC$.

The ultimate fate of this model will depend on the discovery or on the definite proof of the non-existence of Bosonic particles in the normal state of $HT_cSC$. The experimental evidence of such Bosons in the insulating parent compounds of $HT_cSC$ [21] and remnant features of them in the metallic compounds [22] are in strong support of our model.

Although our discussion was essentially based on hole doped cuprates containing apex oxygens, the same reasoning might be well applied to other compounds such as $K_xBa_{1-x}BiO_3$, alkaly-fullerenes and electron doped cuprate oxides. The first tests to be done in this direction in order to verify this supposition would have to be a repetition of the optical measurements [21, 22] carried out so far on the hole doped cuprates $HT_cSC$.

## 5. Conclusion

After several years of intensive experimental research on $HT_cSC$ a consistent picture begins to emerge which gives us hints on the origin of the pairing mechanism as well as on the type of superconducting state.

Strong polaronic features of part of the charge carriers are now well established and the possibility of the existence of bipolarons with reduced lifetime is being actively discussed. This all is in favour of real space pairing via strong electron–phonon interaction within given substructures of these materials.

A large number of physical properties of the normal and superconducting state can seemingly be well described on the basis of a Bose lattice gas model and bipolaronic superconductivity. Yet the existence of a Fermi surface seems to be established, with however possible marginal features of the corresponding Fermi liquid.

Experiments related to doping parent compounds of $HT_cSC$ and to the ordering of dopant atoms accompanied by strong lattice deformations suggest a charge transfer mechanism by which bipolarons (formed in the vicinity of dopant atoms) are exchanged into pairs of electrons in the strongly correlated subsystem of the $CuO_2$ planes. Such a mechanism can be described by a mixture of Bosons and Fermions with an hybridization term between Fermion pairs and Bosons.

This model has features which contain both, the essential physics of BCS superconductors and that of superfluidity of Bosons.

The hall marks of such a picture are:
– a pseudo-gap in the electron density of states around the Fermi level, present in the normal state,
– an opening up of this pseudo-gap into a true BCS-like gap upon entering the superconducting state with a concomitant appearance of collective excitations signaling a condensation of the Bosons in the system. According to that model, changing the number of charge carriers should predominantly influence the number of Bosons (rather than Fermions) in this system. In fact many thermodynamic quantities and $T_c$ turn out to be controlled essentially by the number of Bosons only.

Evidentially the crucial test for this model will be the direct experimental verification of such Bosonic quasi-particles with finite lifetime in the normal phase and of Bosons being locked into a condensate state in the superconducting phase. The existence of Bosons in the non-metallic parent compounds of H$T_c$SC and remnant features of them in the metallic compounds are in favour of such a Boson–Fermion mixture scenario for H$T_c$SC.

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