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Are preformed Cooper pairs the cause for the pseudogap in superconductors?

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A weak-coupling scenario wherein bosonic preformed electron pairs emerge upon cooling from two-electron *correlations* can explain the pseudogap phase consisting of segments where a Bogoliubov-like energy-momentum relation gapped spectrum alternates with a normal ungapped one. Bose–Einstein condensation (BEC) of preformed pairs interacting with the background fermions leads to either d- or s-wave-like superconducting gaps, the result being sensitive to the magnitude of the total number density of pairs n_B at which BEC occurs and becomes possible already for a moderately anisotropic s-wave pairing of fermions repelling each other via isotropic coulombic forces. The present model is compatible with the coexistence of pseudogap and of superconductivity phenomena.

Keywords: pseudogap; preformed pairs; Fermi arcs; gap symmetry

1. Introduction

A growing number of experimental data for pairing above T_c in cuprate superconductors reinforce interest in pseudogap scenarios via the notion of 'pairing without superconductivity.' This notion was introduced in the pioneering work by Eagles [1]; it resurfaced later [2,3] as 'preformed pairs.' Here it is employed to develop a weak-coupling scheme providing a common formalism to account for both pseudogap and superconductivity phenomena observed in cuprates.

Recent angle-resolved-photoemission spectroscopy (ARPES) measurements [4–6] in high-temperature superconductors (HTSCs) *above* their critical temperature T_c suggest that the fermionic dispersion relation in a portion of the Brillouin zone exhibits a gapped spectrum and in the remaining portion behaves as if the samples were a normal metal. Loci of constant energy with normal-metal dispersion in two-dimensional momentum space is commonly known as 'Fermi arcs.'

Some experiments suggest that pairings emerge at temperatures much below a certain T^* (itself much higher than T_c) and below which the pseudogap region characterized by the loss of spectral weight and by certain transport property anomalies develops [7,8].

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However, there are contradictory indications that the 'pseudogap does reflect the formation of preformed pairs of electrons' (see, e.g. in [5,9]) and thus, that pairing fluctuations persist up to a temperature T^*. Whether the pseudogap in cuprates is caused by actual pair formation or reflects some 'hidden' order that competes with superconductivity still awaits a definitive answer. Here, T^* is defined as a temperature below which actual bosonic Cooper pairs (CPs) appear in a system with a nearly filled conductivity band. We discuss the correctness or not of T^* defined in such a manner to describe the peculiarities of cuprate pseudogaps.

Another puzzle relates to the order-parameter pairing symmetry. In spite of the widespread belief that the superconducting order in cuprates is of d-wave symmetry, there are also studies suggesting s (or an $s+d$ mixture) -wave scenarios. For example, in Ref. [10] support is argued for extended s-wave rather than d-wave superconductivity. In contrast, an ingenious experiment [11] was crucial in showing that the superconducting order is predominantly of d-symmetry in YBCO. Interesting too is the fact that the gapped portions of a spectrum are seen not only in HTSCs but *also* in ultracold gases of fermionic atoms. Short coherence lengths as in nearly local CPs in cuprates, as well as the similarity between cuprates and ultracold atomic Fermi gases [12] might suggest a binary [13] (or even *ternary* if hole CPs are included [14–16]) boson-fermion (BF) gas mixture model whereby two-fermionic bound states can be viewed as actual bosonic excitations.

Here it is shown how seemingly inconsistent aspects of HTSCs such as: (i) the qualitatively different behaviours of T^* and T_c as function of doping concentration, specifically, an everywhere *decreasing* T^* in sharp contrast to the well-known *'dome-shaped'* T_c behaviour [17]; (ii) the appearance in **k**-space of alternating regions (the 'Fermi arcs') with either gapped or normal quasiparticle distributions; and (iii) sharply controversial views on the gap symmetry, can all be naturally reconciled already within a *binary* BF gas mixture model containing preformed CPs. Finally, also based on Fermi arcs, an explanation is proposed for a recent observation [18] of *coexisting* pseudogap and superconducting behaviour.

2. Hamiltonian

The Hamiltonian of pairable fermions and composite-boson CPs interacting with each other was initially suggested phenomenologically but it may also be derived from the Anderson model (see refs. in Ref. [19]). Or, it may be postulated to describe processes like the s-channel ones familiar from particle physics [20] or found from the low-energy limit of small-cluster states in a two-dimensional CuO lattice [21]. That Hamiltonian is further generalized to include two important effects: (a) the anisotropy of the pairing interaction and (b) coulombic repulsions between fermions (see, e.g. Ref. [22,23]) in terms of creation/annihilation operators for fermions (a operators) and bosons (b operators). Then, one has

$$\mathcal{H} = \mathcal{H}^o_{el} + \mathcal{H}^o_B + \mathcal{H}_f + \mathcal{H}_U \tag{1}$$

where

$$\mathcal{H}^o_{el} + \mathcal{H}^o_B = \sum_{\mathbf{k},\sigma} \xi_\mathbf{k} a^+_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \sum_\mathbf{K} \mathcal{E}_\mathbf{K} b^+_\mathbf{K} b_\mathbf{K} \tag{2}$$

along with

$$\mathcal{H}_f \equiv \frac{1}{N^{1/2}} \sum_{\mathbf{q},\mathbf{K}} \left(f_\mathbf{q} b^+_\mathbf{K} a_{\mathbf{q}+\mathbf{K}/2\uparrow} a_{-\mathbf{q}+\mathbf{K}/2\downarrow} + h.c. \right) \tag{3}$$

and

$$\mathcal{H}_U \equiv \frac{U}{N} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} a^{+}_{\mathbf{k}+\mathbf{q}/2\uparrow} a^{+}_{-\mathbf{k}+\mathbf{q}/2\downarrow} a_{-\mathbf{k}'+\mathbf{q}/2\downarrow} a_{\mathbf{k}'+\mathbf{q}/2\uparrow}. \tag{4}$$

In (2) fermion $\xi_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} - \mu$ and boson $\mathcal{E}_{\mathbf{K}}$ energies are measured from μ and 2μ, respectively, where $\mathbf{K}$ is the total or centre-of-mass wavevector of the bosonic CP and where the electron chemical potential μ is fixed by the constancy of the total electron number. Its value μ equals the radius of a sphere in energy space with its inner points occupied by the pairable/unpaired fermions. Exterior points of that sphere correspond to two-fermionic states, i.e. CPs, of energies $\mathcal{E}_{\mathbf{K}}$ higher than the lowest energy μ of single-electron excitations [24]. Here N is the number of unit cells in a lattice given by L^d/v_0 where L and v_0 are, respectively, the system size in d dimensions and the 'volume' of each cell.

A possible source in (2) for the term with bosonic energies $\mathcal{E}_{\mathbf{K}}$ is the usual BCS model attraction of strength V to be used throughout this paper. (For tirelessly advocating for the electron-phonon mechanism, even in cuprates, see Refs. [25,26]. A more recent discussion is found in Ref. [27]). As such, the effect of the assumed mutual interfermionic attractions is 'embedded' into the term in (2) with $\mathcal{E}_{\mathbf{K}}$ describing pairing correlations. Indeed, as found (see e.g. Appendix of Ref. [28]), the familiar Cooper equation [29], in addition to the well-known negative-energy solution $\mathcal{E}^{-} \equiv -2\hbar\omega_D(e^{2/\lambda} - 1)^{-1}$ associated with the appearance of bound pairs, where $\lambda \equiv N(0)V$ with $N(0)$, the fermion density of states at the Fermi surface E_F and $\hbar\omega_D$ is the Debye energy, there emerges a second positive-energy solution $\mathcal{E}^{+} \equiv +2\hbar\omega_D(e^{2/\lambda} + 1)^{-1}$. The solution $\mathcal{E}^{-}$ played a key role in understanding the ground state in the BCS theory [30]. However, the scarcely known second solution $\mathcal{E}^{+}$ corresponds to two-fermionic correlations with a total energy higher than the $2E_F$ associated with two individual electrons. It is analogous to the Schafroth [31] resonant modes also found in three dimensional and two dimensional in the more general treatment [32] of Cooper pairing via the Bethe–Salpeter integral equation that does not neglect hole pairs. Those resonances are not bound states and by no means are they CPs either; they have nothing in common with the excited pairs of the original BCS theory. The effect of $\mathcal{E}^{+}$ is expected to be tangible when only few empty states are present in the conductivity band. To understand what new physics emerges from the positive-energy correlations, they are included into (1) as *metastable* composites (of zero total spin) of a bosonic nature. As in the original BCS theory, an attraction of strength V responsible for pairing correlations is considered as an isotropic positive parameter.

The BF vertex interaction hamiltonian H_f in (3) drives mutual transitions between particles of fermionic and bosonic subsystems. The parameter f in H_f (describing formations of paired states from the background fermions followed by their disintegration into two independent fermions) defines the 'efficiency' of those transitions. It depends not only on the strength V of pairing correlations embedded in (2) but also on the peculiarities of the electronic structure, in particular on the direction of a total wavevector $\mathbf{Q}$ of two correlated fermions with momenta wavevectors $-\mathbf{k} + \mathbf{Q}/2$ and $\mathbf{k} + \mathbf{Q}/2$. This is why we believe that transitions between particles of fermionic and bosonic subsystems must occur in line with the symmetry of a 2D (or 3D) Brillouin zone. To account for directional dependency of the efficiency of transitions (associated with the symmetry of background fermions) the BF coupling parameter is taken as $f_{\mathbf{q}} = f\phi_{\mathbf{q}}$ where dimensionless factors $\phi_{\mathbf{q}}$ describe the distribution $f_{\mathbf{q}}$ around an average value [22] f. In order to make perfect contact with BCS theory (but in a *ternary* BF gas *with* hole pairs) the BF vertex coupling constant f

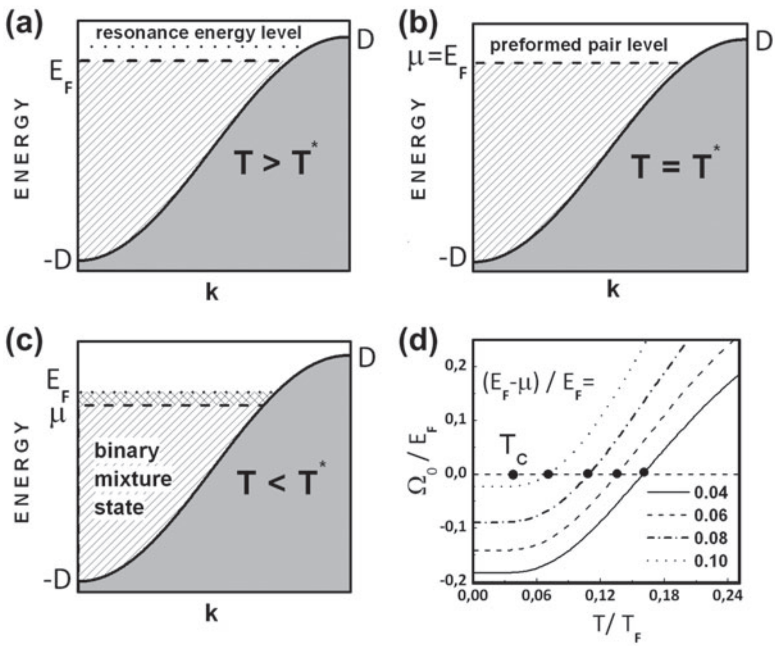

Figure 1. Schematic evolution of an attractively-interacting Fermi gas into a BF binary gas. (a) At $T > T^*$ the *resonances* are separated from the top of the conduction band by a *positive*-energy gap. At these temperatures occupied states are still only of single-particle nature. (b) On lowering T the energy of two-particle states decreases. Boson and unpaired-electron energies equal each other at exactly T^* below which the evolution of the pure Fermi gas of electrons into a *binary* BF gas ensues. (c) Cooling below T^* produces a ground state of single fermions coexisting with preformed CPs which becomes energetically favourable. (d) Dimensionless energy $\Omega_0(\lambda, T)/E_F$ of paired states as a function of T/T_F for several fractional number densities $(E_F - \mu)/E_F$ of bosons showing how non-T-dependent ‘ bare’ bosonic CP energies are renormalized by switching on the BF vertex interaction (3).

has been identified [14] with $\sqrt{2\hbar\omega_D V}$ where V was defined above along with the Debye energy $\hbar\omega_D$. Thus, distracting details of the real interactions like the effect of electronic structure (responsible for the abovementioned ‘efficiency’) are concealed in these so-called, anisotropy factors $\phi_{\mathbf{q}}$. The relation $f = \sqrt{2\hbar\omega_D V}$ allows one to express results in terms of the familiar BCS dimensionless $\lambda \equiv N(0)V$ instead of f.

Lastly, H_U is a coulombic term modelled as a spatially uniform repulsive field of strength U which mimics repulsions between paired electrons within a field of surrounding unpaired electrons.

The central idea behind the various binary BF models [12,19] is that if pairing is strong enough, then single fermions form relatively tightly bound two-particle composites. A new *weak-coupling* scenario different from those strong-coupling models is discussed in Refs. [24,28,33–37]. This scenario relies on the possibility of two fermion *resonances* above the Fermi sea since switching on an attraction between fermions produces two-fermionic resonances of energy $\mathcal{E}_{\mathbf{K}}$ shifted *upwards* from E_F by a *positive* gap (see, e.g. Ref.[28]). At high temperatures, the appearance of positive energy resonances is not advantageous. However, due to (3) the $\mathcal{E}_{\mathbf{K}}$ of individual resonances *renormalizes* to become a T-dependent

$\Omega_{\mathbf{K}}$ which decreases upon cooling (see Figure 1(d)). The pure gas of electrons comes on the verge of forming actual CPs by simultaneous satisfying (i) $\Omega_{\mathbf{0}} = 0$ which is the condition of equality of the resonance energies and the energy of unpaired fermions occurring by a decrease of $\Omega_{\mathbf{K}}$s and (ii) the condition $\mu = E_F$ preventing the survival of paired states above T^*. When $\Omega_{\mathbf{0}} = 0$ the state of single-fermions coexisting with incoherent CPs becomes more favourable than a state of single fermions only. As a result, below T^* two-particle *correlations*, inevitably present in a gas of attractively interacting fermions, become *actual* CPs. The T-behaviour of $\Omega_{\mathbf{0}}$ and relative positions of the two-fermionic level with respect to the top of the nearly filled conductivity band are schematically depicted in Figure 1 showing how the pure gas of electrons evolves into a binary BF gas mixture.

Three remarks are in order here.

First, inspection of terms $b^+_{\mathbf{K}} a_{\mathbf{q}+\mathbf{K}/2\uparrow} a_{-\mathbf{q}+\mathbf{K}/2\downarrow}$ and $b_{\mathbf{K}} a^+_{-\mathbf{q}+\mathbf{K}/2\uparrow} a^+_{\mathbf{q}+\mathbf{K}/2\downarrow}$ in (3) allows distinguishing the limits of nearly-half-filled and almost-full bands. In the former case, electrons act as nearly independent of each other and processes described by H_{int} appear unimportant. However, in the latter case (when the conduction band is crowded with lots of electrons) the role of processes described by H_f in (1) becomes important. Applying the Exclusion Principle one finds that if the band is near half-filling then pair formations rarely occur while pair disintegrations occur readily. For example, for processes $b_{\mathbf{K}} a^+_{-\mathbf{q}+\mathbf{K}/2\uparrow} a^+_{\mathbf{q}+\mathbf{K}/2\downarrow}$ to occur both fermionic states with momenta/spins $-\mathbf{q} + \mathbf{K}/2, \uparrow$ and $\mathbf{q} + \mathbf{K}/2, \downarrow$ must be empty. In contrast, in a nearly full band an abundant creation of paired fermion states are accompanied by their scarce destruction. Thus, the term (3) drives a pure fermionic system into a mixture of single- and two-fermionic objects. But this is especially important only if the band of fermions is nearly full.

Second, generic compounds of cuprates are antiferromagnetic insulators. By introducing holes of composition x onto the CuO_2 planes xN_{Cu} electrons (where N_{Cu} is the number of Cu sites) become mobile. These xN_{Cu} electrons subsist in the repulsive Coulomb field of all other fermions and by assumption interact with each other via the pairing potential of the BCS theory. The competition between electrons to occupy energy levels below E_F so as to minimize the volume of the Fermi sea leads, *in the presence of Coulombic repulsions*, to pushing away from that sea attractively interacting charge-carrier levels. On the other hand, the levels in a band originating from the generic insulating one in cuprates (where due to Coulomb repulsions double occupancy is still rare) are occupied nearly up to the highest energy. Therefore, the effect of a new solution $\mathcal{E}^+$ of the Cooper equation (i.e. pairings above the Fermi sea) and terms $b^+_{\mathbf{K}} a_{\mathbf{q}+\mathbf{K}/2\uparrow} a_{-\mathbf{q}+\mathbf{K}/2\downarrow}$ (along with $b_{\mathbf{K}} a^+_{-\mathbf{q}+\mathbf{K}/2\uparrow} a^+_{\mathbf{q}+\mathbf{K}/2\downarrow}$) in (3) both might be especially significant. It was shown in Ref. [35] how the processes of continual pair formation (above the Fermi sea) and their subsequent disintegration into two unpaired electrons (within that sea) *lowers* the total energy of many-fermion system and leads to a BF gas mixture.

Third, the two-fermionic entities (i.e. short-lived correlated states of two fermions and/or CPs) which inevitably arise at corresponding temperatures in the system of fermions interacting via the pairwise attractive potential V of the BCS model interaction are described in terms of bosonic operators b^+ and b in (3) and these objects satisfy BE statistics, and thus bosonic. This is because they depend *only* on the total $\mathbf{K}$ of the pair of fermions and not also [16] on their *relative* wavevector $\mathbf{k} \equiv \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$ as with BCS pairs [30] which are strictly *not* bosonic arguably since there lacks [16] an exact transformation to construct pure bosonic operators depending *only* on $\mathbf{K}$ from the fermionic ones depending on *both* $\mathbf{K}$ and $\mathbf{k}$.

3. Main formulae

Both fermion and boson spectra in this model are defined as in Ref. [37] where it was shown that below T^* the spectrum of unpaired fermions appears *partially* gapped. The energy $E_{\mathbf{k}}$ of unpaired electrons is found via a generalized energy gap $E_{g\mathbf{k}}(\lambda, T)$ in

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + E_{g\mathbf{k}}^2} \tag{5}$$

where

$$E_{g\mathbf{k}}(\lambda, T) \equiv \begin{cases} f\left(\phi_{\mathbf{k}} - \frac{\Omega_{\mathbf{0}}}{2\hbar\omega_D}\frac{U}{V}\right)\sqrt{N_B(\lambda, T)/N} & \text{for} \quad \phi_{\mathbf{k}} - \frac{\Omega_0}{2\hbar\omega_D}\frac{U}{V} > 0 \\ 0 & \text{for} \quad \phi_{\mathbf{k}} - \frac{\Omega_0}{2\hbar\omega_D}\frac{U}{V} \leq 0. \end{cases} \tag{6}$$

Here $N_B(\lambda, T)/N$ is the *total* bosonic number per cell [37] and $E_{\mathbf{k}}$ fixes the familiar occupation numbers $n_{\mathbf{k}\sigma} = \frac{1}{2}\left[1 - (\xi_{\mathbf{k}}/E_{\mathbf{k}}) \tanh\left(E_{\mathbf{k}}/2k_B T\right)\right]$ of unpaired electrons in each state with wavevector $\mathbf{k}$ and spin σ. Above T^* the numbers $n_{\mathbf{k}\sigma}$ are the same as in a gas of non-interacting fermions distributed around the E_F but below T^* these numbers differ significantly from those in a normal state and become direction-dependent [28] upon including an anisotropy of a pairing interaction. The boson spectrum in the BF mixture gas is found as roots $\Omega_{\mathbf{Q}}$ of the equation [33]

$$\Omega_{\mathbf{Q}} = \mathcal{E}_{\mathbf{Q}} + \left(1 - \frac{U}{N}\sum_{\mathbf{q}} \phi_{\mathbf{q}} \frac{F(\mathbf{q}, \mathbf{Q})}{\Omega_{\mathbf{Q}} - \zeta(\mathbf{q}, \mathbf{Q})}\right)^{-1} \left(\frac{f^2}{N}\sum_{\mathbf{q}} \left|\phi_{\mathbf{q}}\right|^2 \frac{F(\mathbf{q}, \mathbf{Q})}{\Omega_{\mathbf{Q}} - \zeta(\mathbf{q}, \mathbf{Q})}\right) \tag{7}$$

where $\zeta(\mathbf{q}, \mathbf{Q}) \equiv \xi_{-\mathbf{q}+\mathbf{Q}/2} + \xi_{\mathbf{q}+\mathbf{Q}/2}$ and $F(\mathbf{q}, \mathbf{Q}) \equiv 1 - n_{\mathbf{q}+\mathbf{Q}/2\uparrow} - n_{-\mathbf{q}+\mathbf{Q}/2\downarrow}$. For a given μ these roots $\Omega_{\mathbf{Q}}$ determine the average numbers $n_{B\mathbf{Q}}$ of actual bosonic CPs for a wavevector $\mathbf{Q}$ (e.g. in Ref. [33]) to be $n_{B\mathbf{Q}} = \left[\exp(\Omega_{\mathbf{Q}}/k_B T) - 1\right]^{-1}$. In this manner, the total boson number density becomes

$$n_B = N_B/L^d \equiv L^{-d}\sum_{\mathbf{Q}} \left[\exp(\Omega_{\mathbf{Q}}/k_B T) - 1\right]^{-1} \tag{8}$$

with all $\mathbf{Q} \geqslant \mathbf{0}$. In effect it comes from the $n_{B\mathbf{Q}}$ which is determined not by the $\mathcal{E}_{\mathbf{Q}}$ of 'bare' bosons but rather by the T- and coupling-dependent energies of 'dressed' ones defined by (7).

An expression for $\Omega_{\mathbf{Q}}$ was found in Ref. [33] via an infinite chain of equations for two-time retarded Green functions for dynamical operators $b(t)$ and $b^+(t')$ at times t and t' in the Heisenberg representation. Analytical continuation from the real axis to the imaginary axis (by substituting $\Omega \longrightarrow i\omega_n$) makes evident that the contribution to the 'bare boson' energy $\mathcal{E}_{\mathbf{Q}}$ given by the second term in rhs of (7) coincides with the boson self-energy cited in Ref. [23] which was established with a diagrammatic technique for a hamiltonian such as (1) (without H_U) but in an entirely different context.

At sufficiently large n_B the condensation of an indefinite number of CPs into a state with wavevector $\mathbf{Q} = \mathbf{0}$ becomes possible. This occurs when $\Omega_{\mathbf{0}} \to 0$ in (8). The condition $\Omega_{\mathbf{0}} = 0$ satisfied at some $T_c < T^*$ and μ_c which must be sufficiently lower than E_F (to provide a critical n_B) result in an eruption of a BEC in the bosonic subsystem. If one ignores the angular dependence of $\Omega_{\mathbf{Q}}$ and puts $\Omega_{\mathbf{0}}(T_c) = 0$ for all directions $\mathbf{Q} \to \mathbf{0}$ then (6) yields an expression for the superconducting gap that opens at and below T_c which varies over the Fermi surface according to the symmetry of the anisotropy factors $\phi_{\mathbf{k}}$. By decreasing μ from

E_F towards μ_c the pseudogap in the single-particle spectrum converts to a superconducting gap. Through the total number density of CPs n_B and CP energy $\Omega_\mathbf{0}$ the generalized gap Ex. (6) in a single-particle spectrum appears a functional of the two-particle characteristics.

The n_B, which is just half the total number of fermions that are actually paired at temperature T, can be expressed as [24]

$$n_B(\lambda, T) = N(0)(E_F - \mu) \tag{9}$$

where as before $N(0)$ is the density of fermion states per spin and per unit volume at E_F. According to (9) the degree of lowering of μ below E_F defines the composition of single- and two-bound- fermion entities in a BF mixture.

4. Discussion

The T-behaviour of the boson energy $\Omega_\mathbf{0}$ for different boson-number densities n_B is shown in Figure 1(d). Upon switching on the interparticle attraction two-fermionic correlations of energy $\mathcal{E}_\mathbf{0}$ emerge above the Fermi sea of a system of fermions competing to occupy the lowest energy states [28]. This positive contribution $\mathcal{E}_\mathbf{0}$ in (7) enlarges $\Omega_\mathbf{0}$. At high temperatures, the energy $\Omega_\mathbf{0}$ of two-correlated fermions arising at the resonance level seen in Figure 1(a) is higher than the sum of energies of two individual fermions. So the formation of CPs at those temperatures becomes possible *virtually* only. However, due to continual transitions between fermionic and bosonic subsystems, the value of $\Omega_\mathbf{0}$ drops down toward zero upon cooling whereby two-fermionic bound states *actually* materialize. This happens first at T^*, Figure 1(b). The formation of CPs decreases the total energy if T is below T^*. This occurs (i) due to the decrease in the unpaired fermion number contributing to the energy and (ii) due to the lowering of energies $\Omega_\mathbf{Q}$ of each two-particle state. Cooling below T^* leads to the emergence of more and more two-fermionic states: the number of unpaired fermions drops, making the chemical potential μ slide down below E_F, Figure 1(c). Now $\Omega_\mathbf{0}$ measured from 2μ is non-zero but as T is further lowered even more and continues to decrease gives rise of further *bosonization*.

Two-fermionic positive-energy correlations in the assembly of attractively interacting fermions which become actual CPs on cooling is the central idea behind the new weak-coupling scenario developed here and in Refs. [24,28,33–37]. Many different scenarios, e.g. stripe correlations, antiferromagnetism, orbital currents and pairing correlations, the presence of each well supported by experiments on cuprates, can bring on the pseudogap [17]. However, as found from (5)–(9), the notion of preformed pairs results *not only* in gapped fermions above T_c, but also accounts for the striking phenomenon of Fermi arcs alternating with a Bogoliubov-like dispersion of the pseudogapped phase.

Fermi arcs have been studied within a BF model for pairing of d-type symmetry [38] where important aspects of possible relevance for the microscopic origin of superconductivity in cuprates are discussed. In particular, it was shown how the structural instabilities seen in cuprates may suggest a way for fermions to appear either ‘in’ or ‘out’ of (the initially localized) tightly-bound bosonic pairs. Scattering continuously between states of itinerant fermions and states where charge carriers are momentarily trapped led in that paper to an electronic structure consisting of (i) delocalized single fermions and (ii) localized bound bosonic pairs which become itinerant and eventually condense upon cooling. ‘Schizophrenic’ carriers defined there as superpositions of itinerant and localized entities

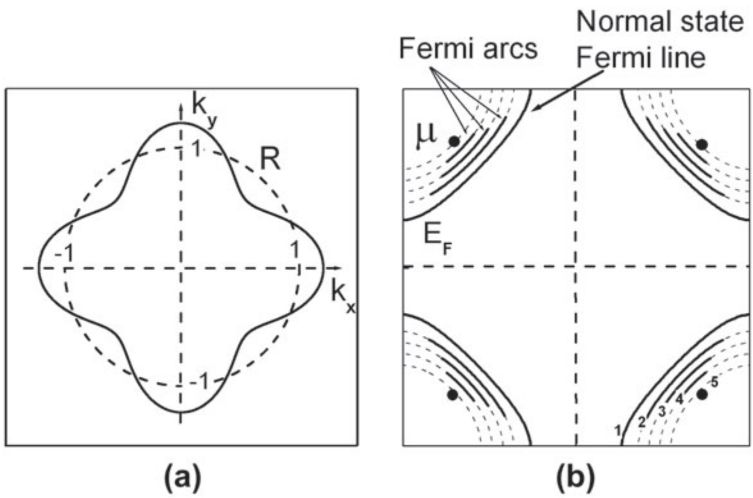

Figure 2. (a) Anisotropy factor $\phi_{\mathbf{k}}$ (full curve) of extended s-symmetry compared with dimensionless Coulomb repulsion R between fermions (dashed curve) that shortens on lowering T. (b) Typical two-dimensional Brillouin zone of hole-doped cuprates. Full curves depict normal Fermi lines. 'Dotted + full' curves enumerated from 2 to 5 show consecutive positions of μ by its lowering below the E_F associated with the reduction in the number of unpaired fermions. Dispersion of fermions is gapless only along the solid portions of those curves.

elucidate there important physics of the transition from the insulating parent compound to the superconducting doping regime. Dispersionless bosonic excitations of the Fermi assembly of energy 2Δ and of polaronic origin used in Ref. [38] which, due to their localized nature, are expected to be far above the Fermi sea. These contrast with the weak-coupling bosons advocated in the present work. Besides, the possibility of getting the Fermi arcs (a phenomenon unique in condensed-matter physics) already for pairing of s-type symmetry, as suggested here, seems intriguing.

The generalized energy gap $E_{g\mathbf{k}}$ in (5) as a function of direction of the wavevector $\mathbf{k}$ is expressed in terms of the factors $\phi_{\mathbf{k}}$ in (3) distributed around 1. These are fitted [28,37] as

$$\phi_{\mathbf{k}}^{\alpha} = \frac{1}{1-\alpha/2}(1 - 4\alpha \sin^2 \varphi \cos^2 \varphi) \tag{10}$$

with the prefactor chosen so as to normalize to unity the mean value of $\phi_{\mathbf{k}}^{\alpha}$ over the azimuthal angle φ determining the direction in $\mathbf{k}$-space of the two-dimensional vector $\mathbf{k}$. Here $0 \leq \alpha \leq 1$ with $\alpha = 0$ for isotropic superconductors. Varying α from 0 to 1 spans all ranges from weak to strong anisotropy. Specifically, we consider the pairing interaction of extended s-symmetry and assume that as the direction of $\mathbf{k}$ varies $\phi_{\mathbf{k}}$ takes on values along the 'distorted circle' obtained by moderately stretching the unit-radius circle along the vertical and horizontal directions, i.e. the $0, \pm\pi$ and $\pm\pi, 0$ directions, and compressing it along the diagonal $\pm\pi, \pm\pi$ directions, as depicted in Figure 2(a) by the full curve (see Ref. [37]). The curve in Figure 2(a) is found by choosing $\alpha = 0.35$ in (10).

The effect of Coulomb repulsions U in (6) depends on the T-dependent pure number $\Omega_0/2\hbar\omega_D$ describing the degree of separation between boson and fermion spectra.

This separation is different for different densities n_B of bosons and diminishes by bosonization, i.e. by raising the factor $E_F - \mu$ in (9) as exhibited in Figure 1(d). The dashed circle in that figure represents the dimensionless $R = (\Omega_0/2\hbar\omega_D)\,(U/V)$ appearing in (6) which diminishes on lowering T as does $\Omega_{\mathbf{0}}$. At sufficiently small T there appear segments of $\mathbf{k}$-space wherein the difference $\phi_{\mathbf{k}} - R$ becomes positive and leads according to (6) to the gapped portions of the E vs $\mathbf{k}$ relation. Results are summarized in Figure 2(b). Full curves, one of which is enumerated as 1 at the right-bottom corner of Figure 2(b), depict normal Fermi lines which might be seen at $T \geq T^*$. At and below T^* the number of the single fermions decreases so that $\mu(T)$ dips below E_F. 'Dotted + full' curves in Figure 2(b) depict the lines of constant energies corresponding to states differing from each other by the numbers of free fermions (panels from 2 to 5 in Figure 2(b) enumerate those isoenergetic lines in order of decreasing μ). According to (6) the single-fermion dispersion is gapless not along the entire 'dotted + full' curves but only along the full portions of those curves whose extensions decrease as T is lowered below T^*. These portions correspond to areas in Figure 2(a) where the factor R in (6) is larger than $\phi_{\mathbf{k}}$. In contrast, along the dotted curves in Figure 2(b) which on cooling, i.e. on even lower $\mu(T)$ below E_F, become broader, the spectrum appears gapped, i.e. of a Bogoliubov type. Disconnected full segments in Figure 2(b) are thus interpreted as the Fermi arcs observed in ARPES experiments [4–6,12]. Along those segments where $\phi_{\mathbf{k}} - R \leq 0$ the T, and hence the factor $\Omega_0(T)/2\hbar\omega_D$ in (6), is still too high to open a gap, thus leading to a dispersion relation as if the sample were a normal metal. The Fermi arcs, i.e. gapless portions of a spectrum in Figure 2(b), are centred on the diagonals of the square Brillouin zone. The lengths of these arcs diminish and vanish completely on further cooling (designated as black dots along the diagonals).

A key finding exhibited in Figure 2(b) is that for any finite U in (6) the resulting dispersion in a pseudogapped state contains fourfold disconnected Fermi arcs alternating with the gapped segments in the entire momentum space, i.e. resembling d-wave symmetry. This result does not depend on the actual pairing symmetry which itself might be d- as well as moderate s-wave-like. As T decreases towards T_c the behaviour of a superconducting gap depends, besides on the factors $\phi_{\mathbf{q}}$, on the $\Omega_{\mathbf{0}}(T)$ in (6). There are two distinct possibilities: *First*, $\Omega_{\mathbf{0}}(T_c)$ becomes zero for all directions of the total momentum $\mathbf{Q} = \mathbf{0}$ of CPs (i.e. BEC occurs upon the opening of a gap over the entire Fermi surface). In this case, as seen by assuming $\Omega_{\mathbf{0}} = 0$ in $E_{g\mathbf{k}}(\lambda, T)$, the symmetry of a superconducting gap is defined *solely* by the symmetry of $\phi_{\mathbf{q}}$. That is, s-like $\phi_{\mathbf{q}}$ drives the gap in a superconducting state into an s-symmetry. Only d-wave-like $\phi_{\mathbf{q}}$ sets below T_c an order of the d-symmetry.

However, starting from the extended s-wave type $\phi_{\mathbf{q}}$ (7) provides a *second* very different possibility to obtain a superconducting gap resembling d-symmetry. The question is really: Can the material superconduct in spite of fermions from portions of $\mathbf{k}$-space still remaining unpaired? The present scenario foresees this possibility. As may be seen [e.g. by substituting $\mathbf{q}' = \pm\mathbf{q} + \mathbf{Q}/\mathbf{2}$ for $\pm\mathbf{q}$ in (7)] $\Omega_{\mathbf{Q}}$ depends not only on a magnitude Q of vector $\mathbf{Q}$ but also on its direction given by the azimuthal angle φ. In the limit of $\mathbf{Q} \to \mathbf{0}$ there appears $\Omega_{\mathbf{0}} \equiv \Omega(0, \varphi)$ in (7) which contains the angle φ. There are a lot of two-particle states with the total momentum $\mathbf{Q} = \mathbf{0}$ differing each from another by the value of φ. For an isotropic pairing interaction all of these pairs are of the same energy $\Omega_{\mathbf{0}}$. However, if the pairing interaction V is direction-dependent [39] then $\Omega_{\mathbf{0}}$ varies in φ. In other words, depending on along which direction the wavenumbers $\mathbf{k}$ and $-\mathbf{k}$ of fermions making up a pair with total momentum $\mathbf{Q} = \mathbf{0}$ are, the energy $\Omega_{\mathbf{0}}$ appears different. Thus, by scanning φ there appear different segments in the $\mathbf{k}$-space where the conditions $\Omega_{\mathbf{0}} = 0$ (necessary to provide a

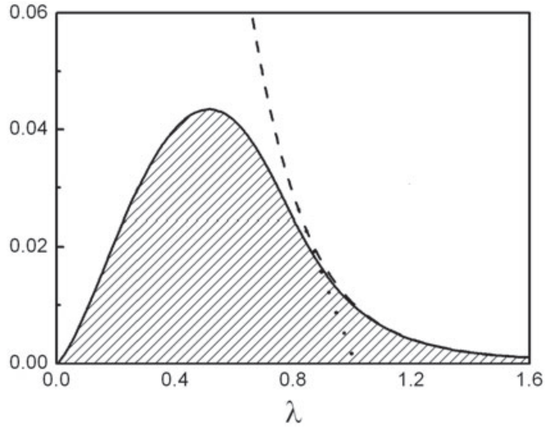

Figure 3. Pseudogap (dashed curve) T^*/T_F and BEC superconducting (full curve) T_c/T_F phase boundaries as functions of λ. Shaded dome-shaped region designates superconducting BEC phase. The normal state lies above the T^*/T_F curve below which the pseudogap phase exists. Dotted curve penetrating *below* superconducting dome depicts a situation which according to widespread belief, if confirmed in observations, might be proof of different origins of superconductivity and the pseudogap. However, this is also possible in a scenario based solely on preformed pairs.

critical density of CPs for BEC to occur) and $\Omega_{\mathbf{0}} \geqslant 0$ [which provide the gapless portions of $E_{g\mathbf{k}}(\lambda, T)$] are satisfied independently. In this situation, the superconducting gap, as well as the pseudogap opening well above T_c, both open only partially. The fourfold portions of momentum space where the superconducting gap opens will alternate with the gapless portions of the dispersion relation and thus resemble a d-wave one, all of this in spite of the assumed extended s-wave symmetry of the pairing interaction.

Hence, the d-symmetry of the order parameter seen in many experiments on cuprates, can be materialized not necessarily by a d-wave-like pairing interaction, but can be alternatively found in terms of extended s-wave symmetry and the density n_B of preformed CPs at which superconductivity begins. What is important is that unlike purely d-symmetry-based models which bypass the possibility of s-wave-like gaps, the present model which operates with n_B embraces both s- and d-wave possibilities. Specifically, experiments probing the surface of cuprates yield d-wave, while experiments probing the bulk point to a substantial s-symmetry (see, e.g. Ref. [40]). If one assumes that the density of paired fermions necessary for surface superconductivity to occur is less than the one necessary for bulk superconductivity, then the results suggested in Ref. [40] may be interpreted in terms of s-symmetry alone.

The scenario just described of the evolution of a pure fermion gas into a binary BF gas mixture allows one to distinguish two critical temperatures, a depairing (or pseudogap) temperature T^* below which preformed CPs appear without coherence, and a BEC critical temperature T_c below which these CPs constitute a coherent fluid. Formulae related to these for finite U were reported in Ref. [33]. Variation of T^* and T_c as functions of the dimensionless BCS attraction parameter $\lambda = N(0)V$ are shown in Figure 3. Correlating λ with the concentration of hole carriers x (in a manner, e.g. as done in Ref. [24]) yields, qualitatively at least, the familiar dome-shaped T_c as well as the well-known monotonically-decreasing T^* with doping parameter x. In Figure 3, the values $\nu \equiv N(0)U = 0.9$ and

$\Theta_D/T_F = 0.35$ are used for illustration purposes where Θ_D and T_F are, respectively, the Debye and Fermi temperatures. It was found that an increase of the dimensionless Coulomb factor ν lowers the maximum T_c and narrows the interval of coupling λ (equivalently doping x) over which superconductivity occurs. But irrespective of the value of ν the T^* and T_c curves always merge together as λ (or x) increases, as seen in Figure 3. Larger Θ_D/T_Fs give higher T_cs while smaller ν makes the dome-shaped structure of T_c vs λ become less prominent.

Many authors contradistinguish BCS and BF regimes of pairings by saying that an increase in λ takes one from the weak-coupling limit (or BCS regime) to a Bose gas. It is also believed that, because of a severe spatially-overlapping wavefunctions of CPs in the BCS regime the conditions for pair formation and quantum coherence of pairs occurs at the same temperature $T^* = T_c$. On the contrary, decrease of pair sizes by increasing λ, allows one to idealize pairs as 'individual molecules.' In this latter Bose regime, the pair formation and their condensation happen [12,41] at different temperatures T^* and T_c with $T^* > T_c$. Because of its intuitive clarity this picture of evolution [42] of fermions from the BCS regime to the limit of a Bose gas is quite popular. However, the present BF model is very different in that already the *weak-couplings* allows for 'individual' bosonic excitations made up two correlated fermions. The criterion for an actual boson must be consistent with Bose–Einstein statistics, i.e. the possibility of condensing an indefinitely large number of pairs into a single ground state. In particular, in the limit of $\lambda \to 0$ this picture leads to different temperatures of pair formation T^* and of their condensation T_c–a result opposite to the prescription of BF models relying on tightly-bound pairs. Furthermore, in contrast to strong-coupling models increased λ leads to pair-formation at much lower temperatures than occurs for smaller λ, as seen in Figure 3.

In sharp contrast to Figure 3, some data suggest a pseudogap existing *below* T_c [43]. Because of the usual condition $T^* \geqslant T_c$ for precursor pairing, an observation of $T^* < T_c$ would apparently rule out models of HTSCs that posit a common origin for both pseudo- and SC-gaps. Observation of $T^* < T_c$ is also reported from resonant ultrasound spectroscopy (RUS) measurements [18]. The smaller of two identified temperatures, 61.6 K and at 68 K, at which the RUS spectra of an overdoped single crystal undergo a discontinuity are interpreted in Ref. [18] as $T^*$and the higher one as T_c.

Some authors, e.g. Ref. [44], tend to interpret $T^* < T_c$ as suggesting a hidden order responsible for the pseudogap phenomenon. However, operating in terms of extended s-wave pairing interaction and the density n_B of preformed CPs merits further discussion on a possible pseudogap below T_c. Indeed, if one assumes that the material superconducts and that this happens in spite of fermions from portions of **k**-space still remaining unpaired, then one can easily see that there must be *no* obvious transitions between unpaired fermions and fermions constituting CPs of the condensate. For transitions to occur a CP must preliminarily disintegrate. Only then can a fermion of the Fermi arc bind with a fermion arising from the disintegration and the result enter the condensate. However, this is related with the appearance of a singly occupied state in the region of states from which a condensate of CPs is made and thus forbidden by energy considerations [30]. Absence of transitions between Fermi-arc fermions and fermions constituting CPs suggests considering the unpaired fermions as independent from those bound up in condensate CPs. Becoming independent below T_c those of the Fermi arcs must undergo their own evolution. In particular, they may pair up and lead to the opening of a new kind of pseudogap in the spectrum of Fermi-arc fermions.

5. Conclusions

It was shown how two-fermionic *positive-energy* correlations in a gas of attractively interacting fermions become *actual* CPs but without the long-range phase coherence one associates with superconductivity. This leads one to develop a weak-coupling scenario for a binary gas mixture of these CPs coexisting with pairable, but unpaired fermions. The mixture reveals a pseudogap phase emerging from pure fermions via small segments alternating with gapless portions of the fermion spectrum. Changing direction the arrowhead of wavevector **k** in two-dimensional momentum space traces so-called nodal lines centred at the diagonals of a square Brillouin zone along which the gap vanishes. As a result, the dispersion consists of disconnected segments resembling d-wave symmetry. Cooling below T^* leads to a broadening of the gapped regions followed by a decrease in the extent of the nodal lines.

Also shown was how the Fermi arcs separated by gapped portions of the energy-momentum relation seen in ARPES experiments may emerge in the present scenario not only for d-wave symmetry but already for a moderately-anisotropic s-wave pairing of fermions repelling each other via isotropic coulombic forces as either d- or s-wave-like gaps, the result being sensitive to the magnitude the value of n_B at which BEC occurs.

Lastly, the present model clarifies the possible coexistence of the pseudogap and of superconductivity. A natural explanation for different, and at first glance incompatible, aspects of cuprates offers important evidence for the preformed-pair scenario in HTSC physics.

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