International Journal of Modern Physics B Vol. 27, No. 29 (2013) 1347002 (16 pages) © World Scientific Publishing Company DOI: 10.1142/S0217979213470024



UNIFORM COULOMB FIELD AS ORIGIN OF "FERMI ARCS" IN AN ANISOTROPIC BOSON-FERMION GAS MIXTURE

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> Received 30 May 2012 Accepted 1 June 2012 Published 3 June 2013

A recent boson-fermion (BF) binary gas mixture model is extended to include: (i) anisotropy of the BF interaction and (ii) momentum-independent Coulomb repulsions. It is applied to account for the peculiarities of the pseudogap observed as function of absolute temperature T and concentration x of holes doped onto the CuO_2 planes and to study the further transformation of the pseudogap into the real superconducting gap, as T is lowered. Using two-time Green functions it is shown that pair breakings depend on the separation between the boson and fermion spectra of the BF mixture. As this separation shrinks, the pair-breaking ability of the Coulomb interaction weakens and disappears at the BEC T_c , i.e., at the T below which a complete softening of bosons occurs. Simultaneous inclusion of both effects (i) and (ii) produces, as T is lowered, "islands" in momentum space of incoherent Cooper pairs above the Fermi sea. These islands grow upon further cooling and merge together just before T_c is reached. The new extended BF model predicts a pseudogap phase in 2D high- T_c superconductors with lines of points, or loci, on the Fermi surface along which the pseudogap vanishes. This explains the origin of T-dependent "Fermi arcs" observed in ARPES experiments.

Keywords: Preformed Cooper pairs; pseudogap; Fermi arcs.

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1. Introduction

Cooper oxides (or cuprates) are compound materials with various phases observed at different absolute temperatures T and compositions x of holes doped into the CuO_2 planes. Such planes are unique structural elements for all Cu -based high- T_c superconductors (HTSC). Phase diagrams, deduced from a vast number of experiments (see e.g., Fig. 1 in Ref. 1), show a varied complexity of physics in those compounds. In particular, clearly seen in that diagram are well-defined regions as an insulating antiferromagnet, a pseudogapped metal, a superconductor and so-called marginal-Fermi-liquid phases. They alternate as x increases. It is widely believed that the complicated and rich physics of cuprates is a result of the combined effect of low-quasi-dimensionality and strong correlations between individual charge carriers. Any comprehensive theory of high- T_c -materials must deduce, within a single unified conception, the dominant interactions underlying the origin of each region of the phase diagram, as well as the crossovers between them. In Ref. 1 special stress is made on so-called "preformed Cooper pairs" as well as "Fermi arcs", both topics to be addressed in the present paper.

The transition from the insulating antiferromagnet phase of the undoped compounds to the metallic state when extra holes are doped into the CuO₂ planes is attributed to the strong on-cite correlations of electrons in quasi-two-dimensional (2D) CuO₂ layers. Their effects are usually described in terms of the extended Hubbard model (see e.g., in Ref. 1). Unfortunately, the central question "is the pairing of charge carriers exclusively of electronic origin or it is conditioned by some combined mechanism involving, e.g., the effect of lattice vibrations" still lacks both an experimental and a theoretical basis. Varied opinions are found in the literature,³ ranging from a complete negation of the role of electron-phonon interactions to the opposite belief that electronic properties and related magnetic-ordering effects are irrelevant for high- T_c materials. Indeed, the dynamical origin of the pairing interaction is a matter of debate. But regardless of the actual dynamics producing pairing, the notion of Cooper pairs (CPs) appears to be an essential ingredient in virtually every theory of superconductivity. A comprehensive theory must account for the presence between the insulating and superconducting phases of a so-called pseudogapped metal domain, the appearance of which is most striking and unprecedented (see, e.g., Ref. 4, Fig. 3). Experiments in cuprates with x spanning this domain exhibit signatures of a suppression of the density of electronic states, i.e., the opening of a gap in the single-particle electronic spectrum below some x-dependent characteristic temperature T^* which can be appreciably higher than T_c . Whether the pseudogap domain is a true thermodynamic phase emerging only for specific compositions x of holes, or is it an "insulator-superconductor crossover" region, remains one of the unsolved questions. Two broad trends are discussed in the literature⁴: First, a pseudogap is basically of the same origin as superconductivity.⁵ In this case it might reflect the presence of preformed pairs, i.e., noncoherent pairs above T_c but below T^* . Or, it is a manifestation of some new order, different from

superconductivity, which may possibly be in competition with the superconducting state. 6

A principal step towards a "complete theory" vitally hinges on which of these two scenarios is correct, or at worst merely dominant. In the absence of such a comprehensive theory, different phenomenological approaches motivated by experimental findings and physical intuitions have appeared that consider various aspects of cuprate physics. Two observations lend credence to boson-fermion (BF) binarygas-mixture models which posit the existence above T_c of actual bosonic CPs of total charge 2e. First, pairs in conventional low- T_c and HTSC differ widely in size, or so-called coherence lengths ζ , compared with the average spacing s between pairs. For conventional superconductors $\zeta \gg s$ and give rise to as many as a million CPs overlapping any single CP. However, according to estimates, the average distance between pairs in CuO₂ planes is approximately 25 Å, i.e., is more than (or of order of) the typical coherence length of pairs observed in cuprates to be of order 20 Å (see, e.g., Ref. 7). Specifically, unlike CPs in low- T_c materials, because ζ and s are comparable in cuprates, pairs in HTSCs by and large occur independently of each other and may therefore be considered as made up of two bound fermions. Second, recent experiments^{8,9} reveal a Bogoliubov quasiparticle spectrum in the pseudogapped-metal domain of the phase diagram which confirms the notion that a pseudogap existing above T_c must be related to pairing.¹⁰ This is perhaps the best evidence for the preformed-pairs scenario. According to these experiments, at temperatures between T_c and T^* dispersion of single-fermions behaves in some directions of the Brilluoin zone as if the sample were a normal metal. It crosses E_F over an extended length forming "Fermi arcs". In contrast, in other directions there is a wavenumber range k near k_F for which the spectrum of free fermions displays a gapped structure. If so, then the question "does the idea of preformed pairs account for all the observed peculiarities of the pseudogap phase as one changes T and x and its subsequent transformation into the actual superconducting gap" becomes relevant.

This paper deals with those aspects of the problem. In Sec. 2 the generalized BF Hamiltonian is introduced; in Sec. 3 the two-time Green-function (GF) technique is applied to obtain the single-fermion occupation numbers $n_{\mathbf{k}\sigma}$ and single-fermion spectrum in the BF mixture; in Sec. 4 the role of renormalized boson energies in the consequent BEC is discussed; in Sec. 5 we analyze the distribution of occupation numbers $n_{\mathbf{k}\sigma}$ along the direction of the 2D wavevector \mathbf{k} as the temperature is reduced; and in Sec. 6 concluding remarks are given.

2. BF Hamiltonian

BF Hamiltonians for *binary* gases were first introduced in Refs. 11–15. A *ternary* model including also hole CPs alongside electron CPs, and capable of making *precise* contact with BCS theory¹⁶ as a special case, appeared later.^{17,18} The binary BF model has been generalized in Ref. 19 to contain terms describing both the

anisotropy of CP formation as well as Coulomb repulsion between fermions. The Hamiltonian is now:

$$\mathcal{H} \equiv \mathcal{H}^o + \mathcal{H}_{eB} + \mathcal{H}_U \,. \tag{1}$$

Here, the first term \mathcal{H}^o in (1) is the sum of Hamiltonians of free (pairable but unpaired) fermions \mathcal{H}_e and of composite-boson CPs \mathcal{H}_B , namely:

$$\mathcal{H}^{o} \equiv \mathcal{H}_{e} + \mathcal{H}_{B} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} a_{\mathbf{k}\sigma}^{+} a_{\mathbf{k}\sigma} + \sum_{\mathbf{K}} \mathcal{E}_{\mathbf{K}} b_{\mathbf{K}}^{+} b_{\mathbf{K}}, \qquad (2)$$

where $a_{\mathbf{k}\sigma}^+$ and $a_{\mathbf{k}\sigma}$ are the usual fermion creation and annihilation operators for individual electrons of momenta \mathbf{k} and spin $\sigma = \uparrow$ or \downarrow while $b_{\mathbf{K}}^+$ and $b_{\mathbf{K}}$ are postulated 17,20 (for a brief review, see Ref. 18) to be bosonic operators associated with CPs of energy $\mathcal{E}_{\mathbf{K}}$ and definite total, or center-of-mass momentum (CMM), wavevector $\mathbf{K} \equiv \mathbf{k}_1 + \mathbf{k}_2$ which is just the sum of the wavevectors of two electrons. In (2) fermion $\mathcal{E}_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$ and boson $\mathcal{E}_{\mathbf{K}}$ energies are measured from μ and 2μ , respectively, where the electronic chemical potential μ is fixed from the constancy of the total electron number. The second term in (1) is the BF vertex interaction

$$\mathcal{H}_{eB} \equiv L^{-d/2} \sum_{\mathbf{q}, \mathbf{K}} (f_{\mathbf{q}} b_{\mathbf{K}}^{\dagger} a_{\mathbf{q} + \mathbf{K}/2\uparrow} a_{-\mathbf{q} + \mathbf{K}/2\downarrow} + \text{h.c.})$$
(3)

and describes processes of boson formation/disintegration where $f_{\bf q}=f\phi_{\bf q}$ is a phenomenological BF coupling constant distributed around its average value f measuring the vertex interaction strength, nonzero only in the electron-energy range $E_F - \hbar \omega_D \leq \epsilon \leq E_F + \hbar \omega_D$ about the Fermi energy E_F of the ideal Fermi gas. To maintain a connection with the electron-phonon Debye energy, the pairing-energy scale is denoted as $\hbar \omega_D$. Also, $f_{\bf q}$ contains so-called anisotropy factors $\phi_{\bf q}=\phi_{\bf -q}$ introduced to account for the anisotropy of the BF interaction associated with CP formation. In the quite general formalism of Refs. 17, 18, which boils down to a ternary BF gas mixture model mentioned earlier that does exclude two-hole CPs unlike binary BF models, one can extract BCS theory as a special case²¹ if one identifies the BF form factor coupling f with $\sqrt{2V\hbar\omega_D}$, where V is the strength of the net attractive pair-forming BCS model interaction. Finally, last term \mathcal{H}_U in (1) is chosen as

$$\mathcal{H}_{U} \equiv U_{0}L^{-d} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} a^{+}_{\mathbf{k}+\mathbf{q}/2\uparrow} a^{+}_{-\mathbf{k}+\mathbf{q}/2\downarrow} a_{-\mathbf{k}'+\mathbf{q}/2\downarrow} a_{\mathbf{k}'+\mathbf{q}/2\uparrow}$$
(4)

and reflects the repulsive Coulomb interaction between fermions modeled as a spatially uniform repulsive field of strength $U_0 \geq 0$. We believe that the inclusion of this term is necessary to prevent the singularities in compressibility which naturally occur in any gas of attractively interacting particles.

Applied to cuprates, (1) implies that 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 which would fill at T=0 the states up to energy $E_F=(\pi\hbar^2N_{\text{Cu}}/m)x$ in a 2D lattice, appear subsisting in a uniform repulsive field

of strength U_0 and interacting with each other via some pairing potential leading to (1). Unfortunately, there is no derivation of (1) based on the electronic structure of CuO_2 planes and the genesis of atomic bonds.^{22,23}

The total electron number whose operator is:

$$N \equiv \sum_{\mathbf{k},\sigma} a_{\mathbf{k}\sigma}^{+} a_{\mathbf{k}\sigma} + 2 \sum_{\mathbf{K}} b_{\mathbf{K}}^{+} b_{\mathbf{K}}$$
 (5)

includes, naturally enough, both the number of unpaired fermions plus twice the number of bosons. It commutes with (1) and is therefore an invariant of motion for the binary BF mixture state. Note that (5) reveals a very different structure of BCS and BF models. Indeed, CPs in the BCS model may appear at temperatures higher than T_c only as superconducting fluctuations. A nonzero equilibrium number density $n_B(T)$ is possible only if $T \leq T_c$. However, within a binary mixture of mutually-converting fermions and bosons, $n_B(T)$ may be nonvanishing on either side of $T = T_c$, reflecting the existence above T_c of incoherent and below T_c of coherent equilibrium pair densities. The temperature and coupling dependent number density $n_B(T)$ of bosonic CPs is proportional²⁴ to the difference $E_F - \mu(T)$ which plays the role of an order parameter in this description. The position of $\mu(T)$ with respect to E_F determines the phase the attractively-interacting fermions reside in, viz., it consists of single fermions only for all $E_F < \mu(T)$ while $E_F = \mu(T)$ provides the condition defining T^* below which the first pairs appear. On the other hand, below T^* the relation $E_F > \mu(T)$ holds. That is, for all $T < T^*$ the attractivelyinteracting fermion gas becomes a binary mixture of interacting fermions and bosons mutually converting into one another. Further decreasing T from T^* to T_c leads to the critical μ at which $E_F - \mu$ and therefore n_B become sufficiently appreciable for Bose–Einstein condensation (BEC) to occur.

It should also be noted that within (1) defining the characteristic $T^* > T_c$ was possible owing solely to the assumption on two-fermion states with a total energy $\geq 2E_F$. This new ingredient in the BF model is discussed in Ref. 25 where it was shown that introducing a net attractive interaction between electrons in the gas of electrons leads to the formation a new type of lower-energy mixture state with bosonic excitations above the Fermi sea of unpaired electrons. This contrasts sharply from BCS theory which is based on CPs with energy $\leq 2E_F$. As shown in the Appendix, the question of two-fermion states with a total energy $\geq 2E_F$ as raised in Refs. 26–29 is resolved, already in terms of the familiar Cooper eigenvalue equation 30 but with a new (scarcely-known "improper" positive-energy) solution. The relation between a Cooper-equation eigenvalue energy $\geq 2E_F$ and a BF model was also discussed in Ref. 25.

3. Single-Particle Spectrum in the BF Mixture

Whatever distribution of free carriers occurs in a superconductor can be addressed by starting from $n_{\mathbf{k},\sigma} \equiv \langle a_{\mathbf{k},\sigma}^{+} a_{\mathbf{k},\sigma} \rangle$. These c-numbers $n_{\mathbf{k},\sigma}$ are then obtained, e.g., from an infinite chain of equations for two-time retarded GF $\langle A(t)|B(t')\rangle$ as

defined in Ref. 31 Eq. (2.1b) for dynamical operators $a_{\mathbf{k}\sigma}(t)$ and $a_{\mathbf{k}'\sigma}^+(t')$ at times t and t' in the Heisenberg representation. If A and B are any two operators, the Fourier transform $\langle\!\langle A|B\rangle\!\rangle_{\omega}$ of $\langle\!\langle A(t)|B(t')\rangle\!\rangle$ satisfies the infinite chain of equations (see, e.g., Eq. (A.2) in Ref. 24).

$$\hbar\omega\langle\langle A|B\rangle\rangle_{\omega} = \langle [A,B]_{\eta}\rangle_{\mathcal{H}} + \langle\langle [A,\mathcal{H}]_{-}|B\rangle\rangle_{\omega}, \qquad (6)$$

where square brackets $[A, B]_{\eta} \equiv AB + \eta BA$ denote the commutator $(\eta = -1)$ or anticommutator $(\eta = +1)$ of operators A and B. Choosing $B \equiv a^+_{\mathbf{k}'\uparrow}$ and $\eta = +1$ we put in (6) first $A \equiv a_{\mathbf{k}\uparrow}$ and then $A \equiv a^+_{\mathbf{k}\downarrow}$. This gives couple of equations which relates the first-order GFs $\langle a_{\mathbf{k}\uparrow} | a^+_{\mathbf{k}'\uparrow} \rangle_{\omega}$ and $\langle a^+_{\mathbf{k}\downarrow} | a^+_{\mathbf{k}'\uparrow} \rangle_{\omega}$ on the left-hand side with higher-order GFs on the right-hand side.

In analogy with the pure Bose gas where the emergence below a critical T_c of nonzero $\langle b_0 \rangle$ and $\langle b_0^+ \rangle$ signals the appearance of superfluidity, here we expect nonzero $\langle b_{\mathbf{K}} \rangle$ and $\langle b_{\mathbf{K}}^+ \rangle$ to presage the BF mixture state that emerges in an attractively-interacting fermion gas. Thus, we put:

$$\langle \langle b_{\mathbf{K}} a_{-\mathbf{k}+\mathbf{K}\downarrow}^{+} | a_{\mathbf{k}'\uparrow}^{+} \rangle \rangle = \langle b_{\mathbf{K}} \rangle \langle \langle a_{-\mathbf{k}+\mathbf{K}\downarrow}^{+} | a_{\mathbf{k}'\uparrow}^{+} \rangle \rangle + \langle \langle (b_{\mathbf{K}} - \langle b_{\mathbf{K}} \rangle) a_{-\mathbf{k}+\mathbf{K}\downarrow}^{+} | a_{\mathbf{k}'\uparrow}^{+} \rangle \rangle$$
(7)

and retain only the term proportional to $\langle b_{\mathbf{K}} \rangle$. Contributions beyond (7) containing the difference $b_{\mathbf{K}}^+ - \langle b_{\mathbf{K}}^+ \rangle$ are neglected.^{24,32} Higher-order GFs, like as $\langle a_{-\mathbf{k}+\mathbf{q}\downarrow}^+ a_{-\mathbf{p}+\mathbf{q}/2\downarrow} a_{\mathbf{p}+\mathbf{q}/2\uparrow} | a_{\mathbf{k}'\uparrow}^+ \rangle_{\omega}$ on the right-hand side of equations for $\langle a_{\mathbf{k}\uparrow} | a_{\mathbf{k}'\uparrow}^+ \rangle_{\omega}$ and $\langle a_{\mathbf{k}\downarrow}^+ | a_{\mathbf{k}'\uparrow}^+ \rangle_{\omega}$ are cast as a linear combination of the first-order GFs and of a so-called irreducible piece which by definition cannot be reduced to lower order GFs. Ignoring all terms leading to the violation of the translational symmetry and to the magnetic ordering and by use of an exact equality:

$$L^{-d/2} \sum_{\mathbf{q}} \phi_{\mathbf{q}} \langle a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} \rangle_{\mathcal{H}} = -f^{-1} \Omega_{\mathbf{Q}} \langle b_{\mathbf{Q}} \rangle_{\mathcal{H}}$$
(8)

and the relation

$$\sum_{\mathbf{q},\mathbf{q}'} \left\langle \frac{b_{\mathbf{q}}^{+}}{L^{d/2}} \right\rangle_{\mathcal{H}} \left\langle \frac{b_{\mathbf{q}'}}{L^{d/2}} \right\rangle_{\mathcal{H}} = L^{-d} \sum_{\mathbf{q},\mathbf{q}'} \langle b_{\mathbf{q}}^{+} b_{\mathbf{q}'} \rangle_{\mathcal{H}} \simeq L^{-d} \sum_{\mathbf{q}} \langle b_{\mathbf{q}}^{+} b_{\mathbf{q}} \rangle_{\mathcal{H}}, \tag{9}$$

which holds *only* for particles obeying Bose statistics in the thermodynamic limit, long calculations the details of which are given in Ref. 19, we reach at the system of linear equations for the first order GFs of view:

$$(\hbar\omega - \xi_{\mathbf{k}})\langle\langle\langle a_{\mathbf{k}\uparrow} | a_{\mathbf{k}'\uparrow}^{+} \rangle\rangle + S_{\mathbf{k}}\langle\langle\langle a_{\mathbf{k}\downarrow}^{+} | a_{\mathbf{k}'\uparrow}^{+} \rangle\rangle = \delta_{\mathbf{k}\mathbf{k}'},$$

$$S_{\mathbf{k}}^{*}\langle\langle\langle a_{\mathbf{k}\uparrow} | a_{\mathbf{k}'\uparrow}^{+} \rangle\rangle + (\hbar\omega + \xi_{\mathbf{k}})\langle\langle\langle a_{\mathbf{k}\downarrow}^{+} | a_{\mathbf{k}'\uparrow}^{+} \rangle\rangle = 0,$$
(10)

where we note that $\xi_{\mathbf{k}} = \xi_{-\mathbf{k}}$ and define $S_{\mathbf{k}} \equiv [f\phi_{\mathbf{k}} - (U_0\Omega_{\mathbf{0}}/f)] \sum_{\mathbf{q}} \langle b_{\mathbf{q}}/L^{d/2} \rangle$. In (8) $\Omega_{\mathbf{Q}}$ is the boson energy $\mathcal{E}_{\mathbf{Q}}$ renormalized due to the BF interaction and the average $\langle \cdots \rangle_{\mathcal{H}}$ is performed over the Hamiltonian (1). Equations (10) immediately give:

$$\langle \langle a_{\mathbf{k}\uparrow} | a_{\mathbf{k}'\uparrow}^{\dagger} \rangle \rangle_{\omega} = \frac{\hbar \omega + \xi_{\mathbf{k}}}{(\hbar \omega)^2 - E_{\mathbf{k}}^2} \delta_{\mathbf{k}\mathbf{k}'},$$
 (11)

$$\langle \langle a_{-\mathbf{k}\downarrow}^+ | a_{\mathbf{k}'\uparrow}^+ \rangle \rangle_{\omega} = -[f\phi_{\mathbf{k}} - (U_0\Omega_{\mathbf{0}}/f)] \frac{\delta_{\mathbf{k}\mathbf{k}'}}{(\hbar\omega)^2 - E_{\mathbf{k}}^2} \sum_{\mathbf{q}} \left\langle \frac{b_{\mathbf{q}}^+}{L^{d/2}} \right\rangle_{\mathcal{H}}.$$
 (12)

Poles of the GFs (11) and (12) occur when:

$$E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + E_{g\mathbf{k}}^2}, \qquad (13)$$

which defines the single-fermion spectrum in the BF mixture phase. The spectrum in the normal phase now appears *gapped* with the generalized gap:

$$E_{g\mathbf{k}}(\lambda, T) \equiv f\left(\phi_{\mathbf{k}} - \frac{\Omega_0}{2\lambda\hbar\omega_D}\nu\right)\sqrt{n_B(\lambda, T)},$$
(14)

where $n_B(\lambda, T)$ is the total number density of electron pairs. This generalizes the principal result Eq. (21) of Ref. 32, namely:

$$E_g(\lambda, T) \equiv f\sqrt{n_B(\lambda, T)}. \tag{15}$$

Recall that the BF coupling parameter f in (14) and (15) was identified ^{17,20} with the net attractive interelectron BCS interaction strength V through the relation $f = \sqrt{2\hbar\omega_D V}$ so as to recover the BCS gap equation as a special case²¹ of the ternary BF model mentioned earlier. Here, we introduce the dimensionless parameters $\lambda \equiv N(0)V$ and, in (14) $\nu \equiv N(0)U_0$, with N(0) the electronic density of states (DOS) for each spin at the Fermi surface. For conventional superconductors, the sign of the order parameter $E_{g\mathbf{k}}(\lambda,T)$ remains positive on the entire Fermi surface, whereas (14) may change sign. If the sign change takes place on a single connected Fermi surface, continuity requires $E_{qk}(\lambda,T)$ to vanish where the sign reversal occurs.³³ Note that $E_{q\mathbf{k}}(\lambda,T)$ is a positively defined gap only for points \mathbf{k} of the momentum space where $f(\phi_{\mathbf{k}} - (\Omega_0/2\lambda\hbar\omega_D)\nu) > 0$ is satisfied. Otherwise, we put $E_{q\mathbf{k}}(\lambda,T)\equiv 0$ assuming that due to the Coulomb repulsion for the directions in the **k** space along which it happens that $f(\phi_{\mathbf{k}} - (\Omega_0/2\lambda\hbar\omega_D)\nu) \leq 0$ so that pairing does not occur. The expression (14) contains an important new physical result, namely, that the pair-breaking ability of the Coulomb repulsion depends on the quantity $\Omega_0/\hbar\omega_D$ describing the degree of separation between boson and fermion spectra. Most affected by the Coulomb repulsion are those pairs that are well separated in energy from the single-fermion continuum.¹⁹

Knowing the two-time GF $\langle \langle a_{\mathbf{k}\uparrow} | a_{\mathbf{k}'\uparrow}^+ \rangle \rangle_{\omega}$ and $\langle \langle a_{-\mathbf{k}\downarrow}^+ | a_{\mathbf{k}'\uparrow}^+ \rangle \rangle_{\omega}$ one can find expressions for the corresponding average values $\langle \langle a_{\mathbf{k}'\uparrow}^+ a_{\mathbf{k}\uparrow} \rangle \rangle_{\mathcal{H}}$ and $\langle \langle a_{\mathbf{k}'\uparrow}^+ a_{-\mathbf{k}\downarrow}^+ \rangle \rangle_{\mathcal{H}}$ from the relation³¹:

$$\langle A(t)B(t')\rangle_{\mathcal{H}} = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega(t-t')} J_{AB}(\omega),$$

where the so-called spectral density $J_{AB}(\omega)$ is in turn determined from:

$$\langle\!\langle A|B\rangle\!\rangle_{\omega+i\varepsilon} - \langle\!\langle A|B\rangle\!\rangle_{\omega-i\varepsilon} = -i(e^{\hbar\omega/k_BT} - 1)J_{BA}(\omega).$$

After some algebra one arrives at the expression:

$$\langle a_{\mathbf{k}\sigma}^{+} a_{\mathbf{k}\sigma} \rangle_{\mathcal{H}} \equiv n_{\mathbf{k}\sigma} = \frac{1}{2} \left[1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2k_{B}T}\right) \right],$$
 (16)

which defines the distribution over the states \mathbf{k} of free carriers which arise as *intrinsic excitations* of a system of paired fermions. To get (16) we rewrite the right-hand side of (11) as:

$$\frac{\hbar\omega + \xi_{\mathbf{k}}}{2E_{\mathbf{k}}} \left(\frac{1}{\hbar\omega - E_{\mathbf{k}}} - \frac{1}{\hbar\omega + E_{\mathbf{k}}} \right) \tag{17}$$

and apply the operator identity

$$\frac{1}{x \pm i\varepsilon} = \frac{1}{x} \mp i\delta(x) \tag{18}$$

to find the spectral density $J_{a_{\mathbf{k}\uparrow}^{+}a_{\mathbf{k}\uparrow}}(\omega)$. For gapless fermions, i.e., when $E_{\mathbf{k}} \equiv \xi_{\mathbf{k}}$, (16) becomes familiar occupation numbers,

$$n_{\mathbf{k}\sigma} = \frac{1}{2} \left[1 - \tanh\left(\frac{\xi_{\mathbf{k}} - E_F}{2k_B T}\right) \right] \tag{19}$$

characteristic for the Fermi–Dirac distribution of interactionless fermions. However, if $E_{\mathbf{k}}$ is gapped then (16) contrasts to the distribution of "normal" fermions. Namely, because of the rapid decrease of $x^{-1} \tanh x$ as x increases in (16), the occupation of high-energy single-fermionic states $E_{\mathbf{k}}$ appears denser than the occupation of states with lower $E_{\mathbf{k}}$. In fact, (16) reflects the occupation-number reduction of single-fermionic states. Such a reduction occurs much more effectively if $E_{\mathbf{k}}$ is small. Some of the fermions now appear involved into paired states. The majority of single-fermions in states close to the Fermi energy pair up and thus lead to a decrease in $n_{\mathbf{k}\sigma}$, explaining the behavior foreseen by (16).

4. Renormalized Boson Energies

Important quantities are the average number densities

$$n_{BQ} = \frac{1}{e^{\Omega_{\mathbf{Q}}/k_B T} - 1} \tag{20}$$

of bosonic CPs at a given two-fermion state Q, where $\Omega_{\mathbf{Q}}$ are energies of those states. However, $\Omega_{\mathbf{Q}}$ in (20) are not the energies $\mathcal{E}_{\mathbf{Q}}$ of "bare bosons" which appear in (2). Now bare bosons appear as "dressed" due to their interaction with fermions so that their energy $\mathcal{E}_{\mathbf{Q}}$ becomes a λ - and T-dependent $\Omega_{\mathbf{Q}}$. The total number-density of composite bosons at any T is then just:

$$n_B \equiv L^{-d} \sum_{\mathbf{Q}} n_{B\mathbf{Q}} \,. \tag{21}$$

Variation in T and/or in λ changes n_{BQ} and thus n_B which are functions of Ω_Q . This precise interpretation of Ω_Q thus defines the peculiarities of the BF system, in particular, the onset temperature T^* of boson formation and the BEC T_c . The condition $E_F = \mu$ yields the T^* below which a transition occurs from normal state with no composite bosons to one with such bosons. At T_c a singularity occurs in the total number density of bosons. This happens as boson energies are softened, i.e., as

 $\Omega_{\mathbf{Q}} \to 0$. In an isotropic model described by (1) without an explicit Coulombic term, an *implicit* equation to determine $\Omega_{\mathbf{Q}}$ was derived in Ref. 24 (see, also Ref. 19), namely:

$$\Omega_{\mathbf{Q}} = \mathcal{E}_{\mathbf{Q}} + f^2 L^{-d} \sum_{\mathbf{k}} \frac{1}{\Omega_{\mathbf{Q}} - 2\xi_{\mathbf{k}}} \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \tanh(E_{\mathbf{k}}/2k_B T).$$
 (22)

with

$$E_{\mathbf{k}} \equiv \sqrt{\xi_{\mathbf{k}}^2 + 2\lambda(\hbar\omega_D)(E_F - \mu)}.$$
 (23)

Here $\mathcal{E}_{\mathbf{Q}}$ are energies of initial interactionless bosons measured from *twice* the fermionic chemical potential μ . An expression for the renormalized $\Omega_{\mathbf{Q}}$ in a BF mixture with a spatially-uniform Coulomb interaction of strength $U_0 \geq 0$ between fermions will be reported elsewhere. To analyze (14) and (20), and to get a qualitative feel of boson formation in establishing electronic properties, we restrict ourselves to (22).

5. Discussion

Figure 1 shows $\Omega_0(\lambda, T)/E_F$ for several fixed values of $(E_F - \mu)/E_F$ (which determines the total boson number density $n_B(\lambda, T)$ Refs. 19 and 24) as a function of T/T_F . The dimensionless interaction parameters λ and $\hbar\omega_D/E_F$ are chosen to be respectively 0.7 and 0.2. By applying Eq. (37) of Ref. 24 for 2D superconductors, this particular choice of λ and $\hbar\omega_D/E_F$ yields for the BEC temperature

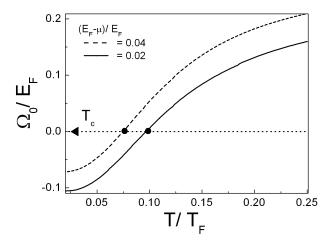


Fig. 1. Dimensionless remormalized bosonic CP energy $\Omega_0(\lambda,T)/E_F$ as function of T/T_F for several fixed fractional number densities $n_B(\lambda,T)/N(E_F)E_F=(E_F-\mu)/E_F$ of bosons. Figure schematically shows how non-temperature-dependent "bare" bosonic CP energies $\mathcal{E}_{\mathbf{K}}$ in (2) are renormalized by "switching-on" the BF vertex interaction. However, the position of $\mathcal{E}_{\mathbf{0}}$ measured from the total energy $2E_F$ of two interactionless fermions that make up a composite CP boson is not shown. Defined in Ref.²⁴ as $\mathcal{E}_{\mathbf{0}}=2[E_F+\hbar\omega_D/\sinh(1/\lambda)]$, it is a coupling-dependent energy, larger than $\Omega_0(\lambda,T)$ over the whole range of temperatures $T\leq T^*$. Here, λ and $\hbar\omega_D/E_F$ are chosen respectively to be 0.7 and 0.2. Black arrowhead marks associated BEC critical temperature.

the value $T_c/T_F = 0.03$. According to Eq. (36) from this latter reference, the deviation of $\mu(\lambda, T)$ from E_F at T_c (in E_F units) necessary for BEC to occur is $(E_F - \mu)/E_F = 0.06$. Specifically, BEC does not occur until the fractional boson density, Eq. (20) in Ref. 24,

$$n_B(\lambda, T)/N(E_F)E_F = (E_F - \mu)/E_F,$$
 (24)

(the ratio of total boson number to the number of available states) reaches the critical value 0.06. Clearly, Ω_0 is positive at higher T. However, for any fixed $n_B(\lambda, T)$ the boson energy $\Omega_0(\lambda, T)$ decreases monotonically upon cooling and passes through zero at a value of T/T_F determined by the value of $n_B(\lambda, T)$ alone. Physically, the composite-boson concentration $n_B(\lambda, T)$ in a BF mixture increases at lower values of T, as expected. From Fig. 1, for larger $n_B(\lambda, T)$ the temperature T at which $\Omega_0(\lambda, T)$ changes sign (indicated by dots in figure) and shifts to lower T. However, BEC cannot occur until $n_B(\lambda, T)$ is at least as large as the critical value $n_B(\lambda, T_c)$. For the parameters chosen in Fig. 1, BEC does not occur whenever $n_B(\lambda, T)/N(E_F)E_F < 0.06$.

In a binary mixture of mutually-converting fermions and bosons $n_B(\lambda, T)$ is not fixed as in Fig. 1. But, since upon cooling thermal dissociations of pairs are reduced, the number of fermions bound into bosons increases and this occurs in accordance with (5). The number $n_B(\lambda, T)$ rises and precisely at T_c it reaches the critical value $n_B(\lambda, T_c)$ required for BEC. Owing to this continuous increase in $n_B(\lambda, T)$, the value of $\Omega_0(\lambda, T)$ does not vanish until T equals T_c , or

$$\lim_{T \to T_c} \Omega_0(T) = 0. \tag{25}$$

Thus, from Fig. 1 one concludes that in a BF mixture with varying boson number density $n_B(\lambda, T)$ the temperature-dependent quantity $\Omega_0(\lambda, T)$ changes sign precisely at the T_c associated with BEC (black arrowhead at $T_c/T_F = 0.03$ in figure). It should be noted that the temperature-dependent behavior of boson energies found here relies on (22) and is thus associated with boson formation/disintegration processes alone.

At the finite temperatures, there are two types of free fermionic charge carriers in the system mutually converting into each other: first, pairable but still unpaired fermions with energies $\xi_{\bf k} \equiv \epsilon_{\bf k} - \mu$ distributed continuously near the Fermi level, and second, single-electron excitations of the condensate of paired fermions (i.e., excitations of the bosonic subsystem sometimes called "bogolons") whose energy spectrum is gapped with a Bogoliubov spectrum (13). In thermodynamic equilibrium we assume that these two different kinds of fermions are distributed in energy as usual, according to

$$n_{\mathbf{k}\sigma} = \frac{1}{2} \left[1 - \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T}\right) \right],$$
 (26)

where $E_{\mathbf{k}}$ is $\xi_{\mathbf{k}}$ for free and $\sqrt{\xi_{\mathbf{k}}^2 + E_{g\mathbf{k}}^2}$ for gapped fermions (the bogolons). The generalized gap $E_{g\mathbf{k}}$ in $E_{\mathbf{k}}$, (13), differs from zero only in specific directions of the

2D vector **k**. Furthermore, for any deviation of k from k_F one expects that $E_{g\mathbf{k}}$ approaches rapidly to zero.

From (14) the behavior of $E_{g\mathbf{k}}$ as a function of the direction of the wavevector \mathbf{k} is expressed in terms of dimensionless anisotropy factors $\phi_{\mathbf{k}}$ whose explicit expression requires a detailed microscopic treatment. However, to extract qualitative features of the effect of actual anisotropic interactions, one may approximate $\phi_{\mathbf{k}}$ by modeling it in line with common symmetry requirements. Specifically, we shall assume that as \mathbf{k} changes the function $\phi_{\mathbf{k}}$ varies in accordance with the symmetry of a 2D square Brillouin zone. It can thus be fitted as:

$$\phi_{\mathbf{k}}^{\alpha} = \frac{1}{1 - \alpha/2} (1 - \alpha \sin^2 2\varphi) \tag{27}$$

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 k-space of the 2D vector \mathbf{k} . Here $0 \le \alpha \le 1$ in general and $\alpha = 0$ for isotropic superconductors. Varying α from 0 to 1 spans all ranges from weak to very strong anisotropy. Note that $\phi_{\mathbf{k}}$ (27) modulates the angular dependence of the anisotropic BF interaction strength $f_{\mathbf{k}} \equiv f\phi_{\mathbf{k}}$ which is assumed to be distributed within the interval $f - \Delta f \le f_{\mathbf{k}} \le f + \Delta f$ of width $2\Delta f$ around its average value f in (1). To illustrate how $\phi_{\mathbf{k}}^{\alpha}$ varies with the direction of \mathbf{k} , i.e., with the azimuthal angle φ , in Fig. 2 it is shown for values $\alpha = 0.25, 0.35$ and 0.45. In our reference calculation we use $\alpha = 0.35$ (full curve in figure).

From (14) $E_{g\mathbf{k}}(\lambda, T)$ is largest along the directions of maximum $\phi_{\mathbf{k}}$. But for any fixed λ and T as the vector \mathbf{k} deviates from the axes along which the gap is maximum, it decreases and turns to zero at points where $\phi_{\mathbf{k}}$ becomes equal or less

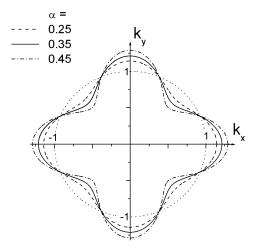


Fig. 2. Anisotropy factors $\phi_{\bf k}^{\alpha}$ defined in (27) as function of direction of the 2D vector $\bf k$ for three different values of $\alpha=0.25,\ 0.35$ and 0.45. Variation of the BF interaction strength $f_{\bf k}$ is modulated in terms of factors $\phi_{\bf k}^{\alpha}$ distributed within an interval of width $2\Delta\phi_{\bf k}^{\alpha}$ around their average value depicted as the dotted circle of radius 1. In the present work we used $\alpha=0.35$ (full curve) in the calculation of Fig. 3.

than the contribution coming from the term $R \equiv (\Omega_0/2\lambda\hbar\omega_D)\nu$ in (14). This $\lambda, \hbar\omega_D$, $\nu \equiv N(0)U_0$ and T dependent, dimensionless parameter R has been introduced in Ref. 19 where it was shown that due to variation of Ω_0 on T, the magnitude of R and therefore the *sizes* of the regions within which quasiparticles exhibit either gapped $\sqrt{\xi_{\mathbf{k}}^2 + E_{g\mathbf{k}}^2}$ or a normal $\xi_{\mathbf{k}}$ behavior, are not constant but rather change with temperature.

Figure 3 shows occupation numbers $n_{\mathbf{k}\sigma}$ of states with least energy $\xi_{\mathbf{k}}=0$ above μ as a function of the azimuthal angle φ determining the direction in k-space of the 2D vector \mathbf{k} for several fixed values of reduced temperature $t=T/T_F$. Comparison is made between $n_{\mathbf{k}\sigma}s$ as temperature is reduced from T^* towards T_c . To get Fig. 3, as in the case of the full curve in Fig. 1, we have used $\lambda=0.7$, $\hbar\omega_D/E_F=0.2$ and the fractional boson density (24) is assumed fixed at 0.04. Regarding the dimensionless Coulomb parameter in Fig. 3 we use $\nu=1.1$. As readily seen from (26), for temperatures $T\geq T^*$, $n_{\mathbf{k}\sigma}$ as a function of $\xi_{\mathbf{k}}\equiv\epsilon_{\mathbf{k}}-\mu$ behaves as in normal metals. Namely, it does not depend on the direction of \mathbf{k} and as the energy $\xi_{\mathbf{k}}$ increases, $n_{\mathbf{k}\sigma}$ drops from 1 to 0 remaining exactly equal to 1/2 for states with least energy. And the width of the energy interval around E_F within which occupation numbers vary from 1 to 0 is $\sim T/T_F$. However, at temperatures below T^* , as seen from Fig. 3, this happens only for disconnected segments of \mathbf{k} wherein the energy gap (14) associated with CP formation vanishes. These segments, whose extension is determined by $\phi_{\mathbf{k}} \leq (\Omega_0/2\lambda\hbar\omega_D)\nu$, trace out

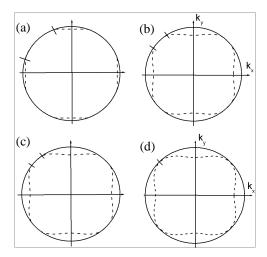


Fig. 3. Occupation numbers $n_{\mathbf{k}\sigma}$ of the least-energy state measured from μ as function of direction of the 2D vector \mathbf{k} . Comparison is made between $n_{\mathbf{k}\sigma}s$ as the temperature (in T_F -units) is reduced from T^* towards to T_c [graphs from Fig. 3(a) to Fig. 3(d)]. Fermi arcs are depicted as segments of azimuthal angle φ between two strokes along $n_{\mathbf{k}\sigma}$ versus φ curves. The reduction in size of Fermi arcs (i.e., extension of segments between consecutive strokes) are clearly seen as T is reduced from T^* towards to T_c . As the BEC is approached, these consecutive strokes join together into a single stroke as, Fig. 3(d).

along the Fermi surface loci called "Fermi arcs". The energy gap (14) along such arcs of the 2D Fermi surface thus disappears. On the other hand, outside these Fermi arcs, i.e., within regions wherein the opposite condition $\phi_{\mathbf{k}} \geq (\Omega_0/2\lambda\hbar\omega_D)\nu$ holds, there are no singly-occupied-fermionic states immediately near the energy equal to μ . Dispersion in such regions is analogous to a Bogoliubov dispersion relation but with the generalized gap (14). Single-fermionic states along such directions are acceptable only for high-energy fermions with $\xi_{\mathbf{k}} \geq E_{g\mathbf{k}}(\lambda, T)$, i.e., for fermions appearing as a result of pair disintegrations in the subsystem of incoherent bosons. Finite, but significantly reduced $n_{\mathbf{k}\sigma}$ seen outside Fermi arcs in Fig. 3 arise from "bogolons" whose energy (least energy $\xi_{\mathbf{k}} = 0$) is higher by $E_{g\mathbf{k}}$ than energy μ around which the fermions from the Fermi arcs are distributed. As a result of the difference in energy scales, where $E_{\mathbf{k}}$ in (26) is either $\xi_{\mathbf{k}}$ or $\sqrt{\xi_{\mathbf{k}}^2 + E_{g\mathbf{k}}^2}$, the occupation of states with wavenumber k directed along various segments appear significantly different.

From Fig. 3, a difference begins to appear on cooling in the distribution of single-fermion states over varying angles φ . First, small "islands" of reduced $n_{\mathbf{k}\sigma}$ emerge in the directions of maximum $\phi_{\mathbf{k}}$. Further lowering T is followed by shortening Fermi arcs, depicted in Fig. 3 as small arcs between two short strokes on $n_{\mathbf{k}\sigma}$ -vs- φ -curves in going from (a) to (b) \cdots to (d). Below the temperature at which the Coulomb factor $R \equiv (\Omega_0/2\lambda\hbar\omega_D)\nu$ passes through the minimum of the anisotropy factor $\phi_{\mathbf{k}}$ the areas with normal distribution of fermions, i.e., Fermi arcs, disappear entirely and the attractively-interacting Fermi gas becomes an anisotropic mixture of coexisting bosons and fermions mutually converting into each other.

The idea of the presence of various charge-carrier groups in HTSCs has been extensively explored in the literature (see, e.g., Ref. 34). In particular, a phenomenological model with Fermi lines on a 2D square-like Fermi surface and regions of momentum space with bosons, originating from fermions paired into a d-wave symmetry state, was proposed in Ref. 35. However, in most studies such as this latter reference, temperature, coupling and the boson-number-density dependences of boson energies which are so important, were missed. The presence of disconnected Fermi arcs in HTSC films is also well-established experimentally.^{8–10,36}

Lastly, we note that in the newly discovered iron-based superconductors such as $BaFe_2(As_{0.7}P_{0.3})$ Zhang *et al.* report³⁷ the discovery of several disconnected Fermi surfaces and ring-like gap nodes on the Fermi surface. These properties are fully consistent with the results of the present paper.

6. Conclusions

Introducing a uniform Coulomb interaction in an anisotropic BF binary gas mixture model reveals, in the pseudogap phase, along with the BF mixture regions (or BF regions where the quasiparticles exhibit a Bogoliubov-dispersion behavior) also the so-called *Fermi arcs* alongside of which a *normal* (i.e., with *no* pseudogap) distribution of free fermions prevails. On cooling, the extent of these Fermi arcs

diminishes, but BF regions grow and merge into one another at temperatures when the Fermi arcs disappear altogether. This occurs because of a softening of the boson energies as one approaches the BEC at lower T. Explanation for the presence of Fermi arcs with the temperature-dependent extension becomes possible owing to the softening of boson energies as one decreases T. Indeed, if (25) did not occur, then the extension of the Fermi arcs would hardly decrease on lowering T. The present work predicts, even in phonon-mediated dynamics, the presence in the energy-momentum dispersion relation of HTSCs of a line of nodal points, i.e., lines in momentum space along which the generalized gap (14) vanishes, and hence, gives rise to Fermi arcs as reported in Refs. 8, 9 and 36.

Acknowledgments

MdeLl thanks UNAM-DGAPA-PAPIIT (Mexico) for partial support through grant IN102011.

Appendix A.

It is well-known that the Cooper equation 30 for the energy eigenvalue $\varepsilon_{\mathbf{0}}$

$$1 = \frac{\lambda}{2} \int_{E_F}^{E_F + \hbar \omega_D} \frac{d\epsilon}{\epsilon - E_F - \varepsilon_0 / 2}$$
 (A.1)

straightforwardly lead to the familiar negative-energy solution of zero-CMM K=0 CPs

$$\varepsilon_{\mathbf{0}}^{-} = -\frac{2\hbar\omega_{D}}{\exp(2/\lambda) - 1} \xrightarrow[\lambda \to 0]{} -2\hbar\omega_{D} \exp(-2/\lambda) < 0. \tag{A.2}$$

Being the energy of two electrons relative to the energy $2E_F$ of a free two-electron state (A.2) implies a bound state of two electrons. This negative-energy solution $\varepsilon_{\mathbf{0}}^{-}$ played a key role in understanding the superconducting state and leads to the BCS theory¹⁶ of SCs. Note that in its original form (A.1) is valid only for negative $\varepsilon_{\mathbf{0}}$ since if $\varepsilon_{\mathbf{0}} \geq 0$ but lying within the interval $0 < \varepsilon_{\mathbf{0}} < 2\hbar\omega_D$ the integrand in (A.1) has a singularity.

It is commonly believed that for $\varepsilon_0 \geq 0$ the two-electron states are simply scattering states.³⁸ However, as reported in Refs. 26–29 two-fermion-states with a total energy $\geq 2E_F$ raised the question of whether there are two-particle solutions with an energy embedded in the continuum of single fermionic states of the attractively-interacting gas of electrons. If so, these might be suggestive of a resonant-like quasi-bound state in the continuum. Here we address this question by showing that if one isolates a simple pole at $\epsilon = E_F + \varepsilon_0/2 \equiv \epsilon_0$ in (A.1) by shifting it onto the complex plane, then such a solution is already present in the Cooper problem. One can substitute the integral on the right-hand side of (A.1) by its principal value to give:

$$2/\lambda = \frac{1}{2} \lim_{\eta \to 0} \int_{E_F}^{E_F + \hbar \omega_D} d\epsilon \left(\frac{1}{\epsilon - \epsilon_0 - i \eta} + \frac{1}{\epsilon - \epsilon_0 + i \eta} \right)$$

$$\begin{split} &=\frac{1}{2}\lim_{\eta\to 0}\int_{E_F}^{E_F+\hbar\omega_D}d\epsilon\frac{2(\epsilon-\epsilon_0)}{(\epsilon-\epsilon_0)^2+\eta^2}\\ &=\frac{1}{2}\lim_{\eta\to 0}\ln\left(\frac{(E_F+\hbar\omega_D-\epsilon_0)^2+\eta^2}{(E_F-\epsilon_0)^2+\eta^2}\right)\\ &=\frac{1}{2}\lim_{\eta\to 0}\ln\left(\frac{[E_F+\hbar\omega_D-(E_F+\varepsilon_0/2)]^2+\eta^2}{[E_F-(E_F+\varepsilon_0/2)]^2+\eta^2}\right)\\ &=\ln\left(\frac{2\hbar\omega_D-\varepsilon_0}{\varepsilon_0}\right). \end{split}$$

This immediately leads to the scarcely-known "improper" positive-energy solution

$$\varepsilon_{\mathbf{0}}^{+} = +\frac{2\hbar\omega_{D}}{\exp(2/\lambda) + 1} \xrightarrow{\lambda \to 0} +2\hbar\omega_{D} \exp(-2/\lambda) > 0 \tag{A.3}$$

reported in Ref. 25 and based exclusively on the elementary fact that $\int x^{-1} dx = \ln |x|$ and not $\ln x$ as commonly assumed.

It should be noted that the shift of a singularity in (A.1) onto complex plane, by substituting $\epsilon_0 \to \epsilon_0 + i\eta$ in (A.1), is physically equivalent to introducing a damping η of two-particle states, ignored entirely in obtaining (A.1). Once raised above the Fermi sea, these positive-energy CPs readily dissipate into two free fermions.

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