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Depairing and Bose–Einstein condensation temperatures in a boson–fermion superconductor model with Coulomb effects

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An extended boson–fermion (BF) model is introduced describing the evolution of attractively interacting single electrons into a binary mixture of unpaired electrons plus incoherent bosonic Cooper pairs as absolute temperature T is lowered. The new model is employed to determine how the system, upon cooling, exhibits critical temperatures for: a) incoherent boson formation below T^* as well as b) for creating a coherent boson fluid below T_c. Critical temperatures T^* and T_c are related with the dynamical parameters of the attractively interacting fermion system. It is shown that the introduction of a uniform Coulomb interaction in an anisotropic BF binary gas mixture model allows finding *not only* a self-consistent description of a pseudogap and a dome-shaped T_c-vs-doping behaviour, but also to predict, even in a phonon-mediated many-electron dynamics, of an energy–momentum dispersion that is either gapped or not depending on direction. This manifests itself in high-T_c superconductors as curves in momentum space along which the superconducting gap vanishes, hence giving rise to the so-called "Fermi arcs" observed in angle-resolved-photoemission spectroscopy experiments.

Keywords: boson–fermion models; boson formation; Bose–Einstein condensation; pseudogap; fermi arcs

1. Introduction

A possible origin for the opening of a so-called *pseudogap* [1] in the electronic spectrum of high-temperature superconductors (HTSCs) is the formation [2] of so-called *preformed* but incoherent Cooper pairs (CPs), well above the critical superconducting temperature T_c below which coherence sets in. A growing number of experimental data for pairing [3–6] above T_c in cuprate superconductors reinforce interest in pseudogap scenarios via the notion of preformed CPs. Unprecedented experimental findings (see, e.g. in Ref. [3]) reveal a dispersion behaving in a portion of the Brillouin zone as if the sample was a normal metal and in the remaining portion exhibiting a Bogoliubov-type gapped spectrum. This bolsters the belief that at temperatures below some T^* in the ground state of HTSCs single fermions coexist with the preformed CPs. Consequently, various boson–fermion (BF) models became natural candidates to describe novel features of HTSCs. Such BF

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models are based on the notion that in the presence of an effective interfermion attractive interaction, the gas of single fermionic charge carriers in an ionic lattice can evolve into both pairable but unpaired (or itinerant) fermions *plus* individual bosonic CPs. A simple enough Hamiltonian, say $\mathcal{H}^o$, describing a binary gas mixture of fermions interacting with bosons was introduced phenomenologically in Ref. [7]. That Hamiltonian was later derived from a model [8] based on the presence of two types of electrons–*wide- and narrow-band*–interacting with each other. Shortly after the discovery of HTSCs, the pairing model proposed in Ref. [7] was applied by many authors (e.g. Refs. [9–23]) to manifest its relevance to HTSCs. The chronological order of the development and perspectives of a mixture model of local pairs coexisting with the quasifree electrons is sketched in Ref. [22]. In particular, these models were generalized (see, e.g. Refs. [19,23,24]) to contain additional terms, $\mathcal{H}_{eB}$ describing anisotropic CP formation as well as Coulomb repulsion $\mathcal{H}_U$ between fermions. This extension of the usual BF models is embodied in the Hamiltonian

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

The first term $\mathcal{H}^o$ includes the sum of Hamiltonians of free (pairable but unpaired) fermions $\mathcal{H}_e$ and of composite-boson CPs $\mathcal{H}_B$, specifically

$$\mathcal{H}^o \equiv \mathcal{H}_e + \mathcal{H}_B = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} a^+_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \mathcal{E}_{\mathbf{k}} b^+_{\mathbf{k}} b_{\mathbf{k}} \tag{2}$$

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 [25,26] (for a brief survey see Ref. [27]) to be bosonic operators associated with CPs of definite total, or centre-of-mass momentum (CMM), wavevector $\mathbf{K} \equiv \mathbf{k}_1 + \mathbf{k}_2$ as the sum of wavevectors of two electrons.

The second term $\mathcal{H}_{eB}$ in (1) is

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

and describes boson formation/disintegration processes where $f_{\mathbf{q}} \equiv f\phi_{\mathbf{q}}$ is a phenomenological BF coupling constant distributed around its average value f, 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. Here, $\hbar\omega_D$ is the ionic crystal Debye energy while $f_{\mathbf{q}}$ contains so-called anisotropy factors $\phi_{\mathbf{q}} = \phi_{-\mathbf{q}}$ introduced to mimic the anisotropy of the BF interaction responsible for CP formation. We note that the Hamiltonian (1) can be derived from the strongly interacting Hubbard model on a square lattice as a low-energy limit of cluster states [28].

Many studies exist supporting either d- or s- (or a $s + d$ mixture) wave scenarios. Experiments probing the surface of cuprates yield d-wave, but experiments probing the bulk suggest a substantial s-symmetry (see, e.g. in Ref. [29]). In Ref. [30] support is argued for extended s-wave rather than d-wave superconductivity in cuprates. In contrast, a clever experiment [31] was crucial in showing that the superconducting order parameter is predominantly of d-symmetry with an admixture of s-symmetry of only about 3% in YBCO. Nonetheless, we note that to describe d-wave superconductivity one needs *no* explicit d-wave symmetry in the underlying pairing interaction as already a moderate anisotropy of the pairing interaction included simultaneously with the uniform Coulomb repulsion

may result in a d-wave-like dispersion of single fermions excited in the superconducting state. This becomes possible owing to the specific temperature dependence of the pair-breaking ability of repulsive Coulomb interaction and, *as shown* in Ref. [24], occurs quite independently of the symmetry of the pairing interaction which may be d- and moderate s-wave-like. Thus, we let $\phi_{\mathbf{q}}$ in (3) to be of both types either s- or d.

In a *ternary* gas formalism that does *not* neglect two-hole CPs alongside the two-electron CPs accounted for in the binary-gas Equations (1)–(3), one can make [25–27] *perfect* contact with both BCS theory and also with the T.D. Lee BF model [10,12,13] if the BF vertex coupling constant f is assumed to be $\sqrt{2\hbar\omega_D V}$ where $V \geq 0$ is the usual BCS model effective attractive interaction between electrons. In fact, both BCS and T.D. Lee theories can be shown to be special cases of the so-called generalized BEC formalism described in Refs. [25–27].

The last term $\mathcal{H}_U$ in (1) is taken as

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

and models the repulsive Coulomb interaction between fermions making up CPs. Here this is assumed to be a uniform repulsive field of strength $U \geq 0$.

In (1) fermion $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$ 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 whose operator is

$$N \equiv \sum_{\mathbf{k},\sigma} a^+_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + 2\sum_{\mathbf{k}} b^+_{\mathbf{k}} b_{\mathbf{k}} \tag{5}$$

and includes both the number of unpaired fermions and, of course, twice the number of bosons. It commutes with (1) and is therefore an invariant of motion for the BF mixture state. In cuprates (1) implies that by introducing holes of concentration x onto the CuO_2 planes N electrons from neighbouring atoms with these hole centres become mobile. Holes are seen by mobile electrons as hopping centres. These electrons which at $T = 0$ would fill states up to the Fermi energy E_F interact with each other via repulsive Coulomb forces plus some pairing attractive interaction due, e.g. to phonons. This results in bosonic CPs. Equation (5) widely introduced (see, e.g. Ref. [13]) in binary BF gas mixture models, contrasts sharply with BCS theory. Indeed, CPs (with CMM $K = 0$) in BCS theory appear at temperatures above T_c only as superconducting fluctuations [32]. And, in fact, nonzero CMM CPs are entirely neglected in BCS theory. However, in a BF binary mixture of bosons and fermions that mutually convert into one another, the temperature- and coupling-dependent *total* number density n_B of bosonic CPs may be different from zero on *either* side of T_c; this suggests the emergence above T_c of *incoherent* and below T_c of *coherent,* equilibrium pair densities.

The main feature of the present model which differs from ordinary binary gas BF models Refs. [9,10,12,13] is that one starts from CPs shifted in energy at zero K from E_F by a *positive* gap. That is, the boson spectrum $\mathcal{E}_{\mathbf{K}}$ in (1) is taken as

$$\mathcal{E}_{\mathbf{K}} = 2(E_F - \mu) + 2\Delta + \varepsilon_{\mathbf{K}} \tag{6}$$

where $\varepsilon_{\mathbf{K}}$ is a nonnegative CP excitation energy that vanishes for $K = 0$. Thus, in (6) $\mathcal{E}_{\mathbf{K}}$ is assumed to be higher than the total energy $2E_F$ of two individual electrons before

confining themselves into bosonic CPs by a positive gap 2Δ. Separation of the initial attractively interacting fermion system into bosons plus (unpaired) fermions with spectra shifted with respect to each other by the coupling-dependent, positive-energy gap of 2Δ is a new ingredient in the present BF model (1) introduced in Refs. [24–26,33–36].

Cuprates have numerous distinct phases observed at different absolute temperatures T and compositions x of holes doped into the CuO_2 planes. Any comprehensive theory of high-T_c-materials should ideally deduce, within a single unified conception, the dominant interactions underlying the origin of each region of the phase diagram (see e.g. Figure 1 in Ref. [2]). As seems to be suggested by that diagram, the normal state of cuprates has very little in common with the ordinary Fermi liquid on which the present paper is based. Therefore, a more natural question is "how can such a simplified model described by (1) address such complicated systems as HTSCs?"

To answer this we note that many researchers seem to agree that HTSCs in their superconducting state obey the standard BCS quasiparticle description. This is the most striking dilemma of high T_c superconductors boldly emphasized by Anderson. Specifically, starting from the Fermi liquid concept he has constructed [37] a transformation which projects the wavefunction of an ordinary Fermi liquid into the wavefunction of HTSC cuprates. Anderson highlights the notion that high-T_c phenomena might be examples of "hidden Fermi liquids" (HFLs) a phrase introduced by him to denote nonFermi liquid states that are related to ordinary Fermi liquids. Quasiparticles of the Fermi liquid emerge in both the superconducting and pseudogap states, the two regions of the complete phase diagram [2] addressed in this paper. In Ref. [2] moreover, special attention is given to so-called "preformed CPs" as well as "Fermi arcs" also addressed in the present paper.

In Section 2, an explicit expression for the boson energies and for total boson number density is derived in a BF mixture with a spatially uniform Coulomb interaction of strength $U \geq 0$ between the fermions bound up in CPs. Those expressions are then applied in Sections 3 and 4 to determine the characteristic temperatures T^* and T_c wherein the role of a uniform Coulomb interaction in forming the BF mixture properties is discussed. In particular, how boson energies given by (6) are feasible is treated in Section 3. In Section 5 concluding remarks are given.

2. Renormalized boson energies and boson number densities

Renormalized boson energies $\Omega_{\mathbf{Q}}$, as function of the CP CMM wavevector $\mathbf{Q}$, in the BF mixture may be found, e.g. by use of an infinite chain of equations for two-time retarded Green functions (GF) $\langle\langle A(t) \mid B(t')\rangle\rangle$ as defined in Equation (2.1b) of Ref. [38] for dynamical operators $A(t)$ and $B(t')$ at times t and t' in the Heisenberg representation. The energy $\hbar\omega$-dependent Fourier transform $\langle\langle A \mid B\rangle\rangle_\omega$ of $\langle\langle A(t) \mid B(t')\rangle\rangle$ then satisfies the infinite chain of equations (see, e.g. Equation (A2) in Ref. [34])

$$\hbar\omega \langle\langle A \mid B\rangle\rangle_\omega = \langle [A, B]_\eta \rangle_{\mathcal{H}} + \langle\langle [A, \mathcal{H}]_- \mid B\rangle\rangle_\omega \tag{7}$$

where the single-angular brackets $\langle X\rangle_{\mathcal{H}}$ of an operator X are T-dependent thermal averages over the Hamiltonian $\mathcal{H}$, while the square brackets $[A, B]_\eta \equiv AB + \eta BA$ denote the commutator ($\eta = -1$) or anticommutator ($\eta = +1$) of operators A and B.

Choosing first $A \equiv b_{\mathbf{Q}}$ and $B \equiv b_{\mathbf{Q}}^{+}$ in (7) with $\eta = -1$ we write (7) as

$$\omega \left\langle\!\left\langle b_{\mathbf{Q}} \mid b_{\mathbf{Q}}^{+} \right\rangle\!\right\rangle_{\omega} = 1 + \left\langle\!\left\langle \left[b_{\mathbf{Q}}, \mathcal{H}\right]_{-} \mid b_{\mathbf{Q}}^{+} \right\rangle\!\right\rangle_{\omega} \tag{8}$$

since $\left[b_{\mathbf{Q}}, b_{\mathbf{Q}}^{+}\right]_{-} = 1$. As is customary in BF models, we assume that fermionic a and bosonic b operators commute with each other. Equation (8) is the first of an infinite chain of equations containing higher order Green functions. An expression for second-order Green function on the rhs of Appendix, Equation (1), can be established if in (7) one takes $\left[b_{\mathbf{Q}}, \mathcal{H}\right]_{-}$ for A and B is still $b_{\mathbf{Q}}^{+}$, namely

$$\hbar\omega \left\langle\!\left\langle \left[b_{\mathbf{Q}}, \mathcal{H}\right]_{-} \mid b_{\mathbf{Q}}^{+} \right\rangle\!\right\rangle_{\omega} = \left\langle \left[\left[b_{\mathbf{Q}}, \mathcal{H}\right]_{-}, b_{\mathbf{Q}}^{+}\right]_{-} \right\rangle_{\mathcal{H}} + \left\langle\!\left\langle \left[\left[b_{\mathbf{Q}}, \mathcal{H}\right]_{-}, \mathcal{H}\right]_{-} \mid b_{\mathbf{Q}}^{+} \right\rangle\!\right\rangle_{\omega}. \tag{9}$$

As to the higher order Green functions on the rhs of (9) for $\left\langle\!\left\langle \left[b_{\mathbf{Q}}, \mathcal{H}\right]_{-} \mid b_{\mathbf{Q}}^{+} \right\rangle\!\right\rangle_{\omega}$ they may be cast as linear combinations of lower order ones [39]. Lengthy manipulations, the details of which are given below in Appendix, lead to the final expression for the single-boson Green function

$$\left\langle\!\left\langle b_{\mathbf{Q}} \mid b_{\mathbf{Q}}^{+} \right\rangle\!\right\rangle_{\omega} = \left\{ \omega - \mathcal{E}_{\mathbf{Q}} - \frac{\frac{f^2}{L^d} \sum_{\mathbf{q}} \left|\phi_{\mathbf{q}}\right|^2 \frac{F(\mathbf{q},\mathbf{Q})}{\omega - \zeta(\mathbf{q},\mathbf{Q})}}{1 - \frac{U}{L^d} \sum_{\mathbf{q}} \phi_{\mathbf{q}} \frac{F(\mathbf{q},\mathbf{Q})}{\omega - \zeta(\mathbf{q},\mathbf{Q})}} \right\}^{-1} \tag{10}$$

where

$$F(\mathbf{q},\mathbf{Q}) \equiv 1 - n_{\mathbf{q}+\mathbf{Q}/2\uparrow} - n_{-\mathbf{q}+\mathbf{Q}/2\downarrow} \quad \text{and} \quad \zeta(\mathbf{q},\mathbf{Q}) \equiv \xi_{-\mathbf{q}+\mathbf{Q}/2} + \xi_{\mathbf{q}+\mathbf{Q}/2}. \tag{11}$$

The former expression is the generalization of Equation (B10) in Ref. [34] for an anisotropic BF mixture with a uniform Coulomb field. Ignoring the Coulomb repulsion between fermions and assuming the system to be isotropic, then (10) takes the same form as Equation (B10) in Ref. [34]. Poles $\omega = \Omega_{\mathbf{Q}}$ of the (10) which are roots of the equation

$$\Omega_{\mathbf{Q}} = \mathcal{E}_{\mathbf{Q}} + \left(1 - \frac{U}{L^d} \sum_{\mathbf{q}} \phi_{\mathbf{q}} \frac{F(\mathbf{q},\mathbf{Q})}{\Omega_{\mathbf{Q}} - \zeta(\mathbf{q},\mathbf{Q})}\right)^{-1} \left(\frac{f^2}{L^d} \sum_{\mathbf{q}} \left|\phi_{\mathbf{q}}\right|^2 \frac{F(\mathbf{q},\mathbf{Q})}{\Omega_{\mathbf{Q}} - \zeta(\mathbf{q},\mathbf{Q})}\right) \tag{12}$$

define the single-boson spectrum in the BF mixture phase. Here $\mathcal{E}_{\mathbf{Q}}$ are energies of the initial noninteracting bosons (6). Energies $\Omega_{\mathbf{Q}}$ determine the average number $n_{B\mathbf{Q}} \equiv \left\langle b_{\mathbf{Q}}^{+} b_{\mathbf{Q}} \right\rangle$ of bosonic CPs for a given CMM wavevector $\mathbf{Q}$; they are found (see, e.g. Equation (12) of Ref. [34]) to be

$$n_{B\mathbf{Q}} = \frac{1}{\exp(\Omega_{\mathbf{Q}}/k_B T) - 1}. \tag{13}$$

These numbers $n_{B\mathbf{Q}}$ yield for the *total* boson number density

$$n_B = L^{-d} \sum_{\mathbf{Q}} n_{B\mathbf{Q}}. \tag{14}$$

Note, however, that $n_{B\mathbf{Q}}$ and n_B are determined not through the energies $\mathcal{E}_{\mathbf{Q}}$ of "bare bosons" appearing in (2) but rather on $\Omega_{\mathbf{Q}}$ given by (12). Indeed, due to interaction with

fermions, bare bosons become renormalized or "dressed" so that their energies $\mathcal{E}_{\mathbf{Q}}$ are replaced with $\Omega_{\mathbf{Q}}$. Hence, the $n_{B\mathbf{Q}}$s and thus n_B turn out to be the λ- and T-*dependent*. Because $n_{B\mathbf{Q}}$ are nonnegative, one must have $\Omega_{\mathbf{Q}} \geqslant 0$ in (13). In analogy to that of a pure boson gas [40], singularities in the behaviour of n_B signal possible anomalies in the system. Because $\varepsilon_{\mathbf{Q}} \geqslant 0$ in (6) the singularity in (14) occurs at complete softening, i.e. $\Omega_{\mathbf{Q}} \to 0$, of a boson energy with $Q = 0$. One such singularity in n_B occurs when $E_F = \mu$, i.e. at the boundary where the transition occurs from the normal state with *no* bosonic CPs to one *with* such pairs. This happens at a specific temperature, say, T^*. Another singularity appears when μ becomes less than E_F. On cooling below T^* the value of μ dips below the E_F. The deviation of μ from E_F is accompanied by further bosonization, i.e. with modification of n_B as given in Ref. [34] by a factor $E_F - \mu$ as

$$n_B(\lambda, T) = N(E_F)\,[E_F - \mu(\lambda, T)] \tag{15}$$

where $N(E_F)$ is the electronic density of states (DOS) (per spin and per unit volume) at the Fermi surface. For sufficiently large $E_F - \mu$ the total number density of bosons n_B reaches a critical value sufficient for BEC to occur. This takes place when the condition $\Omega_{\mathbf{0}}(\mu, T) = 0$ is satisfied, i.e. when (13) and therefore (14) undergoes another singularity at some μ different from E_F .

Therefore, precise interpretation of (12) defines the peculiarities of the BF system. In particular, the condition $\Omega_{\mathbf{0}} = 0$ satisfied at *different fillings* of single-particle states relates, with the parameters of the attractively interacting fermion system, the temperature T^* (below which incoherent CP bosons form) as well as the BEC T_c (below which a coherent bosonic fluid emerges). We employ this idea to determine $T^*$and T_c. Here we note that in an *isotropic* model described by (1) *without* an explicit Coulombic term, an implicit equation to determine $\Omega_{\mathbf{Q}}$ was found in Equation (13) of Ref. [34].

3. Onset temperature T^* for boson formation without coherence

Within the description (1) it was possible to calculate the characteristic $T^* > T_c$ only by assuming two-fermion states to be bosons with total *bare* energies $\geq 2E_F$ (see Ref. [34]). This is sharply distinct from the BCS model based not on actual bosonic CPs but on Cooper *correlations* with energy $\leq 2E_F$. The question "does a system of attractively-interacting fermions possess two-fermion-excitations" has been discussed extensively. It was found (see, e.g. Refs. [35,41–45]) that switching on an attraction between fermions actually produces two-fermionic *resonances* but separated from E_F by a *positive* gap. By virtue of the presence of a gap, however, these resonances hardly become actual states of two correlated fermions, since: (i) the gapped excitations are accompanied by a rise in the system total energy associated with the energy of two coupled fermions and (ii) having an energy higher than the sum of energies of two free electrons, these two-particle states must be unstable rather than stable bound states.

The intriguing question of how, counterintuitively, a state consisting of single-particles and two-fermion excitations above the Fermi sea turns out to be energetically lower compared with the single-component Fermi system of attractively interacting fermions was discussed in Ref. [35]. In particular, assuming single- and bound two-particle objects, not as independent but as continually mutually converting into each other, was decisive for this

energy lowering to occur. To see this, combine (6) and (12) to rewrite (12) as

$$\Omega_{\mathbf{Q}}(T) \equiv \mathring{\Omega}_{\mathbf{Q}}(T) + \varepsilon_{\mathbf{Q}} \tag{16}$$

where

$$\mathring{\Omega}_{\mathbf{Q}}(T) \equiv 2(E_F + \Delta) + \delta\Omega(\mathbf{Q}, T) - 2\mu \tag{17}$$

with

$$\delta\Omega(\mathbf{Q}, T) \equiv \left(1 - \frac{U}{L^d}\sum_{\mathbf{q}} \phi_{\mathbf{q}} \frac{F(\mathbf{q}, \mathbf{Q})}{\Omega_{\mathbf{Q}} - \zeta(\mathbf{q}, \mathbf{Q})}\right)^{-1} \frac{f^2}{L^d}\sum_{\mathbf{q}} \left|\phi_{\mathbf{q}}\right|^2 \frac{F(\mathbf{q}, \mathbf{Q})}{\Omega_{\mathbf{Q}} - \zeta(\mathbf{q}, \mathbf{Q})}. \tag{18}$$

Since $q \gg Q$, where $\mathbf{q}$ and $\mathbf{Q}$ are fermion and boson wavevectors, respectively, one may ignore the Q-dependence in (18) appearing through $\zeta(\mathbf{q}, \mathbf{Q})$ and $F(\mathbf{q}, \mathbf{Q})$ as $\pm\mathbf{q} + \mathbf{Q}/\mathbf{2}$ and put $\mathring{\Omega}_{\mathbf{Q}} \equiv \mathring{\Omega}$ and $\delta\Omega(\mathbf{Q}, T) \equiv \delta\Omega(T)$. Equation (18) defines the magnitude of renormalization of the energy of interactionless bosons (6). In accordance with (16) bosonic excitations $\Omega_{\mathbf{Q}}$ are now separated from the Fermi sea, i.e. from 2μ, not by 2Δ as in (6) but by $\mathring{\Omega}$ which changes with temperature T and coupling λ: it decreases and vanishes upon cooling (see, e.g. Figure 1 in Ref. [24]) allowing to account for how boson energies given by (6) may be feasible.

Indeed, when the new gap $\mathring{\Omega}$ between single- and two-particle spectra disappears, i.e. when boson energy (16) and the energy of unpaired electrons become equal, then the evolution of the pure gas of electrons into a binary BF gas becomes possible. We insert in (17) $\mathring{\Omega}(T^*) = 0$ and $E_F = \mu$ which must be satisfied simultaneously on the verge of boson formation. This yields an equation to determine the temperature T^* at which a transition occurs from the normal state of single fermions into an incoherent binary BF mixture. One then has

$$\frac{1}{2L^d}\sum_{\mathbf{q}} \frac{\phi_{\mathbf{q}}}{\xi_{\mathbf{q}}}\left(\frac{f^2\phi_{\mathbf{q}}^*}{2\Delta} - U\right)\tanh(\xi_{\mathbf{q}}/2k_BT^*) = 1 \tag{19}$$

where $\Delta \equiv \hbar\omega_D/\sinh(1/\lambda)$ is the $T = 0$ BCS energy gap (see discussion in Ref. [34]) with $\lambda \equiv N(0)V$ where $N(0)$ was previously designated as $N(E_F)$. To obtain (19) one writes $\xi_{-\mathbf{q}} \equiv \xi_{\mathbf{q}}$ by symmetry, i.e. $\zeta(q, Q) \equiv 2\xi_{\mathbf{q}}$ and insert this into (18), keeping (11) in mind, where $n_{\mathbf{q}\sigma}(T^*) = \frac{1}{2}[1 - \tanh(\xi_{\mathbf{q}}/2k_BT^*)]$ are the unpaired-electron occupation numbers [34].

The condition $E_F = \mu$ occuring at T^* is equivalent to $n_B = 0$ with n_B vanishing for all $T \geqslant T^*$. Note that (19) is the same as Equations (28) and (29) in Ref. [34] established in an entirely different manner for the *isotropic* BF mixture, i.e. when $\phi_{\mathbf{q}} \equiv 1$ *and* no Coulombic U-term. One then evaluates the sum in (19) as an integral over ξ in the usual way. The DOS $N(\xi)$ is precisely constant in 2D, i.e. energy independent. In 3D $N(\xi) \propto \sqrt{\xi}$ but it varies little over the integration region if $\hbar\omega_D \ll E_F$ so that $N(\xi) \simeq N(0)$. Thus, in either 2D or 3D $N(\xi)$ can be taken outside the integral over ξ. Furthermore, the mean value theorem allows one to replace $\phi_{\mathbf{q}}$ in the lhs of (19) by some constant ϕ from the region of integration over q. Values of $\phi_{\mathbf{q}}$ remain near an averaged value $\bar{\phi} = 1$ of all anisotropy factors over the Fermi surface. Then, substituting $\bar{\phi}$ for ϕ in (19) leaves

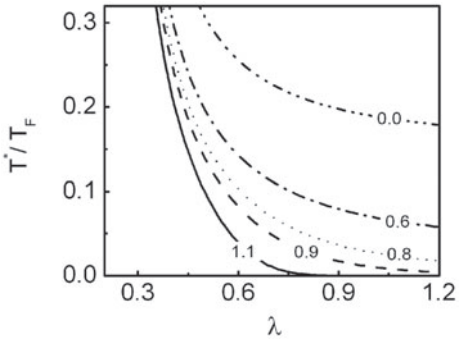

Figure 1. Pseudogap temperature T^* in units of T_F as function of λ for $\Theta_D/T_F = 0.35$ in 2D for different values of $v \equiv N(0)U$.

$$\left(\lambda - \frac{v}{\sinh(1/\lambda)}\right) \int_{-\hbar\omega_D}^{\hbar\omega_D} dx x^{-1} \tanh(x/2k_B T^*) = \frac{2}{\sinh(1/\lambda)} \tag{20}$$

where $\lambda \equiv N(0)V$ and $v \equiv N(0)U$ are both dimensionless. In the absence of reliable estimates for $N(0)U$ below we take v as a phenomenological parameter fitting it to get physically reasonable solutions of (20) and (25).

In Figure 1 the dimensionless depairing temperature T^*/T_F is graphed as a function of λ for $\hbar\omega_D/E_F \equiv \Theta_D/T_F = 0.35$ in 2D for different values of v. The gap 2Δ in the interactionless boson spectrum is smaller for smaller λ. Lesser 2Δ provides satisfaction of $\mathring{\Omega} = 0$ (necessary at the T^*) at higher Ts, thus explaining the rapid decrease of T^*shown in Figure 1. The peculiarities of T^*as a function of λ within a BF mixture model with positive-energy bosons have been discussed in Ref. [34] where the coupling parameter λ was related with the concentration of charge carriers x to explain the empirical behaviour of T^*as x varies. But the new ingredient now is the role of Coulomb repulsion. In a model *without* Coulomb repulsion the appearance of bosons below T^* was possible for any pairing interaction. However, switching on a Coulomb repulsion drastically changes this situation. As seen in Figure 1, T^* rapidly approaches zero as v increases (up to approximately $v \simeq 1$ in Figure 1). In other words, the evolution of single fermions into a BF mixture now becomes possible only for a restricted interval of λ wherein T^*remains nonzero. This in turn explains the "dome-shaped" structure of T_c as observed in HTSC materials (viz. in Figure 2 of Ref. [2]). In the limit of very large λ (i.e. for unreasonably large values of 2Δ) the condition $\mathring{\Omega} = 0$ is satisfied only at $T = 0$. Therefore, pairs might appear only at very low temperatures if λ is sufficiently large.

It is customary to apply the two extreme coupling limits of weak coupling (large pairs) and strong coupling (small pairs). In weak coupling the presence of any, however small, attractive interaction produces an unstable Fermi distribution. This leads to the BCS ground state of pairwise correlated fermions. And when the pairing interaction is strong enough, single fermions devolve into tightly bound two-particle composites. This is the central idea behind the various BF models. However, (6) and (17) provide a new weak-coupling scenario quite different from that of either BCS or strong-coupling BF models. This new scenario relies on the appearance of two-fermion resonances above the Fermi sea which inevitably occur in a system of attractively interacting fermions, followed by their disintegrations. The

frequency of their occurrence is rare at high temperatures but increases due to the gap (16) decrease upon cooling between the least energy of two-fermion resonances and the top of the band of unpaired electrons. They become, when $\mathring{\Omega}(T^*) = 0$, energetically favourable and thus a mixture state appears of single-fermions and two-fermion formations. Note that this coupling scenario does not lead to a departure from the Fermi distribution as occurs in BCS theory. However, due to the decrease in the number of unpaired fermions, the E_F of free fermions moves down to a value $\mu < E_F$. The most prominent manifestation of this coupling scenario is perhaps that found in Figure 1, namely, that T^* is much higher than T_c for small interaction λ.

4. Onset BEC temperature T_c for a coherent fluid

The value of T_c is related implicitly with total number density n_B of bosons at T_c. To consider (14) which is a T- and λ-*dependent* property characterizing a BF mixture, insert into (6) a boson dispersion $\varepsilon_{\mathbf{Q}}$ of general form

$$\varepsilon_{\mathbf{Q}} \equiv C_d\, Q^s \tag{21}$$

where the exponent $s \geqslant 0$ and the dimensionality d- and interaction-dependent coefficient C_d is chosen to match units on both sides of (21). For ordinary bosons of mass m in vacuum $s = 2$ and $C_d = \hbar^2/2m$, while for a CP in the Fermi sea $\varepsilon_{\mathbf{Q}}$ is linearly dispersive (i.e. $s = 1$) and C_d in (21) equals $(\lambda/2\pi)\hbar v_F$ in 2D and $(\lambda/4)\hbar v_F$ in 3D (see, literature cited in Ref. [34]). The sum in (14) is then evaluated as an integral over $\mathbf{Q}$. The volume of a hypersphere of radius Q in $d \geqslant 0$ dimension is $V_d(Q) = \pi^{d/2} Q^d / \Gamma(1 + d/2)$ [46] where $\Gamma(z)$ is the gamma function and $\Gamma(1 + z) \equiv z\Gamma(z)$. For $d = 2$ it is the area πQ^2 of a circle of radius Q and for $d = 3$ it is the sphere volume $4\pi Q^3/3$. Using this for $d > 0$ the summation in (14) over the d-dimensional wavevector $\mathbf{Q}$ becomes

$$\frac{1}{L^d} \sum_{\mathbf{Q}} (\cdots) \longrightarrow \frac{1}{2^{d-1}\pi^{d/2}\Gamma(d/2)} \int (\cdots) Q^{d-1} dQ.$$

The integral form of (14) is then

$$n_B(T) = \frac{1}{(2\pi)^d} \int_{\mathbf{Q}} \frac{d\mathbf{Q}}{\exp(\Omega_{\mathbf{Q}}/k_B T) - 1} = \frac{1}{2^{d-1}\pi^{d/2}\Gamma(d/2)} \int_0^\infty \frac{Q^{d-1} dQ}{A(T)\exp(C_d Q^s/k_B T) - 1} \tag{22}$$

where $A(T) \equiv \exp[\mathring{\Omega}(T)/k_B T]$. In terms of the dimensionless variable $x \equiv C_d Q^s/k_B T$ (22) becomes

$$\int_0^\infty \frac{x^{d/s-1} dx}{A(C_d Q^s/k_B x)\exp x - 1} = 2^{d-1}\pi^{d/2} s^{-1} \Gamma(d/2)\, (C_d/k_B T)^{d/s}\, n_B(T). \tag{23}$$

This relates the *unknown integral* [47] on the lhs to $n_B(T)$. The singularity associated with the condensation of an infinite number of composite bosons into a state with wavevector $\mathbf{Q}$ occurs in (22) when $\Omega_{\mathbf{Q}} \to 0$. Hence, one approaches *momentum-space* condensation temperature as $\mathring{\Omega} = 0$ so that $A = 1$ in (23) for any d. The condition $A(T_c) = 1$ inserted into (23) yields the simple but *implicit* T_c formula for a dispersion (21) and BF mixtures in any dimension d. Namely

$$k_B T_c = C_d [2^{d-1}\pi^{d/2}\Gamma(d/2)]^{s/d} \left(\int_0^\infty \frac{x^{d/s-1} dx}{\exp x - 1} \right)^{-s/d} n_B^{s/d}(T_c).$$

Finally, since $\int_0^\infty x^{d/s-1}[\exp x - 1]^{-1} dx = \Gamma(d/s)\zeta(d/s)$ where $\Gamma(x) \equiv \int_0^\infty \exp(-t) t^{x-1} dt$ and $\zeta(s) \equiv \sum_{n=1}^{\infty} n^{-s}$ is the Riemann Zeta function, one arrives at

$$k_B T_c = C_d \left(\frac{2^{d-1}\pi^{d/2} s \Gamma(d/2)}{\Gamma(d/s)\zeta(d/s)} \right)^{s/d} n_B^{s/d}(T_c). \tag{24}$$

This generalizes T_c for all $d > 0$ and $s > 0$ the linear (i.e. $s = 1$) result for dispersive bosons in $d = 2$ and 3 given by Equations (33) and (34) of Ref. [34]. Note that (24) gives $T_c = 0$ for all $0 < d \leqslant s$ since $\zeta(1) = \infty$. In particular, (24) contains the familiar textbook result of the impossibility of BEC in 2D which is a strictly true only for quadratically dispersive (i.e. $s = 2$) bosons.

It is remarkable that in spite of (24) having been derived for an *interacting* BF-binary mixture with Coulombic repulsions between fermions, it is precisely of the same form as Equation (7) of Ref. [40] valid for a pure boson gas. The reason for this is clear. Let us assume that there exists some unitary transformation $\hat{T}$ separating boson and fermion degrees of freedom in (1). Renormalized energies $\Omega_{\mathbf{Q}}(T)$ found as (16) to (18) actually approximate the energies of "pure bosons" as can be established after such a transformation. However, there is of course a significant difference between BECs in noninteracting bosonic gases and an interacting BF mixture. Indeed, the necessary condition $A(T_c) = 1$ for BEC to occur leads to the important equality connecting the chemical potential μ at the BEC T_c with parameters of the interacting BF mixture such as interelectronic coupling λ, coulombic U, anisotropy factors ϕ, the numbers $n_{\mathbf{k}\sigma}$ of unpaired fermions at T_c and their dispersion $\xi_{\mathbf{k}}$. Setting $Q = 0$ in (23) we find that, in the thermodynamic limit $L^d \to \infty$ and $N \to \infty$ such that N/L^d is constant, the number density n_{B0} of bosons condensed in the state $Q = 0$ becomes appreciable for BEC to occur on cooling whenever

$$E_F - \mu = -\Delta(\lambda) + [1 + \frac{U}{2L^d} \sum_{\mathbf{k}} \frac{\phi_{\mathbf{k}}}{E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T_c} \right)]^{-1} \frac{f^2}{4L^d} \sum_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T_c} \right) \tag{25}$$

is satisfied. In (25) we have used T-dependent occupation numbers $n_{\mathbf{k}\sigma}$ of unpaired electrons in a state with momentum wavevector $\mathbf{k}$ and spin σ, namely

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

where $E_{\mathbf{k}}$ is the unpaired-electron energy. As shown in Ref. [24] at temperatures between the higher T^* and the lower T_c the spectrum of unpaired fermions appears partially gapped via a generalized gap $E_{g\mathbf{k}}$ so that

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + E_{g\mathbf{k}}^2} \tag{26}$$

$$E_{g\mathbf{k}}(\lambda, T) \equiv \begin{cases} f\left(\phi_{\mathbf{k}} - \frac{\Omega_0}{2\hbar\omega_D}\frac{U}{V}\right)\sqrt{n_B(\lambda, T)} & \text{for} \quad \phi_{\mathbf{k}} - \frac{\Omega_0}{2\hbar\omega_D}\frac{U}{V} > 0 \\ 0 & \text{for} \quad \phi_{\mathbf{k}} - \frac{\Omega_0}{2\hbar\omega_D}\frac{U}{V} \leq 0. \end{cases} \tag{27}$$

When applied to (25), because $\Omega_0(T_c) = 0$ at and below T_c, (27) simplifies to

$$E_{g\mathbf{k}}(\lambda, T) = f\phi_{\mathbf{k}}\sqrt{n_{B0}(\lambda, T)} \tag{28}$$

with n_{B0} the condensed boson number density [34]. In Refs. [24] (27) was applied to explain the appearance in angle-resolved-photoemission spectroscopy (ARPES) experiments of so-called "Fermi arcs" in the spectrum of HTSCs (see, e.g. Refs. [3–6]). Fermi arcs are certain curves in momentum space along which the HTSC sample behaves as if it were a normal metal, i.e. is gapless. Equation (27) is found by calculating single-fermion occupation numbers $n_{\mathbf{k}} \equiv \langle a^+_{\mathbf{k}} a_{\mathbf{k}} \rangle$ within the model (1) with the new f (3) and U (4) terms.

According to (26), the dispersion of single particles in a BF state exhibits below T^* an energy gap, but present not over the full Fermi surface. Rather, there exist disconnected segments with temperature dependent extensions along which the gap vanishes. Due to the decreasing Ω_0 in (27) the "sizes" of gapless areas diminish on cooling. These areas disappear at the points of the k-space alongside of which the BF interaction strength $f_{\mathbf{k}} = f\phi_{\mathbf{k}}$ prevails over the pair-breaking ability $R \equiv U\Omega_0/\sqrt{2\hbar\omega_D V}$ of the Coulomb repulsions, as discussed in [24]. If $f_{\mathbf{k}}$ becomes larger than R throughout the Fermi surface then gapless areas vanish entirely.

In Ref. [24] it was crucial to emphasize that Fermi arcs seen in many experiments below T^* appear even for moderate s-wave symmetry of the pairing interaction. We stress here that, if the pairing interaction is of d-symmetry, i.e. if the parameter $f_{\mathbf{k}} = f\phi_{\mathbf{k}}$ vanishes for some specific directions then the conditions for Fermi arcs to disappear *completely* and for BEC to occur are the same, namely $\Omega_0 = 0$. Specifically, for d-wave symmetry of $\phi_{\mathbf{k}}$ Fermi arcs persist for all $T < T^*$ down to T_c and vanish only at and below the T_c for BEC. However, for s-wave symmetry of $f_{\mathbf{k}}$, according to (27), the two specific temperatures a) say, $T_1 \geqslant T_c$, at which Fermi arcs disappear and b) the BEC T_c, are in general distinct. And in the latter case within some temperature interval above the BEC T_c the energy–momentum relation of single fermions in a BF mixture becomes gapped, i.e. exhibit a Bogoliubov dispersion over the entire Fermi surface. We believe that the sole presence, or its absence, immediately above the BEC T_c of a phase with a real gap opening up over the entire Fermi surface may shed light on the question of the gap symmetry in HTSCs.

As done to obtain (20), if the anisotropy factors $\phi_{\mathbf{q}}$ in the sum over $\mathbf{q}$ in (25) are replaced by their average value $\bar{\phi}_{\mathbf{q}} = 1$, and evaluating the sum as an integral over ξ, leaves a closed expression to determine the shift at the BEC T_c of μ from E_F of interactionless fermions, namely

$$E_F - \mu = -\Delta(\lambda) + \frac{\lambda\hbar\omega_D}{2} I\left(1 + \frac{\nu}{2} I\right)^{-1} \tag{29}$$

where we defined

$$I \equiv \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{dx}{\sqrt{x^2 + 2\lambda\hbar\omega_D\,[E_F - \mu(\lambda, T)]}} \tanh\left(\frac{\sqrt{x^2 + 2\lambda\hbar\omega_D\,[E_F - \mu(\lambda, T)]}}{2k_B T_c}\right). \tag{30}$$

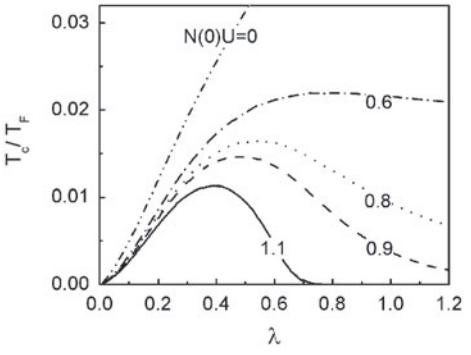

Figure 2. Same as in Figure 1 but for the BEC superconducting T_c/T_F. Increasing λ monotonically increases the magnitude of T_c/T_F for $v \equiv N(0)U = 0$ but maximizes at inordinately large λs. However, inclusion of a uniform Coulomb repulsive field converts the T_c/T_F-*vs*-λ behaviour from monotonically increasing to *dome shaped*. BEC now becomes possible only for a restricted interval of λ values, and increasing v narrows the interval of λ within which BEC occurs.

In actual calculations, from (15) one first extracts T_c/T_F from (24), with $T_F \equiv E_F/k_B$, in terms of $E_F - \mu(\lambda, T)$. Then T_c/T_F is inserted into (25) which gives closed expressions for the BEC T_c as a function of the model microscopic parameters.

In Figure 2 the BEC superconducting T_c/T_F in 2D is shown as function of λ and for different values of $v \equiv N(0)U$ and for $\Theta_D/T_F = 0.35$. For $v \equiv 0$, by increasing λ the magnitude of T_c/T_F increases monotonically and attains a maximum at unusually large λs. However, inclusion of a uniform Coulomb repulsive field converts the T_c/T_F-*vs*-λ curve from monotonically increasing to dome shaped. Now BEC becomes possible only for the restricted interval of λ values. Increasing v narrows the interval of λ within which BEC occurs. Relating the coupling parameter λ with the concentration of charge carriers x providing a qualitative description of the experimental phase diagram (e.g. in Ref. [2]) that includes a pseudogap *as well as* a dome-shaped T_c-vs-doping curve which critically depends on the repulsive Coulomb interaction between fermions confined into CPs. Thus, it becomes possible to describe an onset depairing temperature T^* as well as a BEC T_c, both of which occur by bosonization, in terms of the deviation of $E_F - \mu$. In fact, n_B is proportional [34] to the difference $E_F - \mu$ and plays the role of an order parameter in a BF model description. The position of μ with respect to E_F defines the *phase* in which the attractively interacting fermions appear: it consists of single fermions for all $E_F < \mu$ and when $E_F = \mu$ this condition defines a pseudogap or depairing critical T^* below which pairs first begin to appear so that below T^* one has the relation $E_F > \mu$. Specifically, for all $T \leqslant T^*$ the attractively interacting fermion gas becomes a binary mixture of interacting bosons (both with wavenumbers $K = 0$ *and* $K > 0$) and unpaired fermions. Decreasing T from T^* down to T_c leads to the *critical* μ at which $E_F - \mu$, and thus n_B, first become appreciably large for BEC to be ascertained. Sharp differences in behaviour between T^* and T_c as functions of hole concentrations x such as shown in Figures 1 and 2, is perhaps one reason for ascribing in the literature *different* origins to pseudogap and superconductivity phenomena in HTSCs. However, as shown herewith, both T^* and T_c may be described within the same approach based on bosonic correlations excited above the Fermi sea.

5. Conclusions

A scenario is proposed to describe the evolution of attractively interacting single electrons into a binary BF mixture consisting of unpaired electrons and incoherent bosonic CPs. This is possible owing to two-electron resonances, i.e. continually converting pairs of interacting electrons into correlated states of two fermions and vice versa. Such resonances foreseen in the literature are separated from the top of the single-fermion continuum by a positive energy gap and thus are short-lived states.

However, because of the contribution from continual formations/disintegrations, the magnitude of the gap separating resonances from the single-electron spectrum now becomes temperature- and coupling-dependent and decreases on lowering T. It vanishes at the onset temperature T^* of boson formation, whereby the energies of two-particle and single-particle excitations coincide. Below this temperature positive energy resonances become an actual state of paired electrons continually converting into single independent electrons and vice versa, thus leading to further energy lowering. We have derived an explicit expression for the renormalized boson energies in a BF mixture with a spatially uniform Coulomb interaction of strength $U \geq 0$ between the electrons within CPs. That expression is then applied to determine the characteristic temperatures T^* and T_c wherein the role of a uniform Coulomb interaction in forming the BF mixture properties was discussed. Introducing a uniform Coulomb interaction in an anisotropic BF binary gas mixture model allows one to predict, even in phonon-mediated electron dynamics, the presence in the energy–momentum dispersion relation of HTSCs of a line of nodal points along which the generalized gap (27) vanishes, and hence, gives rise to Fermi arcs as reported from ARPES experiments.

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Appendix

One determines $\left[b_{\mathbf{Q}}, \mathcal{H}\right]_-$ on the rhs of (8) by first splitting it as a sum of terms $I_0 \equiv \left[b_{\mathbf{Q}}, \mathcal{H}^o\right]_-$, $I_{BF} \equiv \left[b_{\mathbf{Q}}, \mathcal{H}_{BF}\right]_-$ and $I_U \equiv \left[b_{\mathbf{Q}}, \mathcal{H}_U\right]_- \equiv 0$ and then finding I_0 and I_{BF} separately. Since $\left[b_{\mathbf{Q}}, b_{\mathbf{k}}\right]_- = 0$ while $\left[b_{\mathbf{Q}}, b^+_{\mathbf{k}}\right]_- = \delta_{\mathbf{Q},\mathbf{K}}$ and $\left[b_{\mathbf{Q}}, b^+_{\mathbf{k}} b_{\mathbf{k}}\right]_- = b_{\mathbf{k}} \delta_{\mathbf{Q},\mathbf{K}}$ one gets, in any dimension d,

$$I_0 \equiv \mathcal{E}_{\mathbf{Q}} b_{\mathbf{Q}} \text{ and } I_{BF} \equiv \frac{1}{L^{d/2}} \sum_{\mathbf{q}} f_{\mathbf{q}} a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}.$$

Combining I_0 and I_{BF} into (8) yields

$$(\omega - \mathcal{E}_{\mathbf{Q}}) \left\langle\!\left\langle b_{\mathbf{Q}} \mid b^+_{\mathbf{Q}} \right\rangle\!\right\rangle_\omega = 1 + \frac{1}{L^{d/2}} \sum_{\mathbf{q}} f_{\mathbf{q}} \left\langle\!\left\langle a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} \mid b^+_{\mathbf{Q}} \right\rangle\!\right\rangle_\omega . \tag{1}$$

An expression for higher order Green functions like $\left\langle\!\left\langle a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} \mid b^+_{\mathbf{Q}} \right\rangle\!\right\rangle_\omega$ on the rhs of (1) can be established if in (7) one takes $a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}$ for A and B is still $b^+_{\mathbf{Q}}$. Thus

$$\omega \left\langle\!\left\langle a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} \mid b^+_{\mathbf{Q}} \right\rangle\!\right\rangle_\omega = \left\langle\!\left\langle \left[a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}, \mathcal{H} \right]_- \mid b^+_{\mathbf{Q}} \right\rangle\!\right\rangle_\omega \tag{2}$$

We first find the commutator $\left[a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}, \mathcal{H} \right]_- = J_0 + J_{BF} + J_U$ where

$$J_0 \equiv \left[a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}, \mathcal{H}_0 \right]_- \tag{3}$$

$$J_{BF} \equiv \left[a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}, \mathcal{H}_{BF} \right]_- \tag{4}$$

$$J_U \equiv \left[a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}, \mathcal{H}_U \right]_- . \tag{5}$$

Straightforward manipulations then give

$$J_0 \equiv \left(\xi_{-\mathbf{q}+\mathbf{Q}/2} + \xi_{\mathbf{q}+\mathbf{Q}/2} \right) a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} \tag{6}$$

$$J_{BF} \equiv \frac{1}{L^{d/2}} \sum_{\mathbf{k}} b_{\mathbf{k}} \left\{ f^*_{\mathbf{q}-\mathbf{Q}/2+\mathbf{K}/2} a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a^+_{\mathbf{q}-\mathbf{Q}/2+\mathbf{k}\uparrow} - f^*_{\mathbf{q}+\mathbf{Q}/2-\mathbf{K}/2} a^+_{-\mathbf{q}-\mathbf{Q}/2+\mathbf{k}\downarrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} \right\} \tag{7}$$

$$J_U \equiv \frac{U}{L^d} \sum_{\mathbf{p}} \left(a^+_{\mathbf{q}-\mathbf{Q}/2+\mathbf{p}\uparrow} a_{\mathbf{q}+\mathbf{Q}/2\uparrow} - a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} a^+_{-\mathbf{q}-\mathbf{Q}/2+\mathbf{p}\downarrow} \right) \left(\sum_{\mathbf{k}'} a_{-\mathbf{k}'+\mathbf{p}/2\downarrow} a_{\mathbf{k}'+\mathbf{p}/2\uparrow} \right) . \tag{8}$$

Let us separate in the summation (7) terms with $\mathbf{K} = \mathbf{Q}$ from those with $\mathbf{K} \neq \mathbf{Q}$, namely

$$J_{BF} \equiv \underbrace{\frac{f^*_{\mathbf{q}}}{L^{d/2}} b_{\mathbf{Q}} \left(1 - \hat{n}_{\mathbf{q}+\mathbf{Q}/2\uparrow} - \hat{n}_{-\mathbf{q}+\mathbf{Q}/2\downarrow}\right)}_{(\mathbf{K}=\mathbf{Q})\text{ coherent term}} + \tag{9}$$

$$\underbrace{\frac{1}{L^{d/2}} \sum_{\mathbf{q},\mathbf{K}\neq\mathbf{Q}} b_{\mathbf{K}} \left(f^*_{\mathbf{q}-\mathbf{Q}/2+\mathbf{K}/2} a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a^+_{\mathbf{q}-\mathbf{Q}/2+\mathbf{K}\uparrow} - f^*_{\mathbf{q}+\mathbf{Q}/2-\mathbf{K}/2} a^+_{-\mathbf{q}-\mathbf{Q}/2+\mathbf{K}\downarrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} \right)}_{(\mathbf{K}\neq\mathbf{Q})\text{ incoherent terms}} .$$

In similar manner, a look at J_U prompts one to separate in the summation (8) over $\mathbf{p}$ terms with $\mathbf{p} = \mathbf{Q}$ from those with $\mathbf{p} \neq \mathbf{Q}$; in the $\mathbf{p} \neq \mathbf{Q}$ contribution one separates terms with $\mathbf{k} = \mathbf{q} - \mathbf{Q}/2 + \mathbf{p}/2$ and $\mathbf{k} = \mathbf{q} + \mathbf{Q}/2 - \mathbf{p}/2$. This gives

$$\begin{aligned} J_U = \frac{U}{L^d} \Bigg[& \underbrace{(\hat{N}_e - \hat{n}_{\mathbf{q}+\mathbf{Q}/2\uparrow} - \hat{n}_{-\mathbf{q}+\mathbf{Q}/2\downarrow}) a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}}_{\textbf{coherent terms}} \\ & + \underbrace{\left(1 - n^+_{\mathbf{q}+\mathbf{Q}/2\uparrow} - n_{-\mathbf{q}+\mathbf{Q}/2\downarrow}\right)}_{\textbf{coherent terms}} \sum_{\mathbf{k}} a_{\mathbf{k}+\mathbf{p}/2\uparrow} a_{-\mathbf{k}+\mathbf{p}/2\downarrow} \\ & + \sum_{\mathbf{p}\neq\mathbf{Q}} \underbrace{\left(a^+_{\mathbf{q}-\mathbf{Q}/2+\mathbf{p}\uparrow} a_{\mathbf{q}+\mathbf{Q}/2\uparrow} - a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} a^+_{-\mathbf{q}-\mathbf{Q}/2+\mathbf{p}\downarrow} \right)}_{\textbf{incoherent terms}} {\sum_{\mathbf{k}}}' a_{-\mathbf{k}+\mathbf{p}/2\downarrow} a_{\mathbf{k}+\mathbf{p}/2\uparrow} \Bigg] . \end{aligned} \tag{10}$$

Here $\hat{n}_{\mathbf{k}\sigma} \equiv a^{+}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}$ is the usual Fermi number operator and the total number operator of unpaired electrons with both $\uparrow$ and $\downarrow$ spins is denoted as $\sum_{\mathbf{k}\sigma} \hat{n}_{\mathbf{k}\sigma} \equiv \hat{N}_e$; the prime "$\prime$" above the summation sign in (10) means that terms with $\mathbf{k} = \mathbf{q} - \mathbf{Q}/2 + \mathbf{p}/2$ and $\mathbf{k} = \mathbf{q} + \mathbf{Q}/2 - \mathbf{p}/2$ *considered separately* are brought outside the summation over $\mathbf{k}$. Further calculations are based on the replacement of number operators $\hat{n}_{\mathbf{q}\sigma}$ and $\hat{N}_e$ in (9) and (10) by their average values $n_{\mathbf{q}\sigma}$ and N_e as well as on the assumption that contributions from so-called "incoherent" terms in J_{BF} and J_U in (2) are negligible compared with contributions of so-called "coherent" terms, allowing one to neglect them entirely. Indeed, in (9) we write

$$\left\langle\left\langle b_{\mathbf{k}} \hat{F} \mid b^{+}_{\mathbf{Q}}\right\rangle\right\rangle_{\omega} \equiv \left\langle\left\langle b_{\mathbf{k}} \left(\hat{F} - \left\langle \hat{F} \right\rangle\right) \mid b^{+}_{\mathbf{Q}}\right\rangle\right\rangle_{\omega} + \left\langle \hat{F} \right\rangle \left\langle\left\langle b_{\mathbf{k}} \mid b^{+}_{\mathbf{Q}}\right\rangle\right\rangle_{\omega} \tag{11}$$

and assume that because of the factor $\hat{F} - \left\langle \hat{F} \right\rangle$ contributions from the first term in (11) approximately vanish by the averaging included in the Green function definitions. This approximation enables writing for coherent term in (9) $\left\langle\left\langle b_{\mathbf{k}} \hat{F} \mid b^{+}_{\mathbf{Q}}\right\rangle\right\rangle_{\omega} \simeq \left\langle \hat{F} \right\rangle \left\langle\left\langle b_{\mathbf{k}} \mid b^{+}_{\mathbf{Q}}\right\rangle\right\rangle_{\omega}$ with $\hat{F}$ constructed from fermion operators. Applied to the "incoherent" terms in J_{BF} , the relation (11) brings in contributions such as $c\left\langle\left\langle b_{\mathbf{k}} \mid b^{+}_{\mathbf{Q}}\right\rangle\right\rangle_{\omega}$ with the prefactor $c \simeq \left\langle a_{\mathbf{q}} a^{+}_{\mathbf{k}} \right\rangle$ with $\mathbf{q} \neq \mathbf{k}$. As regards the higher order Green functions on the rhs of (2) stemming from the "incoherent" terms in J_U (10), they may be cast as linear combinations of lower order ones [39]. Such a decomposition leads to terms with prefactors such as $\left\langle a_{\mathbf{q}} a^{+}_{\mathbf{k}} \right\rangle$ and $\langle a_{\mathbf{q}} a_{\mathbf{k}} \rangle$ where again $\mathbf{q} \neq \mathbf{k}$ as above. Ordinary averages [39]$\left\langle a_{\mathbf{q}} a^{+}_{\mathbf{k}} \right\rangle$ with different q and k must disappear for the systems with translational symmetry. Similarly, for the systems with a number-conservation law, averages with the different numbers of a and a^{+}, like $\langle a_{\mathbf{q}} a_{\mathbf{k}} \rangle$ or $\left\langle a^{+}_{\mathbf{q}} a^{+}_{\mathbf{k}} \right\rangle$, vanish (see details in Ref. [39]). Incidentally, this is the reason which simplify the topological structure of Feynman diagrams, Ref. [39]. That is, substituting $\left\langle a_{\mathbf{q}} a^{+}_{\mathbf{k}} \right\rangle_{\mathcal{H}} \approx \left\langle a_{\mathbf{q}} a^{+}_{\mathbf{k}} \right\rangle_{\mathcal{H}^o}$ where H^o is a Hamiltonian of interactionless particles for which both conservation laws and therefore "selection rules" hold, Ref. [39] we may ignore with the terms with prefactors $\left\langle a_{\mathbf{q}} a^{+}_{\mathbf{k}} \right\rangle$ and $\langle a_{\mathbf{q}} a_{\mathbf{k}} \rangle$ with different q and k assuming these to be small with respect to the "coherent" terms containing the prefactors like $\left\langle a^{+}_{\mathbf{k}} a_{\mathbf{k}} \right\rangle$. Ignoring all incoherent terms and introducing $F(\mathbf{q}, \mathbf{Q}) \equiv 1 - n_{\mathbf{q}+\mathbf{Q}/2\uparrow} - n_{-\mathbf{q}+\mathbf{Q}/2\downarrow}$ one is finally left with

$$J_{BF} = \frac{f^{*}_{\mathbf{q}}}{L^{d/2}} F(\mathbf{q}, \mathbf{Q}) b_{\mathbf{Q}} \tag{12}$$

$$J_U = U\left(n a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} + \frac{F(\mathbf{q}, \mathbf{Q})}{L^d} \sum_{\mathbf{k}} a_{\mathbf{k}+\mathbf{p}/2\uparrow} a_{-\mathbf{k}+\mathbf{p}/2\downarrow}\right) \tag{13}$$

where $n \equiv N_e/L^d$ is the number density of unpaired electrons. Substituting J_0 (6), J_{BF} (12) and J_U (13) into (2) yields

$$\begin{aligned} &\left[\omega - \left(\xi_{-\mathbf{q}+\mathbf{Q}/2} + \xi_{\mathbf{q}+\mathbf{Q}/2} + Un\right)\right] \left\langle\left\langle a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} \mid b^{+}_{\mathbf{Q}}\right\rangle\right\rangle_{\omega} \\ &= F(\mathbf{q}, \mathbf{Q}) \left(\frac{f^{*}_{\mathbf{q}}}{L^{d/2}} \left\langle\left\langle b_{\mathbf{Q}} \mid b^{+}_{\mathbf{Q}}\right\rangle\right\rangle_{\omega} + \frac{U}{L^d} \left\langle\left\langle \sum_{\mathbf{k}} a_{\mathbf{k}+\mathbf{Q}/2\uparrow} a_{-\mathbf{k}+\mathbf{Q}/2\downarrow} \mid b^{+}_{\mathbf{Q}} \right\rangle\right\rangle_{\omega}\right). \end{aligned} \tag{14}$$

In the following the term Un is dropped in (14). It was done by setting $\mu \to \mu - Un/2$ in (14), i.e. by referring the permanent upward shifts of a value $Un/2$ in the single-fermion energy levels $\xi_{\pm\mathbf{q}+\mathbf{Q}/2} \equiv \epsilon_{\pm\mathbf{q}+\mathbf{Q}/2} - \mu$ which appear due to the inclusion of a uniform Coulomb term in (1) to the chemical potential μ. As a result one gets

$$\begin{aligned} &\left\langle\left\langle a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} \mid b^{+}_{\mathbf{Q}}\right\rangle\right\rangle_{\omega} \\ &= \frac{F(\mathbf{q}, \mathbf{Q})}{\omega - \zeta(\mathbf{q}, \mathbf{Q})} \frac{1}{L^{d/2}} \left(f^{*}_{\mathbf{q}} \left\langle\left\langle b_{\mathbf{Q}} \mid b^{+}_{\mathbf{Q}}\right\rangle\right\rangle_{\omega} + \frac{U}{L^{d/2}} \sum_{\mathbf{k}} \left\langle\left\langle a_{\mathbf{k}+\mathbf{Q}/2\uparrow} a_{-\mathbf{k}+\mathbf{Q}/2\downarrow} \mid b^{+}_{\mathbf{Q}}\right\rangle\right\rangle_{\omega}\right) \end{aligned} \tag{15}$$

where $\zeta(\mathbf{q},\mathbf{Q}) \equiv \xi_{-\mathbf{q}+\mathbf{Q}/2} + \xi_{\mathbf{q}+\mathbf{Q}/2}$. Now, (1) allows one to relate the second contribution in double brackets on the rhs of (15) via the single-boson Green functions $\left\langle\!\left\langle b_{\mathbf{Q}} \mid b^{+}_{\mathbf{Q}} \right\rangle\!\right\rangle_{\omega}$. Indeed, anisotropy factors $\phi_{\mathbf{q}}$ in the BF coupling $f_{\mathbf{q}} = f\phi_{\mathbf{q}}$ [exactly $= f$ in (1) if the system is isotropic] vary to modulate the $\mathbf{q}$-dependence of the interaction strength [24]. However, the values of $\phi_{\mathbf{q}}$ remain within an interval near $\bar{\phi} = 1$ which is an averaged value of all $\phi_{\mathbf{q}}$ over the Fermi surface. Substituting $\bar{\phi} = 1$ for $\phi_{\mathbf{q}}$ in (1) renders the last term in double brackets in (15) as

$$\frac{1}{L^{d/2}} \sum_{\mathbf{q}} \left\langle\!\left\langle a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} \mid b^{+}_{\mathbf{Q}} \right\rangle\!\right\rangle_{\omega} = \frac{1}{f} \left[(\omega - \mathcal{E}_{\mathbf{Q}}) \left\langle\!\left\langle b_{\mathbf{Q}} \mid b^{+}_{\mathbf{Q}} \right\rangle\!\right\rangle_{\omega} - 1 \right]. \tag{16}$$

Consequently, (15) becomes

$$\begin{aligned} &\left\langle\!\left\langle a_{\mathbf{q}+\mathbf{Q}/2\uparrow} a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} \mid b^{+}_{\mathbf{Q}} \right\rangle\!\right\rangle_{\omega} \\ &= \frac{f}{L^{d/2}} \frac{F(\mathbf{q},\mathbf{Q})}{\omega - \zeta(\mathbf{q},\mathbf{Q})} \left\{ \phi^{*}_{\mathbf{q}} \left\langle\!\left\langle b_{\mathbf{Q}} \mid b^{+}_{\mathbf{Q}} \right\rangle\!\right\rangle_{\omega} + \frac{U}{f^2} \left[(\omega - \mathcal{E}_{\mathbf{Q}}) \left\langle\!\left\langle b_{\mathbf{Q}} \mid b^{+}_{\mathbf{Q}} \right\rangle\!\right\rangle_{\omega} - 1 \right] \right\}. \end{aligned} \tag{17}$$

Inserting this in (1) gives, after some manipulations, the final expression for the single-boson Green function (10) used in Section 2 to find renormalized boson energies $\Omega_{\mathbf{Q}}$.