Depairing and Bose-Einstein-condensation temperatures in a simple boson-fermion model of superconductors

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(Received 17 July 2006; revised manuscript received 20 November 2006; published 12 March 2007)

Starting from the Friedberg-TD Lee Hamiltonian describing a coexisting and dynamically interacting many-particle binary boson-fermion gas mixture with a coupling (λ)-dependent gap $2\Delta(\lambda)$ in the boson dispersion relation for the *s*-wave Cooper or BCS model interaction, we deduce several observed characteristic features of high-temperature superconductors at the simplest level. Analytic expressions for both the unpaired-fermion and boson number densities, as well for the fermion chemical potential $\mu(\lambda,T)$, all of which vary with the degree of bosonization and with temperature T, are derived in detail using two-time, finite-temperature Green function techniques. Simple implicit formulas are then obtained for both two and three dimensions for the pseudogap T^* and Bose-Einstein condensation T_c temperatures in terms of $\mu(\lambda,T)$ and $2\Delta(\lambda)$. In particular, even at the *s*-wave level we find a self-consistent description of the generic phase diagram observed in cuprates, including the appearance of a pseudogap and a dome-shaped T_c vs doping behavior both of which hinge on the gapped boson spectrum.

DOI: 10.1103/PhysRevB.75.104506 PACS number(s): 74.20.−z, 74.20.Mn, 74.10.+v, 74.25.Dw

I. INTRODUCTION

Boson-fermion (BF) statistical models of superconductivity (SC) as a Bose-Einstein condensation (BEC)[1,2] first began to be studied in the mid-1950s,[3–6] predating even the BCS-Bogoliubov statistical theory.[7–9] Although BCS theory only contemplates the presence of "Cooper correlations" of single-particle states, BF models[3–6,10–21] posit the existence of actual bosonic CPs. The remarkable relation $\Delta(T) \propto \sqrt{n_0(T)}$, with $\Delta(T)$ the BCS gap in the fermion spectrum and $n_0(T)$ the BEC condensate number density of electron pairs, first seems to have appeared in Ref. 19. It resurfaced a year later in the phenomenological BEC BF model that Friedberg and Lee[20,21] (FL) applied to cuprate superconductors. With just *one* adjustable parameter (the ratio of perpendicular to CuO_2-plane boson masses) this theory fitted[21] quasi-2D cuprate T_c/T_F empirical data[22] (see also Ref. 23) rather well. The ratio turned out to be 66 560—just under the 10^5 anisotropy ratio reported[24] almost contemporaneously for $B_{2+x}Sr_{2-y}CuO_{2\pm\delta}$.

The new ingredient here introduced into the FL model is a bosonic CP dispersion relation that is not quadratic, say, $\varepsilon_{\mathbf{K}} = \hbar^2 K^2/2(2m)$ with K the pair center-of-mass wave number and m the single-fermion effective mass, as in Refs. 20 and 21, but rather linear *and* gapped as suggested by a more general treatment[25,26] of Cooper pairing. This additional feature renders the FL model an adjustable-parameter-free theory and is indispensable in reproducing the dome-shaped T_c behavior of cuprates. The FL model has more recently been applied to ultracold fermionic atoms such as ^{6}Li and ^{40}K where pairing into CPs also occurs; for a review see Ref. 27.

In Refs. 10 and 11 a system of electrons interacting pairwise via the familiar Cooper or BCS[7,28] two-parameter *s*-wave model interaction [in either two dimensions (2D) or three dimensions (3D)] is proposed as two coexisting dynamically interacting many-particle subsystems of (a) pairable but unpaired electrons and (b) composite-boson Cooper pairs (CPs) of two mutually confined electrons or holes. Of course, in actual cuprates one expects mixing and interplay between *s*-wave and *d*-wave pairing symmetries but our present paper is meant to provide a first orientation within a sufficiently simple BF binary gas of a BEC scenario. The Cooper or BCS model interaction[7,28] is specified by a negative strength parameter $-V$ whenever the electron energies $\epsilon_{\mathbf{k}}$ lie within the interval $[E_F-\hbar\omega_D, E_F+\hbar\omega_D]$ about the Fermi energy E_F of the ideal Fermi gas, with $\hbar\omega_D$ the Debye energy parameter, and is otherwise zero. This mimicks the electron-phonon mechanism suggested[29] recently as a major, if not sole, component in the pairing dynamics of cuprates.

The FL (Ref. 20) phenomenological Hamiltonian describing our binary BF mixture is written in the form

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} a^+_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \sum_{\mathbf{K}} E(\mathbf{K}) b^+_{\mathbf{K}} b_{\mathbf{K}} + H_{\rm int}, \tag{1}$$

$$H_{\rm int} \equiv \frac{f}{L^{d/2}} \sum_{\mathbf{q},\mathbf{K}} (b^+_{\mathbf{K}} a_{\mathbf{q}+K/2\uparrow} a_{-\mathbf{q}+\mathbf{K}/2\downarrow} + b_{\mathbf{K}} a^+_{-\mathbf{q}+\mathbf{K}/2\downarrow} a^+_{\mathbf{q}+K/2\uparrow}), \tag{2}$$

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 $\sigma=\uparrow,\downarrow$ while $b^+_{\mathbf{K}}$ and $b_{\mathbf{K}}$ are *postulated* (as in Refs. 10

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and 11) to be bosonic operators for the CPs of total, or center-of-mass, momentum (CMM) **K**. The perturbed Hamiltonian describes the formation and disintegration processes of the $2e$-CPs. This postulate is backed by magnetic-flux quantization experiments (see, e.g., Refs. 30–32) that reveal the presence of charge carriers of magnitude $2e$ along with those of e, where e is the electron charge. To our knowledge, no one has yet succeeded in constructing CP creation $b_{\mathbf{K}}^{+}$ and annihilation $b_{\mathbf{K}}$ operators that obey strict Bose commutation relations, starting from fermion operators $a_{\mathbf{k}\sigma}^{+}$ and $a_{\mathbf{k}\sigma}$. However, arguments can be made[33] showing that CPs obey Bose-Einstein statistics. Also, in (1) $\epsilon_{\mathbf{k}} \equiv \hbar^2 k^2/2m$ with m the effective electron mass, $E(\mathbf{K})$ is the CP energy, L is the system size and d its dimensionality. Finally, the BF interaction vertex (*two*-fermion, one-boson) form factor f in (2) is a phenomenological parameter responsible for $2e$-CP formation and/or disintegration processes. If related with the attractive interelectron (*four*-fermion) electron-phonon strength parameter V of the s-wave Cooper or BCS model interaction through

$$f = \sqrt{2\hbar\omega_D V}, \tag{3}$$

the complete BF model[10,11] with $\mathbf{K}=0$ can be shown as a special case to yield the BCS gap equation for all T as well as the BCS $T=0$ condensation energy for all coupling V. The term H_{int} in (1) is chosen in the simplest form that transforms pairs of single electrons into composite-boson CPs with CMM **K**, and vice versa.

Although the vast majority of superconductors have *hole* charge carriers in the normal state,[34] as determined empirically from *positive* Hall coefficients, there are London magnetic-moment measurements[35] establishing—at least according to one interpretation[36]—electron pairs in the condensates of superconductors as diverse as Pb (p type above T_c), $BaPb_{0.8}Bi_{0.2}O_3$ (n type) and $YBa_2Cu_3O_{7-\delta}$ (p type), regardless of whether the single charge carriers in the normal state above T_c are electrons or holes. Related to this there is a wealth of experimental data[37–39] on the Hall-coefficient sign reversal in various cuprates, but we shall not attempt to address in detail this phenomenon here.

The total number of electrons in the system is given by $N=N_1+N_2$ where N_1 is the number of unpairable (i.e., noninteracting or inactive, "spectator") electrons while N_2 is the number of pairable (i.e., interacting or "active") ones. Both N_1 and N_2 are each coupling (V) and temperature (T) dependent. By pairing up some electrons exit the N_2 portion of the fermionic subsystem and enter the bosonic subsystem. As pairing occurs the number of free or unpaired fermions decreases and the chemical potential $\mu(V,T)$ shifts down from its position at $E_F(T) \equiv \mu(0,T)$ for interactionless ($V=0$) fermions at T. Note, at nonzero T, there is temperature smearing of the Fermi distribution and $E_F(T) \equiv \mu(0,T)$ itself shifts[40] down from $E_F(0)$ by an amount of order $(k_B T/2E_F)^2$ and thus negligibly small for reasonable temperatures. Everywhere here we deal with the difference $E_F(T)-\mu(V,T)$ and nowhere use the explicit form of $E_F(T)$ but rather take it simply as E_F. Because of this shift in $\mu(V,T)$, a certain fraction of the N_1 spectator electrons, which is proportional to $E_F - \mu(V,T)$, become active as they begin to feel the attractive pairing interaction $-V$. So, at fixed V and T, N_2 is the sum of the number N_{20} of unpaired (but pairable) fermions plus the actually paired ones $N_2 - N_{20} \equiv 2N_B$, both of which lie within the interaction shell of energy width $\hbar\omega_D$. The decrease or increase in the electron number in the fermionic subsystem must be accompanied by a corresponding increase or decrease in the CP bosonic subsystem particle number N_B. The number conservation law must therefore be

$$N \equiv N_1 + N_2 \equiv N_1 + N_{20} + 2N_B \equiv \left\langle \sum_{\mathbf{k},\sigma} a_{\mathbf{k}\sigma}^{+} a_{\mathbf{k}\sigma} + 2\sum_{\mathbf{K}} b_{\mathbf{K}}^{+} b_{\mathbf{K}} \right\rangle_{\mathcal{H}}, \tag{4}$$

where $\langle X \rangle_{\mathcal{H}}$ of an operator X are T-dependent thermal averages over the Hamiltonian $\mathcal{H} \equiv H - \mu N$ with the electronic chemical potential $\mu(V,T)$ is to be fixed from the constancy of the total electron number N.

The Hamiltonian $\mathcal{H}$ itself is

$$\mathcal{H} \equiv \mathcal{H}_0 + H_{\text{int}} = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu) a_{\mathbf{k}\sigma}^{+} a_{\mathbf{k}\sigma} + \sum_{\mathbf{K}} [E(\mathbf{K}) - 2\mu] b_{\mathbf{K}}^{+} b_{\mathbf{K}} + H_{\text{int}}. \tag{5}$$

Hence, the V- and T-dependent total number of CPs is just $N_B = (N_2 - N_{20})/2$. Variations in the fermion number $N_1 + N_{20}$ will thus determine changes in the boson number N_B due to CP formation and/or disintegration, but with N always constant. The bosonic CPs in (5) cannot strictly be taken as free particles propagating *in vacuo* with a quadratic energy-momentum dispersion relation $\varepsilon_{\mathbf{K}} = \hbar^2 K^2/2(2m)$. In (5) we assume the CPs to be composite bosons with energies $E(\mathbf{K})$ that must be V dependent and gapped at zero K with a V-dependent gap. As we shall see below, this simple assumption leads to pseudogap T^* and superconducting T_c temperature behaving qualitatively as is observed in high-T_c cuprates. These requirements on $E(\mathbf{K})$ are met in Ref. 25 in 3D and Ref. 26 in 2D where it is found that

$$E(\mathbf{K}) \equiv 2E_F + 2\Delta + \varepsilon_{\mathbf{K}}, \tag{6}$$

where $\varepsilon_{\mathbf{K}}$ is the non-negative CP excitation energy which in leading order in K is the *linear* expression arising from the background Fermi sea

$$\varepsilon_{\mathbf{K}} = c_d \hbar v_F K. \tag{7}$$

Here c_d a dimensionality- and interaction-dependent dimensionless coefficient $\lambda/2\pi$ in 2D (Ref. 26) and $\lambda/4$ in 3D,[25] while

$$\Delta = \frac{\hbar\omega_D}{\sinh(1/\lambda)} \xrightarrow[\lambda \to 0]{} 2\hbar\omega_D \exp(-1/\lambda) \tag{8}$$

is the usual $T=0$ BCS energy gap, with $\lambda \equiv g(E_F)V$ and $g(\epsilon)$ is the electronic density of states (DOS) (for each spin). Equations (6)–(8) follow from the Bethe-Salpeter integral equation in the ladder approximation which yielded, in either 2D (Ref. 26) or 3D,[25] *two* different linearly dispersive (in leading order of the CMM wave number K) solutions. First, the dispersion relation (7) for *moving* (i.e., with *nonzero* CMM) $2e$- and $2h$-CPs was obtained as a nontrivial

solution. Second, a trivial solution was present that is associated with the sound mode sometimes known as the Anderson-Bogoliubov-Higgs[9,41,42] excitation. For zero coupling between the fermions this latter mode reduces to the ideal Fermi gas acoustic mode $\hbar v_F K/\sqrt{d}$ with v_F the Fermi velocity and d the system dimensionality. These two "particle" and "acoustic" solutions emerge as clearly *distinct* in the many-fermion system although in the many-boson case they are known[43,44] to be identical.

Specifically, in Refs. 25 and 26 it was shown that the nontrivial solution (a) has a dispersion relation $\varepsilon_{\mathbf{K}}$ for moving $2e$ CPs which in leading order depends linearly on the total momentum K of the pair as in (7); and (b) that the CP energy spectrum is gapped as in (6) above the total energy of two free electrons $2E_F$ by an amount $2\Delta(\lambda)$. So, according to (8), materials with larger couplings λ will allow formation of CPs at energies somewhat higher with respect to $2E_F$. Because of this particular spectral structure, the second term in the last member of (5) describing the contribution of free bosons increases in energy. However, as will be shown elsewhere,[45] the contribution from the interaction term H_{int} in (5) arising from CP formation and/or disintegration processes, is *negative* and at least twice as large in magnitude as the previous term which is the contribution of free pairs. Furthermore, a decrease in the number of unpaired fermions due to pair-formation processes makes the contribution of the first term in (5) to the total energy even smaller. As a result, within a given range of our parameters T and f, the ground state of (5) turns out to be energetically *lower* than the ground state corresponding to the Hamiltonian of interactionless fermions. If $V=0$, or neglecting interelectronic interactions leading to CP formation, then (5) becomes the Hamiltonian of free electrons

$$H^o = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - E_F) a^+_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} \tag{9}$$

since for vanishing $\lambda \equiv g(E_F)V$ both the bosonic $\varepsilon_{\mathbf{K}}$ (7) and Δ vanish so that μ in (5) becomes E_F, ensuring as expected that $\lim_{\lambda\to 0}\mathcal{H}=H^o$.

II. UNPAIRED-ELECTRON AND BOSON NUMBERS

In Eq. (A13) of Appendix A the average number of unpaired electrons in a state $\mathbf{k}$ is found to be

$$n_{\mathbf{k}} = \frac{1}{2}\left(1 - \frac{\epsilon_{\mathbf{k}} - \mu(V,T)}{E_{\mathbf{k}}} \tanh(E_{\mathbf{k}}/2k_BT)\right) \tag{10}$$

in the RPA approximation for all $T \leqslant T^*$ with T^* being the solution of $N_B(T^*) \equiv 0$ and corresponding to a "pseudogap"[46] or "depairing" temperature. Here

$$E_{\mathbf{k}} \equiv \sqrt{[\epsilon_{\mathbf{k}} - \mu(V,T)]^2 + f^2 n_{B0}(T)} \tag{11}$$

with $n_{B0}(T) \equiv N_{B0}(T)/L^d$ being the number density of bosons condensed in the $\mathbf{K}=0$ state. If the boson spectrum is gapped one gets that $T^* \geqslant T_c$, as will be seen.

In Eq. (B14) of Appendix B, we show that the average number of bosonic CPs in a state with a given CMM $\mathbf{K}$ is

$$n_{B\mathbf{K}}(T) = \frac{1}{e^{\Omega_{\mathbf{K}}/k_BT} - 1}, \tag{12}$$

where $\Omega_{\mathbf{K}}$ is a solution of the implicit equation

$$\Omega_{\mathbf{K}} \equiv E(\mathbf{K}) - 2\mu + \frac{f^2}{L^d}\sum_{\mathbf{q}} \frac{1 - n_{\mathbf{q}+\mathbf{K}/2\uparrow} - n_{-\mathbf{q}+\mathbf{K}/2\downarrow}}{\Omega_{\mathbf{K}} - (\xi_{\mathbf{q}+\mathbf{K}/2} + \xi_{-\mathbf{q}+\mathbf{K}/2})} \tag{13}$$

with $\xi_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} - \mu$ and with the $n_{\mathbf{k}}$'s defined by (10). Because of the specific interaction H_{int} in (1) the energy spectrum $\epsilon_{\mathbf{k}}$ of free electrons is renormalized and becomes $E_{\mathbf{k}}$ as given by (11). The $\epsilon_{\mathbf{k}}$ lie in the energy interval $\mu - \hbar\omega_D \leqslant \epsilon_{\mathbf{k}} \leqslant \mu + \hbar\omega_D$ where μ differs from E_F as a result of boson formation. The quantity $E_F - \mu$ in turn determines the value of $n_B(T)$ as will be shown below. Note that the difference between the single-fermion energy levels in the normal and BF-mixture states, i.e., between $\epsilon_{\mathbf{k}} - E_F$ and $E_{\mathbf{k}}$, is both temperature and coupling dependent, changing from zero below T^* and varying according to changes in $E_F - \mu$.

III. NUMBER DENSITY OF COMPOSITE BOSONS

According to (10) the total number of pairable but unpaired fermions $N_{20}(T)$ is given by

$$N_{20}(T) = 2\int_{E_F-\hbar\omega_D}^{E_F+\hbar\omega_D} d\epsilon g(\epsilon) n(\epsilon), \tag{14}$$

where $n(\epsilon) \equiv n_{\mathbf{k}}(\epsilon_{\mathbf{k}})$. Explicitly,

$$N_{20}(T) = \int_{E_F-\hbar\omega_D}^{E_F+\hbar\omega_D} d\epsilon g(\epsilon)\left[1 - \frac{\epsilon - \mu}{\sqrt{(\epsilon-\mu)^2 + f^2 n_{B0}}} \tanh\left(\frac{\sqrt{(\epsilon-\mu)^2 + f^2 n_{B0}}}{2k_BT}\right)\right]. \tag{15}$$

As T decreases below T^* and pairing occurs, μ shifts down from its original value of E_F. As a result, a certain fraction of the spectator electrons now become active due to the downward shift of the interaction shell of energy width $2\hbar\omega_D$ which is fixed in magnitude but centered at μ. If $\hbar\omega_D \gg E_F - \mu$ the number of such electrons, say δN, is much smaller than total number N_2 of active electrons within the shell $\mu - \hbar\omega_D \leqslant \epsilon_{\mathbf{k}} \leqslant \mu + \hbar\omega_D$. In (14) we neglect the contribution coming from such newly joined fermions and the integration there is therefore performed over the interval $[E_F - \hbar\omega_D, E_F + \hbar\omega_D]$.

If we ignore the variation of $g(\epsilon)$ within the (small, if $\hbar\omega_D \ll E_F$) integration region over ϵ and take $g(\epsilon) \simeq g(E_F)$ [which is exact in 2D because $g(\epsilon)$ is constant] then the integration in (15) is easily carried out and yields

$$N_{20}(T) = 2g(E_F)\hbar\omega_D\left[1 - \frac{k_BT}{\hbar\omega_D} \ln\left(\frac{\cosh(A_+/2k_BT)}{\cosh(A_-/2k_BT)}\right)\right], \tag{16}$$

where

$$A_{\pm} \equiv \sqrt{[\hbar\omega_D \pm (E_F - \mu)]^2 + f^2 n_{B0}}. \quad (17)$$

With $N_2 \equiv 2g(E_F)\hbar\omega_D$, the fractional number $N_{20}(T)/N_2$ of pairable (but unpaired) electrons becomes

$$\frac{N_{20}(T)}{N_2} = 1 - (k_B T/\hbar\omega_D) \times \ln\left(\frac{\exp(A_+/2k_BT) + \exp(-A_+/2k_BT)}{\exp(A_-/2k_BT) + \exp(-A_-/2k_BT)}\right). \quad (18)$$

When $f=0$ as in the noninteracting binary BF mixture, (18) reduces to the result established in Eq. 24 of Ref. 14. From (4) the total number of composite bosons $N_B(T)$ is just one-half the total number of fermions that are actually paired at temperature T, or $N_2 - N_{20}$, so that from (18) one gets

$$n_B(T) \equiv N_B(T)/L^d = \frac{N(E_F)}{2} k_B T \ln\left(\frac{\exp(A_+/2k_BT) + \exp(-A_+/2k_BT)}{\exp(A_-/2k_BT) + \exp(-A_-/2k_BT)}\right). \quad (19)$$

Here $N(E_F) \equiv g(E_F)/L^d$ is the electronic DOS (for each spin *and* per unit volume) at the Fermi surface. In the physically important case when both $\hbar\omega_D \gg (E_F - \mu)$ and $\hbar\omega_D \gg f^2 n_{B0}$ are satisfied, the terms $\exp(-A_\pm/2k_BT)$ in the numerator and denominator of (19) may be ignored with respect to the terms $\exp(A_\pm/2k_BT)$. Thus, one can approximate (19) with good accuracy as

$$n_B(\lambda, T) \simeq N(E_F)[E_F - \mu(\lambda, T)], \quad (20)$$

where the explicit λ and T dependence of n_B and μ are now emphasized. This result is now valid for all T as opposed to that obtained in Ref. 47 which is, strictly speaking, valid only for $T=0$. Note that the calculation including the correction associated with the change in E_F in (14) leads to the same result (20). From (11) the term $f^2 n_{B0}$ determines the shift in the free-electron states $\epsilon_{\mathbf{k}}$ due to the interaction (2) in (1). Therefore, the conditions $\hbar\omega_D \gg (E_F - \mu)$ and $\hbar\omega_D \gg f^2 n_{B0}$ just employed assume that the shift in the $\epsilon_{\mathbf{k}}$, as well the change in the position of the Fermi level $E_F - \mu$ due to (2), are much smaller than the bandwidth $2\hbar\omega_D$ within which the interaction takes place. In the normal, i.e., interactionless, state $N(E_F)$ is

$$m/2\pi\hbar^2 \quad (2\mathrm{D}), \quad (21)$$

$$m^{3/2}E_F^{1/2}/2^{1/2}\pi^2\hbar^3 \quad (3\mathrm{D}). \quad (22)$$

In analogy with the E_F of an ideal Fermi gas which depends on the total number of free electrons N, in Ref. 47 we introduced $\mu(V,T)$ which refers instead of N only to the number $N_F \equiv N - 2N_B$ of unpaired electrons in the BF mixture. Assuming that the main contribution to the change in E_F that occurs by switching on H_{int} and that it is associated mainly with variations in the fermion number, it was shown in Ref. 47 that such a choice of $\mu(V,T)$ actually keeps the total electron number N constant. As in 3D in Ref. 47, using $E_F \equiv (\hbar^2/2m)(3\pi^2 N/L^3)^{2/3}$ valid at $T=0$ and $\mu \equiv (\hbar^2/2m) \times (3\pi^2 N_F/L^3)^{2/3}$ (provided the N_F unpaired electrons are interactionless), and then employing (4) as well as the binomial expansion for $E_F - \mu$ for small $2N_B/N$, we immediately get

$$E_F - \mu = \left(\frac{\hbar^2}{2m}\right)(3\pi^2)^{2/3}\left[\left(\frac{N}{L^3}\right)^{2/3} - \left(\frac{N_F}{L^3}\right)^{2/3}\right] = E_F\left[1 - \left(\frac{N_F}{N}\right)^{2/3}\right] = E_F\left[1 - \left(1 - \frac{2N_B}{N}\right)^{2/3}\right] \simeq \frac{4E_F}{3}\frac{N_B}{N}. \quad (23)$$

It is easy to see that (23), first deduced in Ref. 47, written in terms of the number densities $n \equiv N/L^3$ and $n_B \equiv N_B/L^3$ and DOS per spin $N(E_F) = m^{3/2}E_F^{1/2}/2^{1/2}\pi^2\hbar^3$, becomes identical to (20). Here we get an explicit expression (19) for $n_B(\lambda, T)$. The important relation (20) emerges as a special case of (19). Thus (20) directly relates the number density of bosons $n_B(\lambda, T)$ to the shift $E_F - \mu(\lambda, T)$ in the position of the Fermi level. If this shift $E_F - \mu(\lambda, T)$ due to boson formation and/or disintegration and $N(E_F)$ were known, then (20) would serve in finding the total number of bosons in the mixture at any λ and T. We now present a detailed derivation of an equation for $E_F - \mu(\lambda, T)$.

IV. BOSON FORMATION AND FERMION CHEMICAL POTENTIAL

According to (11) when nonzero averages $\langle b_{\mathbf{K}}\rangle_{\mathcal{H}} \neq 0$ and $\langle b_{\mathbf{K}}^+\rangle_{\mathcal{H}} \neq 0$ appear the spectrum of unpaired electrons begins to differ from the spectrum $\epsilon_{\mathbf{k}}$ of free electrons. This is readily seen if we set $n_{B,\mathbf{K}} \simeq \langle b_{\mathbf{K}}^+\rangle_{\mathcal{H}}\langle b_{\mathbf{K}}\rangle_{\mathcal{H}}$ in (11) for $\mathbf{K}=0$ and recall the identity

$$\langle [A, \mathcal{H}]\rangle_{\mathcal{H}} \equiv \mathrm{Tr}[(A\mathcal{H} - \mathcal{H}A)\exp(-\beta\mathcal{H})] = 0, \quad (24)$$

where A is *any* dynamical operator and the average of the commutator $[A, \mathcal{H}] \equiv A\mathcal{H} - \mathcal{H}A$ is performed over the Hamiltonian $\mathcal{H}$. The above relation is proved straightforwardly by doing a cyclic permutation under the trace. Setting $A \equiv b_{\mathbf{Q}}^+$ in (24) we get, since $\langle [b_{\mathbf{Q}}^+, \mathcal{H}]\rangle_{\mathcal{H}} = 0$, that

$$\langle b_{\mathbf{Q}}^+\rangle_{\mathcal{H}} = -\frac{1}{E(\mathbf{Q}) - 2\mu}\frac{f}{L^{d/2}}\sum_{\mathbf{q}}\langle a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}^+ a_{\mathbf{q}+\mathbf{Q}/2\uparrow}^+\rangle_{\mathcal{H}}. \quad (25)$$

In Eqs. (A14)–(A16) of Appendix A we show how the averages on the right-hand side (rhs) of (25) are evaluated to relate to the $\langle b_{\mathbf{Q}}^+\rangle_{\mathcal{H}}$ on the left-hand side (lhs). This leads to a closed expression, the solution of which determines the value of $E_F - \mu(\lambda, T)$. Since $\xi_{\mathbf{k}} \equiv \xi_{-\mathbf{k}}$, from (A14)–(A16) we have for $\mathbf{K}=0$,

$$\langle a_{\mathbf{q}\uparrow}^+ a_{-\mathbf{q}\downarrow}^+\rangle_{\mathcal{H}} = \frac{f}{2L^{d/2}}\frac{\langle b_0^+\rangle}{\sqrt{(\epsilon_{\mathbf{q}} - \mu)^2 + f^2 n_{B0}}} \times \tanh\frac{\sqrt{(\epsilon_{\mathbf{q}} - \mu)^2 + f^2 n_{B0}}}{2k_BT}. \quad (26)$$

When substituted into (25) with $\mathbf{Q}=0$ this leads to

$$1 = \frac{f^2}{E(0) - 2\mu} \frac{1}{2L^d} \sum_{\mathbf{q}} \frac{1}{\sqrt{(\epsilon_{\mathbf{q}} - \mu)^2 + f^2 n_{B0}}} \times \tanh \frac{\sqrt{(\epsilon_{\mathbf{q}} - \mu)^2 + f^2 n_{B0}}}{2k_B T}. \quad (27)$$

The sum in (27) becomes an integration over the free-electron energy states ϵ. Using (3), (6), and (20) and integrating over the interval $[\mu - \hbar\omega_D, \mu + \hbar\omega_D]$ one can rewrite (27) as

$$E_F - \mu(\lambda, T) = -\Delta(\lambda) + \frac{\lambda\hbar\omega_D}{2} \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{dx}{\sqrt{x^2 + f^2 n_{B0}(T)}} \times \tanh \frac{\sqrt{x^2 + f^2 n_{B0}(T)}}{2k_B T}. \quad (28)$$

This equation must be satisfied for any temperature $T \leqslant T^*$. In particular, the solution of (28) for T with $E_F = \mu$ yields a temperature T^* at which a transition occurs from the normal state with *no composite bosons* to one *with such bosons*, i.e., to the incoherent binary BF mixture. The condition $E_F = \mu$ is equivalent to $n_B(T^*) = 0$ which implies $n_{B0}(T) = 0$ in (28) since $0 < n_{B0}(\lambda, T) < n_B(\lambda, T)$. Furthermore, $n_{B0}(\lambda, T)$ vanishes for all $T > T_c$. For materials with λ and ω_D such that $k_B T^* \ll \hbar\omega_D$, setting $E_F - \mu(\lambda, T) = 0$ in (28) immediately gives

$$k_B T^* \simeq 1.134\hbar\omega_D \exp(-\Delta/2\lambda\hbar\omega_D) \quad \text{if } k_B T^* \ll \hbar\omega_D. \quad (29)$$

This should be compared with the weak-coupling BCS formula $k_B T_c \simeq 1.134\hbar\omega_D \exp(-1/\lambda)$ which in turn is *less* than (29), as of course it should be, provided only that $\Delta < \hbar\omega_D$. Thus, for $k_B T^* \ll \hbar\omega_D$ (29) gives a temperature T^* below which some of the electrons begin to pair up. For fixed $T \leqslant T^*$ the solution of (28) determines the value of $E_F - \mu(\lambda, T)$ which gives the shift in $\mu(\lambda, T)$ with respect to E_F of the normal metal due to boson formation.

V. BOSE-EINSTEIN-CONDENSATION TRANSITION TEMPERATURE

The total number $N_B(\lambda, T)$ of bosons in the system is now determined from (12), namely

$$N_B(\lambda, T) \equiv \sum_{\mathbf{K}} n_{B\mathbf{K}}(\lambda, T) = \sum_{\mathbf{K}} (e^{\Omega_{\mathbf{K}}/k_B T} - 1)^{-1} \quad (30)$$

where a singularity occurs at $\Omega_{\mathbf{K}} \to 0$. Fortuitously, this singularity defines the Bose-Einstein-condensation (BEC) transition temperature T_c for the BF mixture in perfect analogy to that of a *pure* boson gas.[14] Setting $\mathbf{K} = 0$ and $\Omega_0 = 0$ in (13) and substituting (6) into it, we find that in the thermodynamic limit $L^d \to \infty$ and $N \to \infty$ the number density $n_{B0}(\lambda, T) = N_{B0}(\lambda, T)/L^d$ of condensed bosons in the state $\mathbf{K} = 0$ *just ceases to be negligible* upon cooling whenever

$$E_F - \mu(\lambda, T_c) \equiv -\Delta(\lambda) + \frac{f^2}{4L^d} \sum_{\mathbf{q}} \frac{1 - n_{\mathbf{q}\uparrow} - n_{-\mathbf{q}\downarrow}}{\epsilon_{\mathbf{q}} - \mu(T_c)} \quad (31)$$

is satisfied. The sum in (31) can be evaluated as an integral over ϵ. The 2D DOS $N(\epsilon)$ is exactly constant. In 3D $N(\epsilon) \propto \sqrt{\epsilon}$ but its variation is small within the integration region if $\hbar\omega_D \ll E_F$ so that $N(\epsilon) \simeq N(E_F)$ in (31) in either 2D or 3D. Inserting the fermion occupation numbers $n_{\mathbf{k}}$ (10) and using (3) we rewrite (31) as

$$E_F - \mu(\lambda, T_c) \equiv -\Delta(\lambda) + \frac{\lambda\hbar\omega_D}{2} \int_{-\hbar\omega_D}^{\hbar\omega_D} dx \frac{\tanh(x/2T_c)}{x}. \quad (32)$$

Note that this is the same result as (28) with $n_{B0}(T_c) \equiv 0$. Clearly then, $E_F - \mu(\lambda, T)$ will depend on $\Delta(\lambda)$ which from (6) is one-half the boson formation energy over and above the Fermi energy; it also depends on the redistribution of single-particle levels caused by boson formation. Equation (32) is a necessary condition for BEC to take place. For the linear dispersion law (7) and spherical symmetry over $\mathbf{K}$, integration over K itself in (30) is easily performed [see, e.g., Ref. 14, Eq. (12)]. For our 2D and 3D BF mixtures one then obtains the simple but *implicit* T_c formulas

$$k_B T_c = c_2 2\sqrt{3}\pi^{-1/2}\hbar v_F n_B(\lambda, T_c)^{1/2} \quad \text{(2D)}, \quad (33)$$

$$k_B T_c = c_3 \pi^{2/3} \zeta(3)^{-1/3} \hbar v_F n_B(\lambda, T_c)^{1/3} \quad \text{(3D)}, \quad (34)$$

where $\zeta(3) \simeq 1.202$ is the Riemann zeta function of order 3. Since $N(E_F)$ is given by (21) and (22), substituting (20) into (33) and (34) leaves

$$k_B T_c / E_F = \begin{cases} 2\sqrt{3}\pi^{-1} c_2 [1 - \mu(\lambda, T_c)/E_F]^{1/2} & \text{(2D)}, \\ 2^{1/3}\zeta(3)^{-1/3} c_3 [1 - \mu(\lambda, T_c)/E_F]^{1/3} & \text{(3D)}. \end{cases} \quad (35)$$

These two implicit T_c formulas are the main result of this paper. They were obtained differently in Ref. 47 where their derivation was merely sketched.

In actual calculations we first express $[1 - \mu(\lambda, T_c)/E_F]$ in (35) in terms of T_c/T_F with $T_F \equiv E_F/k_B$, i.e., we write

$$1 - \mu(\lambda, T_c)/E_F = (B_d T_c/\lambda T_F)^d, \quad (36)$$

where the d-dependent parameters B_d are determined by using the specific values of $c_2 = \lambda/2\pi$ and $c_3 = \lambda/4$ mentioned before.[25,26] One gets $B_2 \simeq 5.698$ and $B_3 \simeq 3.376$. Thus (32) yields the implicit equations

$$(B_d T_c/\lambda T_F)^d - (\lambda\hbar\omega_D/2E_F) \int_{-\hbar\omega_D/E_F}^{\hbar\omega_D/E_F} dx \frac{\tanh(xT_F/2T_c)}{x} + \Delta(\lambda)/E_F = 0 \quad (d = 2 \text{ or } 3) \quad (37)$$

which can be solved numerically for either d. The pseudogap phenomenon, therefore definition of finite T^*, within the present theory is only possible in the gapped structure of the boson spectrum $E(\mathbf{K})$ originally assumed in (5). To determine T^* we must set $E_F = \mu$, i.e., $n_B(T^*) = 0$, in (28). In fact, if there were no gap $2\Delta(\lambda)$ in $E(\mathbf{K})$ then from (28) we imme-

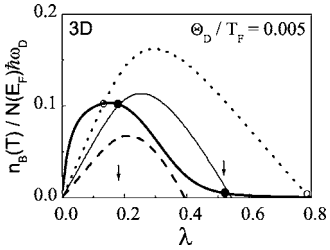

FIG. 1. Fractional density of pairable electrons that become composite bosons, as function of dimensionless electron-phonon coupling λ in 3D for reduced temperatures $T/T_F=0.0025$ dotted curve, 0.004 thin full curve, and 0.006 dashed curve, all for the typical value of Θ_D/T_F shown. Shaded region is where no BEC has yet appeared in the incoherent BF mixture. Unshaded region corresponds to the superconducting BEC coherent phase that occurs in the BF mixture.

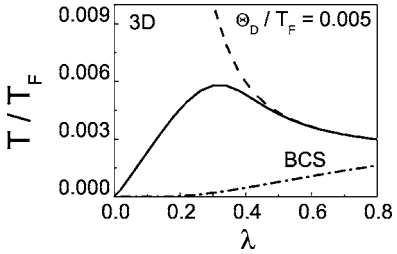

FIG. 2. BEC superconducting (full curve) T_c/T_F and pseudogap (dashed curve) T^*/T_F phase boundaries, as functions of λ for $\Theta_D/T_F=0.005$ in 3D. Shaded region designates the superconducting BEC phase of the BF mixture. The normal state lies above the pseudogap phase boundary defined by the reduced depairing temperature T^*/T_F (dashed curve) below which the pseudogap phase exists. Dotted-dashed curve is the BCS value from $T_c/T_F \simeq 1.134(\Theta_D/T_F)\exp(-1/\lambda)$.

diately get two noninteraction dependent and thence unphysical trivial solutions: (a) $T^*=0$ and (b) $T^*=\infty$. Solution (a) precludes boson formation processes at any finite temperature while solution (b) implies that bosons must be formed at arbitrarily large T. A gapped boson dispersion ensures finite, nonzero values for T^*. But it should be emphasized that the density of bosons $n_B(\lambda,T)$ as given by (20) and (28), can be obtained regardless of the precise form of a $E(\mathbf{K})$.

VI. RESULTS AND DISCUSSION

In Fig. 1 the fractional density of pairable electrons that are composite bosons $n_B(\lambda,T)/N(E_F)\hbar\omega_D$ is shown for $\Theta_D/T_F=0.005$ as a function of $\lambda=N(E_F)V$ in 3D for three reduced temperatures $T/T_F=0.0025$, 0.004, and 0.006, respectively, designated by dotted, thin, and dashed curves. Here $N(E_F)\hbar\omega_D$ is one-half the total number of pairable fermions. The thick curve is the critical such fractional density, say, n_B^o above which a BEC occurs in the incoherent BF mixture. Bold and open circles are points where $n_B(\lambda,T)$ achieves that critical value n_B^o. Note from Fig. 1 that BEC never occurs in the region where $n_B(\lambda,T)<n_B^o$. For example, over the entire range of λ values and for $T/T_F=0.006$ (dashed curve) the density $n_B(\lambda,T)$ never reaches the value n_B^o. Therefore, this BF mixture never becomes superconducting at temperatures as high as $0.006T_F$. Two features are noteworthy in the figure. First, the system of free fermions becomes unstable when the smallest attractive interaction between charge carriers appears. Namely, for an infinitesimal pairing interaction $\lambda=0^+$ the boson density $n_B(\lambda,T)$ begins differing from zero. In other words, the system of interactionless electrons becomes an incoherent BF mixture for any $\lambda>0$. The highest temperature below which the system remains an incoherent BF mixture depends on the actual value of λ. As to the magnitude of $n_B(\lambda,T)$, it rapidly decreases with increasing temperature as seen from the curves for $T/T_F=0.0025$, 0.004, and 0.006. Second, the boson density $n_B(\lambda,T)$ decreases considerably for larger values of λ. Numerically at least, one sees that if there were no term $2\Delta(\lambda)$ in the dispersion relation (6) of composite bosons, then $n_B(\lambda,T)$ would be a monotonically increasing function of λ. Because the formation of bosons energetically situated well above the Fermi level is associated with a substantial change in the ground-state energy, such processes occur rarely in the system and this explains the decrease in $n_B(\lambda,T)$ with λ. The figure also shows that lowering T/T_F increases the interval in λ (marked by vertical arrows) over which superconductivity occurs.

This explains the nonmonotonic "dome-shaped" behavior of T_c vs λ shown in Fig. 2 where T_c/T_F (full curve) and T^*/T_F (dashed curve) are drawn as functions of λ for the same $\Theta_D/T_F=0.005$ in 3D. The dashed curve separates the normal phase at all temperatures above T^* from the BF mixture phase emerging from the interacting-fermion system below T^*. By lowering T below T_c (where $T_c<T^*$) BEC occurs in the interacting BF mixture. Some peculiarities in the figure should be noted: (a) the behavior of T_c vs λ is nonmonotonic, rising at first as λ increases from zero, maximizing at $\lambda\sim 0.35$, then dropping off by more than by a factor of 2 from its maximum value, and finally decreasing to zero very slowly for larger λ; (b) T^* and T_c are drastically different at small λ but then merge into one another as λ increases.

If we associate the dimensionless interaction parameter $\lambda=N(E_F)V$ with the concentration of charge carriers x (ignoring the antiferromagnetic region in generic cuprates, not addressed here) then Fig. 2 becomes the typical dome-shaped phase diagram[48] of high-T_c superconductors. This x vs λ correlation can be justified, at least qualitatively, from McMillan's expression[49] for the dimensionless electron-phonon interaction parameter

$$\lambda = \frac{N(E_F)\langle J^2\rangle_{FS}}{M\langle\omega^2\rangle_{ph}} \tag{38}$$

with J and ω, respectively, being an electron-ion interaction matrix element and a phonon frequency; M is the ionic mass. Here, $\langle\cdots\rangle_{FS}$ and $\langle\cdots\rangle_{ph}$ denote average values over the Fermi surface and phonon spectrum, respectively. The term $M\langle\omega^2\rangle_{ph}$ in the denominator is sometimes called the lattice "stiffness." Since in 3D $N(E_F)\propto\sqrt{E_F}$ with $E_F=(\hbar^2/2m)\times(3\pi^2 n)^{2/3}$ and as before n the total density of single

charged carriers, then in (38) $N(E_F) \propto n^{1/3}$. Varying the doping parameter x changes the density of charged carriers and therefore $N(E_F)$, which in turn leads to variations in λ from (38). As to $\langle J^2 \rangle_{FS}$, it depends on local (atomic) properties of the material rather than on n. However, in the presence of a *denser* electron liquid, phonons become *softer*[50] so that the term in the denominator in (38) will *decrease* with n, thus enhancing the x vs λ correlation. In 2D systems where $N(E_F)$ is independent of E_F and thus of n, the x vs λ correlation still holds if one assumes that by varying x the lattice stiffness $M\langle \omega^2 \rangle_{ph}$ changes. In fact, formula (38) obtained for the phonon-mediated-pairing mechanism and used here to justify the "x vs λ" correlation cannot be applied to a nonphonon pairing mechanism. Recent experiments,[29] however, suggest that phonons play an important if not decisive role in high-T_c superconductors. Nevertheless, a less rigorous justification of the "x vs λ " association follows directly from the expression $\lambda = N(E_F)V$ and applies for any pairing mechanism if one ignores the variation of V with x.

The rapid decrease of T^* with λ in Fig. 2 is important. It shows that composite bosons formed in materials with large λ are broken up more easily at higher temperatures, or, that the T below which a boson with a larger value of 2Δ appears is lower than that at which a boson with smaller 2Δ is formed. In other words, bosons energetically closer to Fermi surface, namely those formed with smaller λ, turn out to be better "protected" against thermal disruptions and thus survive over a wider temperature range. At first glance, this curious T^* vs λ behavior may be understood in terms of the *gapped* dispersion relation (6). In fact, for this breakup to occur fermionic levels that are occupied by electrons resulting from bosonic breakup, must be empty. However, the expectation that the single-fermion $\mathbf{k}$ states needed to be occupied as a result of a breakup are empty, is smaller if these $\mathbf{k}$ states are situated in the sea of densely populated fermion states or near it [see expression for occupation numbers (10)]. By contrast, bosons propagating with energies *above* E_F break up into unpaired fermions more easily because there are many admissible states to be occupied above E_F. Experimentally,[48] T_c in cuprates vanishes as x increases beyond some threshold value, say, x_{crit}. Ignoring for a moment the fact that T_c vanishes for $x \geqslant x_{\mathrm{crit}}$ and instead of λ set x on the horizontal axis in Fig. 2, then (1) a rapidly decreasing T^* vs λ and (2) the merging of T^* with T_c at large λ, qualitatively explain the empirical phase diagram for high-temperature superconductors (see discussion below on why T^* vanishes at large λ).

We emphasize that the appearance in Fig. 2 of a pseudogap phase, namely an incoherent (i.e., *without* BEC) BF mixture phase, is a direct consequence of the gapped spectrum of the composite boson dispersion relation (6). Indeed, the T^* phenomena in the present theory arises solely because of the term 2Δ in (6). As to the magnitude of T^* at very small λ, widespread opinion holds that it must vanish in this limit, e.g., Ref. 27. This would certainly be the case for two free electrons interacting via an attractive potential in the absence of the Fermi sea of other particles, i.e., *in vacuo*, in keeping with the *gapless* quadratic dispersion used for the bosons used in Ref. 27 (as well as in Refs. 6, 10, 11, 20, and 21 among many others) so that in the limit of zero interaction a composite state breaks up into independent states of two electrons. This does not happen here. For *gapless* bosonic excitations it was argued in Ref. 20 that the decay of composite bosons is more difficult at temperatures below T_c and that at $T=0$ it cannot take place *at all* because of the exclusion principle. Applying this idea here we see that composite bosons persist up to T^* as soon as an interelectronic attractive interaction $-V$ is different from zero. This is similar to that of the BCS scenario where the slightest *infinitesimal* attractive interaction leads to the creation of pairs below some threshold temperature (here below T^*). But the unexpected outcome here is that the temperature T^* below which bosons first appear must be higher for smaller λ (i.e., when the gap 2Δ in the boson spectrum is smaller) than T^* for larger λ. As a result, bosons created in the $\lambda \to 0$ limit, i.e., pairs emerging within the Fermi sea, appear to be stable up to much high temperatures than bosons created for larger λ. We believe that this reflects the fact that as soon as λ differs from zero, pair fluctuations in the electron medium become possible. Of course, thermal fluctuations will break these pairs up. However, independently of how large T is, this mode of pair formation will always differ from zero. This feature has no analogy either in conventional superconductors, as in the BCS model where the "hardness" of pairs is associated with large λ, nor in BF models[20] with a gapless boson dispersion curve. It seems to be an inherent property of a BF mixture with an *interaction-dependent* gap such as 2Δ in its composite-boson spectrum.[25,26] To understand this result intuitively, note that in BF mixture models pair stability (or CP lifetime) depends not only on how large the interaction parameter λ is but also on the degree to which the corresponding bosonic states are energetically separated from the Fermi surface. The latter is determined by the energy gap 2Δ in the dispersion relation (6) and plays a decisive role in confining two electrons to form a CP with a finite lifetime. Indeed, increasing λ increases the separation of the bosonic states from the Fermi sea, thus making pairs more loosely bound, e.g., with respect to decay by thermal effects as discussed above. There will always be pair-creation in the medium of attractively interacting electrons. However, formation of bosons well-separated from the Fermi sea (i.e., with large 2Δ) is reduced. Therefore, the conditions for such pairs to appear (i.e., pairs formed at large λ) must be more restrictive and therefore are more easily satisfied at lower temperatures.

The many-particle contributions to pairing[25] lead not only to the gap 2Δ in the CP boson spectrum, which explains the pseudogap state and its peculiarities. They also yield linearly dispersive boson energies allowing BEC superconductivity not only in 3D but also in 2D systems[14] where it would be forbidden with quadratically dispersive pairs that occur *in vacuo*. As to the zero-temperature gap 2Δ in (6) it needs to be generalized to finite temperatures, a task for future work. The merging of T^* with T_c for large λ may be also easily understood if one considers the conditions $n_B(\lambda, T^*)=0$ and $n_{B0}(\lambda, T_c)=0$ with $n_B(\lambda, T)$ and $n_{B0}(\lambda, T)$, respectively, the total number density of bosons and number density of condensed bosons. To ascertain that T^* and T_c become nearly the same in the large λ limit, we note that the condition $n_B(\lambda, T^*)=0$ that determines T^* and the condition $n_{B0}(\lambda, T_c)$

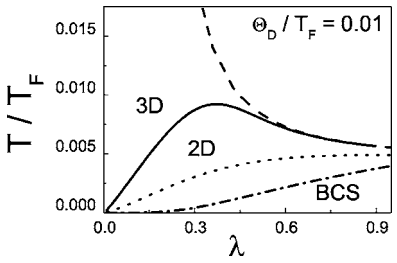

FIG. 3. Comparison of results in 2D (short-dashed curve) of the T_c/T_F phase boundary with those in 3D (full) curve of Fig. 2 but for $\Theta_D/T_F=0.01$ instead of 0.005. Long-dashed curve is again T^*/T_F. Dotted-dashed curve is the (d-independent) BCS value as in Fig. 2.

$=0$ determining T_c coincide for large λ as seen in Fig. 1. In fact, T^* is a temperature at which incoherent pairs first emerge in the normal state but, as shown in Fig. 1, the critical density of bosons above which BEC occurs also vanishes for large λ. The condition $n_B(\lambda,T_c)\simeq n_B(\lambda,T^*)=0$ [and therefore $n_{B0}(\lambda,T_c)=0$] satisfied at large λ drives T^* to merge with T_c in this limit. Last, $n_B(\lambda,T_c)\to 0$ for large λ is directly related to the gapped boson dispersion relation (6). This is because the number of pairs excited much above E_F, i.e., pairs associated with larger λ and therefore larger values of the boson gap 2Δ, are much less likely.

In Fig. 3 the BEC T_c vs λ in 2D and 3D systems with the same $\Theta_D/T_F=0.01$ are compared. Within a wide range of λ values the 2D BEC temperature T_c (dotted curve) is bounded from above by the 3D value of T_c (full curve). However, the threshold temperature for pair formation T^* (dashed curve) does not depend on dimensionality d. This suggests that T^* depends only on the local pairing interaction between fermions which for the Cooper or BCS model interaction is itself independent of d. The two T_c curves for 2D and 3D approach each other as λ increases, eventually merging together as well as with T^*. Therefore, at least within the present simplified BF model and *in the limit of large* λ the BEC of a BF mixture is largely controlled by the magnitude of Θ_D and does not depend on dimensionality, with T_c larger for materials with larger Θ_D. This is clear from (37) for 2D and 3D in the large λ limit if one assumes $T_c<\Theta_D$.

It should be noted that in the present work a well-defined domed structure in T_c vs λ is maintained in 3D only for Θ_D/T_F up to about 0.01. However, this result is very sensitive to the form of $2\Delta(\lambda)$. It was seen in our numerical calculations that the variation of $2\Delta(\lambda)$, apart from its monotonic increase with λ, leads to a considerable change in the critical value of Θ_D/T_F below which the domed structure in T_c vs λ first occurs. If the λ dependence of 2Δ in (6) were stronger than that given by (8), e.g., of the form $\lambda^{1+\alpha}\hbar\omega_D$ or $\lambda^{\alpha}\Delta(\lambda)$ with $\alpha\simeq 1$ and this substituted for $2\Delta(\lambda)$ in (6), then for the broad range of Θ_D/T_F from 0.05 to 0.14 appropriate in cuprates[51] one may easily get in 2D: (a) the well-defined domed shape of T_c vs λ; (b) the merging of T^* and T_c as λ increases; and (c) T_c values almost within the experimental range for cuprates. Therefore, it is extremely important to ascertain an accurate expression for the CP spectrum $E(\mathbf{K})$ starting from the many-particle electron-ion interactions which take place in the cuprates.

Experimentally, e.g., in $La_{2-x}Sr_xCuO_4$ (Refs. 52 and 53) T_c first rises with doping x (underdoped region). It then maximizes (optimal doping), and drops to zero as x is further increased (overdoped region). Because of our λ vs x correlation, the same behavior is expected for T_c as a function of λ, that is, we predict that superconductivity eventually vanishes at larger λ. However, at least within the present simplified BF model, T_c never strictly vanishes when $\lambda\to\infty$. It continues to fall with increasing λ but very slowly. The extinction of superconductivity in highly overdoped oxides established by experiment may be accounted for as a result of lattice instability that sets in as λ increases indefinitely.[54] The instability with increasing λ (or, because of our λ vs x correlation, with increasing x) should not be discarded as a possible explanation for the vanishing of T_c at large x. Of course, there may be other physical reasons for this in the overdoped cuprates, e.g., in terms of composite-boson localization effects as suggested in Ref. 27.

VII. CONCLUSIONS

We started from the Friedberg-Lee Hamiltonian describing a boson-fermion model of two coexisting and dynamically interacting many-particle subsystems, unpaired fermions and composite bosons but with a coupling (λ)-dependent gap $2\Delta(\lambda)$ in the boson dispersion relation *instead* of the usual quadratic one appropriate of composite bosons propagating in vacuum. Using two-time (or, retarded) finite-temperature Green functions, analytic expressions for the coupling (λ)- and temperature (T)-dependent unpaired-fermion and boson number densities were obtained, as well as the fermion chemical potential $\mu(\lambda,T)$, all of which vary with boson formation and temperature. Relating a depairing temperature T^* and the BEC T_c with $\mu(\lambda,T)$ and $2\Delta(\lambda)$ provides a qualitative but self-consistent description of the generic experimental cuprate phase diagram that includes a pseudogap as well as a dome-shaped T_c-vs-doping behavior, in spite of the simplicity of a boson-fermion model with only s-wave pairing.

ACKNOWLEDGMENTS

One of the authors (T.A.M.) thanks the Institute of Physics of Azerbaijan for granting him academic leave at the Baskent University of Turkey. One of the authors (M.deLl.) acknowledges DGAPA-PAPIIT (UNAM, Mexico) Grant No. IN106401, and CONACyT (Mexico) Grant No. 41302F, as well as the Texas Center for Superconductivity, University of Houston, Houston, TX 77204 for partial support, as well as the Royal Society (UK) and the Academia Mexicana de Ciencias (Mexico) for a joint program.

APPENDIX A: UNPAIRED-ELECTRON NUMBER

Here we derive (10) for the number of unpaired electrons $n_{\mathbf{k},\sigma}\equiv\langle a^+_{\mathbf{k},\sigma}a_{\mathbf{k},\sigma}\rangle$ in a state with momentum $\mathbf{k}$ and spin σ in full detail; this was only outlined before in Ref. 55. Starting from the grand canonical Hamiltonian $\mathcal{H}$ we write it as a sum of two pieces, $\mathcal{H}_0$ and $H_{\rm int}$ (5). Two-time retarded Green

functions at times t and t' for dynamical operators $A(t)$ and $B(t')$ are defined[56] with double-angular brackets as

$$\langle\langle A(t)|B(t')\rangle\rangle \equiv \theta(t-t')\langle[A(t),B(t')]_\eta\rangle_{\mathcal{H}},$$

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, and $\theta(x)$ is the Heaviside unit step function. In this formalism any dynamical operator $X(t)$ is in the Heisenberg representation, i.e., is of the form $X(t) = \exp(i\mathcal{H}t)X\exp(-i\mathcal{H}t)$. It is not difficult to see that Green functions $\langle\langle A(t)|B(t')\rangle\rangle$ satisfy the equation[56]

$$i\frac{d}{dt}\langle\langle A(t)|B(t')\rangle\rangle = i\delta(t-t')\langle[A(t),B(t')]\rangle + \langle\langle[A(t),H]|B(t')\rangle\rangle. \tag{A1}$$

Inserting

$$\langle\langle A|B\rangle\rangle_\omega \equiv \frac{1}{2\pi}\int_{-\infty}^{\infty}\langle\langle A(t)|B(t')\rangle\rangle e^{i\omega(t-t')}d(t-t')$$

into (A1) immediately gives the chain of equations

$$\omega\langle\langle A|B\rangle\rangle_\omega = \langle[A,B]_\eta\rangle_{\mathcal{H}} + \langle\langle[A,\mathcal{H}]_-|B\rangle\rangle_\omega \tag{A2}$$

for the Fourier transform $\langle\langle A|B\rangle\rangle_\omega$ of $\langle\langle A(t)|B(t')\rangle\rangle$ in ω. To find values for $n_{\mathbf{k},\sigma}$ we set $\eta=+1$ in Eq. (A2). Choosing *first* $A\equiv a_{\mathbf{k}\uparrow}$ and *then* $A\equiv a^+_{\mathbf{k}\downarrow}$ and setting B equal to $a^+_{\mathbf{k}'\uparrow}$, one obtains

$$(\omega-\epsilon_{\mathbf{k}}+\mu)\langle\langle a_{\mathbf{k}\uparrow}|a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega = \delta_{\mathbf{k}\mathbf{k}'} - \frac{f}{L^{d/2}}\sum_{\mathbf{K}}\langle b_{\mathbf{K}}\rangle \times\langle\langle a^+_{-\mathbf{k}+\mathbf{K},\downarrow}|a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega, \tag{A3}$$

$$(\omega+\epsilon_{\mathbf{k}}-\mu)\langle\langle a^+_{\mathbf{k}\downarrow}|a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega = -\frac{f}{L^{d/2}}\sum_{\mathbf{K}}\langle b^+_{\mathbf{K}}\rangle\langle\langle a_{-\mathbf{k}+\mathbf{K},\uparrow}|a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega. \tag{A4}$$

To calculate the commutators on the rhs of (A2) the relations $[a_{\mathbf{k}\sigma},a^+_{\mathbf{k}'\sigma'}]_+=\delta_{\mathbf{k}k'}\delta_{\sigma\sigma'}$, $[a^+_{\mathbf{k}\sigma},a^+_{\mathbf{k}'\sigma'}]_+=0$ and $[a_{\mathbf{k}\sigma},a_{\mathbf{k}'\sigma'}]_+=0$ are used. Furthermore, in establishing (A3) and (A4) the higher-order Green functions $\langle\langle BC|a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega$ which come from $\langle\langle[A,\mathcal{H}]_-|B\rangle\rangle_\omega$ in (A2) are put into the form

$$\langle\langle BC|a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega = \langle B\rangle\langle\langle C|a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega + \langle\langle(B-\langle B\rangle)C|a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega, \tag{A5}$$

where $B=b_{\mathbf{K}}$ or $b^+_{\mathbf{K}}$, i.e., it is a pure *boson* operator, while $C=a_{\mathbf{k}\alpha}$ or $a^+_{\mathbf{k}\alpha}$ is a pure *fermion* operator. Terms of the type $\langle\langle(B-\langle B\rangle)C|a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega$ are then considered small contributions in (A3) and (A4) and hence neglected. Now, replacing the index $\mathbf{K}$ in (A4) by $\mathbf{Q}$, index $\mathbf{k}$ by $-\mathbf{k}+\mathbf{K}$ and substituting (A4) into (A3) we have

$$(\omega-\epsilon_{\mathbf{k}}+\mu)\langle\langle a_{\mathbf{k}\uparrow}|a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega = \delta_{\mathbf{k}\mathbf{k}'} + \frac{f^2}{L^d}\sum_{\mathbf{K},\mathbf{Q}}\frac{\langle b_{\mathbf{K}}\rangle\langle b^+_{\mathbf{Q}}\rangle}{\omega+\epsilon_{-\mathbf{k}+\mathbf{K}}-\mu}\langle\langle a_{\mathbf{k}-\mathbf{K}+\mathbf{Q}\uparrow}|a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega. \tag{A6}$$

We assume that functions such as $\langle\langle a_{\mathbf{k}\uparrow}a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega$ are diagonal in $\mathbf{k}$ and $\mathbf{k}'$, as in lowest-order two-time Green functions[57] due to translational symmetry. Keeping only terms with $\mathbf{Q}=\mathbf{K}$ in (A6) then gives

$$\langle\langle a_{\mathbf{k}\uparrow}|a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega \simeq \delta_{\mathbf{k}\mathbf{k}'}\left(\omega-\epsilon_{\mathbf{k}}+\mu-\frac{f^2}{L^d}\sum_{\mathbf{K}}\frac{\langle b_{\mathbf{K}}\rangle\langle b^+_{\mathbf{K}}\rangle}{\omega+\epsilon_{-\mathbf{k}+\mathbf{K}}-\mu}\right)^{-1}. \tag{A7}$$

Separating terms with $\mathbf{K}=0$ from $\mathbf{K}\neq 0$, restricting ourselves to terms $O(f^2)$, and writing $\epsilon_{\mathbf{k}}=\epsilon_{-\mathbf{k}}$ by symmetry, one obtains after some tedious algebra that

$$\langle\langle a_{\mathbf{k}\alpha}|a^+_{\mathbf{k}'\alpha}\rangle\rangle_\omega = \frac{\omega+\epsilon_{\mathbf{k}}-\mu}{\omega^2-E^2_{\mathbf{k}}}\left(1+\frac{1}{L^d}\frac{f^2}{\omega-\epsilon_{\mathbf{k}}+\mu}\times\sum_{\mathbf{K}\neq\mathbf{0}}\frac{\langle b^+_{\mathbf{K}}\rangle\langle b_{\mathbf{K}}\rangle}{\omega+\epsilon_{-\mathbf{k}+\mathbf{K}}-\mu}\right)\delta_{\mathbf{k}\mathbf{k}'}, \tag{A8}$$

where

$$E_{\mathbf{k}} \equiv \sqrt{(\epsilon_{\mathbf{k}}-\mu)^2+f^2\langle b^+_0\rangle\langle b_0\rangle}. \tag{A9}$$

In particular, by substituting (A8) in (A4) it is not difficult to arrive at

$$\langle\langle a^+_{-\mathbf{k}+\mathbf{K}/2\downarrow}|a^+_{\mathbf{k}+\mathbf{K}/2\uparrow}\rangle\rangle_\omega = -\frac{f}{L^{d/2}}\frac{\omega+\xi_{\mathbf{k}+\mathbf{K}/2}}{\omega+\xi_{-\mathbf{k}+\mathbf{K}/2}}\frac{\langle b^+_{\mathbf{K}}\rangle}{\omega^2-E^2_{\mathbf{k}+\mathbf{K}/2}} + O(f^3). \tag{A10}$$

Knowing the two-time Green functions $\langle\langle a_{\mathbf{k}\alpha}|a^+_{\mathbf{k}'\alpha}\rangle\rangle_\omega$ and $\langle\langle a^+_{-\mathbf{k}\downarrow}|a^+_{\mathbf{k}'\uparrow}\rangle\rangle_\omega$ one can find expressions for the corresponding average values $\langle a^+_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha}\rangle_{\mathcal{H}}$ and $\langle a^+_{\mathbf{k}\uparrow}a^+_{-\mathbf{k}'\downarrow}\rangle_{\mathcal{H}}$ from the relation[56]

$$\langle A(t)B(t')\rangle_{\mathcal{H}} = \frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega e^{i\omega(t-t')}J_{AB}(\omega), \tag{A11}$$

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

$$\{\langle\langle A|B\rangle\rangle_{\omega+i\varepsilon} - \langle\langle A|B\rangle\rangle_{\omega-i\varepsilon}\} = -i(e^{\hbar\omega/k_BT}-\eta)J_{BA}(\omega). \tag{A12}$$

After some algebra one obtains

$$\langle a^+_{\mathbf{k}\alpha}a_{\mathbf{k}\alpha}\rangle_{\mathcal{H}} \equiv n_{\mathbf{k}} = \frac{1}{2}\left(1-\frac{\epsilon_{\mathbf{k}}-\mu}{E_{\mathbf{k}}}\tanh(E_{\mathbf{k}}/2k_BT)\right) \tag{A13}$$

which proves (10).

One also finds, to be used in proving (25) via (26), that

$$\langle a^+_{\mathbf{k}+\mathbf{K}/2\uparrow}a^+_{-\mathbf{k}+\mathbf{K}/2\downarrow}\rangle_{\mathcal{H}} = \frac{f}{2L^{d/2}}\frac{\langle b^+_{\mathbf{K}}\rangle}{E_{\mathbf{k}+\mathbf{K}/2}}\{Z_1(\mathbf{k},\mathbf{K}) - Z_2(\mathbf{k},\mathbf{K})\}, \tag{A14}$$

where we defined

$$Z_1(\mathbf{k},\mathbf{K}) \equiv \left(1 - \frac{(\xi_{\mathbf{k}+\mathbf{K}/2} - \xi_{-\mathbf{k}+\mathbf{K}/2})\xi_{-\mathbf{k}+\mathbf{K}/2}}{E^2_{\mathbf{k}+\mathbf{K}/2} - \xi^2_{-\mathbf{k}+\mathbf{K}/2}}\right)\tanh\frac{E_{\mathbf{k}}}{2k_BT}, \tag{A15}$$

$$Z_2(\mathbf{k},\mathbf{K}) \equiv \frac{(\xi_{\mathbf{k}+\mathbf{K}/2} - \xi_{-\mathbf{k}+\mathbf{K}/2})E_{\mathbf{k}+\mathbf{K}/2}}{E^2_{\mathbf{k}+\mathbf{K}/2} - \xi^2_{-\mathbf{k}+\mathbf{K}/2}}\tanh\frac{\xi_{-\mathbf{k}+\mathbf{K}/2}}{2k_BT} \tag{A16}$$

with $\xi_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} - \mu$.

APPENDIX B: BOSON NUMBER

Here we derive (13) that determines the boson number-density $n_{B\mathbf{K}}(T)$ given by (12) for fixed CMM $\mathbf{K}$. The total number of composite bosons at any temperature T is just $N_B(T) \equiv \Sigma_{\mathbf{Q}} n_{B\mathbf{Q}}(T)$ with $n_{B\mathbf{Q}}(T) \equiv \langle \hat{n}_{B\mathbf{Q}}\rangle$ and $\hat{n}_{B\mathbf{Q}} \equiv b^+_{\mathbf{Q}}b_{\mathbf{Q}}$. Changing T and/or λ will change $N_B(T)$. Choosing first $A \equiv b_{\mathbf{Q}}$ and $B \equiv b^+_{\mathbf{Q}}$ in (A2) with $\eta = -1$ we write (A2) as

$$\omega\langle\langle b_{\mathbf{Q}}|b^+_{\mathbf{Q}}\rangle\rangle_\omega = 1 + \langle\langle[b_{\mathbf{Q}},\mathcal{H}]_-|b^+_{\mathbf{Q}}\rangle\rangle_\omega \tag{B1}$$

since $[b_{\mathbf{Q}}, b^+_{\mathbf{Q}}]_- = 1$. We determine $[b_{\mathbf{Q}},\mathcal{H}]_-$ on the rhs of (B1) by first splitting it as a sum of two terms $I_0 \equiv [b_{\mathbf{Q}},\mathcal{H}_0]$ and $I_{\text{int}} \equiv [b_{\mathbf{Q}}, H_{\text{int}}]$, and then finding I_0 and I_{int} separately. As is customary in boson-fermion models, we assume that a and b operators commute with each other. Since $[b_{\mathbf{Q}}, b_{\mathbf{K}}]_- = 0$ while $[b_{\mathbf{Q}}, b^+_{\mathbf{K}}]_- = \delta_{\mathbf{Q},\mathbf{K}}$ and $[b_{\mathbf{Q}}, b^+_{\mathbf{K}}b_{\mathbf{K}}]_- = b_{\mathbf{K}}\delta_{\mathbf{Q},\mathbf{K}}$ we get

$$I_0 = [E(\mathbf{Q}) - 2\mu]b_{\mathbf{Q}} \quad \text{and} \quad I_{\text{int}} = \frac{f}{L^{d/2}}\sum_{\mathbf{q}} a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}.$$

Combining I_0 and I_{int} into (B1) yields

$$[\omega - E(\mathbf{Q}) + 2\mu]\langle\langle b_{\mathbf{Q}}|b^+_{\mathbf{Q}}\rangle\rangle_\omega \times = 1 + \frac{f}{L^{d/2}}\sum_{\mathbf{q}}\langle\langle a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}|b^+_{\mathbf{Q}}\rangle\rangle_\omega. \tag{B2}$$

This is the first of an infinite chain of equations containing higher-order Green functions. An expression for higher-order Green functions like $\langle\langle a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a_{-\mathbf{Q}+\mathbf{Q}/2\downarrow}|b^+_{\mathbf{Q}}\rangle\rangle_\omega$ on the rhs of (B2) can be established if in (A2) 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

$$\omega\langle\langle a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}|b^+_{\mathbf{Q}}\rangle\rangle_\omega = \langle\langle[a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a_{-\mathbf{q}+\mathbf{Q}/2\downarrow},\mathcal{H}]_-|b^+_{\mathbf{Q}}\rangle\rangle_\omega. \tag{B3}$$

We first find the commutator $[a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a_{-\mathbf{q}+\mathbf{Q}/2\downarrow},\mathcal{H}]_- \equiv J_0 + J_{\text{int}}$ with $J_0 \equiv [a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a_{-\mathbf{q}+\mathbf{Q}/2\downarrow},\mathcal{H}_0]$ and $J_{\text{int}} \equiv [a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}, H_{\text{int}}]$. Straightforward manipulations yield

$$J_0 = (\epsilon_{-\mathbf{q}+\mathbf{Q}/2} + \epsilon_{\mathbf{q}+\mathbf{Q}/2} - 2\mu)a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} \tag{B4}$$

and

$$J_{\text{int}} = \frac{f}{L^{d/2}}\sum_{\mathbf{K}} b_{\mathbf{K}}(a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a^+_{\mathbf{q}-\mathbf{Q}/2+\mathbf{K}\uparrow} - a^+_{-\mathbf{q}-\mathbf{Q}/2+\mathbf{K}\downarrow}a_{-\mathbf{q}+\mathbf{Q}/2\downarrow}). \tag{B5}$$

In the summation in (B5), let us separate terms with $\mathbf{K} = \mathbf{Q}$ from those with $\mathbf{K} \neq \mathbf{Q}$, namely

$$J_{\text{int}} = \frac{f}{L^{d/2}}b_{\mathbf{Q}}\underbrace{(a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a^+_{\mathbf{q}+\mathbf{Q}/2\uparrow} - a^+_{-\mathbf{q}+\mathbf{Q}/2\downarrow}a_{-\mathbf{q}+\mathbf{Q}/2\downarrow})}_{\text{coherent terms}} + \underbrace{\sum_{\mathbf{K}\neq\mathbf{Q}} b_{\mathbf{K}}(a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a^+_{\mathbf{q}-\mathbf{Q}/2+\mathbf{K}\uparrow} - a^+_{-\mathbf{q}-\mathbf{Q}/2+\mathbf{K}\downarrow}a_{-\mathbf{q}+\mathbf{Q}/2\downarrow})}_{\text{incoherent terms}}.$$

Setting J_0 and J_{int} into (B3) leads to the high-order Green functions of the type $\langle\langle b_{\mathbf{K}}\hat{F}|b^+_{\mathbf{Q}}\rangle\rangle_\omega$ with

$$\hat{F} \equiv \begin{cases} a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a^+_{\mathbf{q}-\mathbf{Q}/2+\mathbf{K}\uparrow} - a^+_{-\mathbf{q}-\mathbf{Q}/2+\mathbf{K}\downarrow}a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} & \text{for coherent terms,} \\ a_{\mathbf{q}+\mathbf{Q}/2\uparrow}a^+_{\mathbf{q}-\mathbf{Q}/2+\mathbf{K}\uparrow} - a^+_{-\mathbf{q}-\mathbf{Q}/2+\mathbf{K}\downarrow}a_{-\mathbf{q}+\mathbf{Q}/2\downarrow} & \text{for incoherent terms.} \end{cases}$$

Then we write

$$\langle\langle b_{\mathbf{K}}\hat{F}|b^+_{\mathbf{Q}}\rangle\rangle \equiv \langle\langle b_{\mathbf{K}}(\hat{F} - \langle\hat{F}\rangle)|b^+_{\mathbf{Q}}\rangle\rangle + \langle\hat{F}\rangle\langle\langle b_{\mathbf{K}}|b^+_{\mathbf{Q}}\rangle\rangle \tag{B6}$$

and assume that because of the factor $\hat{F} - \langle\hat{F}\rangle$, the contribution coming from the first term in (B6) approximately vanishes by averaging included into the definition of the Green functions. This approximation lets us write $\langle\langle b_{\mathbf{K}}\hat{F}|b^+_{\mathbf{Q}}\rangle\rangle \simeq \langle\hat{F}\rangle\langle\langle b_{\mathbf{K}}|b^+_{\mathbf{Q}}\rangle\rangle$ with $\hat{F}$ being constructed from the fermion operators. Applied to the so-called "noncoherent" terms in J_{int} this decomposition procedure allows us to neglect with all of them. Indeed, the relation (B6) applied to the noncoherent terms in J_{int} brings to the contributions of the type $c\langle\langle b_{\mathbf{K}}|b^+_{\mathbf{Q}}\rangle\rangle$ with the prefactors $c \sim \langle a_{\mathbf{q}}|a^+_{\mathbf{k}}\rangle$. Because of the relations $\mathbf{K} \neq \mathbf{Q}$ and $\mathbf{q} \neq \mathbf{k}$ this kind of terms appears to be small with respect to the so-called "coherent terms." Using Fermi anticommutators in the first term and ignoring all incoherent terms one is finally left with

$$J_{\rm int} \simeq \frac{f}{L^{d/2}} b_{\mathbf{Q}}(1 - a^{+}_{\mathbf{q+Q/2}\uparrow} a_{\mathbf{q+Q/2}\uparrow} - a^{+}_{\mathbf{-q+Q/2}\downarrow} a_{\mathbf{-q+Q/2}\downarrow})$$

$$\equiv \frac{f}{L^{d/2}} b_{\mathbf{Q}}(1 - \hat{n}_{\mathbf{q+Q/2}\uparrow} - \hat{n}_{\mathbf{-q+Q/2}\downarrow}), \tag{B7}$$

where $\hat{n}_{\mathbf{k},\sigma}$ are the usual Fermi number operators. Substituting J_0 (B4) and $J_{\rm int}$ (B7) into (B3) yields

$$\langle\langle a_{\mathbf{q+Q/2}\uparrow} a_{\mathbf{-q+Q/2}\downarrow} | b^{+}_{\mathbf{Q}} \rangle\rangle_{\omega}$$

$$= \frac{f}{L^{d/2}} \frac{\langle\langle b_{\mathbf{Q}}(1 - \hat{n}_{\mathbf{q+Q/2}\uparrow} - \hat{n}_{\mathbf{-q+Q/2}\downarrow}) | b^{+}_{\mathbf{Q}} \rangle\rangle_{\omega}}{\omega - (\epsilon_{\mathbf{-q+Q/2}} + \epsilon_{\mathbf{q+Q/2}} - 2\mu)}. \tag{B8}$$

Using in the rhs of (B8) the approximation (B6) we may write

$$\langle\langle a_{\mathbf{q+Q/2}\uparrow} a_{\mathbf{-q+Q/2}\downarrow} | b^{+}_{\mathbf{Q}} \rangle\rangle_{\omega}$$

$$= \frac{1 - n_{\mathbf{q+Q/2}\uparrow} - n_{\mathbf{-q+Q/2}\downarrow}}{\omega - (\epsilon_{\mathbf{-q+Q/2}} + \epsilon_{\mathbf{q+Q/2}} - 2\mu)} \frac{f}{L^{d/2}} \langle\langle b_{\mathbf{Q}} | b^{+}_{\mathbf{Q}} \rangle\rangle_{\omega}. \tag{B9}$$

The assumption made in (B9) can be justified via the definition of the Green functions along with the commutativity of $b^{+}_{\mathbf{Q}}$ and $n_{\mathbf{q}\sigma}$ in the random-phase approximation (RPA). The expression $\langle 1 - \hat{n}_{\mathbf{q+Q/2}\uparrow} - \hat{n}_{\mathbf{-q+Q/2}\downarrow} \rangle$ is denoted as $1 - n_{\mathbf{q+Q/2}\uparrow} - n_{\mathbf{-q+Q/2}\downarrow}$. Finally, substituting (B9) into (B2) leads to the solution

$$\langle\langle b_{\mathbf{Q}} | b^{+}_{\mathbf{Q}} \rangle\rangle_{\omega} = \left(\omega - E(\mathbf{Q}) + 2\mu - \frac{f^2}{L^d} \sum_{\mathbf{q}} \frac{F(q,Q)}{\omega - \zeta(q,Q)} \right)^{-1} \tag{B10}$$

where $F(q,Q) \equiv 1 - n_{\mathbf{q+Q/2}\uparrow} - n_{\mathbf{-q+Q/2}\downarrow}$ and $\zeta(q,Q) \equiv \epsilon_{\mathbf{-q+Q/2}} + \epsilon_{\mathbf{q+Q/2}} - 2\mu$.

Once calculated, (B10) determines $n_{B\mathbf{Q}}(T) \equiv \langle b^{+}_{\mathbf{Q}} b_{\mathbf{Q}} \rangle_{\mathcal{H}}$ via the identity

$$\langle b^{+}_{\mathbf{Q}} b_{\mathbf{Q}} \rangle_{\mathcal{H}} = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega J_{b^{+}_{\mathbf{Q}} b_{\mathbf{Q}}}(\omega), \tag{B11}$$

where

$$J_{b^{+}_{\mathbf{Q}} b_{\mathbf{Q}}}(\omega) = i(e^{\omega/k_B T} - 1)^{-1} \{ \langle\langle b_{\mathbf{Q}} | b^{+}_{\mathbf{Q}} \rangle\rangle_{\omega + i0} - \langle\langle b_{\mathbf{Q}} | b^{+}_{\mathbf{Q}} \rangle\rangle_{\omega - i0} \}$$

is the so-called spectral density. In operator form, using (B10) one first writes for small ε,

$$\langle\langle b_{\mathbf{Q}} | b^{+}_{\mathbf{Q}} \rangle\rangle_{\omega \pm i\varepsilon} \equiv \frac{1}{A \pm i\varepsilon B} = \frac{1}{B} \{ P(B/A) \mp i\pi \delta(A/B) \}, \tag{B12}$$

where the operator identity $(x \pm i\varepsilon)^{-1} = P(x^{-1}) \mp i\pi\delta(x)$ was used with P denoting the principal value of the integral, while in (B12) we have set

$$A \equiv \omega - E(\mathbf{Q}) + 2\mu - \frac{f^2}{L^d} \sum_{\mathbf{q}} \frac{F(q,Q)}{\omega - \zeta(q,Q)},$$

$$B \equiv 1 + \frac{f^2}{L^d} \sum_{\mathbf{q}} \frac{F(q,Q)}{[\omega - \zeta(q,Q)]^2 + \varepsilon^2}.$$

Setting (B12) into (B11) yields

$$J_{b^{+}_{\mathbf{Q}} b_{\mathbf{Q}}}(\omega) = 2\pi (e^{\omega/k_B T} - 1)^{-1} \frac{1}{B} \delta[A(\omega,Q)/B(\omega,Q)]. \tag{B13}$$

Finally, inserting this into (B11) gives

$$n_{B\mathbf{Q}}(T) \equiv \langle b^{+}_{\mathbf{Q}} b_{\mathbf{Q}} \rangle = \frac{1}{B} \int_{-\infty}^{\infty} d\omega (e^{\omega/k_B T} - 1)^{-1}$$

$$\times \delta[A(\omega,Q)/B(\omega,Q)] = \frac{1}{B} (e^{\Omega_{\mathbf{Q}}/k_B T} - 1)^{-1}, \tag{B14}$$

where $\Omega_{\mathbf{Q}}$ is the root of the equation $A(\Omega,Q)/B(\Omega,Q) = 0$, i.e.,

$$\left(\omega - E(\mathbf{Q}) + 2\mu - \frac{f^2}{L^d} \sum_{\mathbf{q}} \frac{F(q,Q)}{\omega - \zeta(q,Q)} \right)$$

$$\times \left(1 + \frac{f^2}{L^d} \sum_{\mathbf{q}} \frac{F(q,Q)}{[\omega - \zeta(q,Q)]^2} \right)^{-1} = 0.$$

Since the second factor is nonzero, the first factor must vanish; this gives (13) for insertion in the BE distribution (12) of a pure boson gas.

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