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Volume 453, Issues 1-2, 15 March 2007
Complete volume

ISSN 0921-4534



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The BCS–Bose crossover theory

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Received 5 August 2006; received in revised form 18 October 2006; accepted 13 December 2006

Available online 20 December 2006

Abstract

We contrast *four* distinct versions of the BCS–Bose statistical crossover theory according to the form assumed for the electron–number equation that accompanies the BCS gap equation. The four versions correspond to explicitly accounting for two-hole-(2h) as well as two-electron-(2e) Cooper pairs (CPs), or both in equal proportions, or only either kind. This follows from a recent generalization of the Bose–Einstein condensation (GBEC) statistical theory that includes not boson–boson interactions but rather 2e- and also (without loss of generality) 2h-CPs interacting with unpaired electrons and holes in a single-band model that is easily converted into a two-band model. The GBEC theory is essentially an extension of the Friedberg–Lee 1989 BEC theory of superconductors that excludes 2h-CPs. It can thus recover, when the numbers of 2h- and 2e-CPs in both BE-condensed and non-condensed states are separately equal, the BCS gap equation for all temperatures and couplings as well as the zero-temperature BCS (rigorous-upper-bound) condensation energy for all couplings. But ignoring either 2h- or 2e-CPs it can do neither. In particular, only *half* the BCS condensation energy is obtained in the two crossover versions ignoring either kind of CPs. We show how critical temperatures T_c from the original BCS–Bose crossover theory in 2D require unphysically large couplings for the Cooper/BCS model interaction to differ significantly from the T_c s of ordinary BCS theory (where the number equation is substituted by the assumption that the chemical potential equals the Fermi energy).

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PACS: 74.20.-z; 74.20.Mn; 05.30.Fk; 05.30.Jp

Keywords: Bose–Einstein condensation statistical model; BCS–Bose crossover theory

1. Introduction

Boson–fermion (BF) statistical models of superconductivity (SC) as a Bose–Einstein condensation (BEC) [1,2] began to be seriously studied in the mid-1950’s [3–6], pre-dating even the BCS–Bogoliubov statistical theory [7–9]. Although BCS theory only contemplates the presence of “Cooper correlations” of single-particle states, BF models [3–6,10–18] posit the existence of actual bosonic CPs. A drawback of early BF models is the notorious absence of

an electronic gap $\Delta(T)$, with T the absolute temperature. Perhaps the first BF model *with* a gap was introduced in Ref. [19]. Somewhat later, the remarkable relation $\Delta(T) \propto \sqrt{n_0(T)}$, with $n_0(T)$ the BEC condensate number density of electron-pairs, first seems to have appeared [20]. It resurfaced a year later in the BEC BF model in 3D of Friedberg and Lee [21,22] applied to cuprate superconductors. With just *one* adjustable parameter (the ratio of perpendicular to CuO_2 -plane boson masses) this theory fitted [22] quasi-2D cuprate T_c/T_F empirical values [23] rather well. The ratio turned out to be 66,560 – just under the 10^5 anisotropy ratio reported for $B_{2+x}\text{Sr}_{2-y}\text{CuO}_{2\pm\delta}$ [24] almost contemporaneously.

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An extension of the work in Refs. [21,22] is a generalized BEC (GBEC) statistical single-band theory whereby a superconducting BCS condensate was recently suggested [10], and subsequently confirmed [11] (but only to lowest order in the BF coupling), to be precisely a Bose–Einstein condensate (BEC) of equal numbers of bosonic two-electron (2e) and two-hole (2h) Cooper pairs (CPs), at least inasmuch as the GBEC reproduces the same BCS gap equation for all temperature and coupling as well as the same $T = 0$ condensation energy found from BCS theory. The holes that make up the 2h-CPs originate precisely from the Fermi sea associated with the N-electron system in the simple single-band model studied here. One advantage of the single-band model is that it allows recovering, among other theories, the BCS theory as a special case. The distinction (Ref. [25] pp. 70–72) between *single* particles and holes is, in a sense, trivial. Not so for particle-pairs and hole-pairs, as will be seen shortly.

The BF coupling assumed appears in an interaction many-body Hamiltonian H_{int} which defines the GBEC theory. Added to H_{int} is an unperturbed Hamiltonian H_0 describing a free *ternary* gas of unpaired electrons plus 2e-CPs plus 2h-CPs. The noninteracting ternary gas represents the normal state of the original, strongly-correlated many-electron system under study, and is a viable candidate for a so-called “non-Fermi-liquid.” The new GBEC theory embodied in $H = H_0 + H_{\text{int}}$ is in essence a *complete* BF (statistical) single-band model that, however, admits departure [11] from the perfect 2e-/2h-CP symmetry that constrains BCS theory by construction. It can be diagonalized via a Bogoliubov canonical transformation *exactly* if one neglects nonzero center-of-mass-momentum (CMM) CPs in H_{int} as is done in BCS theory but *not* in H_0 which in BCS theory represents a pure electron gas. The GBEC theory is *complete* only in the sense that 2h-CPs are not ignored. It reduces to all the known statistical theories of superconductors (SCs), including the BCS–Bose “crossover” picture in the four versions to be distinguished below. Its practical impact is that it yields [12,13] robustly higher T_c 's than BCS theory without abandoning electron–phonon dynamics, when one departs from the perfect 50/50 symmetry of 2e-/2h-CPs in the condensate.

In the literature, electron–phonon dynamics have been widely mimicked by the s-wave BCS/Cooper model interaction $V_{\mathbf{k},\mathbf{k}'}$ [7,26]. It is a nonzero negative constant $-V$, if and only if single-particle energies $\epsilon_{\mathbf{k}}, \epsilon_{\mathbf{k}'}$ lie within the energy interval $[\max\{0, \mu - \hbar\omega_D\}, \mu + \hbar\omega_D]$ where μ is the electron chemical potential and ω_D the Debye frequency. We employ this model interaction here. Other pairing symmetries beyond pure s-wave can also be accommodated. Although it sheds considerable light on different possible crossover schemes, our single-band picture where single-electron and single-holes are assumed to have the same effective mass is not as realistic in describing real materials as a *multiband* (say, a valence-like band for holes and a conduction-like one for electrons) theory where these two masses can differ, as will be discussed later.

A fundamental drawback of early [3–6] BF models, which took 2e-CPs as analogous to diatomic molecules in a classical atom–molecule binary gas mixture, is the cumbersome introduction of an electron energy gap $\Delta(T)$. “Gapless” models, however, are useful [15,16] in locating transition-temperature singularities if approached from *above*, i.e., from the *normal* state where $T > T_c$.

The “ordinary” CP problem [26] for two distinct inter-fermion interactions (the δ -potential well [17,18] or the Cooper/BCS model [7,26] interactions) neglects the effect of 2h-CPs treated on an equal footing with 2e [or, in general, two-particle (2p)] CPs. On the other hand, Green's functions [25] can naturally deal with hole propagation and thus accommodate both 2e- and 2h-CPs via, e.g., the Bethe–Salpeter equation [27,28]. In addition to the generalized CP problem, a crucial result [10,11] as already mentioned is that the BCS condensate consists of equal numbers of 2e- and 2h-CPs. This was implicitly already suggested from the perfect symmetry about electron energy $\epsilon = \mu$ of the well-known Bogoliubov [29] $v^2(\epsilon)$ and $u^2(\epsilon)$ coefficients, with the tail of $v^2(\epsilon)$ *above* $\epsilon = \mu$ representing 2e correlations and that of $u^2(\epsilon)$ *below* $\epsilon = \mu$ refers to 2h correlations.

In this paper, we show how: (a) four versions of the BCS–Bose statistical crossover theory can be obtained by ignoring either 2h- or 2e-CPs or by including both; (b) for only two of the four versions can the precise BCS gap equation for all temperatures T be derived; (c) crossover picture T_c s, defined self-consistently by *both* the gap and fermion–number equations, requires unphysically large couplings (at least for the Cooper/BCS model interaction in 2D SCs) to differ significantly from the T_c of ordinary BCS theory defined *without* the number equation since here the chemical potential is assumed equal to the Fermi energy; and (d) the full $T = 0$ BCS condensation energy follows from one crossover version but only *half* of it from the two versions ignoring either kind of CPs. The condensation energy is simply related to the ground-state energy of the many-fermion system, which in the case of BCS is a rigorous-upper-bound to the exact many-body value for the given Hamiltonian as BCS theory starts from a variational wave function for the superconductor ground state. These results, with the exception of (c) which does not apply as such, are expected to hold also for neutral-fermion superfluids (SFs) – such as liquid ^3He [30,31], neutron matter and trapped ultra-cold fermion atomic gases [32–43] – where the pair-forming two-fermion interaction, of course, differs from the Cooper/BCS one for SCs.

2. Generalized BEC theory (GBEC)

The GBEC theory is described in detail in Refs. [10–13]; here we summarize its main equations. It applies in d dimensions and is defined by a Hamiltonian of the form $H = H_0 + H_{\text{int}}$. The unperturbed Hamiltonian H_0 should ideally be, to quote Leggett [44] “an appropriate ‘zeroth-order’ starting point” accounting for “pairs of electronic

excitations with charge $2e$ that all have the same ground-state wavefunction.” Thus, our H_0 corresponds to a non-Fermi-liquid “normal” state which, besides just fermions, is an ideal (i.e., noninteracting) ternary gas mixture of unpaired fermions *and* both types of CPs namely, $2e$ and $2h$, the latter introduced without loss of generality. Specifically

$$H_0 = \sum_{\mathbf{k}_1, s_1} \epsilon_{\mathbf{k}_1} a_{\mathbf{k}_1, s_1}^+ a_{\mathbf{k}_1, s_1} + \sum_{\mathbf{K}} E_+(K) b_{\mathbf{K}}^+ b_{\mathbf{K}} - \sum_{\mathbf{K}} E_-(K) c_{\mathbf{K}}^+ c_{\mathbf{K}}, \quad (1)$$

where $\mathbf{K} \equiv \mathbf{k}_1 + \mathbf{k}_2$ is the CMM wavevector of the pair, while $\epsilon_{\mathbf{k}_1} \equiv \hbar^2 k_1^2 / 2m$ are the single-electron, and $E_{\pm}(K)$ the $2e$ -/ $2h$ -CP *phenomenological*, energies. Here $a_{\mathbf{k}_1, s_1}^+$ ($a_{\mathbf{k}_1, s_1}$) are creation (annihilation) operators for fermions and similarly $b_{\mathbf{K}}^+$ ($b_{\mathbf{K}}$) and $c_{\mathbf{K}}^+$ ($c_{\mathbf{K}}$) for $2e$ - and $2h$ -CP bosons, respectively. These b and c operators depend only on \mathbf{K} and so are *distinct* from the BCS operators depending on both \mathbf{K} *and* the relative $\mathbf{k} \equiv \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$ discussed in Ref. [7] Eqs. (2.9)–(2.13) for the particular case of $\mathbf{K} = 0$ and shown there *not* to satisfy the ordinary Bose commutation relations. But because two pairs cannot exactly overlap in real space without violating the Pauli principle, they are often considered “hard-core bosons,” albeit of hard-core radii 0^+ . For this reason, one can probably not expect to be able to construct the b and c operators directly from the a operators in order to establish that b and c obey Bose commutation relations precisely. Nonetheless, these pairs stand for objects that can easily be seen to obey Bose–Einstein statistics as, in the thermodynamic limit, an indefinitely large number of \mathbf{k} values correspond to a given \mathbf{K} value defining an energy level $E_+(K)$ or $E_-(K)$. This is all that is needed to ensure the BEC (or macroscopic occupation of a given state that appears below a certain fixed $T = T_c$) found [10–13] numerically *a posteriori* in the GBEC theory. Furthermore, being noninteracting (except for the Pauli principle restriction mentioned), CPs satisfy the Ehrenfest–Oppenheimer [45] criteria for two clusters of charges to conserve a specific kind of statistics, either Bose or Fermi. These assumed properties are justified *a posteriori* when in the GBEC theory: (a) the BCS gap equation is recovered for equal numbers of both kinds of pairs, both in the $\mathbf{K} = 0$ state and in all $\mathbf{K} \neq 0$ states taken collectively, and in weak-coupling, regardless of CP overlaps; and (b) the precise familiar BEC T_c formula emerges [10] when (i) $2h$ -CPs are ignored, the Friedberg–Lee model [21,22] equations are recovered and (ii) one switches off the BF interaction. The only difference in the recovered BEC T_c formula is that the boson number density now depends on T_c , as expected in a boson–fermion mixture where populations are T -dependent. Finally, we note that fermion scattering terms [46] are not included in (1) as they are not expected to be substantial, say, in the BCS limit of high electron-density where they would be the most effective, which in turn is included in the GBEC model as a special case.

Two-hole CPs in (1) are postulated to be *distinct* and *kinematically independent* from both the $2e$ -CPs and the unpaired electrons, i.e., operators a , b and c are assumed to commute with each other. This postulate is grounded on magnetic-flux-quantization measurements establishing the presence of *pair* charge carriers in both conventional [47,48] as well as cuprate [49] superconductors, and on the fact that no experiment has yet been done, to our knowledge [50], that distinguishes between electron and hole CPs. The latter uncertainty further motivates a Hamiltonian such as (1) with *both* kinds of CPs.

The interaction Hamiltonian H_{int} in the expression $H = H_0 + H_{\text{int}}$ describes the formation and disintegration of CPs, respectively, from and into unpaired electrons and holes. It is further simplified by dropping all $\mathbf{K} \neq 0$ terms. This is also done in BCS theory in its full Hamiltonian $H = H_0 + H_{\text{int}}$, but *kept* in the GBEC theory in its unperturbed H_0 portion (1). The GBEC H_{int} is made up of four distinct BF interaction vertices each with two-fermion/one-boson creation and/or annihilation operators. These vertices depict how unpaired electrons (subindex $+$) [or holes (subindex $-$)] are involved in the formation and disintegration of the $2e$ - (and $2h$ -) $\mathbf{K} = 0$ CPs in the d -dimensional system of size L , namely

$$H_{\text{int}} = L^{-d/2} \sum_{\mathbf{k}} f_+(k) \{ a_{\mathbf{k}, \uparrow}^+ a_{-\mathbf{k}, \downarrow}^+ b_0 + a_{-\mathbf{k}, \downarrow} a_{\mathbf{k}, \uparrow} b_0^+ \} + L^{-d/2} \sum_{\mathbf{k}} f_-(k) \{ a_{\mathbf{k}, \uparrow}^+ a_{-\mathbf{k}, \downarrow}^+ c_0^+ + a_{-\mathbf{k}, \downarrow} a_{\mathbf{k}, \uparrow} c_0 \}, \quad (2)$$

where $\mathbf{k} \equiv \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$ is again the relative wavevector of a CP. The interaction vertex form factors $f_{\pm}(k)$ in (2) are essentially the Fourier transforms of the $2e$ - and $2h$ -CP intrinsic wavefunctions, respectively, in the relative coordinate of the two fermions. The GBEC theory is thus reminiscent of the Sommerfeld theory of the electron gas combined with the Debye picture of the phonon gas which together give a binary mixture of noninteracting electrons and phonons, a picture which describes low- T specific heats in metals and insulators. But to explain either resistance and superconductivity, they must then be allowed to interact via the Fröhlich electron–phonon interaction [51] of a form analogous to (2) but without hole terms. In contrast, the full BCS Hamiltonian $H_0^{\text{BCS}} + H_{\text{int}}^{\text{BCS}}$ consists of only the first (electron) term on the rhs of (1) namely

$$H_0^{\text{BCS}} = \sum_{\mathbf{k}_1, s_1} \epsilon_{\mathbf{k}_1} a_{\mathbf{k}_1, s_1}^+ a_{\mathbf{k}_1, s_1} \quad (3)$$

and

$$H_{\text{int}}^{\text{BCS}} = \sum_{\mathbf{k}_1, l_1} V_{\mathbf{k}_1, l_1} a_{\mathbf{k}_1, \uparrow}^+ a_{-\mathbf{k}_1, \downarrow}^+ a_{-\mathbf{l}_1, \downarrow} a_{\mathbf{l}_1, \uparrow}. \quad (4)$$

The BCS H_0^{BCS} thus represents a Fermi-liquid normal state.

In order to eventually recover BCS theory, in Refs. [10–13] the corresponding energy form factors were picked as

$$f_+(\epsilon) = \begin{cases} f & \text{for } E_f < \epsilon < E_f + \delta\epsilon, \\ 0 & \text{otherwise,} \end{cases} \quad (5)$$

$$f_-(\epsilon) = \begin{cases} f & \text{for } E_f - \delta\epsilon < \epsilon < E_f, \\ 0 & \text{otherwise.} \end{cases} \quad (6)$$

This is after one introduces the quantities E_f and $\delta\epsilon$ as *new* phenomenological dynamical energy parameters (in addition to the positive BF vertex coupling parameter f) that replace the previous phenomenological CP energy parameters $E_{\pm}(0)$, through the definitions

$$E_f \equiv \frac{1}{4}[E_+(0) + E_-(0)] \quad \text{and} \quad \delta\epsilon \equiv \frac{1}{2}[E_+(0) - E_-(0)] \geq 0, \quad (7)$$

where $E_+(0)$ and $E_-(0)$ are the (empirically unknown) zero-CMM energies of the 2e- and 2h-CPs, respectively. Note that $2E_f$ lies midway between $E_+(0)$ and $E_-(0)$. Alternately, instead of (7) one can write the two inverse relations

$$E_{\pm}(0) = 2E_f \pm \delta\epsilon. \quad (8)$$

The quantity E_f serves as a convenient energy scale; it is not to be confused with the Fermi energy $E_F = \frac{1}{2}mv_F^2 \equiv k_B T_F$ where T_F is the Fermi temperature. The Fermi energy E_F equals $\pi\hbar^2 n/m$ in 2D and $(\hbar^2/2m)(3\pi^2 n)^{2/3}$ in 3D, with $n \equiv N/L^d$ the total number density of charge-carrier mobile electrons, while E_f is of the same form but with n replaced by, say, n_f , which in turn serves as convenient electron-density scale. The quantities E_f and E_F coincide *only* when perfect 2e/2h-CP symmetry holds, i.e., when $n = n_f$.

The grand potential Ω for the full Hamiltonian $H = H_0 + H_{\text{int}}$ given by (1) and (2) is then constructed via (Ref. [25] Eq. (4.14)) the definition

$$\Omega(T, L^d, \mu, N_0, M_0) = -k_B T \ln [\text{Tr} e^{-\beta(H - \mu\hat{N})}], \quad (9)$$

where “Tr” stands for “trace” and $\beta \equiv 1/k_B T$ with T the absolute temperature. It is related to the system pressure P , internal energy E and entropy S by $\Omega = -PL^d = F - \mu N = E - TS - \mu N$, where F is the Helmholtz free energy. Following the Bogoliubov prescription [52], one sets b_0^+ , b_0 equal to $\sqrt{N_0}$ and c_0^+ , c_0 equal to $\sqrt{M_0}$ in (2), where N_0 is the T -dependent number of zero-CMM 2e-CPs and M_0 likewise for 2h-CPs. This allows *exact* diagonalization for any coupling, through a Bogoliubov transformation of the a^+ , a fermion operators, giving [53] after some algebra

$$\begin{aligned} \Omega(T, L^d, \mu, N_0, M_0)/L^d &= \int_0^\infty d\epsilon N(\epsilon) [\epsilon - \mu - E(\epsilon)] \\ &\quad - 2k_B T \int_0^\infty d\epsilon N(\epsilon) \ln \{1 + \exp[-\beta E(\epsilon)]\} + [E_+(0) - 2\mu] n_0 \\ &\quad + k_B T \int_{0^+}^\infty d\epsilon M(\epsilon) \ln \{1 - \exp[-\beta\{E_+(0) + \epsilon - 2\mu\}]\} \\ &\quad + [2\mu - E_-(0)] m_0 \\ &\quad + k_B T \int_{0^+}^\infty d\epsilon M(\epsilon) \ln \{1 - \exp[-\beta\{2\mu - E_-(0) + \epsilon\}]\}. \end{aligned} \quad (10)$$

Here $N(\epsilon)$ and $M(\epsilon)$ are respectively the electronic and bosonic density of states, while

$$\begin{aligned} E(\epsilon) &\equiv \sqrt{(\epsilon - \mu)^2 + \Delta^2(\epsilon)} \\ &\equiv \sqrt{(\epsilon - \mu)^2 + n_0 f_+^2(\epsilon) + m_0 f_-^2(\epsilon)}, \end{aligned} \quad (11)$$

since $\Delta(\epsilon) \equiv \sqrt{n_0} f_+(\epsilon) + \sqrt{m_0} f_-(\epsilon)$ and $f_+(\epsilon) f_-(\epsilon) \equiv 0$ from (5) and (6) with $n_0(T) \equiv N_0(T)/L^d$ and $m_0(T) \equiv M_0(T)/L^d$ being the 2e-CP and 2h-CP number densities, respectively, of BE-condensed (i.e., with $K = 0$) bosons.

Minimizing F with respect to N_0 and M_0 , while simultaneously fixing the total number N of electrons by introducing the electron chemical potential μ in the usual way, namely

$$\frac{\partial F}{\partial N_0} = 0, \quad \frac{\partial F}{\partial M_0} = 0, \quad \text{and} \quad \frac{\partial \Omega}{\partial \mu} = -N \quad (12)$$

ensures an *equilibrium thermodynamic state* of the system with volume L^d at temperature T and chemical potential μ . Evidently, N includes both paired and unpaired CP electrons. Some algebra then leads [53] to the three coupled integral Eqs. (7)–(9) of Ref. [10] which, since from (5) and (6) one has that $f_+(\epsilon) f_-(\epsilon) \equiv 0$, can be simplified to the two “gap-like equations”

$$\begin{aligned} [2E_f + \delta\epsilon - 2\mu(T)] &= \frac{1}{2} f^2 \int_{E_f}^{E_f + \delta\epsilon} d\epsilon N(\epsilon) \frac{\tanh \frac{1}{2} \beta \sqrt{[\epsilon - \mu(T)]^2 + f^2 n_0(T)}}{\sqrt{[\epsilon - \mu(T)]^2 + f^2 n_0(T)}}, \end{aligned} \quad (13)$$

$$\begin{aligned} [2\mu(T) - 2E_f + \delta\epsilon] &= \frac{1}{2} f^2 \int_{E_f - \delta\epsilon}^{E_f} d\epsilon N(\epsilon) \frac{\tanh \frac{1}{2} \beta \sqrt{[\epsilon - \mu(T)]^2 + f^2 m_0(T)}}{\sqrt{[\epsilon - \mu(T)]^2 + f^2 m_0(T)}} \end{aligned} \quad (14)$$

and a single “*number equation*” (that guarantees charge conservation)

$$2n_B(T) - 2m_B(T) + n_f(T) = n, \quad (15)$$

where

$$n_f(T) \equiv \int_0^\infty d\epsilon N(\epsilon) \left[1 - \frac{\epsilon - \mu}{E(\epsilon)} \tanh \frac{1}{2} \beta E(\epsilon) \right] \quad (16)$$

is clearly the number of unpaired electrons. This is identical with $2 \sum_{\mathbf{k}} v_k^2(T)$ with $v_k^2(T)$ the well-known T -dependent Bogoliubov v^2 -coefficient. In (15) $n \equiv N/L^d$ is the number density of electrons while $n_B(T)$ and $m_B(T)$ are, respectively, the number densities of 2e- and 2h-CPs in *all* bosonic states (both $K = 0$ as well as $K > 0$). The “complete” number Eq. (15) can be rewritten more explicitly as

$$\begin{aligned} 2n_0(T) + 2n_{B^+}(T) - 2m_0(T) - 2m_{B^+}(T) + n_f(T) \\ = n \quad \text{crossover version A,} \end{aligned} \quad (17)$$

where $n_B(T)$ is [13]

$$n_B(T) \equiv n_0(T) + n_{B+}(T);$$

$$n_{B+}(T) \equiv \int_{0+}^{\infty} d\varepsilon M(\varepsilon) [\exp \beta \{E_+(0) + \varepsilon - 2\mu\} - 1]^{-1} \quad (18)$$

and similarly for $m_B(T)$ which is

$$m_B(T) \equiv m_0(T) + m_{B+}(T);$$

$$m_{B+}(T) \equiv \int_{0+}^{\infty} d\varepsilon M(\varepsilon) [\exp \beta \{2\mu - E_-(0) + \varepsilon\} - 1]^{-1}. \quad (19)$$

Clearly, $m_{B+}(T)$ are precisely the number of “pre-formed” $K > 0$ 2h-CPs, and $n_{B+}(T)$ that of 2e-CPs. These CPs are non-condensed in contrast with the $K = 0$ CPs which are BE-condensed. Evaluating the integrals requires knowing the bosonic density-of-states $M(\varepsilon)$ of CPs of energy ε , which in turn requires knowing the dispersion relation ε vs. K , e.g., as has been determined via the Bethe–Salpeter equation in the ladder approximation in 3D [27] and in 2D [28].

Self-consistent (at worst, numerical) solution of the three coupled integral Eqs. (13), (14) and (17) then yields the three thermodynamic variables of the GBEC theory

$$n_0(T, n, \mu), \quad m_0(T, n, \mu), \quad \text{and} \quad \mu(T, n). \quad (20)$$

Fig. 1 displays the three BE-condensed phases – labelled $s+$, $s-$ and ss – along with the normal phase n , that emerge [11] from the GBEC theory. Phase $s+$ stands for a pure 2e-CP BE condensate, $s-$ for a pure 2h-CP such condensate and ss denotes a mixed phase. Only the two pure phases were found [11] to display T_c values higher than the corresponding BCS value, while the mixed phase occurs below this value.

For the two pure phases one can, in principle, shift from the single-band model implied so far to a *two*-band model by allowing the particle (e) masses to differ from hole (h) masses; this can be done by introducing two different Fermi energies E_F^c and E_F^h that differ precisely by these two masses.

The GBEC theory contains [13] the key equations of all *five* distinct statistical theories as special cases. These range

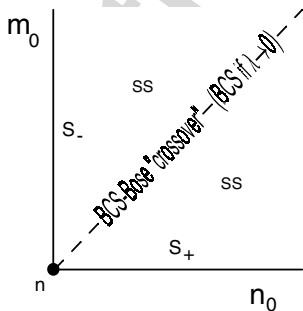


Fig. 1. Illustration in the n_0 – m_0 plane of three GBEC theory condensed phases (the pure 2e-CP $s+$ and pure 2h-CP $s-$ BE condensate phases and a mixed phase ss) along with the normal (ternary BF non-Fermi-liquid) phase n that corresponds to the origin at $n_0 = 0 = m_0$.

from ordinary BCS to ordinary BEC theories, which are thereby completely unified by the GBEC theory. Perfect 2e-/2h-CP symmetry signifies equal numbers of 2e- and 2h-CPs, more specifically, $n_B(T) = m_B(T)$ as well as $n_0(T) = m_0(T)$. This implies that $n_{B+}(T) = m_{B+}(T)$ for all T , meaning that the exponents in (18) and (19) coincide so that with (8) this makes $E_f = \mu$. The GBEC theory then reduces to the gap and number equations [viz., in 2D for $T = T_c$ both (28) and (29)] of the original [55] BCS–Bose crossover picture with the Cooper/BCS model interaction – if its parameters V and $\hbar\omega_D$ are identified with the BF interaction GBEC Hamiltonian H_{int} parameters $f^2/2\delta\varepsilon$ and $\delta\varepsilon$, respectively. This one-to-one correspondence between H_{int} and $H_{\text{int}}^{\text{BCS}}$ defined in (2) and (4) justifies the particular choice of form factors (5) and (6) for the BF interaction.

The original crossover picture for unknowns $\Delta(T)$ and $\mu(T)$ is now supplemented by the central relation

$$\Delta(T) = f\sqrt{n_0(T)} = f\sqrt{m_0(T)}. \quad (21)$$

All three functions $\Delta(T)$, $n_0(T)$ and $m_0(T)$ have the familiar “half-bell-shaped” forms. Namely, they are zero above a certain critical temperature T_c , and rise monotonically upon cooling (lowering T) to maximum values $\Delta(0)$, $n_0(0)$ and $m_0(0)$ at $T = 0$. The energy gap $\Delta(T)$ is the order parameter describing the superconducting (or superfluid) condensed state, while $n_0(T)$ and $m_0(T)$ are the BEC order parameters depicting the macroscopic occupation that occurs below T_c in a BE condensate. This $\Delta(T)$ is precisely the BCS energy gap if the boson–fermion coupling f is made to correspond to $\sqrt{2V\hbar\omega_D}$ within the GBEC formalism. Evidently, the BCS and BEC T_c s are the same. Writing (21) for $T = 0$ and dividing this into (21) gives the much simpler f -independent relation involving order parameters *normalized* to unity in the interval $[0,1]$

$$\Delta(T)/\Delta(0) = \sqrt{n_0(T)/n_0(0)}$$

$$= \sqrt{m_0(T)/m_0(0)} \begin{cases} \longrightarrow 1 & T \rightarrow 0 \\ \longrightarrow 0 & T \geq T_c \end{cases} \quad (22)$$

The first equality, apparently first obtained in Ref. [20], connects in a simple way the two heretofore unrelated “half-bell-shaped” order parameters of the BCS and the BEC theories. The second equality implies [10,11] that a BCS condensate is precisely a BE condensate of equal numbers of 2e- and 2h-CPs. Since (22) is *independent* of the particular two-fermion dynamics of the problem, it can be expected to hold for either SCs and SFs.

3. Gap equation

The standard procedure in all SC and SF theories of many-fermion systems is to *ignore* dealing explicitly with 2h-CPs altogether. Neglecting in (10) all terms containing $m_0(T)$, $E_-(0)$ and $f_-(\varepsilon)$ leaves an $\Omega(T, L^d, \mu, N_0)$ defining a *binary*, instead of ternary, BF model. Minimizing the

associated Helmholtz free energy $F(T, L^d, \mu, N_0) = \Omega(T, L^d, \mu, N_0) + \mu N$ over N_0 (for fixed total electron number N) requires that $\partial F/\partial N_0 = 0 = \partial F/\partial n_0$, which becomes

$$\int_0^\infty d\epsilon N(\epsilon) \left[-1 + \frac{2 \exp\{-\beta E(\epsilon)\}}{1 + \exp\{-\beta E(\epsilon)\}} \right] \frac{dE(\epsilon)}{dn_0} + [E_+(0) - 2\mu] = 0$$

or

$$2[2E_f + \delta\epsilon - 2\mu] = f^2 \int_{E_f}^{E_f + \delta\epsilon} d\epsilon N(\epsilon) \frac{1}{E(\epsilon)} \tanh \frac{1}{2} \beta E(\epsilon). \quad (23)$$

Using (8) yields precisely the BCS gap equation for all T , Eq. (3.27) of Ref. [7], provided one picks $E_f = \mu$, namely

$$1 = \lambda \int_0^{\hbar\omega_D} d\xi \frac{1}{\sqrt{\xi^2 + \Delta^2(T)}} \tanh \frac{1}{2} \beta \sqrt{\xi^2 + \Delta^2(T)}, \quad (24)$$

where $\xi \equiv \epsilon - \mu$, since $\lambda \equiv N(E_f)V = f^2 N(E_f)/2\delta\epsilon$ while $\delta\epsilon = \hbar\omega_D$ [see relation between V and f stated just above (21)], and provided $N(\epsilon)$ can be taken outside the integral sign in (23). This last operation is exact in 2D when $N(\epsilon)$ is independent of ϵ and is otherwise a good approximation if $\hbar\omega_D \ll \mu$.

However, the choice $E_f = \mu$ cannot be justified, to our knowledge, without assuming within the GBEC that $n_B(T) = m_B(T)$ as well as $n_0(T) = m_0(T)$, i.e., by explicitly recognizing the existence of 2h-CPs along with 2e-CPs and taking them in equal or 50–50 proportions.

4. Number equation

Besides the normal phase consisting of the ideal BF ternary gas described by H_0 , three different stable BEC phases emerge [11] when solving all three Eqs. (13), (14) and (17): two pure phases, a pure 2e-CP BEC and a pure 2h-CP BEC, as well as a mixed phase consisting of both types of BECs in varying proportions. For a half-and-half mixed phase, i.e., $n_0(T) = m_0(T)$ and $n_{B+}(T) = m_{B+}(T)$, all the boson number density terms in (17) cancel and the BCS number equation

$$n = n_f(T) \quad \text{crossover version B (special case of A)} \quad (25)$$

is recovered, with $n_f(T)$ defined by (16). Crossover version B does not explicitly neglect either kind of CP, nor does it draw a distinction between them. It is the version applied below in 2D to obtain (28)–(30) and the results of Fig. 2. This is the original crossover version first presented in 1967 in Ref. [55].

If 2h-CPs are ignored altogether, the companion number equation follows from the last equation of (12) as

$$n = n_f(T) + 2n_B(T) \quad \text{crossover version C} \quad (26)$$

where $n_f(T)$ is interpreted as the number density of unpaired but BCS-correlated electrons and is given by (16).

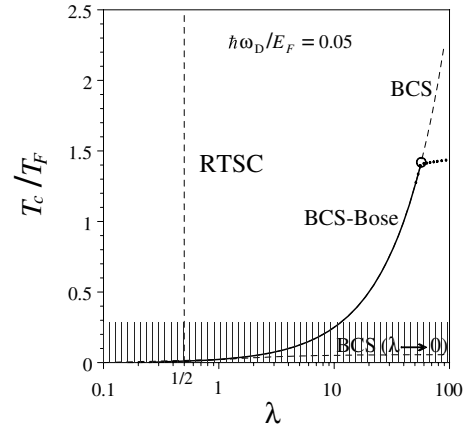


Fig. 2. Critical SC temperatures T_c in units of T_F for the BCS–Bose crossover theory (full curve) in 2D compared with the BCS value from the exact implicit T_c equation (see e.g., Ref. [25], p. 447) $1 = \lambda \int_0^{\hbar\omega_D/2k_B T_c} dx x^{-1} \tanh x$ (upper dashed curve) valid for any $d > 0$ in any coupling λ , and its weak-coupling explicit solution $T_c \simeq 1.134 \hbar\omega_D \exp(-1/\lambda)$ (lower dashed curve). The dot-dashed “appendage” signals a breakdown in the BCS/Cooper interaction model when $\mu(T_c)$ turns negative, as the Fermi surface at μ then washes out and the interaction model becomes meaningless. The value of $\lambda = 1/2$ marked is the maximum possible value allowed just short of lattice instability in 3D for this interaction model, at least by one criterion [59]. Unshaded region refers to room-temperature superconductivity (RTSC) for SCs with $T_F \lesssim 10^3$ K.

In perhaps the first attempt [19] to discuss BEC in 1969 within the BCS–Bose crossover picture, Eagles [54] imposed (26) to accompany the gap equation in what was perhaps the first BF model with a gap. This differs from the much simpler number equation of crossover version B, which gave (29) below as a special case for $T = T_c$ when $\Delta(T_c) = 0$ is substituted into (25) and (16) if one uses the identity $1 - \tanh(x/2) \equiv 2/(\exp x + 1)$. It is this version that corresponds to the Friedberg–Lee model [21,22].

Similarly, ignoring 2e-CPs and keeping only 2h-CPs leads to $\Omega(T, L^d, \mu, M_0)$ from which to minimize $F(T, L^d, \mu, M_0)$ over M_0 requires that one set $\partial F/\partial M_0 = 0 = \partial F/\partial m_0$. Noting that $E(\xi) \equiv E(-\xi)$, this also leads to the gap Eq. (24) provided, again, one picks $E_f = \mu$, but now with the companion number equation

$$n = n_f(T) - 2m_B(T) \quad \text{crossover version D} \quad (27)$$

instead of (26) but with the same $n_f(T)$ as in (16).

5. BCS–Bose crossover T_c compared with BCS T_c in 2D

The original crossover theory [55] is defined by two simultaneous coupled equations, the BCS gap and number equations, without the BCS assumption that the chemical potential μ equals the Fermi energy E_F . For subsequent extensions of the original version, see reviews in Refs. [56,57]. The critical temperature T_c is defined by $\Delta(T_c) = 0$, and is to be determined self-consistently with $\mu(T_c)$ by solving both gap and number equations. Because

of its interest in quasi-2D cuprate superconductors [58], in this section we concentrate on 2D only. For the Cooper/BCS model interaction, if $\lambda \equiv N(E_F)V$ where $N(E_F) = m/2\pi\hbar^2$, the two crossover equations to be solved self-consistently reduce to

$$1 = \lambda \int_0^{\hbar\omega_D/2k_B T_c} dx \frac{\tanh x}{x} \quad (\text{if } \mu > \hbar\omega_D);$$

$$1 = \lambda \int_{-\mu(T_c)/2k_B T_c}^{\hbar\omega_D/2k_B T_c} dx \frac{\tanh x}{2x} \quad (\text{if } \mu < \hbar\omega_D) \quad (28)$$

$$\int_0^\infty \frac{d\epsilon}{\exp\{[\epsilon - \mu(T_c)]/2k_B T_c\} + 1} = E_F. \quad (29)$$

The last integral can be done analytically and leaves the explicit expression

$$\mu(T_c) = k_B T_c \ln(e^{E_F/k_B T_c} - 1), \quad (30)$$

which is then eliminated symbolically from (28) to render T_c as an implicit function of λ alone. Using $\hbar\omega_D/E_F = 0.05$ as a typical value for cuprates, increasing λ makes $\mu(T_c)$ decrease from its weak-coupling (where $T_c \rightarrow 0$) value of E_F down to $\hbar\omega_D$ when $\lambda \simeq 56$, an unphysically large value as it well exceeds the Migdal ionic-lattice stability upper limit [59] of 1/2, although [60] “there is no universally accepted, simple, and quantitative stability criterion”.

Fig. 2 displays T_c (in units of T_F) as function of λ . Note that room-temperature SCs (RTSC) are predicted by BCS–Bose crossover theory but only for λ values definitely larger than about 10 that are still too unphysical.

6. Condensation energy

The $T = 0$ condensation energy per unit volume according to the GBEC theory, given (10), is

$$\frac{E_s - E_n}{L^d} = \frac{\Omega_s(T=0) - \Omega_n(T=0)}{L^d}, \quad (31)$$

since for any T the Helmholtz free energy $F \equiv E - TS = \Omega + \mu N$, with S the entropy, and μ is the same for either superconducting s or normal n phases with internal energies E_s and E_n , respectively. In the normal phase $n_0(T) = 0$, $m_0(T) = 0$ so that $\Delta(T) = 0$ for all $T \geq 0$, so that (10) reduces to

$$\frac{\Omega_n(T=0)}{L^d} = \int_0^\infty d\epsilon N(\epsilon)(\epsilon - \mu - |\epsilon - \mu|)$$

$$= 2 \int_0^\mu d\epsilon N(\epsilon)(\epsilon - \mu) = 2 \int_{-\mu}^0 d\xi N(\xi)\xi. \quad (32)$$

For the superconducting phase, and when $n_0(T) = m_0(T)$ and $n_B(T) = m_B(T)$ hold, i.e., crossover scenario B, one deduces from (8) and (10) that $\mu = E_f$. Putting $\Delta(T=0) \equiv \Delta$ in (10) as well as $\delta\epsilon \equiv \hbar\omega_D$, while using (8), gives

$$\frac{\Omega_s(T=0)}{L^d} = 2\hbar\omega_D n_0(0) + \int_{-\mu}^\infty d\xi N(\xi) \left(\xi - \sqrt{\xi^2 + \Delta^2} \right)$$

$$= 2\hbar\omega_D n_0(0) + 2 \int_{-\mu}^{-\hbar\omega_D} d\xi N(\xi)\xi$$

$$- 2 \int_0^{\hbar\omega_D} d\xi N(\xi) \sqrt{\xi^2 + \Delta^2}. \quad (33)$$

The first factor of 2 in the last line comes precisely from the condition $n_0(T) = m_0(T)$ while the last two factors of 2 arise from the condition that according to (5) and (6) the magnitudes of $f_+(\epsilon)$ and $f_-(\epsilon)$ are the same and equal f . Subtracting (32) from (33) and putting $N(\xi) \cong N(0)$, the density of electronic states at the Fermi surface [designated before as $N(E_F)$] yields

$$\frac{E_s - E_n}{L^d} = 2\hbar\omega_D n_0(0) + 2N(0) \int_0^{\hbar\omega_D} d\xi \left(\xi - \sqrt{\xi^2 + \Delta^2} \right)$$

$$= 2\hbar\omega_D n_0(0) + N(0) \left[(\hbar\omega_D)^2 - \hbar\omega_D \sqrt{(\hbar\omega_D)^2 + \Delta^2} \right.$$

$$\left. + \Delta^2 \ln \frac{\Delta}{\hbar\omega_D + \sqrt{(\hbar\omega_D)^2 + \Delta^2}} \right] (\text{GBEC}) \quad (34)$$

exactly, by standard integrations [61]. Using the expression that follows from (24) for $T = 0$ gives Eq. (2.40) of Ref. [7], namely

$$\Delta = \frac{\hbar\omega_D}{\sinh(1/\lambda)}, \quad (35)$$

where λ is related to GBEC BF interaction parameter f through

$$\lambda \equiv VN(0) = f^2 N(0)/2\hbar\omega_D.$$

This makes the first term on the rhs of (34) exactly equal to $\Delta^2 N(0)/\lambda$ which in turn can be shown to cancel exactly against the log term if one recalls the hyperbolic-function identity $\sinh^2 x + 1 \equiv \cosh^2 x$. Thus, the GBEC theory condensation energy (34) is identical for any coupling to that of BCS theory, Eq. (2.42) of Ref. [7], namely

$$\frac{E_s - E_n}{L^d} = N(0)(\hbar\omega_D)^2 \left[1 - \sqrt{1 + (\Delta/\hbar\omega_D)^2} \right] \quad (\text{BCS})$$

$$\xrightarrow{\lambda \rightarrow 0} -\frac{1}{2} N(0) \Delta^2 \left[1 - \frac{1}{4} \left(\frac{\Delta}{\hbar\omega_D} \right)^2 + \mathcal{O} \left(\frac{\Delta}{\hbar\omega_D} \right)^4 \right]. \quad (36)$$

This energy, associated with the expectation value of the BCS trial wavefunction gives a rigorous-upper-bound to the exact ground-state energy of the BCS Hamiltonian. Empirically, for niobium (Nb, bcc, $T_c \simeq 9.3$ K, critical magnetic field $H_c \simeq 160$ kA/m) the condensation energy to be compared with the BCS result (36) works out to be just 2×10^{-6} eV/atom [62]. The equivalence of (34) and (36) seems to suggest that, as in the GBEC theory, there are no pair–pair interactions in the BCS theory either, as is evident from Hamiltonians (1), (2) and (4).

What happens on ignoring *either* 2e- or 2h-CPs, as seems to be common practice in theories of SCs and SFs? This gives crossover versions C and D. Starting from (10) for $T = 0$, and following a similar procedure to arrive at (33) but *without* 2h-CPs such that $f_- = 0$, $m_0(0) = 0$ and $n_0(0) = \Delta^2/f^2$, one gets

$$\left[\frac{Q_s(T=0)}{L^d} \right]_+ = \hbar\omega_D n_0(0) + 2 \int_{-\mu}^0 d\xi N(\xi) \xi + N(0) \int_0^{\hbar\omega_D} d\xi \left(\xi - \sqrt{\xi^2 + \Delta^2} \right). \quad (37)$$

Subtracting (32) from (37) gives

$$\left[\frac{E_s - E_n}{L^d} \right]_+ = \hbar\omega_D n_0(0) + N(0) \int_0^{\hbar\omega_D} d\xi \left(\xi - \sqrt{\xi^2 + \Delta^2} \right), \quad (38)$$

which is just *half* the full GBEC theory result (34). Furthermore, if $[(E_s - E_n)/L^d]_-$ is the contribution from 2h-CPs alone we may assume that $f_+ = 0$ and $n_0(0) = 0$ and eventually arrive at precisely the rhs of (38) but with $m_0(0) = \Delta^2/f^2$ in place of $n_0(0) = \Delta^2/f^2$. Hence

$$\begin{aligned} \left[\frac{E_s - E_n}{L^d} \right]_+ &= \left[\frac{E_s - E_n}{L^d} \right]_- \\ &= \frac{1}{2} N(0) (\hbar\omega_D)^2 \left[1 - \sqrt{1 + (\Delta/\hbar\omega_D)^2} \right] \\ &\xrightarrow{\lambda \rightarrow 0} -\frac{1}{4} N(0) \Delta^2 \left[1 - \frac{1}{4} \left(\frac{\Delta}{\hbar\omega_D} \right)^2 + O\left(\frac{\Delta}{\hbar\omega_D} \right)^4 \right] \end{aligned} \quad (39)$$

which again is just one-half the full GBEC theory condensation energy (34) that was found to be identical to the full BCS condensation energy (36). Though not too surprising as the function $E(\epsilon) \equiv \sqrt{(\epsilon - \mu)^2 + \Delta^2(\epsilon)}$, where $\Delta(\epsilon) \equiv \sqrt{n_0 f_+(\epsilon) + m_0 f_-(\epsilon)}$, becomes “half-gapless” in either crossover versions C or D, this one-half difference occurs precisely because either n_0 or m_0 , and $f_+(\epsilon)$ or $f_-(\epsilon)$, have been deleted. Including *both* 2e- and 2h-CPs gave similarly striking conclusions on generalizing via the Bethe–Salpeter equation the ordinary [26] CP problem from unrealistic infinite-lifetime pairs to the physically expected finite-lifetime ones of Refs. [27,28].

7. Conclusions

The recent generalized BEC (GBEC) statistical single-band theory was employed to distinguish four different versions of the BCS–Bose crossover picture. One of these is the original BCS–Bose crossover theory with number Eq. (25), crossover version B. For the Cooper/BCS model interaction predicts in 2D virtually the same T_c s to well beyond physically unreasonable values of coupling, as the (allegedly less general) BCS statistical theory where the number equation becomes trivial on assuming that

the electron chemical potential $\mu = E_F$, the Fermi energy. However, T_c s much higher than those of the BCS–Bose crossover theory have been obtained [63] via the GBEC number Eq. (17), designated here as crossover version A, that includes both electron- or hole-pair bosons explicitly but in *different* proportions.

The GBEC statistical theory also reveals that the BCS gap equation for all temperatures follows rigorously only when *neither* hole- nor electron-pairs are ignored and occur in *equal* proportions, separately for zero- and non-zero-CMM pairs, and that the resulting GBEC $T = 0$ condensation energy equals the entire (rigorous-upper-bound) BCS value for *any* coupling. But that it is only *half as large* when either kind of pair is ignored. Hence, if a BEC theory that reduces properly to BCS theory is at all relevant in SCs and SFs taken as many-fermion systems where pairing into bosonic CPs can occur, two-hole CPs must play an unambiguously crucial role.

Acknowledgements

M.de.Ll thanks J.F. Annett, D.M. Eagles, M. Fortes, J. Javanainen, T.A. Mamedov, J.P. Rodríguez, O. Rojo, V.V. Tolmachev, J.A. Wilson and G.M. Zhao for discussions. M.de.Ll and M.A.S acknowledge UNAM-DGAPA-PAP-IIT (Mexico) for Grants IN106401 and IN111405, and CONACyT (Mexico) Grants 41302F and 43234F, for partial support. M.de.Ll also thanks 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 fellowship.

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