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Is BCS Related with BEC?

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Abstract We present the complete phase diagram implied by the generalized Bose-Einstein condensation (GBEC) formalism that in essence is a ternary boson-fermion (BF) model with *three* constituents: two bosonic [two-electron Cooper pairs (2e-CPs) and two-hole Cooper pairs (2h-CPs)] along with unpaired electrons whose number naturally vanishes in the limit of infinite e-e coupling. There arise three coupled transcendental equations to be solved self-consistently: two gap-like equations (one for each kind of CPs) and a third which guarantees charge conservation via the number equation for the total electron number density of the system. The unknown variables are the chemical potential as well as the number density of zero-momentum 2e-CPs and 2h-CPs, each depending on coupling as well as absolute temperature. The GBEC subsumes as special cases all statistical theories of superconductors including BCS and BEC. It also subsumes the BCS-Bose "crossover" theory which in turn relates BCS with BEC. The GBEC formalism yields a substantial increase in critical temperature compared with BCS theory even with only electron-phonon dynamics.

Keywords Generalized Bose-Einstein Condensation · High-T_c superconductors · BCS theory · Cooper pairs

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1 Introduction

It is well-known that high T_c superconductivity remains unexplained by BCS [1] theory. Nevertheless, with a new formalism that generalizes Bose-Einstein condensation (GBEC) [2–6] with its explicit inclusion of two-hole (2h) Cooper pairs (CPs) sizably increases T_c with respect to BCS. This new formalism is essentially a statistical *ternary* boson-fermion (BF) model—contrasting with the more familiar pioneering *binary* models of, e.g., Eagles [7], Ranninger et al. [8], Friedberg et al. [9], and others. The ternary-BF-gas [6–11] GBEC formalism subsumes ordinary BEC [12, 13] and was proposed to describe superconductors in general. In the new formalism, the fermions are unpaired electrons (e) and, without loss of generality, also holes (h); the bosons are CPs of both the e and h oppositely charged fermions. The GBEC formalism yields three condensed chemically and thermodynamically stable phases [14]: two pure BEC phases, one for 2e-CPs, and other one for 2h-CPs, along with a mixed phase in arbitrary proportions of each of the two pure phases.

Besides including as special cases all known statistical models of superconductors [2–6], also subsumed by the GBEC is the BCS-Bose "crossover" [4] theory which in turn includes BCS as a special case when coupling is so weak that the chemical potential μ can safely be replaced by the Fermi energy E_F as was originally assumed by BCS [1].

Moreover, GBEC predicts T_cs as high as room temperature without abandoning electron-phonon dynamics [15], as illustrated in the full phase diagram presented here for the first time. Also discussed for the first time is the physical interpretation of the unpaired fermions and their contribution to the associated critical temperature in each phase.

2 GBEC Formalism

The GBEC [2–6] total Hamiltonian H consists of two parts, $H = H_0 + H_{int}$. An unperturbed Hamiltonian

$$H_0 = \sum_{\mathbf{k}_1,s_1} \boldsymbol{\varepsilon}_{\mathbf{k}_1} a^{\dagger}_{\mathbf{k}_1,s_1} a_{\mathbf{k}_1,s_1} + \sum_{\mathbf{K}} E_+(K) b^{\dagger}_{\mathbf{K}} b_{\mathbf{K}} - \sum_{\mathbf{K}} E_-(K) c^{\dagger}_{\mathbf{K}} c_{\mathbf{K}} \quad (1)$$

describing a ternary BF ideal gas in 3D where $\mathbf{K} \equiv \mathbf{k}_1 + \mathbf{k}_2$ is the total or center-of-mass momentum (CMM) wave-vector and $\varepsilon_{k_1} \equiv \hbar^2 k_1^2/2m$ the energy of each electron of effective mass m [15] while $E_{\pm}(K) \equiv E_{\pm}(0) \pm \hbar^2 K^2/4m$ are phenomenological energies of 2e-/2h-CPs each of mass $2m$. Here, $a^{\dagger}_{\mathbf{k}_1,s_1}(a_{\mathbf{k}_1,s_1})$ are the creation (annihilation) operators for fermions and similarly $b^{\dagger}_{\mathbf{K}}(b_{\mathbf{K}})$, $c^{\dagger}_{\mathbf{K}}(c_{\mathbf{K}})$ for bosonic 2e- and 2h-CPs, respectively. The first term in (1) accounts for unpaired electrons while the second and the third correspond to bosonic 2e-CPs and 2h-CPs, respectively.

To our knowledge, no one has yet constructed, from Fermi operators, such b and c operators obeying Bose commutation rules. However, it is clear [16] that operators depending only on **K**—and not *also* on relative **k** as BCS-pair operators do—lead to states obeying *Bose statistics*.

Though the postulated Hamiltonian (1) has defied all efforts to be deduced from the ab initio one of effectively attractive electrons alone, it is apparently vindicated when seen to *explicitly* reproduce as special cases the BCS-Bose crossover [4] theory which in turn includes BCS when coupling is weak, as well as ordinary BEC theory when it is so strong that no unpaired electrons remain in the original ternary BF mixture.

The second part H_{int} of the full Hamiltonian describes interactions via four distinct BF interaction vertices each with two unpaired fermions and one boson operator of creation (annihilation) that represent how unpaired electrons (subindex +) or holes (subindex -) are involved in the formation and disintegration of the 2e-/2h-CPs. Specifically,

$$\begin{aligned} H_{\text{int}} = {} & L^{-3/2} \sum_{\mathbf{k},\mathbf{K}} f_+(k) \\ & \times \left(a^{\dagger}_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow} a^{\dagger}_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow} b_{\mathbf{K}} + a_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow} a_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow} b^{\dagger}_{\mathbf{K}} \right) \\ & + L^{-3/2} \sum_{\mathbf{k},\mathbf{K}} f_-(k) \\ & \times \left(a^{\dagger}_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow} a^{\dagger}_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow} c^{\dagger}_{\mathbf{K}} + a_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow} a_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow} c_{\mathbf{K}} \right) \end{aligned} \quad (2)$$

where $f_{\pm}(k)$ are BF coupling terms of electrons and holes, respectively. One can simplify H_{int} by ignoring $K \neq 0$ terms in the interaction but *not* in the unperturbed Hamiltonian as done in BCS theory. Ignoring interactions between unpaired electrons and *excited* $K \neq 0$ bosons the simplified total dynamical operator becomes

$$\begin{aligned} \hat{H} - \mu\hat{N} \simeq {} & \sum_{\mathbf{k}_1,s_1} [\boldsymbol{\varepsilon}(k_1) - \mu]\, a^{\dagger}_{\mathbf{k}_1,s_1} a_{\mathbf{k}_1,s_1} \\ & + [E_+(0) - 2\mu] N_0 + \sum_{\mathbf{K}\neq 0} \left[E_+(K) - 2\mu\right] b^{\dagger}_{\mathbf{K}} b_{\mathbf{K}} \\ & + [2\mu - E_-(0)] M_0 + \sum_{\mathbf{K}\neq 0} \left[2\mu - E_-(K)\right] c^{\dagger}_{\mathbf{K}} c_{\mathbf{K}} \\ & + \sum_{\mathbf{k}} \left[\sqrt{n_0} f_+(k) + \sqrt{m_0} f_-(k)\right] \\ & \times \left(a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow} + a_{\mathbf{k}\downarrow} a_{-\mathbf{k}\uparrow} \right) \end{aligned} \quad (3)$$

where $E_{\pm}(0)$ is the phenomenological energy of the bosonic 2e-/2h-CPs with $K = 0$, $\hat{N}$ is the operator of the total number of fermions including the unpaired fermions. Here, one applies the Bogoliubov recipe [18], valid below T_c, of replacing each creation (annihilation) operator for bosons $b^{\dagger}_0, b_0$ by the number $\sqrt{N_0}$ where N_0 is the number of composite-boson 2e-CPs with $K = 0$ and similarly for $c^{\dagger}_0, c_0$ by the number $\sqrt{M_0}$ where M_0 is the number of composite-bosons 2h-CPs with $K = 0$. The full simplified Hamiltonian can then be diagonalized [5]. This simplification can be lifted (see [19] where excited bosons with $K \neq 0$ are not excluded in the interaction Hamiltonian of (3)).

The dynamical operator (3) can now be exactly diagonalized via a Bogoliubov-Valatin transformation [18, 20]. Thus, the well-known grand canonical ensemble relation

$$\Omega(T, L^3, \mu, N_0, M_0) = -k_B T \ln \left[Tr\, e^{-\beta(\hat{H} - \mu\hat{N})} \right] \quad (4)$$

can be evaluated explicitly, where *Tr* stands for "trace." Here, T is the absolute temperature and $\beta \equiv 1/k_B T$, k_B the Boltzmann constant, and μ are the chemical potential of the many-electron subsystem. From (4), one can find all the thermodynamic properties of the system such as pressure $P(T, n) = -\Omega/L^3$, entropy $S(T, n)/L^3 = -k_B \partial(\Omega/L^3)/\partial T$ and the Helmholtz free energy $F(T, L^3, N, M) \equiv \Omega + \mu N$. Taking the partial derivative of (4) with respect to chemical potential and minimizing $F(T, L^3, N, M) \equiv \Omega + \mu N$ over N_0, M_0 gives

$$\frac{\partial\Omega}{\partial\mu} = -N \qquad \frac{\partial F}{\partial N_0} = 0 \qquad \frac{\partial F}{\partial M_0} = 0. \quad (5)$$

The first relation is the well-known result of statistical mechanics and here ensures the net charge conservation of the GBEC formalism, i.e., *gauge invariance*, in contrast with BCS theory which lacks it. After some algebra, one arrives at the three transcendental coupled equations that determine the GBEC formalism, a "number equation"

$$n = 2n_0(T) + 2n_{B+}(T) - 2m_0(T) - 2m_{B+}(T) + n_f(T) \quad (6)$$

where $n_{B+}(T)$ and $m_{B+}(T)$ are the non-condensed-boson number densities for $2e$- and $2h$-CPs, respectively, with $n \equiv N/L^3$ where L is the length of the "box" of volume L^3, and $n_f(T)$ refers to the unpaired electrons of the system at any T and turns out to be

$$n_f(T) = \int_0^\infty d\epsilon N(\epsilon)\left[1 - \frac{\epsilon - \mu}{E(\epsilon)} \tanh \frac{1}{2}\beta E(\epsilon)\right]. \quad (7)$$

The last two requirements of (5) lead to two "gap-like equations" for 2e-CPs and for 2h-CPs [2, 4], with $E(\epsilon) \equiv \sqrt{(\epsilon - \mu)^2 + \Delta^2(\epsilon)}$ where the T-dependent gap $\Delta(\epsilon) \equiv \sqrt{n_0(T)} f_+(\epsilon) + \sqrt{m_0(T)} f_-(\epsilon)$, and $N(\boldsymbol{\epsilon}) \equiv m^{3/2}\sqrt{\boldsymbol{\epsilon}}/2^{1/2}\pi^2\hbar^3$ the electron density of states. Here, $n_0 \equiv N_0/L^3$ and $m_0 \equiv M_0/L^3$ are the number densities of condensed 2e-/2h-CPs respectively. The strength functions $f_+(\boldsymbol{\epsilon})$ and $f_-(\boldsymbol{\epsilon})$ can be constructed as in [2, 3].

3 GBEC Phases

One has from (6) the single number equation which guarantees charge conservation, here $n_0(T)$ is the number density of condensed 2e-CPs and $n_{B+}(T)$ is the number density of uncondensed 2e-CPs can be expressed as

$$n_{B+}(T) \equiv \int_{0+}^\infty d\boldsymbol{\varepsilon} M(\boldsymbol{\varepsilon}) \left[\exp \beta\{E_+(0) + \boldsymbol{\varepsilon} - 2\mu\} - 1\right]^{-1} \quad (8)$$

a typical Bose-Einstein forms are clearly recovered, as expected, and $m_{B+}(T)$ as

$$m_{B+}(T) \equiv \int_{0+}^\infty d\boldsymbol{\varepsilon} M(\boldsymbol{\varepsilon}) \left[\exp \beta\{2\mu - E_-(0) + \boldsymbol{\varepsilon}\} - 1\right]^{-1} \quad (9)$$

is the number density of uncondensed 2h-CPs. Here, $E_\pm(0) = 2E_f \pm \delta\boldsymbol{\varepsilon}$ (see [3] p. 551) where E_f is the interaction energy width of bosons and $\delta\boldsymbol{\varepsilon}$ is a shell energy about E_f, this energy being the so-called *pseudo-Fermi energy*. Again, $N(\epsilon)$ and $M(\boldsymbol{\varepsilon})$ are the electronic and bosonic density of states, respectively.

For the two pure phases, one can generalize from the *single-band model* used 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 E_f^e and E_f^h differing precisely by the two masses.

In Fig. 1, we plot the total dimensionless T_c/T_F vs dimensionless number density n/n_f for the pure 2e-CP phase with no 2h-CPs in the ground state, as well as the pure 2h-CP phase with no 2e-CPs in the ground state, where T_F is the actual Fermi-energy-related temperature. These two curves are compared with BEC and BCS. Also plotted is the dotted thin curve for perfect symmetry between the number of 2h-CPs and 2e-CPs (50-50 mixture), namely

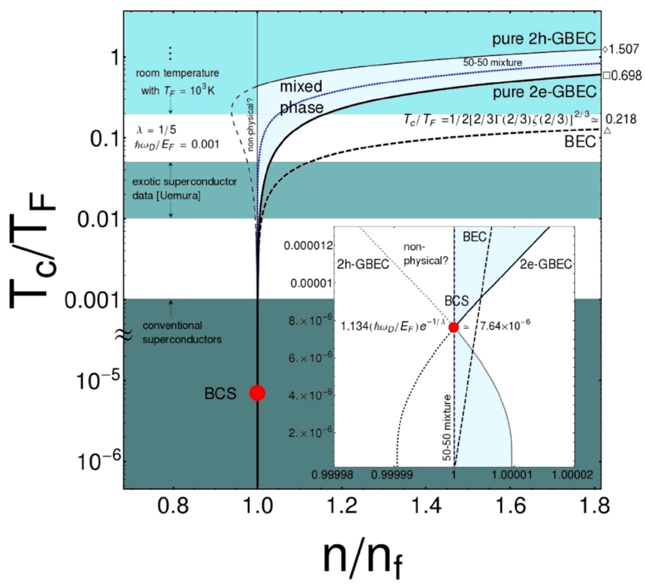

Fig. 1 Dimensionless T_c/T_F versus n/n_f for pure GBEC phases 2h-/2e-CPs and the ordinary BEC (*black dashed curve*) in 3D, extrapolating for $n_f \to 0$ to the familiar limit 0.218. *Inset* shows the intersection between the pure phase 2e-CP and the pure phase 2h-CP when $n/n_f = 1$ which implies $T_c/T_F = 7.64 \times 10^{-6}$ given by the BCS T_c weak-coupling formula $k_BT_c \simeq 1.134\hbar\omega_D \exp(1/\lambda)$ using $\lambda = 1/5$ and $\hbar\omega_D/E_F = 0.001$, where $\hbar\omega_D$ is the Debye energy of the lattice. The *red dot* marks the critical BCS temperature. The *blue dotted thin curve* (online) corresponds to perfect symmetry between 2e-/2h-CPs, i.e., $n_0(T) = m_0(T)$ and $n_{B+}(T) = m_{B+}(T)$. For $n/n_f < 1$, the pure phases curves are marked as dotted, but are thus far with no physical meaning. Symbols *diamond*, *square*, and *triangle* are the limit of the two pure-phase GBEC and single BEC curves, respectively, when $n/n_f \to \infty$, i.e., when $n_f(T \to 0) \equiv n_f$ (see §4). Uemura's exotic data are taken from [21]

$n_0(T) = m_0(T)$ and $n_{B+}(T) = m_{B+}(T)$ implying [6] that $\mu = E_f$. Furthermore, in the inset of Fig. 1, the BCS value of $T_c/T_F = 7.64 \times 10^{-6}$ is indicated by the red dot with a number density $n/n_f = 1$; it follows from the standard BCS theory weak-coupling formula $k_BT_c \simeq 1.134\hbar\omega_D \exp(1/\lambda)$ for $\lambda = 1/5$ and $\hbar\omega_D = 10^{-3}E_F$. The light blue shaded area between the two pure 2h-/2e-CP curves corresponds to *the mixed phase of GBEC with arbitrary proportions between 2h-/2e-CPs* , as well as below the BCS point (inset in Fig. 1). Clearly, *GBEC can enhance T_c values compared with BCS as high as room temperature and higher* employing the BCS model interaction mimicking the electron-phonon attraction overwhelming the Coulomb e-e repulsions.

The total dimensionless number density of the pure phase 2e-GBEC of 2e-CPs and 2h-GBEC of 2h-CPs has a definite limit when $n/n_f \to \infty$ in which limit all there are no unpaired electrons whatsoever leading to an ideal BF gas mixture without mutual interactions. The number of unpaired fermions $n_f(T)$ at precisely $T = 0$ leads to

$n_f \equiv n_f(T=0) = (2mE_f)^{3/2}/2^{1/2}\pi^2\hbar^3$, the first equality to be derived in next section.

4 Unpaired Electrons and Meaning of n_f as $n_f(T=0)$

The total number of unpaired electrons (7) at any T can be decomposed as

$$\begin{aligned} n_f(T) &= \int_0^{E_f-\delta\epsilon} d\epsilon N(\epsilon)\left[1-\frac{\epsilon-\mu}{|\epsilon-\mu|}\tanh\left(\frac{\epsilon-\mu}{2k_BT}\right)\right] \\ &+\int_{E_f+\delta\epsilon}^{\infty} d\epsilon N(\epsilon)\left[1-\frac{\epsilon-\mu}{|\epsilon-\mu|}\tanh\left(\frac{\epsilon-\mu}{2k_BT}\right)\right] \\ &+\int_{E_f-\delta\epsilon}^{E_f+\delta\epsilon} d\epsilon N(\epsilon)\left[1-\frac{\epsilon-\mu}{\sqrt{(\epsilon-\mu)^2+\Delta^2}}\right. \\ &\left.\times\tanh\left(\frac{\sqrt{(\epsilon-\mu)^2+\Delta^2}}{2k_BT}\right)\right] \\ &\underset{T\to 0}{=} \left(2mE_f\right)^{3/2}/2^{1/2}\pi^2\hbar^3 \equiv n_f \end{aligned} \tag{10}$$

Consider the dimensionless number density of unpaired electrons $n_f(T)/n_f$ at $T = T_c$ where the energy gap is $\Delta = 0$. If one takes the limit $T \to 0$, then $\mu \simeq E_f$ since $E_+(0) = E_-(0)$ so that $n_f(T \to 0)$ becomes in the rhs of (10) simply n_f, meaning that n_f is just *the number density of unpaired electrons* at $T = 0$. This result is illustrated in Fig. 2. The highest T_c/T_F occurs in each case precisely when the number of unpaired electrons at $T = 0$ vanishes $n_f \to 0$, meaning that $n/n_f \to \infty$, as in this limit, all electrons are strongly coupled yielding a purely bosonic system.

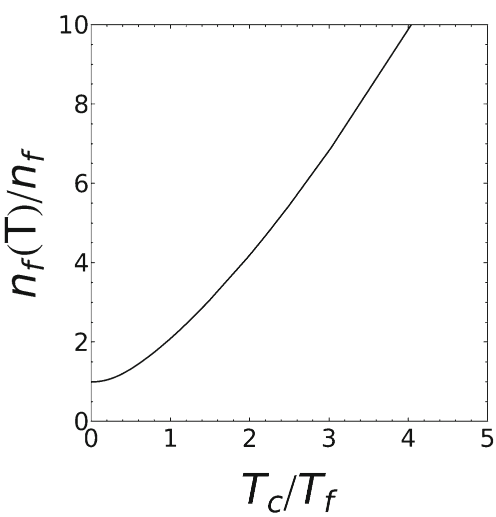

Fig. 2 Here, we plot of (10) the dimensionless number density of the unpaired electrons $n_f(T)/n_f$ vs T/T_f. As $T \to 0$ one clearly gets that $n_f(T)/n_f = 1$—or that n_f is precisely the number density of unpaired electrons at $T = 0$. On the other hand, as $T \to \infty$ one must have $n_f(T)/n_f \to \infty$ since the number of unpaired electrons increases without limit as temperature increases

5 Conclusions

The GBEC formalism describes a superconductor via a ternary BF gas with unpaired electrons as well as bosonic 2e-CPs and 2h-CPs. In GBEC, one finds two pure BEC phases and a mixed phase with arbitrary proportions of 2e-/2h-CPs. Within this mixed phase is the phase-boundary curve with perfect symmetry (50-50 mixture). In GBEC, the BCS theory is subsumed when one has this perfect symmetry; also subsumed is the BCS-Bose "crossover" theory reduces to BCS where $\mu = E_F$. The results presented in the phase diagram enable one to find a much higher T_c than predicted by standard BCS theory. Furthermore, considering a pure phase, e.g., 2h-GBEC, T_c increases dramatically with respect to BCS without abandoning electron-phonon dynamics. We found that a minor change in the number density of the system can substantially enhance T_c. The physical interpretation of the unpaired electrons in the limit of very strong coupling leads one to a purely bosonic system. The uncondensed pairs of either electrons or holes play an important, albeit elusive, role to describe high-T_c superconductivity. The *precise* role of 2h-CPs in this formalism may shed light on high-T_c superconductivity.

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