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ORIGINAL PAPER

Multicondensate Superconductivity in a Generalized BEC Formalism with Hole Cooper Pairs

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Abstract We sketch the generalized Bose-Einstein condensation (GBEC) formalism of a *ternary* boson-fermion (BF) model to study the critical transition temperature T_c of a superconductor. This ternary model contrasts with the more familiar *binary* models of, e.g., Eagles, Ranninger et al., T.D. Lee et al., etc. The fermions are unpaired electrons (e) or, without loss of generality, holes (h); the bosons are Cooper pairs (CPs) each of both these fermions. In essence, the GBEC is a statistical model, as is the Bardeen-Cooper-Schrieffer (BCS) theory also, and yields three condensed chemically- and thermodynamically-stable phases: two pure phases, one for electron Cooper pairs (2e-CPs), and the other for hole Cooper pairs (2h-CPs), along with a mixed phase in arbitrary proportions of each of the two pure phases. The *explicit* inclusion of 2h-CPs *dramatically increases* the T_c of a superconductor with respect to BCS besides including as special cases all known statistical models of superconductors.

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

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1 Introduction

It's been said that in the twentieth century, there were three central paradigms in condensed-matter physics (i) the band theory of solids [1]; (ii) the Landau theory of Fermi liquids [2]; and (iii) the BCS theory of superconductivity (SC) [3]. One might also add (binary) boson-fermion (BF) models to describe SC. These were pioneered in 1969 by Eagles [4], in the late 1970s by Leggett [5], in the mid to late 1980s by Ranninger et al. [6], T.D. Lee et al. [7, 8], and others. Nonetheless, high-T_c superconductivity remained altogether unexplained.

A newer approach, based on a *ternary* BF model with explicit inclusion of two-hole (2h) Cooper pairs (CPs) leads to a formalism that generalizes Bose-Einstein condensation (GBEC) [9–13] and is vastly more general with sizeable increases in T_c with respect to those predicted by BCS. The ternary-BF-gas [4, 6–8, 13–15] GBEC formalism subsumes BCS theory as well as ordinary BEC [16, 17] and was proposed to describe SC in general.

Three crucial elements characterizing GBEC are (i) CPs, which obey Bose statistics [13], are considered as real bosons—as opposed to BCS pairs which are strictly not bosonic as they do not obey Bose commutation relations [3]; (ii) BF vertex interactions (similar to electron-phonon vertices) which drive formation/disintegration of CPs; and (iii) 2h-CPs explicitly accounted for along with two-electron (2e) CPs. Besides, including as special cases, all known statistical models of superconductors [9–13] the GBEC formalism also subsumes the BCS-Bose "*crossover*" [11] theory which in turn includes BCS as a special case.

It is noteworthy that Hirsch [18] has strenuously emphasized that upon cooling a SC with either 2h-CPs or 2e-CPs in its normal phase (as the case may be with a given material) CPs first emerge as *preformed* CPs above T_c but that only actual 2e-CPs appear *below* T_c.

2 GBEC Equations

The GBEC [9–13] total Hamiltonian H consists of two parts $H_0 + H_{int}$. An unperturbed Hamiltonian

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

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) wavevector of a CP and $\varepsilon_{k_1} \equiv \hbar^2 k_1^2/2m$ the energy of each electron of effective mass m [19] while $E_\pm(K) \equiv E_\pm(0) \pm \hbar^2 K^2/4m$ are *phenomenological* energies of the bosonic 2e-/2h-CPs each of effective 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 the 2e-CPs and 2h-CPs, respectively.

The second part H_{int} of the full GBEC 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

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

where $f_\pm(k)$ are BF coupling terms of electrons and holes, respectively. This is depicted in Fig. 1. One can simplify H_{int} by ignoring $\mathbf{K} \neq 0$ terms in the interaction but *not* in the unperturbed Hamiltonian as done in BCS theory [3]. Ignoring *excited* $\mathbf{K} \neq 0$ terms in (2), a simplified, readily diagonalizable, total dynamical operator $\hat{H} - \mu\hat{N}$ as appears in Ref. [9, 10] where μ is a Langrange multiplier and $\hat{N}$ is the operator for total number of electrons including

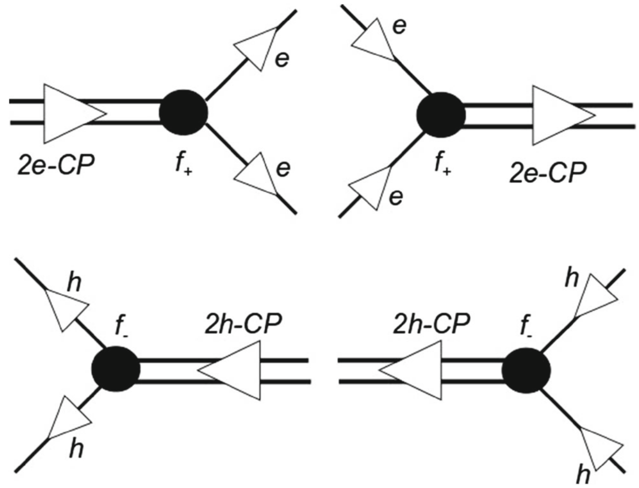

Fig. 1 The BF hamiltonian interaction (2) consists of 4-vertices each with two-fermion/one-boson creation-anihilation operators representing how unpaired electrons (+) and/or holes (−) bind to form 2e- or 2h-CPs, and disintegrate into two unpaired fermions

the unpaired electrons. Applying the Bogoliubov "recipe" of replacing $b_0^{\dagger}(b_0)$ and $c_0^{\dagger}(c_0)$, respectively, by $\sqrt{N_0}$ and $\sqrt{M_0}$, where N_0 and M_0 are the number of composite-boson 2e/2h-CPs with $K = 0$, leads below T_c to a full simplified Hamiltonian which is then exactly diagonalizable [12] via a Bogoliubov-Valatin transformation [20, 21]. This simplification can be lifted—see Ref. [22–25] where excited bosons with $\mathbf{K} \neq 0$ are *not* excluded in the interaction Hamiltonian of $\hat{H} - \mu\hat{N}$ which can then be dealt with via two-time Green functions.

The simplified dynamical operator $\hat{H} - \mu\hat{N}$ can now be exactly diagonalized. Thus, the well-known grand canonical ensemble definition of the grand (or Landau) potential

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

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 is the chemical potential of the many-electron subsystem. The Helmholtz free energy below T_c is $F(T, L^3, N_0, M_0) \equiv \Omega + \mu N$. Taking the partial derivative of (3) with respect chemical potential and minimizing $F(T, L^3, N_0, M_0)$ over N_0, M_0 gives

$$\frac{\partial \Omega}{\partial \mu} = -N \qquad \frac{\partial F}{\partial N_0} = 0 \qquad \frac{\partial F}{\partial M_0} = 0. \quad (4)$$

The first relation is the familiar 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. The last two relations are necessary to define a stable thermodynamic state.

After some algebra, one arrives at the three transcendental coupled equations that determine the GBEC formalism: a "*number equation*" for the electron number density

$$n = 2n_0(T) + 2n_{B+}(T) - 2m_0(T) - 2m_{B+}(T) + n_f(T). \quad (5)$$

Here, $n_0 \equiv N_0/L^3$ and $m_0 \equiv M_0/L^3$ are the number densities of condensed bosonic 2e-/2h-CPs, respectively, while $n_{B+}(T)$ and $m_{B+}(T)$ are the uncondensed-boson number densities for $2e$- and $2h$ -CPs, respectively. Also, $n \equiv N/L^3$ where L is the length of the "box" of volume L^3, and $n_f(T)$ refers to the unpaired-electron number density of the system at any T which turns out to be

$$n_f(T) = \int_0^\infty d\epsilon N(\epsilon)\left[1 - \frac{\epsilon - \mu}{E(\epsilon)} \tanh \frac{1}{2}\beta E(\epsilon)\right]. \quad (6)$$

Here, $E(\epsilon) \equiv \sqrt{(\epsilon - \mu)^2 + \Delta^2(\epsilon)}$ where the T-dependent gap$\Delta(\epsilon) \equiv \sqrt{n_0(T)} f_+(\epsilon) + \sqrt{m_0(T)} f_-(\epsilon)$. The strength functions $f_+(\varepsilon)$ and $f_-(\varepsilon)$ can be constructed as in Ref. [9, 10]. The last two requirements of (4) lead to two "*gap-like equations*" associated with 2e-CPs and 2h-CPs [6–8].

Figure 2 shows the five statistical theories that are subsumed as special cases in the GBEC formalism. Keeping only 2e-CPs eventually leads to ordinary BEC theory. On the other hand, if one assumes perfect symmetry between 2e-CPs and 2h-CPs, one obtains the BCS theory of SC, insofar as the precise gap equation and $T = 0$ condensation energy are recovered [13].

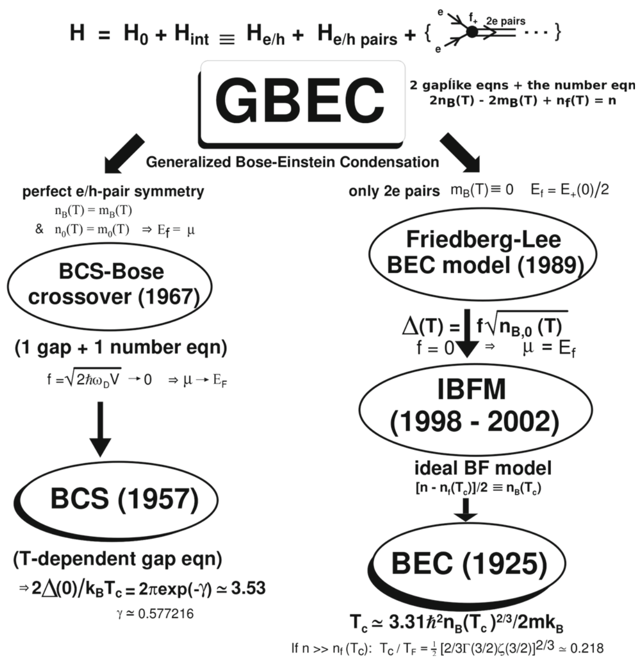

Fig. 2 Flowchart illustrating conditions under which the GBEC formalism reduces to, or subsumes, all five statistical theories of superconductivity (*ovals*). Here ideal boson-fermion model (IBFM) is the *binary* case of GBEC corresponding to the unperturbed hamiltonian (1). Here $\zeta(3/2) \simeq 2.612$ is the zeta function of order 3/2

3 2h-CPs in GBEC Multiphases and High T_c

In Fig. 3, we plot the total dimensionless T_c/T_F versus dimensionless number density n/n_f (where n_f is the number density of unpaired electrons at $T = 0$, see Fig. 2 below) 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 temperature related to the actual Fermi energy E_F in the normal state. These two curves are compared with ordinary BEC and BCS. Also plotted is the thin-dotted curve for perfect symmetry between the number of 2h-CPs and 2e-CPs (50–50 mixture), namely $n_0(T) = m_0(T)$ *and* $n_{B+}(T) = m_{B+}(T)$ implying [13] that $\mu = E_f$. In the larger Inset of Fig. 3, the BCS value of $T_c/T_F = 7.64 \times 10^{-6}$ is recovered and marked by the red dot (online) with a number density $n/n_f = 1$ and follows from the standard BCS theory weak-coupling formula $k_B T_c \simeq 1.134\hbar\omega_D \exp(1/\lambda)$ for $\lambda = 1/5$ and $\hbar\omega_D = 10^{-3} E_F$, the values used in the figure. The light-blue (online) shaded area between the two pure 2h-/2e-CP curves corresponds to the *mixed phase of GBEC* with arbitrary proportions of bosonic 2h-/2e-CPs, as well as below the BCS point (larger Inset in Fig. 3). Clearly, *GBEC can enhance T_c values compared with BCS as high as room temperature and higher,* employing only the BCS model interaction mimicking the electron-phonon attraction that overwhelms Coulomb e-e repulsions. Note that with a minor change in the number density around $n/n_f = 1$, the system T_c/T_F can change substantially, increasing or decreasing as the case may be.

It has been shown that in the relativistic ideal Bose gas (RIBG) [26], the inclusion of *anti*bosons produces higher critical temperatures with respect to an RIBG without antibosons. In SCs, a dramatic increase of T_c with the GBEC occurs if one includes the 2h-CPs, their intriguing role having been discussed [27] as a "background" effect in enhancing T_c.

However, in Fig. 3, the pure 2e-GBEC phase at T_c is described by $n = 2n_{B+}(T_c) - 2m_{B+}(T_c) + n_f(T_c)$ which contains unpaired electrons as well as uncondensed 2e-/2h-CPs bosons; we found that uncondensed 2e-CPs predominate over uncondensed 2h-CPs. In ordinary BEC (dashed-curve in Fig. 3), one has a condensate gas composed of 2e-CPs bosons in which one completely ignores pairs of holes (rhs of Fig. 2). As expected, the BEC curve is in the $n/n_f > 1$ region where uncondensed 2e-CPs bosons predominate, this also being seen in large Inset of Fig. 3, the BEC curve *always remaining* in the $n/n_f > 1$ region. Thus, the physical interpretation when $n/n_f > 1$ is that uncondensed 2e-CPs bosons predominate over uncondensed 2h-CPs bosons.

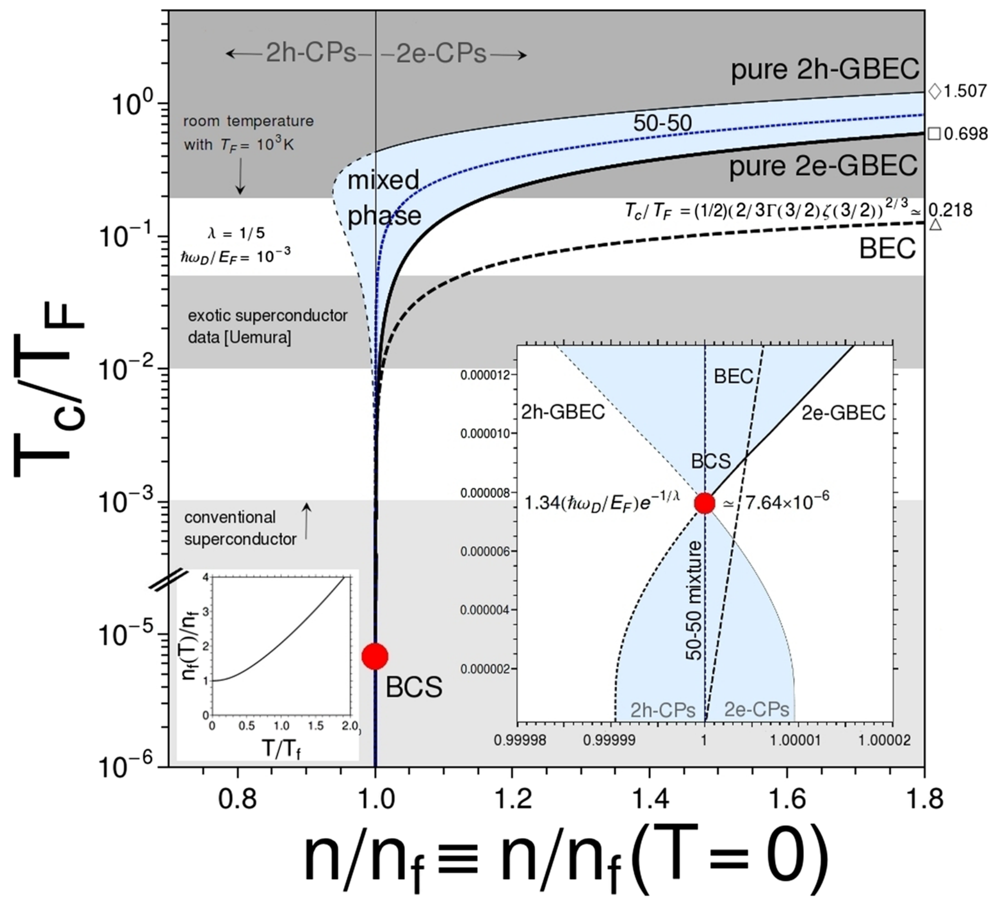

Fig. 3 Dimensionless T_c/T_F versus n/n_f for pure GBEC phases 2h-/2e-CPs and the ordinary BEC in 3D (*thick dashed curve*), extrapolating for $n_f \to 0$ to the familiar limit 0.218. Compared are three bands encompassing conventional, exotic [28] and room-temperature empirical T_c values. *Larger Inset* is a blow up around $n/n_f = 1$ where the intersection reproduces the BCS value $T_c/T_F = 7.64 \times 10^{-6}$ given by the BCS T_c weak-coupling formula $k_B T_c \simeq 1.134\hbar\omega_D \exp(1/\lambda)$ for $\lambda = 1/5$ and $\hbar\omega_D = 10^{-3}E_F$, where $\hbar\omega_D$ is the Debye energy of the lattice. *Red dot* (online) marks the critical BCS temperature. *Blue thin dashed curve* (online) marked 50-50, corresponds to perfect symmetry between 2e-/2h-CPs. The *blue shaded area* (online) is a mixed phase with arbitrary proportions of 2e-/2h-CPs, as well as in the larger Inset below the BCS dot. For $n/n_f < 1$ the pure-phase curves are marked as *short-dashed*, in this region uncondensed 2h-CPs bosons predominate while in the $n/n_f > 1$ region (*pure-phase solid curves*) uncondensed 2e-CPs bosons predominate. Symbols ◇, □, △ mark the limit of the two pure-phase GBEC and BEC curves, respectively, when $n/n_f \to \infty$, i.e., when $n_f(T) \to 0$, meaning that all unpaired electrons are paired. *Smaller Inset* shows plot of the dimensionless number density $n_f(T)/n_f$ of unpaired electrons (6) and its $T = 0$ limit n_f, see Ref. [29]

Also, this can be explained with the pure phase 2h-GBEC at T_c, described by $n = 2n_{B+}(T_c) - 2m_{B+}(T_c) + n_f(T_c)$. In this phase, one sees that uncondensed 2h-CPs predominate over uncondensed 2e-CPs and T_c/T_F increases dramatically wrt BCS (red dot–online Fig. 3). A slight change in number density around $n/n_f < 1$ gives a substantial increase in T_c. In perfect symmetry (50–50 mixture) one has the same number between 2e-CPs and 2h-CPs and the blue dotted curve (online) in Fig. 3 goes towards the $n/n_f > 1$ region, this being due to the contribution of 2e-CPs from $n_f(T)$, namely $n/n_f \to \infty$ when $n_f(T) \to 0$ meaning that all electrons in the system are paired, as expected if one has only 2e-CPs when $n/n_f > 1$.

In this study, one has phases with both types of 2e-/2h-CPs bosons, the physical interpretation of the two associated regions in the phase diagram of Fig. 3 is that there are precise amounts of unpaired electrons or unpaired holes that contribute to electron-/hole-pairing to enhance the superconducting transition temperature. This behavior might be associated with electron-electron as opposed to electron-ion interactions as defined by Hirsch [18].

4 Conclusions

The GBEC formalism describes a superconductor via a *ternary* BF gas with unpaired electrons *as well as* bosonic

2e-CPs and 2h-CPs. It gives two pure GBEC phases and a mixed phase with arbitrary proportions of 2e-/2h-CPs. Within this mixed phase is the phase-boundary curve with perfect (50–50 mixture) symmetry. In the GBEC, the BCS theory is subsumed when one has this perfect symmetry; also subsumed is the BCS-Bose "*crossover*" theory which in turn reduces to BCS when $\mu = E_F$. Note our designation of "BCS-Bose" instead of the more common usage "BCS-BEC" since BEC is impossible in 1D where, however, the "*crossover*" itself *can* occur [30] in 1D.

The results in phase diagram Fig. 3 illustrate a much higher T_c than predicted by standard BCS theory. Furthermore, considering, e.g., a pure 2h-GBEC phase, T_c increases dramatically with respect to BCS, *without abandoning electron-phonon dynamics* [31–33]. A minor change in number density of the system around $n/n_f = 1$ substantially enhances T_c, i.e., slightly changing the number of unpaired electrons/holes in the system gives a sizeable T_c increase. The physical interpretation of unpaired electrons in the limit of very strong coupling leads to a purely bosonic system composed only of 2e-CPs. The GBEC formalism admits different phases with different proportions of 2e-CP and 2h-CP bosons.

The unpaired electrons as well as also uncondensed pairs of either electrons or holes play an important role in describing high-T_c superconductivity. In particular, the *precise* role of 2h-CPs in this formalism may shed further light in high-T_c superconductivity.

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