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ORIGINAL PAPER

Generalized Bose–Einstein Condensation in Superconductivity

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Abstract Unification of the BCS and the Bose–Einstein condensation (BEC) theories is surveyed via a generalized BEC (GBEC) finite-temperature statistical formalism. Its major difference with BCS theory is that it can be diagonalized *exactly*. Under specified conditions it yields the precise BCS gap equation for all temperatures as well as the precise BCS zero-temperature condensation energy for all couplings, thereby suggesting that a BCS condensate is a BE condensate in a *ternary* mixture of kinematically independent unpaired electrons coexisting with equally proportioned weakly-bound two-electron and two-hole Cooper pairs. Without abandoning the electron–phonon mechanism in moderately weak coupling it suffices, in principle, to reproduce the unusually high values of T_c (in units of the Fermi temperature T_F) of 0.01–0.05 empirically reported in the so-called "exotic" superconductors of the Uemura plot, including cuprates, in contrast to the low values of $T_c/T_F \leq 10^{-3}$ roughly reproduced by BCS theory for conventional (mostly elemental) superconductors.

Keywords Cooper pairs · Hole Cooper pairs · Bose–Einstein condensation

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1 Introduction

Boson–fermion (BF) models of superconductivity (SC) as a Bose–Einstein condensation (BEC) go back to the mid-1950's [1–4], pre-dating even the BCS–Bogoliubov theory [5, 6]. Although BCS theory only contemplates the presence of "Cooper correlations" of single-particle states, BF models [1–4, 7–19] posit the existence of actual bosonic CPs. With two [18, 19] exceptions, however, all BF models neglect the effect of *hole* CPs included on an equal footing with electron CPs to give the "complete" *ternary* (instead of binary) BF model that constitutes the generalized Bose–Einstein condensation (GBEC) theory to be analyzed here in greater detail.

2 The Hamiltonian

The GBEC [18, 19] is described by the Hamiltonian $H = H_0 + H_{\text{int}}$ where

$$H_0 = \sum_{\mathbf{k}_1, s_1} \epsilon_{\mathbf{k_1}} a^+_{\mathbf{k}_1, s_1} a_{\mathbf{k}_1, s_1} + \sum_{\mathbf{K}} E_+(K) b^+_{\mathbf{K}} b_{\mathbf{K}} - \sum_{\mathbf{K}} E_-(K) c^+_{\mathbf{K}} c_{\mathbf{K}} \tag{1}$$

and $\mathbf{K} \equiv \mathbf{k_1} + \mathbf{k_2}$ is the CP center-of-mass momentum (CMM) wavevector. Here $\epsilon_{\mathbf{k}_1} \equiv \hbar^2 k_1^2/2m$ are the single-electron, and $E_\pm(K)$ the 2e-/2h-CP *phenomenological,* energies. Also, $a^+_{\mathbf{k}_1, s_1}$ ($a_{\mathbf{k}_1, s_1}$) are creation (annihilation) operators for electrons and similarly $b^+_{\mathbf{K}}$ ($b_{\mathbf{K}}$) and $c^+_{\mathbf{K}}$ ($c_{\mathbf{K}}$) for 2e- and 2h-CP bosons, respectively. As suggested by the original Cooper-pair problem [20], the b and c operators proposed depend only on $\mathbf{K}$ and so are *distinct* from the BCS-pair operators depending on both $\mathbf{K}$ *and* the relative wavevector $\mathbf{k} \equiv \frac{1}{2}(\mathbf{k_1} - \mathbf{k_2})$; see [5, (2.9) to (2.13)] for the particular case of $\mathbf{K} = 0$ and shown there *not* to satisfy the ordinary Bose commutation relations. Nonetheless, CPs are objects easily be seen to obey Bose–Einstein statistics as, in the thermodynamic limit, an indefinitely large number of distinct $\mathbf{k}$ values correspond to a given $\mathbf{K}$ value characterizing the energy levels $E_+(K)$ or $E_-(K)$ given in (1). Only this is needed to ensure a BEC (or macroscopic occupation of a given state that appears below a certain fixed $T = T_c$). This was found [18, 19] numerically a posteriori in the GBEC theory. Also, the BCS gap equation is recovered for equal numbers of both kinds of pairs, in the $\mathbf{K} = 0$ state and in all $\mathbf{K} \neq 0$ states taken collectively, and in weak coupling, regardless of CP overlaps. The precise familiar BEC T_c formula emerges [18] in strong coupling when (i) 2h-CPs are ignored (whereupon the Friedberg-T.D. Lee model [12–16] equations are recovered) and (ii) one switches off the BF interaction defined below in (2). The 2e- and 2h-CPs postulated in (1) are idealized objects with the same mass but opposite charges. Thus, they do not include the crucial effects on them of the ionic-crystalline band-structure such as the "dressing" and "undressing" properties connecting particles and holes extensively discussed by Hirsch [21] as a fundamental property of matter that he calls "electron-hole asymmetry".

The interaction Hamiltonian H_{int} consists of four distinct BF interaction *single* vertices each with two-fermion/one-boson creation or annihilation operators. Each vertex is reminiscent of the Fröhlich electron-phonon interaction. Here H_{int} depicts how unpaired electrons (or holes) combine to form the 2e- (and 2h-CPs) assumed in a d-dimensional system of size L, namely

$$
\begin{aligned}
H_{\text{int}} = {} & L^{-d/2}\sum_{\mathbf{k},\mathbf{K}} f_+(k)\big\{a^+_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow}a^+_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow}b_{\mathbf{K}} \\
& + a_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow}a_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow}b^+_{\mathbf{K}}\big\} \\
& + L^{-d/2}\sum_{\mathbf{k},\mathbf{K}} f_-(k)\big\{a^+_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow}a^+_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow}c^+_{\mathbf{K}} \\
& + a_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow}a_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow}c_{\mathbf{K}}\big\}.
\end{aligned} \tag{2}
$$

The energy form factors $f_\pm(k)$ in (2) are taken as in [18, 19] where the associated quantities E_f and $\delta\varepsilon$ are *new* phenomenological dynamical energy parameters (in addition to the positive BF vertex coupling parameter f) that replace the previous such $E_\pm(0)$, through the relations $E_f \equiv \frac{1}{4}[E_+(0) + E_-(0)]$ and $\delta\varepsilon \equiv \frac{1}{2}[E_+(0) - E_-(0)] \geq 0$ where $E_\pm(0)$ are the (empirically *un*known) zero-CMM energies of the 2e- and 2h-CPs, respectively. We refer to E_f as the "pseudoFermi" energy. It serves as a convenient energy scale and is not to be confused with the usual 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 the total number-density of charge-carrier electrons, while E_f is similarly related to another density n_f which serves to scale the ordinary density n. The two quantities E_f and E_F, and consequently also n and n_f, coincide *only* when perfect 2e/2h-CP symmetry holds as in the BCS instance.

3 Reduced Hamiltonian and Its Diagonalization

The interaction Hamiltonian (2) can be further simplified by keeping only the $\mathbf{K} = 0$ terms, namely

$$
\begin{aligned}
H_{\text{int}} \simeq {} & L^{-d/2}\sum_{\mathbf{k}} f_+(k)\big\{a^+_{\mathbf{k}\uparrow}a^+_{-\mathbf{k}\downarrow}b_{\mathbf{0}} + a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow}b^+_{\mathbf{0}}\big\} \\
& + L^{-d/2}\sum_{\mathbf{k}} f_-(k)\big\{a^+_{\mathbf{k}\uparrow}a^+_{-\mathbf{k}\downarrow}c^+_{\mathbf{0}} + a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow}c_{\mathbf{0}}\big\}
\end{aligned} \tag{3}
$$

which allows *exact* diagonalization as follows. One can now apply the Bogoliubov "recipe" (see e.g. [22], p. 199 ff.) of replacing in the full Hamiltonian (1)–(2) all zero-CMM 2e- and 2h-CP boson creation and annihilation operators by their respective c-numbers $\sqrt{N_0(T)}$ and $\sqrt{M_0(T)}$, where $N_0(T)$ and $M_0(T)$ are the number of zero-CMM 2e- and 2h-CPs, respectively. One eventually seeks the highest temperature, say T_c, above which e.g. $N_0(T_c)$ or $M_0(T_c)$ vanish and below which one and/or the other is nonzero. Note that T_c calculated thusly can, in principle, turn out to be zero, in which case there is no BEC, but this will not turn out to be for the BCS model interaction to be employed here. If the number operator is

$$
\hat{N} \equiv \sum_{\mathbf{k}_1,s_1} a^+_{\mathbf{k}_1,s_1}a_{\mathbf{k}_1,s_1} + 2\sum_{\mathbf{K}} b^+_{\mathbf{K}}b_{\mathbf{K}} - 2\sum_{\mathbf{K}} c^+_{\mathbf{K}}c_{\mathbf{K}} \tag{4}
$$

the simplified $\hat{H} - \mu\hat{N}$ is now entirely *bilinear* in the a^+ and a operators, as it already was in the boson operators b and c. It can thus be diagonalized exactly via a Bogoliubov–Valatinv transformation [23, 24]

$$
a_{\mathbf{k},s} \equiv u_k\alpha_{\mathbf{k},s} + 2s v_k\alpha^\dagger_{-\mathbf{k},-s} \tag{5}
$$

to new operators $\alpha^\dagger$ and α and where $s = \pm\frac{1}{2}$. The transformation (5) *exactly* diagonalizes (1) plus (3) to the fully bilinear form

$$
\begin{aligned}
\hat{H} - \mu\hat{N} \\
\simeq {} & \sum_{\mathbf{k},s} \underbrace{\left[\xi_k\left(u_k^2 - v_k^2\right) + 2\Delta_k u_k v_k\right]}_{\equiv E_k}\alpha^\dagger_{\mathbf{k},s}\alpha_{\mathbf{k},\mathbf{s}} \\
& + \sum_{\mathbf{k},s} 2s\left[\overbrace{\xi_k u_k v_k - \frac{1}{2}\Delta_k\left(u_k^2 - v_k^2\right)}^{\equiv 0}\right]
\end{aligned}
$$

$$\times\left(\alpha^{\dagger}_{\mathbf{k},s}\alpha^{\dagger}_{-\mathbf{k},-\mathbf{s}}+\alpha_{\mathbf{k},s}\alpha_{-\mathbf{k},-\mathbf{s}}\right)$$
$$+\sum_{\mathbf{k},s}2\left[\xi_k v_k^2+\Delta_k u_k v_k\right]+\left[E_+(0)-2\mu\right]N_0$$
$$+\sum_{\mathbf{K}\neq 0}\left[E_+(K)-2\mu\right]b^{\dagger}_{\mathbf{K}}b_{\mathbf{K}}+\left[2\mu-E_-(0)\right]M_0$$
$$+\sum_{\mathbf{K}\neq 0}\left[2\mu-E_-(K)\right]c^{\dagger}_{\mathbf{K}}c_{\mathbf{K}} \qquad (6)$$

with $\xi_k\equiv\epsilon_k-\mu$. The term set equal to zero in (6) is justified as this merely fixes the coefficient, say v_k, that was restricted only by $u_k^2+v_k^2=1$ which in turn follows from the requirement that both the *a and* α operators obey Fermi anticommutation relations. There are no products such as $\alpha^{\dagger}_{\mathbf{k},s}\alpha^{\dagger}_{-\mathbf{k},-\mathbf{s}}$ remaining, nor any other nonbilinear terms, as with [25] the BCS two-vertex, *four*-fermion Hamiltonian [5] that neglects other than $K=0$ pairings

$$H=\sum_{\mathbf{k},s}\epsilon_k a^{+}_{\mathbf{k},s}a_{\mathbf{k},s}-V\sum_{\mathbf{k},\mathbf{k}',s}a^{+}_{\mathbf{k}',s}a^{+}_{-\mathbf{k}',-s}a_{-\mathbf{k},-s}a_{\mathbf{k},s}, \qquad (7)$$

where $-V\leq 0$ and the second summation is restricted by $E_F-\hbar\omega_D\leq\hbar^2k^2/2m\equiv\epsilon_k,\epsilon_{k'}\leq E_F-\hbar\omega_D$.

Thus, the GBEC formalism is *not* restricted to weak coupling. Eigenstates of the now fully diagonalized simplified $\hat{H}-\mu\hat{N}$ given by (6) are

$$|\ldots n_{\mathbf{k},s}\ldots N_{\mathbf{K}}\ldots M_{\mathbf{K}}\ldots\rangle$$
$$=\prod_{\mathbf{k},s}\left(\alpha^{\dagger}_{\mathbf{k},s}\right)^{n_{\mathbf{k},s}}\prod_{\mathbf{K}\neq 0}\frac{1}{\sqrt{N_K!}}\left(b^{\dagger}_{\mathbf{K}}\right)^{N_{\mathbf{K}}}\prod_{\mathbf{K}\neq 0}\frac{1}{\sqrt{M_K!}}\left(c^{\dagger}_{\mathbf{K}}\right)^{M_{\mathbf{K}}}|\mathbf{O}\rangle$$

where the three exponents $n_{\mathbf{k},s}$, $N_{\mathbf{K}}$ and $M_{\mathbf{K}}$ are occupation numbers. Here $|\mathbf{O}\rangle$ is the vacuum state for the "bogolon" fermion quasiparticles created by $\alpha^{\dagger}_{\mathbf{k},s}$ with the gapped dispersion energy rewritten below in (10). It is simultaneously a vacuum state for 2e-CP and 2h-CP boson, creation and annihilation operators—which is to say that $|\mathbf{O}\rangle$ is defined by $\alpha_{\mathbf{k},s}|\mathbf{O}\rangle\equiv b_{\mathbf{K}}|\mathbf{O}\rangle\equiv c_{\mathbf{K}}\mid\mathbf{O}\rangle\equiv 0$.

4 Thermodynamic Potential

With the Hamiltonian explicitly diagonalized, one can now straightlyforwardly construct the thermodynamic potential $\Omega\equiv -PL^d$ for the GBEC, with L^d the system "volume" and P its pressure, which is defined as [22, p. 228]

$$\Omega\left(T,L^d,\mu,N_0,M_0\right)=-k_BT\ln\left[\operatorname{Tr}\exp\left\{-\beta(H-\mu\hat{N})\right\}\right], \qquad (8)$$

where "Tr" stands for "trace." Inserting (1) plus (2) into (8) [18] one obtains after some algebra an explicit expression for $\Omega(T,L^d,\mu,N_0,M_0)/L^d$ (see [26, (10)]). In $d=3$ one usually has

$$N(\epsilon)\equiv\frac{m^{3/2}}{2^{1/2}\pi^2\hbar^3}\sqrt{\epsilon}\quad\text{and}\quad M(\varepsilon)\equiv\frac{2m^{3/2}}{\pi^2\hbar^3}\sqrt{\varepsilon} \qquad (9)$$

for the (one-spin) fermion DOS at energies $\epsilon=\hbar^2k^2/2m$ and the boson DOS for an *assumed quadratic* [1] boson dispersion $\varepsilon=\hbar^2K^2/2(2m)$, respectively. The latter is an assumption to be lifted later so as to include Fermi-sea effects which change the boson dispersion relation from quadratic to *linear* as mentioned before. Finally, the relation between the resulting fermion spectrum $E(\epsilon)$ and fermion energy gap $\Delta(\epsilon)$ is of the form

$$E(\epsilon)=\sqrt{(\epsilon-\mu)^2+\Delta^2(\epsilon)}, \qquad (10)$$
$$\Delta(\epsilon)\equiv\sqrt{n_0}f_+(\epsilon)+\sqrt{m_0}f_-(\epsilon). \qquad (11)$$

This last expression for the gap $\Delta(\epsilon)$ implies a simple T-dependence rooted in the 2e-CP $n_0(T)\equiv N_0(T)/L^d$ and 2h-CP $m_0(T)\equiv M_0(T)/L^d$ number densities of BE-condensed bosons, i.e.,

$$\Delta(T)=\sqrt{n_0(T)}f_+(\epsilon)+\sqrt{m_0(T)}f_-(\epsilon).$$

If hole pairs are ignored the resulting relation $\Delta(T)=f\sqrt{n_0(T)}$ has recently been generalized [27] to include nonzero-$\mathbf{K}$ pairs beyond the expression (3). This leads to a generalized gap $E_g(\lambda,T)$ defined as

$$E_g(\lambda,T)=\sqrt{2\hbar\omega_D V n_B(\lambda,T)}\equiv f\sqrt{n_B(\lambda,T)}, \qquad (12)$$

where $n_B(\lambda,T)$ is the *net* number density of CPs, both in and above the condensate, in the BF mixture which in [27] for simplicity was taken as a binary one. The generalized gap $E_g(\lambda,T)$ accommodates pseudogap phenomena [28].

5 Helmholtz Free Energy

The Helmholtz free energy is by definition

$$F\left(T,L^d,\mu,N_0,M_0\right)\equiv\Omega\left(T,L^d,\mu,N_0,M_0\right)+\mu N. \qquad (13)$$

Minimizing it with respect to N_0 and M_0, and simultaneously fixing the total number N of electrons by introducing the electron chemical potential μ in the usual way, specifies an *equilibrium state* of the system at fixed volume L^d and temperature T. The necessary conditions for an equilibrium state are thus

$$\partial F/\partial N_0=0,\qquad \partial F/\partial M_0=0,$$
$$\text{and}\quad \partial\Omega/\partial\mu=-N \qquad (14)$$

where N evidently includes both paired and unpaired CP fermions.

6 Three GBEC Equations

Some algebra then leads to the three coupled transcendental (7)–(8) of [18]. These can be rewritten somewhat more transparently as: (a) two "*gap-like equations*"

$$\big[2E_f + \delta\varepsilon - 2\mu(T)\big] = \frac{1}{2}f^2 \int_{E_f}^{E_f+\delta\varepsilon} d\epsilon\, N(\epsilon) \frac{\tanh \frac{1}{2}\beta\sqrt{[\epsilon-\mu(T)]^2 + f^2 n_0(T)}}{\sqrt{[\epsilon-\mu(T)]^2 + f^2 n_0(T)}} \tag{15}$$

and

$$\big[2\mu(T) - 2E_f + \delta\varepsilon\big] = \frac{1}{2}f^2 \int_{E_f-\delta\varepsilon}^{E_f} d\epsilon\, N(\epsilon) \frac{\tanh \frac{1}{2}\beta\sqrt{[\epsilon-\mu(T)]^2 + f^2 m_0(T)}}{\sqrt{[\epsilon-\mu(T)]^2 + f^2 m_0(T)}} \tag{16}$$

as well as (b) a single "*number equation*"

$$2n_B(T) - 2m_B(T) + n_f(T) = n. \tag{17}$$

This last relation ensures charge conservation in the ternary mixture. In general $n \equiv N/L^d$ is the total number density of electrons, $n_f(T)$ that of the *unpaired* electrons, while $n_B(T)$ and $m_B(T)$ are respectively those of 2e- and 2h-CPs in *all* bosonic states, ground plus excited. The latter turn out to be

$$n_B(T) \equiv n_0(T) + \int_{0+}^{\infty} d\varepsilon\, M(\varepsilon) \times \big(\exp\beta[2E_f + \delta\varepsilon - 2\mu + \varepsilon] - 1\big)^{-1} \tag{18}$$

$$m_B(T) \equiv m_0(T) + \int_{0+}^{\infty} d\varepsilon\, M(\varepsilon) \times \big(\exp\beta[2\mu + \varepsilon - 2E_f + \delta\varepsilon] - 1\big)^{-1} \tag{19}$$

which are clear manifestations of the bosonic nature of both kinds of CPs. One also obtains for the number density of unpaired electrons at any T

$$n_f(T) \equiv \int_0^{\infty} d\epsilon\, N(\epsilon)\left[1 - \frac{\epsilon-\mu}{E(\epsilon)} \tanh \frac{1}{2}\beta E(\epsilon)\right] = 2\sum_{\mathbf{k}} v_k^2(T), \tag{20}$$

where $v_k^2(T) \equiv \frac{1}{2}[1 - (\epsilon_k - \mu)/E_k] \underset{T\to 0}{\longrightarrow} v_k^2$ with E_k being given by (10) is precisely the BCS–Bogoliubov T-dependent coefficient that is linked with $u_k(0) \equiv u_k$ through $v_k^2 + u_k^2 = 1$ of the BCS trial wavefunction

$$|\mathbf{O}\rangle \equiv \prod_{\mathbf{k}} \big(u_{\mathbf{k}} + v_{\mathbf{k}} a^+_{\mathbf{k}\uparrow} a^+_{-\mathbf{k}\downarrow}\big)|O\rangle, \tag{21}$$

where $|O\rangle$ is the ordinary vacuum. The zero-T version of the two amplitude coefficients v_k and u_k originally appeared in (21) and shortly afterwards in the Bogoliubov–Valatinv canonical transformation. Next, one picks $\delta\varepsilon = \hbar\omega_D$ as well as identifies nonzero $f_+(\epsilon)$ and nonzero $f_-(\epsilon)$ with $f \equiv \sqrt{2\hbar\omega_D V}$ but such that $f_+(\epsilon) f_-(\epsilon) = 0$. Assuming $n_0(T) = m_0(T)$ and adding together (15) and (16) gives the precise BCS gap *provided* one can identify E_f with μ. This in turn is guaranteed if $n_B(T) = m_B(T)$, namely, if (18) and (19) are set equal to each other so that the arguments of the two exponentials become identical.

Self-consistent (at worst, numerical) solution of the *three coupled equations* (15) to (17) yields the three thermodynamic variables of the GBEC formalism

$$n_0(T, n, \mu), \qquad m_0(T, n, \mu) \quad \text{and} \quad \mu(T, n). \tag{22}$$

Proving *a posteriori* the existence of a *nonzero* T_c associated with these expressions vindicates the GBEC theory.

All told, the three GBEC equations (15) to (17) subsume *five* different theories as special cases, see flowchart in Fig. 1. The vastly more general GBEC theory has been applied and gives sizeable enhancements in T_c's over BCS theory that emerge [29] by admitting, apparently for the first time, departures from the very special case of perfect 2e/2h-pair symmetry in the mixed phase.

7 Conclusions

In conclusion, five statistical continuum theories of superconductivity, including both the BCS and BEC theories, are contained as special limiting cases within a single generalized Bose–Einstein condensation (GBEC) model. This model includes, for the first time, along with unpaired electrons, both two-electron and two-hole pair-condensates in freely variable proportions. The BCS and BEC theories are thus completely *unified* within the GBEC. The BCS condensate emerges directly from the GBEC *as a BE condensate* through the condition for phase equilibria when both total 2e- and 2h-pair number, as well as their condensate, densities are *equal* at a given T and coupling—provided the coupling is weak enough so that the electron chemical potential μ roughly equals the Fermi energy E_F. The ordinary BEC T_c-formula, on the other hand, is recovered from the GBEC when hole pairs are completely neglected,

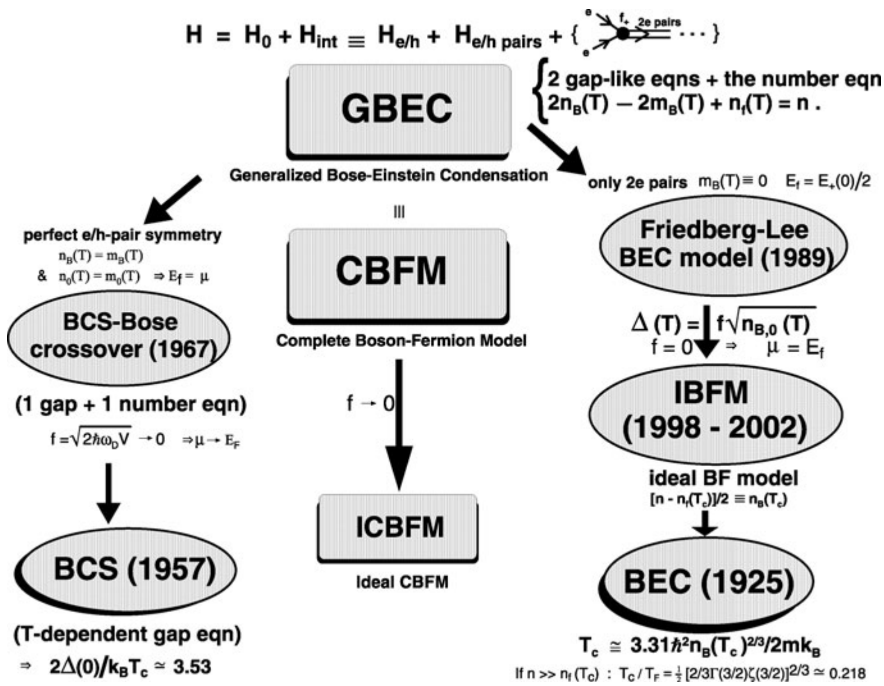

Fig. 1 Flowchart outlining conditions under which the GBEC formalism reduces to all five statistical theories of superconductivity (*ovals*). The GBEC formalism has alternately been called the "complete boson-fermion model" (CBFM) in that hole pairs are not ignored

the BF coupling f is made to vanish, and the limit of zero unpaired electrons is taken, this implying very strong inter-electron coupling. The practical outcome of the BCS-BEC unification via the GBEC is *enhancement* in T_c, by more than two orders-of-magnitude in 3D. These enhancements in T_c fall within empirical ranges for 2D and 3D "exotic" SCs, whereas BCS T_c values remain low and within the empirical ranges for conventional, elemental SCs using standard interaction-parameter values. Lastly, room temperature superconductivity is possible for a material with a Fermi temperature $T_F \lesssim 10^3$ K, with the *same* interaction parameters used in BCS theory for conventional SCs.

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