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Generalized BEC and crossover theories of superconductors and ultracold Fermi gases

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ABSTRACT

The generalized Bose–Einstein condensation (GBEC) formalism of superconductivity hinges on *three* separate new ingredients: (a) treatment of Cooper pairs as real bosons, (b) inclusion of two-hole pairs on an equal footing with two-electron ones, and (c) inclusion in the resulting ternary ideal boson–fermion gas of boson–fermion vertex interactions that drive formation/disin-tegration processes. Besides subsuming both BCS and BEC theories as well as the well-known crossover picture as special cases, GBEC leads to several-order-of-magnitude enhancement in the critical superconducting temperature T_c.

The crossover picture is applicable also to ultracold atomic clouds, both bosonic and fermionic. But low-density expansions involving the interatomic scattering length a diverge term-by-term around the so-called unitary zone about the Feshbach resonance. However, expanding a in powers of the attractive part of the interatomic potential renders smooth, divergence-free low-density expansions.
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1. Introduction

Since its theoretical prediction by Einstein in 1925 based on the work in 1924 by Bose on photons, and after many decades languishing as a mere academic exercise in textbooks, Bose–Einstein condensation (BEC) was finally observed in laser-cooled, magnetically-trapped ultra-cold bosonic atomic clouds of $^{87}_{37}$Rb [1]. Within weeks other observations were reported, with $^{7}_{3}$Li [2], $^{23}_{11}$Na [3], $^{1}_{1}$H [4], $^{85}_{33}$Rb [5], $^{4}_{2}$He [6], $^{41}_{19}$K [7], $^{133}_{55}$Li [8], $^{52}_{24}$Cr [9], and in two-electron systems such as alkaline-earth and ytterbium atoms $^{174}_{70}$Yb [10–12]. Also, BEC was most recently found in $^{84}_{38}$Sr [13].

BEC has been detected as well in *fermionic* atomic gases of $^{40}_{19}$K [14] and $^{6}_{3}$Li [15] as a result, presumably, of some of the fermions Cooper-pairing [16] into bosons.

Sometime ago Leggett [17] derived the *two* basic equations associated with the so-called BCS–BEC crossover [18–20] picture at $T = 0$ for any many-fermion system of particles of mass m whose pair interactions are described by the S-wave scattering length a between pairs of fermionic atoms a. Specifically, he obtained a *number equation*

$$\frac{4}{3} = \int_0^\infty d\tilde{\epsilon}\sqrt{\tilde{\epsilon}}\left[1 - \frac{\tilde{\epsilon}-\tilde{\mu}}{\sqrt{(\tilde{\epsilon}-\tilde{\mu})^2 + \tilde{\Delta}^2)}}\right] \tag{1}$$

where the tildes signify in units of $E_F \equiv \hbar^2 k_F^2/2m$, with μ and Δ being the zero-T fermionic chemical potential and gap, as well as a *gap equation*

$$\frac{\pi}{k_F a} = \int_0^\infty d\tilde{\epsilon}\left[\frac{1}{\sqrt{\tilde{\epsilon}}} - \frac{\sqrt{\tilde{\epsilon}}}{\sqrt{(\tilde{\epsilon}-\tilde{\mu})^2 + \tilde{\Delta}^2)}}\right]. \tag{2}$$

An alternate derivation of these two equations has been reported in Ref. [21].

Both equations are coupled transcendental equations which must be solved self-consistently for μ and Δ, with Δ depending (explicitly) on a and μ on Δ and so that μ depends implicitly on a. These two equations are valid for any coupling, weak or strong. For weak coupling $\mu \simeq E_F$ as assumed by BCS in their epoch-making 1957 paper [22] on superconductivity described by a *single* equation, the celebrated gap equation. However, for very strong coupling $\mu \simeq B_2/2$ with B_2 being the two-body (positive) binding energy of a pair *in vacuo* provided the two-body potential supports one and only one bound state as, e.g., the BCS model interaction can be shown [23] to effectively do so.

In 2D Miyake [24] solved the two crossover equations *exactly* at $T = 0$ for an attractive delta interaction potential between pairs of fermions. He obtains $\Delta = \sqrt{2E_F B_2}$ and $\mu = E_F - \frac{1}{2}B_2$ which evidently reduces in weak coupling to E_F and in strong to $-B_2/2$. Indeed, a 2D [25] as well as a 3D delta-potential well supports an infinite number of bound-state levels; this alone would suffice to collapse the many-fermion ground state to infinite binding and density. Although not mentioned explicitly, this author must have implied

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use of a *regularized* delta, namely, one constructed [26] so as to possess one and only one bound state. Besides avoiding possible collapse, a 3D regularized delta potential allows conveniently describing [27] the entire range from weak- to strong-coupling smoothly in terms of the dimensionless coupling parameter $1/k_Fa$ from $-\infty$ ($a = 0^-$) through 0 to $+\infty$ ($a = 0^+$) and with only *one* zero.

For many-fermion superconducting states the role of *hole* Cooper pairs, accounted for or not along with the usual electron Cooper pairs, has been explored [28–33] within a generalized BEC (GBEC) scenario with striking implications. In particular, it was shown [32] to subsume the BCS–BEC crossover equations for $\mu(T)$ and $\Delta(T)$ at *finite* temperatures $T \geqslant 0$. The GBEC formalism has thus far only employed the BCS model interaction between individual charges. This interaction is familiar; it is characterized by two parameters: the maximum energy $\hbar\omega_D$ of a phonon exchanged between the charges and the net attractive interaction strength V due to repulsive Coulomb and attractive electron–phonon interactions. The latter is usually expressed in the well-known BCS dimensionless coupling parameter $\lambda \equiv VN(E_F)$ where $N(E_F)$ is the density of electron states at the Fermi surface.

A different two-body interaction applies, of course, in ultracold fermionic gases such as the aforementioned $^{40}_{19}$K and $^{6}_{3}$Li, e.g., a Lennard–Jones interatomic potential for which the S-wave scattering length a applies. Expansions of a in powers of the strength of the attractive part of a number of such potentials have been determined numerically [34]. We argue how this is an ideal way of treating the unitarity region around a Feshbach resonance where a diverges. This divergence is entirely averted in low-density expressions that depend not on a but rather on the attractive part of the interatomic interaction. This is equivalent to expanding not about the ideal (boson or fermion) gas but about the corresponding purely repulsive gas in order to generate the well-known low-density expansions but now as a power series in the attractive part of the interatomic potential.

2. Generalized BEC and superconductors

Boson–fermion (BF) models of superconductivity (SC) as a Bose–Einstein condensation (BEC) go back to the mid-1950s [35–38], pre-dating even the BCS-Bogoliubov theory [39,40]. Although BCS theory only envisions the presence of "Cooper correlations" of single-electron states, BF models [35–38,41–50] posit the existence of actual bosonic Cooper pairs (CPs). With a single exception [28], however, all BF models neglect the effect of *hole* CPs included on an equal footing with electron CPs to give the "complete" BF model at the heart of the generalized Bose–Einstein condensation (GBEC) formalism. This formalism is described by the Hamiltonian $H = H_0 + H_{int}$.

First, one has an *ideal* ternary gas mixture described by

$$H_0 = \sum_{\mathbf{k}_1,s_1} \epsilon_{k_1} a^+_{\mathbf{k}_1,s_1} a_{\mathbf{k}_1,s_1} + \sum_{\mathbf{K}} E_+(K) b^+_{\mathbf{K}} b_{\mathbf{K}} - \sum_{\mathbf{K}} E_-(K) c^+_{\mathbf{K}} c_{\mathbf{K}} \tag{3}$$

where $\mathbf{K} \equiv \mathbf{k}_1 + \mathbf{k}_2$ is the CP total or center-of-mass-momentum (CMM) wavevector of two-electron- and two-hole-CPs, while $\epsilon_{k_1} \equiv \hbar^2 k_1^2/2m$ 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 electrons and similarly $b^+_{\mathbf{K}}$ ($b_{\mathbf{K}}$) and $c^+_{\mathbf{K}}$ ($c_{\mathbf{K}}$) for 2e- and 2h-CP bosons, respectively. As originally implied in the work of Cooper [16], the b and c CP operators depend only on $\mathbf{K}$ as the CP eigenvalue appears in a summation over the relative wavevector $\mathbf{k} \equiv \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$. Hence, CPs are *distinct* from BCS pairs described by operators depending on both $\mathbf{K}$ *and* $\mathbf{k}$ as displayed in Ref. [22], Eqs. (2.9–2.13), for the particular case of $\mathbf{K} = 0$ and shown there *not* to satisfy the ordinary Bose commutation relations. However, CPs are objects easily 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 defining energy eigenvalues $E_+(K)$ or $E_-(K)$. This is sufficient to ensure a BEC (or, a macroscopic occupation of a given state that appears below a certain fixed $T = T_c$). This was found [28] numerically *a posteriori* in the GBEC theory. Also, the BCS gap equation is recovered exactly 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 [29] of CP overlaps. The precise familiar BEC T_c formula emerges [28] when: (i) 2h-CPs are ignored (whereupon the Friedberg–T.D. Lee model [46–49] equations are recovered) and (ii) one switches off the BF interaction but under strong interelectron coupling whereby no unpaired electrons survive in the remaining binary mixture which now becomes a pure ideal boson gas.

Secondly, one switches on a boson–fermion (BF) interaction among the three species of the originally ideal ternary gas represented by (3). This interaction is given by the Hamiltonian H_{int} consisting 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 with CPs replacing phonons. Here H_{int} depicts how unpaired electrons (or holes) combine to form the 2e- (and 2h-CPs), and viceversa, assumed in a d-dimensional system of size L, namely

$$H_{int} = L^{-d/2} \sum_{\mathbf{k},\mathbf{K}} f_+(k) \left[a^+_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow} a^+_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow} b_{\mathbf{K}} + a_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow} a_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow} b^+_{\mathbf{K}} \right] \tag{4}$$

$$+ L^{-d/2} \sum_{\mathbf{k},\mathbf{K}} f_-(k) \left[a^+_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow} a^+_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow} c^+_{\mathbf{K}} + a_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow} a_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow} c_{\mathbf{K}} \right]. \tag{5}$$

Defining a simpler H_{int} by neglecting nonzero K terms on the rhs renders an exactly diagonalizable expression via a Bogoliubov transformation. (These terms were later restored via two-time Green functions, albeit without 2hCPs, and eventually lead [51,52] to a pseudogap.) The energy form factors $f_\pm(k)$ in (5) are taken as in Refs. [28,30] 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 introduced in Refs. [28,30]) that replace the previous such $E_\pm(0)$, through the relations $E_f \equiv \frac{1}{4}[E_+(0) + E_-(0)]$ and $\delta\varepsilon \equiv \frac{1}{2}[E_+(0) - E_-(0)] \geqslant 0$ where $E_\pm(0)$ are the (empirically *un*known) zero-CMM energies of the 2e- and 2h-CPs, respectively. Putting $E_f = E_F$ and $\delta\varepsilon = \hbar\omega_D$ leads [28–33] *exactly* to the BCS gap equation.

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 $E_F = \frac{1}{2} m v_F^2 \equiv k_B T_F$ where T_F is the Fermi temperature. If n is the total number-density of charge-carrier electrons of effective mass m, 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, while E_f is similarly related to another density n_f which serves to scale the ordinary electron-number density $n \equiv N/L^d$. 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.

The GBEC formalism leads to three coupled transcendental equations for the three functions determining the phase diagram of thermodynamic equilibrium associated with three condensed phases, in addition to the normal phase of the ideal ternary gas described by (3). The condensed phases are two pure BEC phases, one for 2e-CPs the other for 2h-CPs, and a mixed phase. The three functions for which one solves numerically based on the three coupled transcendental equations are the electron chemical potential $\mu(T)$ along with the 2e-CP and 2h-CP BE condensate densities $n_0(T)$ and $m_0(T)$, respectively. Of those three coupled transcendental equations two are "gap-like" equations and the third is a "number equation" which guarantees charge conservation and therefore gauge invariance (in contrast with BCS theory), namely

$$n = 2n_B(T) - 2m_B(T) + n_f(T) \quad (6)$$

where $n_f(T)$ corresponds to the *unpaired* electrons, while $n_B(T)$ and $m_B(T)$ are respectively the number densities of 2e- and 2h-CPs in *all*-bosonic states, ground plus excited, i.e., condensed and noncondensed. The latter turn out to be

$$n_B(T) \equiv n_0(T) + \int_{0+}^{\infty} d\varepsilon M(\varepsilon)(\exp\beta[2E_f + \delta\varepsilon - 2\mu + \varepsilon] - 1)^{-1} \quad (7)$$

$$m_B(T) \equiv m_0(T) + \int_{0+}^{\infty} d\varepsilon M(\varepsilon)(\exp\beta[2\mu + \varepsilon - 2E_f + \delta\varepsilon] - 1)^{-1} \quad (8)$$

where the Bose distributions 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

$$n_f(T) \equiv \int_0^{\infty} d\epsilon N(\epsilon)\left[1 - \frac{\epsilon - \mu}{E(\epsilon)}\tanh\frac{1}{2}\beta E(\epsilon)\right]. \quad (9)$$

In (40–42) $N(\epsilon)$ and $M(\epsilon)$ are respectively the electronic and bosonic density of states, while

$$E(\epsilon) = \sqrt{(\epsilon - \mu) + \Delta^2(\epsilon)} \quad (10)$$

is the familiar gapped Bogoliubov fermionic dispersion relation. Perfect 2e/2h symmetry in (6) of the GBEC formalism means $2n_B(T) = 2m_B(T)$ which in turn implies

$$n = n_f(T). \quad (11)$$

At zero-temperature the number Eq. (9) simplifies to

$$n_f(T) = \int_0^{\infty} d\epsilon N(\epsilon)\left[1 - \frac{\epsilon - \mu}{E(\epsilon)}\right] \quad (12)$$

which is easily seen to reduce to (1).

Fig. 1 shows the phase boundaries for the specific set of BCS model-interaction parameter $\lambda = 1/2$ and $\hbar\omega_D = 10^{-3}E_F$. As one lowers temperature, the first thermodynamically-stable GBEC phase encountered is the one consisting of two-hole rather than two-electron CPs. This is quite probably related to the apparently universal property of superconductors as emphasized most brilliantly by Hirsch (Ref. [54] S6) and corroborated with experiments, namely, that regardless of the sign of individual charge carriers in the normal state (i.e., above T_c), below T_c they are always two-electron CPs. In addition, he interprets these empirical findings in terms of the "hole theory of superconductivity [55,56]" he has been espousing over the years.

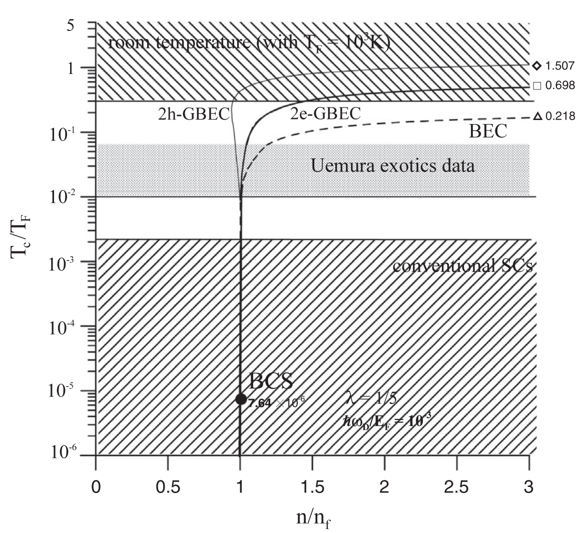

Fig. 1. Phase boundaries of pure GBEC of 2h-CPs (thin curve) and of 2e-CPs (thick full curve) compared to the standard BEC curve (dashed) and the BCS, for a BCS model interaction creating the CPs, all for BCS model interaction dimensionless parameters $\lambda = 1/5$ and $\hbar\omega_D/E_F = 10^{-3}$ vs. dimensionless charge-carrier densities n/n_f with n_f as defined in text and roughly corresponds to the number density of unpaired fermions. Exotics data are from Ref. [53]. Here and in text $\hbar\omega_D$ is the Debye energy associated with the ionic lattice while E_F is the Fermi energy of the electron gas. Values indicated by the diamond, square and triangle symbols, correspond to the limit values of T_c obtained for $n/n_f \longrightarrow \infty$ at which limit there are no unpaired fermions left.

Finally, we note that the 2eCP GBEC phase boundary more than triply enhances T_c with respect to an ordinary pure 2eCP BEC in which all the electrons are assumed paired in bosons and giving the familiar $T_c/T_F \equiv \frac{1}{2}[2/3\Gamma(3/2)\zeta(3/2)]^{2/3} \simeq 0.218$ where Γ and ζ are gamma and zeta functions.

3. Ultracold atomic clouds

3.1. Bosons

The ground-state equation-of-state for a many-boson gas of identical bosons of mass m, number density $n = N/V$, and with pair interactions giving rise to an S-wave scattering length a, the ground-state energy per particle is known to be given by the low-density expansion [57–59]

$$\frac{E}{N}\underset{na^3 \ll 1}{=} \frac{2\pi\hbar^2}{m} na[1 + C_1(na^3)^{1/2} + C_2(na^3)\ln(na^3) + C_3(na^3) + O(na^3)^{3/2}\ln(na^3)] \quad (13)$$

$$C_1 \equiv \frac{128}{15\sqrt{\pi}} \qquad C_2 \equiv 8\left(\frac{4}{3}\pi - \sqrt{3}\right) \qquad C_3 = unknown.$$

Each term contains the dimensionless smallness parameter na^3 but it *diverges* in the unitarity region, i.e., around the Feshbach resonance. Obviously, the entire low-density series will then diverge in this region as well.

For the simple two-body hard-core-square-well (HCSW) potential

$$v(r) = \begin{cases} +\infty & (r < c) \\ -v_0 & (c < r < R) \\ 0 & (r < R) \end{cases} \quad (14)$$

where r is the interparticle separation, the scattering length is exactly analytical

$$\frac{a}{c} = 1 + \alpha\left(1 - \frac{\tan\sqrt{\lambda}}{\sqrt{\lambda}}\right) \quad (15)$$

$$\alpha \equiv \frac{R - c}{c} \qquad \lambda \equiv \frac{mv_0}{\hbar^2}(R - c)^2. \quad (16)$$

Calling the smallness parameter $(nc^3)^{1/2} \equiv x$ some computer algebra gives for the energy per boson the double series

$$\frac{E}{N} \equiv \epsilon(x, \lambda) = \sum_{i=0} \epsilon_i(x)\lambda^i \quad (17)$$

where the coefficients $\epsilon_i(x)$ would be known for $x \ll 1$. Since from (16) λ is proportional to the attractive part of the two-boson interaction *in vacuo* then $\epsilon(x, \lambda = 0)$ is of precisely the same form as (13) with a replaced by c. This energy represents the energy-per-boson not of an ideal boson gas (which of course vanishes) but of a boson gas of hard spheres of diameter c, with attraction treatable perturbatively to any order. The double series is divergence-free even in the unitarity region.

3.2. Fermions

For fermions, the expansion for the ground-state energy per particle is given exactly through the low-density expansion [58]

$$\frac{E}{N}\equiv\frac{3}{5}\frac{\hbar^2k_F^2}{2m}\left[1+C_1k_Fa+C_2(k_Fa)^2+\left\{\frac{1}{2}C_3\frac{r_0}{a}+C_4\frac{A_1(0)}{a^3}+C_5\right\}(k_Fa)^3 +C_6(k_Fa)^4\ln|k_Fa|+\left\{\frac{1}{2}C_7\frac{r_0}{a}+C_8\frac{A_0''(0)}{a^3}+C_9\right\}(k_Fa)^4+O\{(k_Fa)^4\}\right] \quad (18)$$

where k_F is the Fermi wavenumber while r_0 is the effective range of the two-fermion interaction having scattering length a and the coefficients $C_1, \dots, C_9$ are known [58]. It too diverges in the unitarity region since each term in the dimensionless smallness-parameter k_Fa. diverges there. Here, the fermion number density is

$$n = N/V = \nu k_F^3/6\pi^2 \quad (19)$$

with $\nu$the number of intrinsic degrees of freedom [60] if any, such as spin and isospin.

For the HCSW potential (14) the exact result (15) expands in powers of λ, e.g., with a computer-algebra program such as MACSYMA or REDUCE [61], as

$$k_Fa = x\left[1-\alpha\left(\frac{1}{3}\lambda+\frac{2}{15}\lambda^2+\frac{17}{315}\lambda^3+\frac{62}{2835}\lambda^4+\frac{1382}{155925}\lambda^5+\frac{21844}{6081075}\lambda^6+\cdots\right)\right]. \quad (20)$$

For other interfermion potentials such as the Lennard–Jones interatomic potential $V(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]$ with $\epsilon$and σ convenient energy and length parameters one can separate it as a repulsive-core plus attractive part and redefine the latter as the parameter λ. Coefficients such as those in (20) have been determined numerically [34] for a variety of two-body interatomic potentials in current used.

4. Conclusions

A ternary boson–fermion superconducting gas model leads to a generalized Bose–Einstein condensation formalism which, assuming quadratically-dispersive two-electron- or two-hole Cooper pairs already leads to a phase diagram with three condensed phases (two pure 2e-CP and 2h-CP BECs plus a mixed phase) at temperatures cooler than the ubiquitous normal phase of an ideal ternary gas of both types of CPs plus unpaired electrons. Enhanced T_cs of several orders of magnitude emerge in comparison with the BCS result which is the highest T_c associated with the mixed phase.

For ultracold quantum gases low-density expansions of point particles, whether boson or fermion, involving the S-wave scattering length a associated with the free-pair interaction diverge term-by-term around the Feshbach resonance whenever the strength of the interaction attraction is large enough to bind the pair. This divergence can be averted altogether by redefining the expansion to be associated instead with purely-repulsive *extended* particles, e.g., the hard cores of a hard-core-square-well potential, or the soft cores associated with interatomic potentials such as the Lennard–Jones potential.

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