J Supercond Nov Magn (2016) 29:691–695
DOI 10.1007/s10948-015-3288-y

ORIGINAL PAPER

Generalized BEC and Crossover Theories of Superconductors and Ultracold Bosonic and Fermionic Gases

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Received: 10 October 2015 / Accepted: 19 November 2015 / Published online: 14 December 2015

Abstract The generalized Bose-Einstein condensation (GBEC) theory of superconductivity hinges on *three* distinct 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) insertion in the resulting ternary ideal boson-fermion gas of boson-fermion vertex interactions that drive formation/disintegration processes. Besides subsuming both BCS and BEC theories as well as the well-known crossover picture as special cases, GBEC leads to several-orders-of-magnitude enhancements in the critical superconducting temperature T_c. The crossover picture is applicable also to ultracold atomic clouds, both bosonic and fermionic. But known low-density expansions involving the interatomic scattering length a diverge term-by-term around the so-called unitary zone about the Feshbach resonance where a itself diverges. However, expanding a in powers of the attractive part of the interatomic potential renders smooth, divergence-free low-density expansions whose convergence can be accelerated with Padé approximants.

Keywords Cooper pairing · Boson-fermion models · Bose-Einstein condensation · Superconductors · BEC in ultracold quantum gases

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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], $^{85}_{37}$Rb [5], $^{4}_{2}$He [6], $^{41}_{19}$K [7], $^{133}_{55}$Cs [8], $^{52}_{24}$Cr [9] nuclei, and in two-electron systems such as alkaline-earth and ytterbium atoms $^{174}_{70}$Yb [10–12] as well as with $^{84}_{38}$Sr [13]. It has also been detected 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-Bose 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. Specifically, he obtained two zero-temperature dimensionless

(i) *Number equation*
$4/3 = \int_0^\infty d\widetilde{\epsilon}\sqrt{\widetilde{\epsilon}}\left[1 - (\widetilde{\epsilon} - \widetilde{\mu})/\sqrt{(\widetilde{\epsilon} - \widetilde{\mu})^2 + \widetilde{\Delta}^2}\right]$
where the tildes signify in units of the Fermi energy $E_F \equiv \hbar^2 k_F^2/2m$ of the ideal Fermi gas, with μ and Δ being the zero-T fermionic chemical potential and energy gap, as well as

(ii) A *gap equation*
$\pi/k_F a = \int_0^\infty d\widetilde{\epsilon}\left[1/\sqrt{\widetilde{\epsilon}} - \sqrt{\widetilde{\epsilon}}/\sqrt{(\widetilde{\epsilon} - \widetilde{\mu})^2 + \widetilde{\Delta}^2}\right]$.

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

Expansions of a in powers of the strength of the attractive part of a number of two-fermion potentials have been determined numerically [22]. We argue how this is an ideal way of treating the unitarity region around a Feshbach resonance where a diverges. This divergence is then 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 associated purely repulsive gas in order to generate low-density expansions without a being explicit but now as a power series in the attractive part of the interatomic potential. The convergence of these power series can be accelerated via Padé approximants as surveyed, e.g., in ref. [23].

2 Generalized BEC Equations

Boson-fermion (BF) models of superconductivity (SC) as a Bose-Einstein condensation (BEC) go back to the mid-1950s [24–27], pre-dating even the BCS-Bogoliubov theory [28, 29]. Although BCS [30] theory only envisions the presence of "Cooper correlations" of single-electron states, BF models [24–27], [31–40] posit the existence of *actual* bosonic Cooper pairs (CPs). With a single exception [41], however, all BF models neglect the explicit 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) theory. The GBEC theory [41–43] 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 [41]. The condensed phases are two pure GBEC 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 above-mentioned three equations are the electron chemical potential $\mu(T)$ along with the 2e-CP and 2h-CP GBEC densities $n_0(T)$and $m_0(T)$, respectively. Among those three equations is a "number equation" which guarantees charge conservation and therefore gauge invariance [44] (in contrast with BCS [30] theory which does not) and two are "gap-like" equations [41]. Specifically,

$$2\sqrt{n_0}[E_+(0) - 2\mu] = \int_0^\infty d\epsilon N(\epsilon)\frac{\Delta(\epsilon) f_+(\epsilon)}{E(\epsilon)}\left[1 - \frac{2}{\exp[\beta E(\epsilon)] + 1}\right] \quad (1)$$

and

$$2\sqrt{m_0}[2\mu - E_-(0)] = \int_0^\infty d\epsilon N(\epsilon)\frac{\Delta(\epsilon) f_-(\epsilon)}{E(\epsilon)}\left[1 - \frac{2}{\exp[\beta E(\epsilon)] + 1}\right] \quad (2)$$

where $\mu(T)$ are the chemical potential of unpaired electrons, $E_\pm(0)$ are the energy of bosonic 2e-CP and 2h-CP, respectively, with center-of-mass momentum $K = 0$ and $\beta = 1/k_B T$ with k_B the Boltzmann constant. Here, $E(\epsilon) \equiv \sqrt{(\epsilon - \mu)^2 + \Delta^2(\epsilon)}$ is the familiar gapped Bogoliubov fermionic dispersion relation, and $\Delta(\epsilon) = f_+\sqrt{n_0(T)} + f_-\sqrt{m_0(T)}$ with $f_\pm(\varepsilon)$ the boson-fermion interaction strength as defined in ref. [41]. Note the explicit presence of a Fermi-Dirac distribution function.

The number density is

$$n = 2n_0(T) + 2n_{B+}(T) - 2m_0(T) - 2m_{B+}(T) + n_f(T) \quad (3)$$

where $n = N/V$, N the total number of particles, V the volume of the system, $n_f(T)$ corresponds to the *unpaired* electrons, while $n_0(T)$ and $m_0(T)$ are, respectively, the number densities of 2e- and 2h-CPs in bosonic condensates and $n_{B+}(T)$ and $m_{B+}(T)$ are, respectively, the number densities of 2e- and 2h-CPs in *excited* bosonic states, i.e., *noncondensed*. The latter turn out to be

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

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

where $M(\varepsilon)$ is bosonic density of states. And here, one notes explicit Bose-Einstein distribution functions, as expected. The number density $n_f(T)$ of *unpaired* electrons at any T turns out to be

$$n_f(T) = \int_{0^+}^{\infty} d\epsilon N(\epsilon)\left[1 - \frac{\epsilon - \mu}{E(\epsilon)}\left(1 - \frac{2}{\exp[\beta E(\epsilon)] + 1}\right)\right] \quad (4)$$

where $N(\epsilon)$ is the electronic density of states for one spin.

2.1 Crossover and GBEC Phases

GBEC theory is an *extended* crossover theory since it gives *two* gap-like equations and a single number equation, all to be solved self-consistently. It has three different stable BEC phases that emerge when solving all three (1) to (3) and is thus equivalent to a new, more general version of the crossover, which leads to (i) a pure 2e-GBEC phase, solving (1) and (3), (ii) a pure 2h-GBEC phase, solving (2) and (3), and (iii) a mixed phase with different proportions of 2e- and 2h-CPs solving (1), (2), and (3). This is then a generalized or extended crossover with a mixed phase of an ideal 50–50 proportion between 2e- and 2h-CPs, i.e., $n_0(T) = m_0(T)$ and $n_{B+}(T) = m_{B+}(T)$.

All possible GBEC phases are plotted in Fig. 1 at T_c normalized with the Fermi temperature T_F. Version (iii) of the crossover corresponds to the blue shaded area (mixed phase) along with the GBEC phase-boundary curves. Also plotted is the ordinary BEC curve (dashed black). The red dot is the

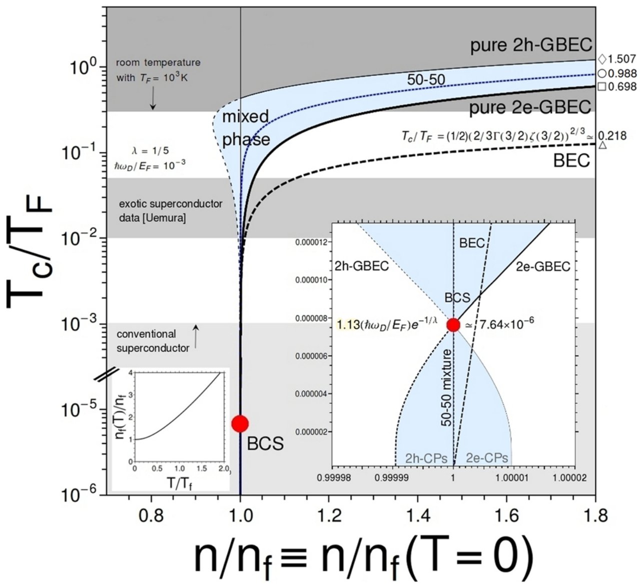

Fig. 1 Dimensionless T_c/T_F versus n/n_f for pure GBEC phases of 2h-/2e-CPs and the ordinary BEC in 3D (*thick dashed curve*). Note that extrapolating to $n_f \to 0$ gives the familiar limit 0.218, as expected. These results are displayed in a background with three horizontal bands corresponding to conventional and exotic [45] empirical values and expected room-temperature values. Larger 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 quoted in text using $\lambda = 1/5$ and $\hbar\omega_D = 10^{-3}E_F$ where $\hbar\omega_D$ is the Debye energy of the lattice. *Red dot* marks the critical BCS temperature. *Blue thin dashed curve* (online) marked 50–50 corresponds to perfect symmetry between 2e-/2h-CPs, i.e., $n_0(T) = m_0(T)$ and $n_{B+}(T) = m_{B+}(T)$. Symbols *diamondsuit*, *square*, *circle*, and *triangle* are the limits of the two pure-phase GBEC, 50–50 mixed phase and ordinary BEC curves, respectively, when $n/n_f \to \infty$, i.e., when $n_f(T_c) \to 0$ implying not unpaired electrons. Smaller inset shows number density of unpaired electrons $n_f(T)$ (4) and its $T = 0$ limit $n_f(T \to 0) \equiv n_f$

BCS critical temperature via the familiar weak-coupling formula $k_B T_c \simeq 1.134\hbar\omega_D \exp(-1/\lambda)$. All results correspond to the fixed BCS model-interaction parameter $\lambda = 1/2$ and for $\hbar\omega_D = 10^{-3}E_F$.

3 Ultracold Atomic Clouds

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, is known to be given by the *exact* low-density expansion [46, 47]

$$\frac{E}{N} \underset{na^3<<1}{=} \frac{2\pi\hbar^2}{m} na \Big[1 + C_1(na^3)^{1/2} + C_2(na^3)\ln(na^3) + C_3(na^3) + \mathcal{O}(na^3)^{3/2}\ln(na^3)\Big] \quad (5)$$

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

Each expansion term contains the dimensionless smallness parameter na^3 but *diverges* in the unitarity region, i.e., around the Feshbach resonance, due to the appearance of a bound state there making a itself diverge. Obviously, the entire low-density series will then diverge term by term in this region as well.

For the simple two-body hard-core-square-well (HCSW) potential $v(r) = +\infty\ (r < c);\ -v_0\ (c < r < R);\ 0\ (r < R)$ where r is the interparticle separation, the scattering length is *exactly* analytical [48] $a/c = 1 + \alpha\left(1 - \tan\sqrt{\lambda}/\sqrt{\lambda}\right)$, $\alpha \equiv (R-c)/c,\ \lambda \equiv m v_0 \hbar^{-2}(R-c)^2$. Calling the smallness parameter $(nc^3)^{1/2} \equiv x$ some computer algebra gives for the energy per boson the double series

$$\frac{E}{N} \equiv \epsilon(x,\lambda) = \sum_{i=0} \epsilon_i(x)\lambda^i \quad (6)$$

where the coefficients $\epsilon_i(x)$ would be known for $x << 1$. Since dimensionless λ for the HCSW 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 (5) with a replaced by c. This 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 series (6) is clearly *divergence-free* even in the unitarity region.

For **fermions**, the expansion for the ground-state energy per particle is given exactly through the low-density expansion [49]

$$\frac{E}{N} \equiv \frac{3}{5}\frac{\hbar^2 k_F^2}{2m}\Big[1 + C_1 k_F a + C_2(k_F a)^2 + \left(\frac{1}{2}C_3\frac{r_0}{a} + C_4\frac{A_1(0)}{a^3} + C_5\right) \times (k_F a)^3 + C_6 (k_F a)^4 \ln|k_F a| + \left(\frac{1}{2}C_7\frac{r_0}{a} + C_8\frac{A_0''(0)}{a^3} + C_9\right) \times (k_F a)^4 + \mathcal{O}\left(\{k_F a\}^5\right)\Big] \quad (7)$$

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 $C_1, \cdots, C_9$ are known [49]. It too diverges term by term in the unitarity region since each term in the dimensionless smallness-parameter $k_F a$ diverges there. Here, the fermion number density is $n = N/V = \nu k_F^3/6\pi^2$ with ν the number of intrinsic degrees of freedom [50] if any, such as spin and isospin.

For the HCSW potential, the exact result for a/c expands in powers of λ, e.g., with a computer-algebra program such as MATHEMATICA [51], as

$$k_F a = x\left[1-\alpha\left(\frac{1}{3}\lambda+\frac{2}{15}\lambda^2+\frac{17}{315}\lambda^3+\cdots\right)\right]. \qquad (8)$$

For other interfermion potentials such as the Lennard-Jones interatomic potential $V(r) = 4\epsilon\left[(\sigma/r)^{12}-(\sigma/r)^6\right]$, with ϵ and σ convenient energy and length parameters, one can separate them as a *soft* repulsive-core plus attractive part and redefine the latter with the parameter λ. Coefficients such as those in (8) have been determined numerically [22] for a variety of two-body interatomic potentials in current use. Note that these are not rational as in (8).

4 Conclusions

An extended BCS-Bose crossover theory can be extracted from the *ternary* boson-fermion superconducting gas model at the heart of the generalized Bose-Einstein condensation (GBEC) theory. Assuming quadratically-dispersive two-electron or two-hole Cooper pairs, it already leads to a phase diagram with three condensed phases (two pure 2e-CP and 2h-CP GBECs plus a mixed phase) at temperatures cooler than for the normal phase of the initial 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 for the same electron-phonon interaction parameters.

For ultracold quantum gases, low-density expansions of point particles, whether bosons or fermions, 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 a pair and make a diverge. This divergence can be averted altogether by redefining an expansion related 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.

Acknowledgments IC thanks CONACyT (Mexico) for postgraduate grant 260978, MG acknowledges partial support from UNAM-DGAPA-PAPIIT (Mexico) grant IN116914 and MdeLl from UNAM-DGAPA-PAPIIT (Mexico) grant IN100314.

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