International Journal of Modern Physics B
Vol. 31, No. 25 (2017) 1745004 (6 pages)

DOI: 10.1142/S0217979217450047

Role of superconducting energy gap in extended BCS-Bose crossover theory

I. Chávez*, L. A. García and M. de Llano
Instituto de Investigaciones en Materiales, UNAM,
Circuito Exterior, Ciudad Universitaria,
Coyoacán 04510, Mexico City, Mexico
**israelito@ciencias.unam.mx*

M. Grether
Facultad de Ciencias, UNAM,
Circuito Exterior, Ciudad Universitaria,
Coyoacán 04510, Mexico City, Mexico

Accepted 11 July 2017
Published 18 August 2017

The generalized Bose–Einstein condensation (GBEC) theory of superconductivity (SC) is briefly surveyed. It hinges on three distinct new ingredients: (i) Treatment of Cooper pairs (CPs) as actual bosons since they obey Bose *statistics*, in contrast to BCS pairs which do not obey Bose *commutation relations*; (ii) inclusion of two-hole Cooper pairs (2hCPs) on an equal footing with two-electron Cooper pairs (2eCPs), thus making this a *complete* boson–fermion (BF) model; and (iii) inclusion in the resulting ternary ideal BF gas with particular BF vertex interactions that drive boson formation/disintegration processes. GBEC subsumes as special cases both BCS (having its 50–50 symmetry of both kinds of CPs) and ordinary BEC theories (having no 2hCPs), as well as the now familiar BCS-Bose crossover theory. We extended the crossover theory with the explicit inclusion of 2hCPs and construct a phase diagram of T_c/T_F versus n/n_f, where T_c and T_F are the critical and Fermi temperatures, n is the total number density and n_f that of unbound electrons at $T = 0$. Also, with this extended crossover one can construct the energy gap $\Delta(T)/\Delta(0)$ versus T/T_c for some elemental SCs by solving at least *two* equations numerically: a gap-like and a number equation. In 50–50 symmetry, the energy gap curve agrees quite well with experimental data. But ignoring 2hCPs altogether leads to the gap curve falling substantially below that with 50–50 symmetry which already fits the data quite well, showing that 2hCPs are indispensable to describe SCs.

Keywords: Hole Cooper pairs; BCS-Bose crossover.

*Corresponding author.

1. Introduction

The energy gap Δ is an important result of BCS[1] theory; it was discovered experimentally around the same time when the 1957 BCS theory was formulated. The energy 2Δ is needed to break a Cooper pair (CP) at the Fermi energy[2] E_F. In weak coupling $\lambda \ll 1$, gap simplifies to $\Delta = 2\hbar\omega_D \exp(-1/\lambda)$ where $\hbar\omega_D$ is the Debye energy of the lattice and λ is a dimensionless electron–phonon coupling constant. According to BCS theory a *universal ratio* involving the gap at $T = 0$ and the critical temperature T_c, namely $2\Delta(0)/k_B T_c \simeq 3.53$, must hold for all superconductors. BCS theory is characterized by an energy-gap equation while the electronic chemical potential μ assumed fixed as $\mu = E_F$. In 1963, Schrieffer[3] observed that one must simultaneously solve *two* coupled equations to determine the gap Δ *and* the chemical potential μ. In 1967, Friedel *et al.*[4] wrote that "*two equations must be solved in the BCS formalism to obtain the gap equation at* $T = 0$." A bit later Eagles[5] studied *two* simultaneous equations for the BCS gap Δ and its associated chemical potential μ. Solutions of these two equations for T_c came to define the so-called "*BCS-BEC crossover.*" Leggett[6] (see also Ref. 8) later derived the two basic equations associated with this crossover picture at $T = 0$[7] for *any* many-identical-fermion system each fermion of mass m and whose pair interaction is described by its S-wave scattering length a. We denote the crossover by "BCS-Bose" instead of by the more familiar "BCS-BEC" since a BEC cannot occur in either 2D nor in 1D[9] whereas bosons *can* form in both instances.

2. Extended Crossover Theory Subsumed in the GBEC Formalism

The GBEC formalism describes an *ideal BF ternary* gas in 3D consisting of unbound electrons along with two-electron CPs (2eCPs) as well as two-hole CPs (2hCPs), both as actual bosons, plus very particular BF interactions. This formalism is fully described in Refs. 10–13. The GBEC formalism through equilibrium conditions[10,11] leads to three coupled, transcendental equations bearing three condensed phases: Two *pure* BEC phases, one for 2eCPs and the other for 2hCPs, and a mixed phase of arbitrary proportions of both kinds of CPs. These three phases are determined numerically by solving the ensuing three equations, and formally depend on three unknown functions, all as functions of absolute temperature T: the electron chemical potential $\mu(T)$, along with the 2eCP and 2hCP BE condensate number-densities $n_0(T)$ and $m_0(T)$, respectively. One then has the two gap-like equations[10]

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

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

where $N(\epsilon)$ is the electronic density of states, $E_\pm(0)$ are phenomenological energies of the bosonic CPs with center-of-mass momentum wavenumber $K = 0$, $E(\epsilon) \equiv \sqrt{(\epsilon-\mu)^2 + \Delta^2(\epsilon)}$ is the familiar gapped Bogoliubov fermionic dispersion

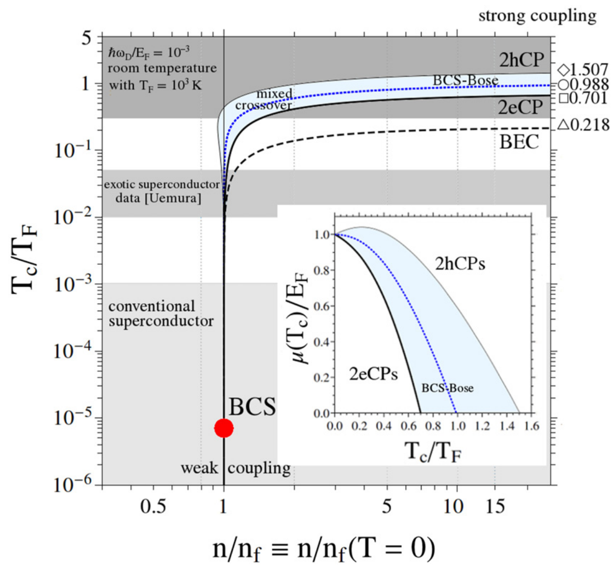


Fig. 1. (Color online) T_c/T_F versus n/n_f for the three equilibrium phases. Thick curve labeled 2eCP phase is obtained by simultaneously solving (1) with (3); thin curve 2hCP phase by solving (2) with (3) and short-dashed curve by solving (1) plus (2) and (3) with 50–50 symmetry, i.e., the *unextended* BCS-Bose crossover. Blue (online) shaded area marks the mixed crossover region with arbitrary proportions between 2eCPs and 2hCPs. Long-dashed curve is ordinary BEC curve graphed here for comparison purposes. Also shown are three temperature bands corresponding to conventional SCs, exotic SCs (Uemura data[16]) and a possible room temperature SC with $T_F = 10^3$ K. Inset shows the chemical potential $\mu(T_c)/E_F$ versus T_c/T_F where one notes that if $T_c/T_F \to 0$ all curves tend to $\mu \to E_F$ (weak-coupling extreme). On the other hand, strong-coupling limits for T_c/T_F marked with symbols (○, △, ◇ and □), i.e., $n/n_f \to \infty$ or $n_f \to 0$, implying that $\mu \to 0$ and one is at the strong-coupling extreme.

relation and $\Delta(\epsilon) \equiv f_+\sqrt{n_0(T)} + f_-\sqrt{m_0(T)}$ and $f_\pm(\epsilon)$ are the BF vertex-function interactions as defined in Refs. 10 and 11. In addition, from the well-known result of statistical mechanics to conserve the net charge of the system, one obtains the total number-density equation

$$n \equiv 2n_0(T) + 2n_{B+}(T) - 2m_0(T) - 2m_{B+}(T) + n_f(T), \tag{3}$$

where $n_f(T)$ is that of the *unbound* electrons while $2n_0(T)$ and $2m_0(T)$ are respectively those bound into 2eCPs and 2hCPs in *all* ground bosonic states as well as with excited ones $2n_{B+}(T)$ and $2m_{B+}(T)$.

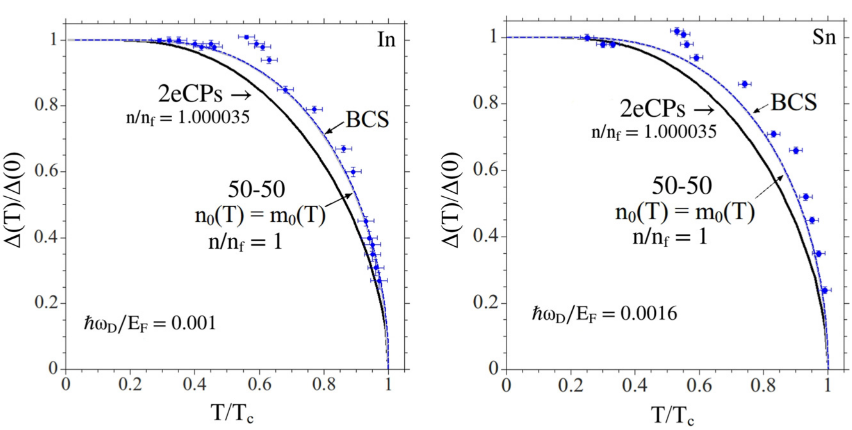
An *extended* BCS-Bose crossover then emerges as one has *explicitly* included bosonic 2hCPs in addition to the 2eCPs. For perfect symmetry between 2eCPs and 2hCPs, i.e., with half-and-half proportions, as $n_0(T) = m_0(T)$ and $n_{B+}(T) = m_{B+}(T)$ (so that $n/n_f = 1$ for 50–50 symmetry) but for $\mu \neq E_F$ one recovers the familiar BCS-Bose crossover. From Fig. 1 one sees that two coupling regimes are present. Weak coupling is around $n/n_f \simeq 1$ but in this regime one has very low T_c/T_Fs as with BCS theory. This extreme is found assuming $\mu = E_F$ with 50–50 symmetry so that only *one* equation now requires solving, the gap equation. On the other hand, strong coupling corresponds to $n/n_f \to \infty$, e.g., $n_f \to 0$ as in this extreme all electrons are bound, thus leaving a pure noninteracting Bose gas implying no interaction ($f = 0$) between unbound electrons. This leads one to solve only the number equation (3). As T increases the entire system is driven into a crossover region and finally to the strong-coupling regime where there remain no unbound electrons leaving only a binary gas of bosonic 2eCPs and 2hCPs. The dramatic T_c enhancement is due to the *mere presence* of 2hCPs, a behavior analogous to the relativistic ideal Bose gas[14] where the mere presence of antibosons, created at higher and higher temperatures, increases T_c with respect to that with no antibosons present.

Energy Gap in the Extended BCS-Bose Crossover

The original BCS-Bose crossover picture for the electronic gap $\Delta(T)$ is

$$\Delta(T) = f\sqrt{n_0(T)} = f\sqrt{m_0(T)} \tag{4}$$

where f is a boson–fermion vertex interaction coupling constant inherent to the GBEC theory. All three functions $\Delta(T)$, $n_0(T)$ and $m_0(T)$ have common "half-bell-shaped" forms. Namely, they vanish above a certain critical temperature T_c, and rise monotonically upon cooling (i.e., lowering T) to maximum values $\Delta(0)$, $n_0(0)$ and $m_0(0)$ at $T = 0$. The energy gap $\Delta(T)$ is the order parameter describing the SC condensed state, while $n_0(T)$ and $m_0(T)$ are the BEC order parameters



(a) (b)

Fig. 2. Energy-gap curves $\Delta(T)/\Delta(0)$ versus T/T_c of extended BCS-Bose crossover for (a) In and for (b) Sn with $n/n_f = 1$, i.e., the 50–50 symmetry, which coincides precisely with BCS energy-gap curve. The 2eCPs curve is obtained by simultaneously solving (1) and (3), with $n/n_f = 1.000035$, i.e., slightly different from the 50–50 symmetry. Note that the 2eCPs curve now falls substantially *below* the 50–50 curve agreeing quite well with the data. Here, experimental values of $\hbar\omega_D/E_F$ for In and Sn as well as gap experimental data were taken from Ref. 17.

depicting the macroscopic occupation that occurs below T_c in a BE condensate. This $\Delta(T)$ is *precisely* the BCS energy gap if the GBEC theory coupling is taken as $f \equiv \sqrt{2V\hbar\omega_D}$ where V and $\hbar\omega_D$ are the two parameters of the BCS model interelectronic interaction. Evidently then, the BCS and BEC T_cs are essentially equivalent.

Writing (4) for $T = 0$ and dividing this into (4) gives the much simpler f-*independent* relation involving order parameters, as well as temperatures T, normalized to unity in the interval $[0, 1]$, namely $\Delta(T)/\Delta(0) = \sqrt{n_0(T)/n_0(0)} = \sqrt{m_0(T)/m_0(0)}$. The first equality, apparently first obtained in Ref. 15, connects in a simple way the two heretofore unrelated "half-bell-shaped" order parameters of the BCS and the BEC theories. The second equality implies that a BCS condensate is precisely a BE condensate of equal numbers of 2eCPs and 2hCPs.

Here we solve at least two equations of the extended crossover instead just one as in the BCS theory, this giving the energy gap $\Delta(T)/\Delta(0)$ versus T/T_c for any superconductor with a specific value of n/n_f. Figure 2 shows energy-gap curves for In and Sn and compared with experimental data.[17] It shows the BCS curve corresponding with 50–50 symmetry obtained by solving (1) plus (2) with (3) when $n/n_f = 1$. Also shown in Fig. 2 is the 2eCP case when $\Delta(T) = f\sqrt{n_0(T)}$ while one ignores 2hCPs altogether, namely $m_0(T) = 0$, this case was used $n/n_f = 1.000035$, this curve falling *below* the 50–50 case. Clearly then, 2hCPs play an indispensable, albeit intriguing,[18] role in describing SCs. Lastly, the T-dependence of the upper critical magnetic field is analyzed in Ref. 11, p. 546, Fig. 7.

3. Conclusion

GBEC theory describes SCs starting with an ideal BF ternary gas made up of unbound electrons as well as bosonic 2e/2hCPs. It subsumes BCS theory for 50–50 symmetry between both kinds of CPs. One also recovers the usual *un*extended BCS-Bose crossover theory. With the BCS-Bose crossover extended with 2hCPs one finds a phase diagram with substantially higher T_cs with respect to BCS theory. One obtains two coupling extremes: when $n/n_f \to 1$ one has weak coupling; when $n/n_f \to \infty$ one has strong coupling and, of course, intermediate coupling whenever $1 < n/n_f < \infty$. The extended crossover predicts superconducting energy gaps for some elemental SCs by solving *three* equations when $n/n_f = 1$ which coincides precisely with BCS. Ignoring 2hCPs altogether the energy gap lies *below* the 50–50 curve, thus implying that 2hCPs are indispensable in describing SCs.

Acknowledgments

We thank F. Marsiglio for calling Ref. 3 to our attention. IC and LAG thanks CONACyT (Mexico) for postgraduate grant 291001 and 403765, respectively. MG and MdeLl thank PAPIIT-DGAPA-UNAM (Mexico) for research grant IN116914 and IN100314, respectively.

References

1. J. Bardeen, L. N. Cooper and J. R. Schrieffer, *Phys. Rev.* **108**, 1175 (1957).
2. J. F. Annett, *Superconductivity, Superfluids and Condensates* (Oxford University Press, New York, 2004), p. 127.
3. J. R. Schrieffer, *Theory of Superconductivity* (Benjamin, New York, 1963), p. 41.
4. J. Labbé, F. Barisic and J. Friedel, *Phys. Rev. Lett.* **19**, 1039 (1967).
5. D. M. Eagles, *Phys. Rev.* **186**, 456 (1969).
6. A. J. Leggett, *J. Phys. (Paris). Colloq.* **41**, C7–19 (1980).
7. M. Randeria, *Bose–Einstein Condensation*, eds. A. Griffin *et al.*(Cambridge University, Cambridge, 1995), p. 355.
8. R. M. Carter *et al.*, *Phys. Rev. B* **52**, 16149 (1995).
9. R. M. Quick, C. Esebbag and M. de Llano, *Phys. Rev. B* **47**, 11512 (1993).
10. V. V. Tolmachev, *Phys. Lett. A* **266**, 400 (2000).
11. M. de Llano and V. V. Tolmachev, *Physica A* **317**, 546 (2003).
12. M. de Llano and V. V. Tolmachev, *Ukrain. J. Phys.* **55**, 79 (2010).
13. M. Grether, M. de Llano and V. V. Tolmachev, *Int. J. Quant. Chem.* **112**, 3018 (2012).
14. M. Grether, M. de Llano and G. A. Baker, Jr., *Phys. Rev. Lett.* **99**, 200406 (2007).
15. J. Ranninger, R. Micnas and S. Robaszkiewicz, *Ann. Phys. Fr.* **13**, 455 (1988).
16. Y. J. Uemura, *J. Phys. Cond. Mat.* **16**, S4515 (2004) and more recently in *Physica B* **1**, 374 (2006).
17. I. Giaver and K. Megerle, *Phys. Rev.* **122**, 1101 (1961); P. Richards and M. Tinkham, *Phys. Rev.* **119**, 575 (1960); P. Townsend and J. Sutton, *Phys. Rev.* **128**, 591 (1962).
18. M. Grether *et al.*, *Int. J. Mod. Phys. B* **22**, 4367 (2008).