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BCS-Bose crossover theory extended with hole Cooper pairs

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Applying the generalized Bose–Einstein condensation (GBEC) formalism, we extend the BCS-Bose crossover theory by explicitly including hole Cooper pairs (2hCPs). From this follows a phase diagram with two pure phases, one with 2hCPs and the other with electron Cooper pairs (2eCPs), plus a mixed phase with arbitrary proportions of 2eCPs and 2hCPs. One has a special-case phase when there is perfect symmetry (i.e., with ideal 50–50 proportions between 2eCPs and 2hCPs). Explicitly including 2hCPs leads to an *extended* BCS-Bose crossover which predicts T_c/T_F values for some well-known conventional superconductors (SCs) (i.e., assuming electron–phonon dynamics). These compare reasonably well with experimental data. We compare with experimental T_c/T_F values for some conventional SCs associated with the new dimensionless number density n/n_f with theoretical curves associated with the extended crossover for the special case of perfect symmetry. They all obey the Bogoliubov *et al.* upper limit, thus vindicating it.

Keywords: Boson-fermion models; generalized Bose–Einstein condensation; BCS-Bose crossover; hole Cooper pairs.

1. Introduction

In 1963, Schrieffer[1] declared that one must simultaneously solve *two* equations to determine the energy-gap parameter Δ *and* the chemical potential μ, that in BCS[2] theory was put equal to the Fermi energy E_F, which depends only on the electron number density. In the mid-1960s, for the first time, Keldysh *et al.*[3] argued that the weak Coulomb interaction corresponds to the assumption that the mean correlation

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energy is much less than E_F, this condition being satisfied for the relatively small electron number-densities of $n \sim 10^{18} - 10^{19}$ cm^{-3}. A year later, Popov[4] suggested a theory of a Bose gas made up of bound pairs of Fermi particles which in the small density limit describes a system behaving as a Bose gas whose particles should form a Bose condensate at low enough temperatures. In 1967, Friedel *et al.*[5] proposed that "*two equations must be solved in the BCS formalism to obtain the gap equation at* $T = 0$." A couple of years later, Eagles[6] studied *two* simultaneous equations for the BCS gap Δ and its associated fermionic chemical potential μ. Solutions of these two simultaneous equations for T_c thus defined the so-called *BCS–BEC crossover*. Leggett[7] later derived the *two* basic equations associated with this crossover picture at $T = 0$ (see Ref. 8) for *any* many-fermion system of identical particles each of mass m and whose pair interaction is described by its S-wave scattering length a. At absolute temperature $T = 0$, these two equations were alternately derived as reported in Ref. 9. Note that we refer to the crossover as "BCS-Bose" instead of the usual "BCS–BEC" since a BEC cannot occur in either 2D or in 1D.[10]

Boson-fermion (BF) models of SCs as a BEC go back to the mid-1950s[11,13] predating even the BCS-Bogoliubov theory.[2–14] These models, see Ref. 15 and references therein, posit the existence of *actual* bosonic CPs. With a single exception,[16] *all* BF models neglect the explicit effect of *hole* CPs included on an equal footing with electron CPs to give a *complete* BF model[16–18] which we here call the GBEC theory. This enables one to easily deal with nonzero T.

2. GBEC Formalism

The GBEC formalism describes an *ideal BF ternary* gas in 3D consisting of unbound electrons along with Cooper pairs of electrons (2eCP) and *also* of holes (2hCP) as bosons, plus very particular BF interactions. It is fully described in Refs. 16–18.

The thermodynamic (or Landau) potential in the grand canonical ensemble is $\Omega(T, L^3, \mu, N_0, M_0)$ and the Helmholtz free energy *below* T_c is $F(T, L^3, \mu, N_0, M_0) \equiv \Omega + \mu N$ where $N_0(T)$ and $M_0(T)$ are, respectively, the numbers of condensed 2eCPs and 2hCPs, where μ is the chemical potential of the many-electron subsystem. Taking the negative partial derivative of Ω with respect to chemical potential, and also minimizing F wrt N_0, M_0, gives the three requirements: $-(\partial\Omega/\partial\mu) = N$, $(\partial F/\partial N_0) = 0$ and $(\partial F/\partial M_0) = 0$, where N is the total number of electrons in the system. The first relation is familiar from grand-canonical statistical mechanics; here it ensures the net charge conservation of the GBEC formalism, i.e., *gauge invariance*[19] — in contrast with BCS theory which lacks of it. The last two requirements define a stable thermodynamic state.

These three conditions lead to three coupled transcendental equations. From $(\partial F/\partial N_0) = 0$ and $(\partial F/\partial M_0) = 0$, one obtains two gap-like equations[16]

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

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

where $\beta \equiv 1/k_BT$, $E_\pm(0)$ are the phenomenological energies of the 2e/2hCPs with center-of-mass momentum (CMM) $K = 0$, $E(\epsilon) \equiv \sqrt{(\epsilon-\mu)^2 + \Delta^2(\epsilon)}$ with $\Delta(\epsilon) \equiv f_+\sqrt{n_0(T)} + f_-\sqrt{m_0(T)}$, $N(\epsilon)$ is the electronic density of states and $f_\pm(\epsilon)$ are the BF vertex-function interactions as defined in Refs. 16 and 17. In addition, $(\partial\Omega/\partial\mu) = -N$ yields the total number-density equation

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

where $n_0(T)$ and $m_0(T)$ are, respectively, those of 2e and 2hCPs in the ground state along with excited $2n_{B+}(T)$ and $2m_{B+}(T)$, i.e., condensed and noncondensed. The number density of *unbound* electrons at any T turns out to be $n_f(T) \equiv \int_0^\infty d\epsilon N(\epsilon)[1 - (\epsilon - \mu/E(\epsilon))\tanh\{\frac{1}{2}\beta E(\epsilon)\}]$ and taking $T \to 0$ in turn gives $n_f(0) = (2mE_f)^{3/2}/3\pi^2\hbar^3 \equiv n_f$ as reported in Ref. 20. Here, E_f is a "pseudo-Fermi" energy of the unbound-electron system; from 3, it coincides precisely with E_F only when $n_B(T) = m_B(T)$ *and* $n_{B+}(T) = m_{B+}(T)$ (i.e., 50-50 symmetry).

3. Extended BCS-Bose Crossover

The *extended* BCS-Bose crossover emerges from GBEC when one *explicitly* postulates bosonic 2hCPs, i.e., $m_0(T)$ and $m_{B+}(T)$ in addition to the 2eCPs. For 50-50 symmetry (with μ *unspecified*), one recovers the original BCS-Bose crossover.

Figure 1(a) shows two coupling regimes. A useful coupling constant that is interaction-model-independent (in contrast with the λ of BCS theory, λ_{BCS}) is the dimensionless number density n/n_f where n is the total number density of the system and n_f the number density of unbound electrons at $T = 0$. Thus, the weak-coupling extreme is around $n/n_f \simeq 1$ but here one gets very low T_c/T_Fs as implied by BCS who assumed $\mu = E_F$ with $n/n_f = 1$ so that one needs to solve just one (the gap) equation. On the other hand, strong coupling corresponds to $n/n_f \to \infty$, viz. $n_f \to 0$ as in this extreme all electrons are bound and thus a pure noninteracting Bose gas with no unbound electrons left. Besides the gap equation, this requires also solving a number equation.

Figure 1(b) shows experimental T_c/T_Fs (fourth column in Table 1) as function of $\Delta n \equiv n/n_f - 1$, compared with two pairs of theoretical curves from the extended crossover: (a) top pair of curves labeled $\lambda_{\mathrm{BCS}} = 1/2$ corresponds to the Bogoliubov *et al.* upper limit and $\hbar\omega_D/E_F = 0.002$, (b) bottom pair of curves is for $\lambda_{\mathrm{BCS}} = 1/5$ and $\hbar\omega_D/E_F = 0.001$. The values of $\hbar\omega_D/E_F$ are typical for conventional SCs. Black dots refer to experimental values of T_c/T_F for each SC associated with 50-50 symmetry, i.e., $\Delta n = 0$. Note that all SC empirical data for T_c/T_F fall within the two theoretical extended-crossover curves.

Table 1 lists elemental superconductors Nb, Hg, Al, In, Pb, and Sn showing extended-crossover T_c/T_F-values, compared with experimental and with BCS theory values. Extended-crossover T_c/T_F values (sixth column) were obtained by

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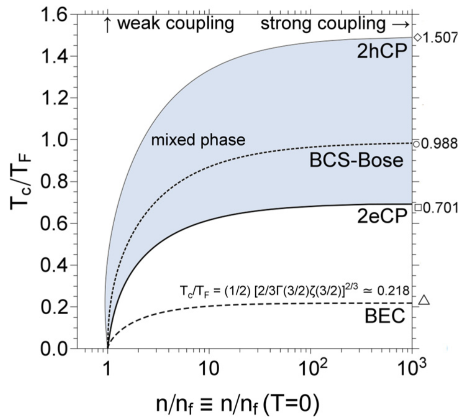
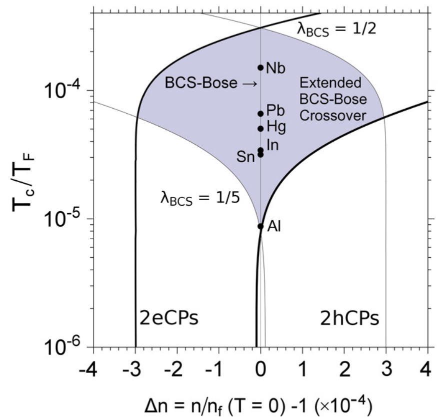


(a)



(b)

Fig. 1. (Color online) (a) Phase diagram of T_c/T_F versus n/n_f with 2eCP curve resulting by simultaneously solving (1) with (3) and 2hCP curve by solving (2) with (3). Blue (online) shaded area arises from solution of *all three* equations (1), (2) and (3). Symbols at right mark the T_c/T_F limit values when $n/n_f \to \infty$. Curve labeled BEC is shown here only for comparison. (b) Theoretical curves from extended-crossover compared with T_c/T_F experimental values for aforementioned SCs. Thick curves labeled 2eCPs phase is obtained by simultaneously solving (1) with (3); 2hCPs thin curves by solving (2) with (3). Black dots mark experimental T_c/T_F values at 50-50 symmetry (fourth column in Table 1). Error bars fall within dot sizes. Top pair of curves labeled $\lambda_{\rm BCS} = 1/2$ were found following by the Bogoliubov *et al.*[21] upper limit, with $\hbar\omega_D/E_F = 0.002$, while bottom pair of curves are for $\lambda_{\rm BCS} = 1/5$ with $\hbar\omega_D/E_F = 0.001$, where $\hbar\omega_D$ are Debye energies typical for conventional SCs.

Table 1. Experimental data for some conventional (i.e., presumed electron-phonon) superconductors compared with the *extended* BCS-Bose crossover subsumed in the GBEC formalism.

			$T_c/T_F(\times 10^{-5})$		
	T_c	$T_F(\times 10^5)$	Expt	BCS	Extd. Cross.
Al	1.17	1.36	0.87	0.77	0.87
In	3.41	1.00	3.41	3.45	3.40
Sn	3.72	1.18	3.15	3.08	3.14
Hg	**4.15**	**0.83**	**5.00**	**6.16**	**5.01**
Pb	**7.20**	**1.10**	**6.55**	**8.02**	**6.55**
Nb	9.25	0.62	14.97	16.24	15.00

Notes: Debye, Fermi and critical temperatures are in kelvin units (K).[23,24] The BCS gap-T_c ratio formula $2\Delta(0)/k_BT_c \simeq 3.53$ was used to calculate the BCS T_c/T_F, using experimental data[25] of the energy gap at $T = 0$. The T_c/T_F values of the extended crossover are taken with $n/n_f = 1$. In **bold** are marked the "bad" actors[22] of the BCS theory.

solving self-consistently two equations simultaneously, namely, the 2eCP case using (1) and (3) (thick curve) and 2hCP case solving (2) with (3) (thin curve), these curves crossing precisely at $n/n_f = 1$ and the T_c/T_F value marked by a black dot in Fig. 1(b). Note that the extended crossover predicts T_c values for aforementioned SCs quite well, even for the so-called BCS theory "bad" actors.[22] Here, we solved two equations just as suggested by Keldysh *et al.*,[3] Popov,[4] Friedel *et al.*,[5] Eagles[6]

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and finally Leggett,[7] rather than just one (the gap) equation with $\mu = E_F$ as assumed in BCS theory.

4. Conclusion

The GBEC formalism contains as a special case a BCS-Bose crossover theory extended with explicit inclusion of 2hCPs. Starting from an ideal BF ternary gas with particular BF vertex interactions, the extended crossover is defined by two thermodynamic-equilibrium requirements along with a well-known result from grand-canonical statistical mechanics that guarantees charge conservation. The Bogoliubov *et al.*[21] upper limit of $\lambda_{\rm BCS} \leq 1/2$ is seen vindicated by the extended crossover theory. Finally, for all six SCs, and for perfect ideal symmetry between 2eCPs and 2hCPs, it predicts T_c/T_F values agreeing reasonably well with experimental data.

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