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# GENERALIZED BCS-BOSE CROSSOVER PICTURE OF SUPERCONDUCTIVITY

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A recent unification of the BCS theory with that of the Bose–Einstein condensation (BEC) through a "complete" boson-fermion model is discussed as a generalization of the "BCS-Bose crossover" picture of superconductivity. Good first-principles $T_c$ predictions in 2D are calculated with no adjustable parameters for the so-called "exotic" cuprate superconductors of the "Uemura plot", without abandoning the phonon interaction mechanism. The only condition is that one depart moderately from the perfect electron-/hole-Cooper-pair symmetry to which BCS (as well as the "crossover") theory are restricted by construction.

Efforts to unify both the Bardeen, Cooper & Schrieffer (BCS) and Bose–Einstein condensation (BEC) pictures of superconductivity in terms of a "*complete* boson-fermion (BF) model" (CBFM), that in essence is a generalized "BCS-Bose crossover" theory,[1] have recently been reviewed.[2] The CBFM reduces in special cases to all the main continuum (as opposed to "spin") statistical theories of superconductivity. We have found[3] that the crossover theory, characterized by an electron chemical potential $\mu$ which is *not* set equal to the Fermi energy $E_F$ as in BCS theory, but solved for via the number equation along with the gap equation, is a very minor improvement over BCS theory since it takes a dimensionless coupling constant $\lambda$ (to be defined below) as unphysically large as 8 in the crossover theory for $\mu/E_F$ to drop from 0.999 to 0.998.

The CBFM, on the other hand, is "complete" in the sense that not only two-electron (2e) but also two-hole (2h) Cooper pairs (CPs) are allowed in *arbitrary* proportions, as opposed to *equal* proportions as in the BCS or crossover condensates by construction. Unfortunately, there is apparently no experiment yet that distinguishes between electron- and hole-CPs, nor that measures their relative proportions, either above or below $T_c$. With two[4,5] exceptions, moreover, all BF models neglect the effect of *hole* CPs formulated on an equal footing with electron CPs to give us a complete BF model (CBFM) consisting of *both* bosonic CP species coexisting with *unpaired* electrons. Here we apply the CBFM to exhibit how the BCS model interaction for the electron-phonon dynamical mechanism is sufficient to predict the unusually high values[6] of $T_c$ (in units of the material Fermi temperature $T_F$) of $\simeq 0.01 - 0.1$ of the so-called "exotic" superconductors[7] — relative to the low values of $\lesssim 10^{-3}$ more or less correctly predicted by BCS theory for conventional, elemental superconductors.

We first list several common "myths" in the theory of superconductivity that we tacitly *disbelieve* (for the reasons given in parentheses) and which have severely hindered theoretical progress in the field.

**1.** With the electron-phonon dynamical mechanism transition temperatures $T_c \lesssim 45$ K at most. For higher $T_c$'s one needs magnons or excitons or plasmons or other electronic mechanisms. (Fig. 1 below illustrates how this is not so).

**2.** Cooper pairs (CPs): **(a)** consist of negative-energy stable (i.e. stationary) bound states[8] (this neglects hole CPs which if included give positive-energy resonant states[9]); **(b)** propagate in the Fermi sea with energy $\hbar^2K^2/2(2m)$ where $\hbar K$ is the total or center-of-mass momentum (CMM) of the composite pair (this is only true in perfect vacuum[10]); **(c)** may have a linear dispersion $E \propto v_F\hbar K$, with $v_F$ the Fermi velocity, but it is then merely the acoustic mode in the ideal Fermi gas (+ interactions) with sound speed $v_F/\sqrt{d}$ in any dimensionality $d$ (the acoustic and actual "moving CP" solutions are *distinct*[9]); **(d)** "... with $K \neq 0$ represent states with net current flow"[11] (true only for $K$ in a definite direction to give a "drift" velocity); **(e)** are *not* bosons (Ref. 12, p. 38) (BCS pairs are not bosons while CPs are as they satisfy BE statistics). And most notoriously, that:

**3.** BEC is impossible in 2D.[13]

**4.** Superconductivity is unrelated to BEC (the opposite has now been shown to be the case[4]).[14]

The CBFM[4,5] is described by $H = H_0 + H_{int}$ where the unperturbed Hamiltonian $H_0$ corresponds to an *ideal* (i.e. noninteracting) gas mixture of fermions and both types of CPs, two-electron (2e) and two-hole (2h), namely

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

where $\mathbf{K} \equiv \mathbf{k_1} + \mathbf{k_2}$ is the CMM wavevector $[\mathbf{k} \equiv \frac{1}{2}(\mathbf{k_1} - \mathbf{k_2})$ is the relative wavevector, to be referred to later$]$ while $\varepsilon_{\mathbf{k}} \equiv \hbar^2k^2/2m$ are the electron and $E_\pm(K)$

the 2e-/2h-CP energies. Here $a^+_{\mathbf{k}_1,s_1}$ $(a_{\mathbf{k}_1,s_1})$ are creation (annihilation) operators for fermions and similarly $b^+_{\mathbf{K}}$ $(b_{\mathbf{K}})$ and $c^+_{\mathbf{K}}$ $(c_{\mathbf{K}})$ for 2e- and 2h-CP bosons, respectively. We distinguish between our CPs (which are Cooper's original objects, characterized *only* by $K$) that satisfy BE statistics and BCS pairs (characterized by *both* $K$ and $k$) which do not obey BE commutation relations. The interaction Hamiltonian $H_{int}$ consists of four distinct interaction vertices, each with two-fermion/one-boson creation or annihilation operators, depicting how unpaired electrons (subindex $+$) [or holes (subindex $-$)] combine to form the 2e- (and 2h-CPs) assumed in the $d$-dimensional system of size $L$, namely

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

$$+ L^{-d/2}\sum_{\mathbf{k},\mathbf{K}} f_-(k)\{a^+_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow}a^+_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow}c^+_{\mathbf{K}} + a_{-\mathbf{k}+\frac{1}{2}\mathbf{K},\downarrow}a_{\mathbf{k}+\frac{1}{2}\mathbf{K},\uparrow}c_{\mathbf{K}}\}\,, \quad (2)$$

where the $f_\pm(k)$ are taken as step functions involving certain[5] phenomenological dynamical energy parameters $E_f$ and $\delta\varepsilon$ (in addition to the positive coupling parameter $f$). The quantity $E_f$ will serve as a convenient energy scale and is not to be confused with the Fermi energy $E_F = \frac{1}{2}mv_F^2 \equiv k_BT_F$ where $T_F$ is the Fermi temperature. The Fermi energy $E_F$ equals $\pi\hbar^2 n/m$ when $d = 2$, with $n$ the total number-density of charge-carrier electrons. The quantities $E_f$ and $E_F$ coincide *only* when perfect 2e/2h-CP symmetry holds. The interaction Hamiltonian (2) can be further simplified by keeping only the $\mathbf{K} = 0$ terms. One then applies the Bogoliubov "recipe" of replacing in the full hamiltonian $H = H_0 + H_{int}$ all zero CMM creation and annihilation operators by c-numbers: $\sqrt{N_0}$ and $\sqrt{M_0}$ for 2e- and 2h-CP operators, where $N_0(T)$ and $M_0(T)$ are the number of zero-CMM 2e- and 2h-CPs, respectively. Minimizing the so-called thermodynamic (or grand) potential associated with the full Hamiltonian $H$ with respect to the independent variables $N_0$ and $M_0$, as well as keeping the total number of electrons fixed and thereby introducing the electron chemical potential $\mu(T)$, yields a set of three coupled, transcendental, integral equations [Ref. 4, Eqs. (7) and (8)]. These three equations define the CBFM. Two of these are coupled "gap-like" equations involving the 2e-CP and 2h-CP BE-condensed boson number densities $n_0(T) \equiv N_0(T)/L^d$ and $m_0(T) \equiv M_0(T)/L^d$, linked together through an electron energy gap $\Delta(T)$. The third equation can be cast as a number equation of the form

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

involving both 2e and 2h boson number-densities but now for all energy states, where $n_f(T)$ is the number-density of unpaired electrons. Most significantly, these three equations contain the *five* different statistical continuum theories of superconductivity (including the "BCS-Bose crossover" picture) as special cases; see flow chart in Fig. 1 of Ref. 2.

From the general BEC $T_c$-formula for noninteracting bosons in $d$-dimensions of energy $\varepsilon_K = C_s K^s$, $s > 0$, and recalling that

$$k_B T_F = \hbar^2 k_F^2/2m \quad \text{with} \quad k_F = [2^{d-2}\pi^{d/2} d\Gamma(d/2)n]^{1/d},$$

then, if $m_B = 2m$ and $n_B = n/2$ (all electrons paired) for $s = 2$, one gets

$$T_c/T_F = \frac{1}{2}[2/d\Gamma(d)g_{d/2}(1)]^{2/d} = 0 \quad \text{for} \quad d \leq 2$$

since the "Bose integral" $g_{d/2}(1) = \infty$ for $d/2 \leq 1$. For $d = 3$ we arrive at the familiar result

$$T_c/T_F = \frac{1}{2}\,[2/3\Gamma(3/2)\zeta(3/2)]^{2/3} \simeq 0.218$$

since the Riemann Zeta function $\zeta(3/2) \simeq 2.612$; see dashed line in "Uemura plot" of Ref. 6 (Fig. 2). We now focus on $s = 1$ . For the boson excitation energy $\eta$ to be used the leading term in the many-body Bethe–Salpeter (BS) CP dispersion relation is *linear*, i.e. $\eta \simeq (\lambda/2\pi)\hbar v_F K$ [see Ref. 9 for the derivation in 3D which gives $\eta \simeq (\lambda/4)\hbar v_F K$]. Here $\lambda \equiv VN(E_F)$ where $N(E_F)$ is the electron density of states (DOS) (for one spin) at the Fermi surface. Note that the boson energy $\eta$ is *linear* in CMM $K$ — and *not* the quadratic $\hbar^2K^2/4m$ appropriate for a composite boson of mass $2m$ moving not in the Fermi sea but in vacuum. The quadratic holds only when $E_F$ is *strictly* zero,[10] i.e. when no Fermi sea is present. But the above results with $\eta \propto \lambda\hbar v_F K$ in fact refer to actual "moving" (or "excited") CPs *in the Fermi sea. Both* kinds of *distinct* soundwave-like solutions — moving CPs and ABH phonons — appear in the many-body BS ladder-summation scheme of Ref. 9. Thus again with $n_B = n/2$, for $s = 1$ and $C_1 = (\lambda/2\pi)\hbar v_F$ one gets in 2D that $T_c/T_F = (\sqrt{3}/\pi^2)\lambda$ since $\zeta(2) = \pi^2/6$, which for $\lambda = 1/2$ and $1/4$ is $\simeq 0.088$ and $0.044$, respectively. These two values for $T_c/T_F$ appear as the black squares in Fig. 1; they mark the BEC limiting values if *all* electrons in our 2D many-electron system were imagined paired into noninteracting bosons formed with the BCS model inter-electron interaction.

We now apply the very general CBFM to exhibit the sizeable enhancements in $T_c$s over BCS theory that emerge for moderate departures from perfect 2e/2h-pair symmetry for the *same* interaction model. Remarkably, the pair-fermion interaction (2) bears a one-to-one correspondence with the more familiar "direct" inter-fermion electron-phonon interaction, mimicked, e.g. in the BCS model interaction (whose double Fourier transform is a negative constant $-V$ nonzero only within an energy shell $2\hbar\omega_D$ about the Fermi surface, with $\omega_D$ the Debye frequency) if we set $f^2/2\delta\varepsilon \equiv V$ and $\delta\varepsilon \equiv \hbar\omega_D$.[4,5] The familiar dimensionless BCS model interaction parameters $\equiv N(E_F)V$ and $\hbar\omega_D/E_F$ are then recovered. The three coupled equations of the CBFM determining the $d$-dimensional BE-condensate number-densities $n_0(T)$ and $m_0(T)$ of 2e- and 2h-CPs, respectively, as well as the fermion chemical potential $\mu(T)$, were solved numerically in Ref. 5 in 3D for $\lambda = 1/5$ and $\hbar\,\omega_D/E_F = 0.001$ assuming a quadratic boson dispersion relation $\eta = \hbar^2K^2/4m$. Besides the

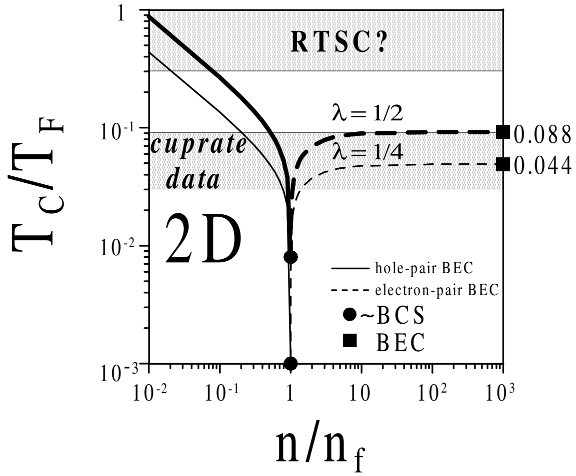


Fig. 1. Phase diagram in 2D for temperature (in units of $T_F$) and electron density (in units of $n_f$ as defined in text) showing the phase boundaries of $T_c$'s for the pure 2e-CP BEC phases (dashed curves) determined by $\Delta(T_c) = f\sqrt{n_0(T_c)} \equiv 0$, and the pure 2h-CP BEC phase given by $\Delta(T_c) = f\sqrt{m_0(T_c)} \equiv 0$ for $\lambda = 1/4$ and $1/2$ with $\hbar\omega_D/E_F = 0.05$. Intersections corresponding to $n_0(T_c) = m_0(T_c)$ locating the approximate BCS $T_c$ are marked by black dots, while black squares locate the linearly-dispersive BEC limit where all electrons are imagined paired into 2e-CP bosons, as detailed in Ref. 2. The upper shaded region labelled "RTSC?" refers to $T_c \simeq 300$ $K$ superconductivity for materials with $T_F \leq 1000$ $K$.

*normal* phase consisting of the ideal BF gas described by $H_0$, three different types of stable (plus several metastable, i.e. of higher Helmholtz free energy) BEC-like phases emerged. These are two *pure* phases of *either* 2e- *or* 2h-CP BE-condensates, and a lower temperature *mixed* phase with arbitrary proportions of 2e- *and* 2h-CPs. Of greater physical interest are the two higher-$T_c$ *pure* phases so that we focus below only on them. Note that Ref. 5 corrects a small discrepancy related to the correct gap-to-$T_c$ and specific heat jump universal ratios of 3.53 and 1.43, respectively, in Figs. 3 and 4, which incidentally are switched, of Ref. 4. A more exhaustive study within the CBFM is in progress of these ratios *away* from the BCS limit $n = n_f$.

We examine the two extreme values of $\lambda = 1/4$ (lower set of curves in Fig. 1) and $\lambda = 1/2$ (upper set of curves), and $\hbar\omega_D/E_F = 0.05$ (a typical value for cuprates), to compute the $T_c/T_F$ versus $n/n_f$ phase boundaries graphed in the figure for both the 2e-CP (dashed curves) and 2h-CP (full curves) pure, stable BEC-like phases. The value $n/n_f = 1$ corresponds to perfect 2e/2h-CP symmetry characterizing, in addition to weak coupling, BCS theory. The $T_c$ value where both curves

$$n_0(T_c) = m_0(T_c) = 0$$

intersect is marked by the large dots in the figure; these values are consistent with those gotten from the familiar BCS expression $T_c/T_F \simeq 1.134(\hbar\omega_D/E_F)\exp(-1/\lambda)$ $\simeq 0.001$ for $\lambda = 1/4$, and $\simeq 0.008$ for $\lambda = 1/2$, for $\hbar\omega_D/E_F = 0.05$. Cuprate data empirically[15] fall within the range (shadowed in the figure) $T_c/T_F \simeq 0.03 - 0.09$.

Thus, moderate departures from perfect 2e/2h-CP symmetry enable the CBFM to reach quasi-2D cuprate empirical $T_c$ values, *without abandoning electron-phonon dynamics* — contrary to popular belief. Compelling evidence for a strong, if not sole, phonon dynamical component in cuprates has recently been reported[16] from angle-resolved-photoemission data. And room temperature superconductivity (labelled rtsc in the figure) is allowed.

We conclude that the practical outcome of the BCS-BEC unification via the CBFM, which is essentially a generalized "BCS-Bose crossover" theory and which unlike BCS theory is *not a priori limited to weak coupling*, produces *enhancements* in $T_c$ over BCS values by more than an order-of-magnitude in 2D — provided only that one departs moderately from the perfect 2e/2h-pair symmetry to which BCS theory is intrinsically restricted. These enhancements in $T_c$ fall within empirical ranges for quasi-2D cuprate "exotic" superconductors.

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