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High T_c's from BCS and BEC unification

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Abstract

Without abandoning the electron–phonon mechanism, relatively large superconducting transition temperatures T_c are herewith shown to result in 2D from a recent unification of BCS theory with that of Bose–Einstein condensation (BEC) in terms of the "*complete* boson–fermion (BF) model" that allows departing from the perfect electron- and hole-pair symmetry of the BCS condensate.

We report new calculations in 2D with a recent "*complete* boson–fermion (BF) model" (CBFM) [1,2]. Arguably the broadest generalization of BCS theory to date, the model reduces in special cases to all the main continuum (as opposed to "spin") statistical theories of superconductivity. It is "complete" in that not only two-electron (2e) but also two-hole (2h) Cooper pairs (CPs) are present in arbitrary proportions. In contrast, BCS—derivable as the theory of a mixture of unpaired electrons, 2e- and 2h-CPs—allows only equal (50–50%) mixtures of the two kinds of CPs, regardless of the actual predominance above T_c of either charge of *single* unpaired carriers as Hall measurements suggest. The CBFM with the simple BCS model interaction suffices to predict the unusually high values [3] of T_c (in units of the Fermi temperature) of $\simeq$0.03–0.09 exhibited by quasi-2D cuprate superconductors, relative to the low values of $<10^{-3}$ roughly predicted by BCS theory for conventional, elemental superconductors.

The CBFM reduces, in the appropriate limits, to the special cases: (i) BCS theory; (ii) BEC theory; (iii) BCS–Bose crossover theory; (iv) the Lee et al. (1989) [4] BEC theory of superconductors; and (v) to the ideal BF model [5].

The CBFM is described by $H = H_0 + H_{\rm int}$ where H_0 corresponds to an *ideal* (i.e., noninteracting) gas mixture of fermions and both types of 2e- and 2h-CPs, namely

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

where $\mathbf{K} \equiv \mathbf{k_1} + \mathbf{k_2}$ is the center-of-mass momentum (CMM) wavevector, $\mathbf{k} \equiv \frac{1}{2}(\mathbf{k_1} - \mathbf{k_2})$ the relative one, while $\varepsilon_{\mathbf{k}} \equiv \hbar^2 k^2/2m$ 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 e and h fermions, and similarly $b^+_{\mathbf{K}}$ ($b_{\mathbf{K}}$) and $c^+_{\mathbf{K}}$ ($c_{\mathbf{K}}$) for 2e- and 2h-CP bosons, respectively. We make the nontrivial distinction between Cooper pairs (characterized only by $\mathbf{K}$) and BCS pairs (characterized by *both* $\mathbf{K}$ and $\mathbf{k}$). The former are bosons whereas the latter are not.

The $H_{\rm int}$ is a Fröhlich-like expression with fermion–CP terms (instead of phonons) in a system of size L,

$$H_{\rm int} = L^{-d/2} \sum_{\mathbf{k}} f_+(k) \{ a^+_{\mathbf{k}\uparrow} a^+_{-\mathbf{k}\downarrow} b_{\mathbf{0}} + a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} b^+_{\mathbf{0}} \} + L^{-d/2} \sum_{\mathbf{k}} f_-(k) \{ a^+_{\mathbf{k}\uparrow} a^+_{-\mathbf{k}\downarrow} c^+_{\mathbf{0}} + a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} c_{\mathbf{0}} \}. \tag{2}$$

Besides a BF coupling constant f ($\equiv \sqrt{2\hbar\omega_D V}$ with $\hbar\omega_D$ and V the BCS interaction parameters, see below), the

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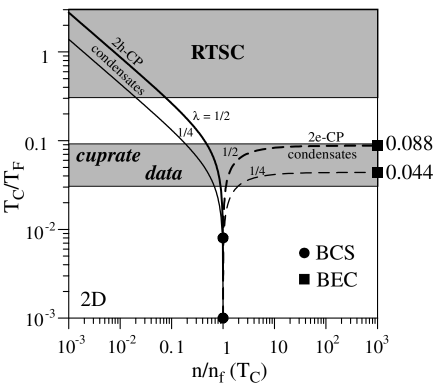

Fig. 1. Phase diagram (for $n/n_f \to 0$) in 2D for temperature (in units of T_F) vs electron density n [in units of $n_f(T_c)$ as defined in text] showing phase boundaries of T_c's for pure 2e-CP (dashed curves) and 2h-CP (full curves) BEC phases for $\lambda = 1/4$ and 1/2 with $\hbar\omega_D/E_F = 0.05$. Black squares mark the BEC limit where all electrons are imagined [6] paired into 2e-CP bosons, which in 3D for quadratic bosons would be the familiar value $\simeq$0.218. Large dots are the BCS $T_c/T_F \simeq 1.134(\hbar\omega_D/E_F)\exp(-1/\lambda) \simeq$ 0.001 for $\lambda = 1/4$, and 0.008 for $\lambda = 1/2$.

$f_\pm(k)$ are given [6] in terms of energy parameters $E_f \equiv \frac{1}{4}[E_+(0) + E_-(0)]$ and $\delta\varepsilon \equiv \frac{1}{2}[E_+(0) - E_-(0)]$, where $E_\pm(0)$ are the (empirically *unknown*) zero-CMM energies of the 2e- and 2h-CPs, respectively. Clearly $E_\pm(0) = 2E_f \pm \delta\varepsilon$, with E_f serving as a convenient energy scale not to be confused with the Fermi energy $E_F = \frac{1}{2}mv_F^2 \equiv k_B T_F$; E_F equals $\pi\hbar^2 n/m$ in 2D with n the total number-density of electrons, and coincides with E_F *only* when perfect 2e/2h-CP symmetry holds.

For the 2D boson energy $E_\pm(K) \equiv E_\pm(0) + \eta$ the many-body Bethe–Salpeter (BS) equation gives CPs propagating in the Fermi sea with a *linear* dispersion leading term, viz., $\eta \simeq (\lambda/2\pi)\hbar v_F K$ [7] in terms of the BCS $\lambda \equiv VN(E_F)$ where $N(E_F)$ is the electron density of states (DOS) (for one spin) at the Fermi surface. Clearly, η is *not* the quadratic $\hbar^2K^2/4m$ appropriate for a composite boson of mass $2m$ moving in vacuum [1,2,8], so that $T_c \neq 0$ in 2D. We use $E_f \equiv \pi\hbar^2 n_f/m = k_B T_f$ as energy/density/temperature scaling factors, and the relation $n/n_f = E_F/E_f$. For the two extreme values of $\lambda = 1/4$ (thin curves in Fig. 1) and $= 1/2$ (thick curves), and $\hbar\omega_D/E_F = 0.05$ (a typical value for cuprates), we computed the T/T_F vs. $n/n_f(T)$ phase diagram for both 2e-CP (dashed curves) and 2h-CP (full curves) pure, stable BEC phases. Here $n_f(T_c)$ (in general $\neq n_f$) is the number density of unpaired electrons at T_c, so that $(1/2)[n - n_f(T_c)]$ is the *total* number of excited (*i.e., all* with $K > 0$) 2e-CPs if $n/n_f(T_c) > 1$, or *minus* the number of excited 2h-CPs if $n/n_f(T_c) < 1$. Such excited pairs might well be the "preformed CPs" widely conjectured. Note that $n/n_f(T_c) = 1$ for perfect 2e/2h-CP symmetry at T_c. The BEC limits [6] (black squares in figure) can be shown to follow analytically from the CBFM equations for the 2e-CP condensate when $n/n_f(T_c) \to \infty$, provided one chooses $n/n_f \to 0$.

Hence, the CBFM reproduces quasi-2D cuprate empirical T_c values, and predicts room temperature superconductivity (RTSC in Fig. 1) but only via *hole*-pair BE condensates.

To conclude, the practical outcome of the BCS–BEC unification via the CBFM yields *enhancements* in T_c by more than an order-of-magnitude in 2D for the same electron–phonon dynamics mimicked by the BCS model interaction—provided only that one departs moderately from the perfect 2e/2h-pair symmetry to which BCS theory is intrinsically restricted.

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