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Superconductivity as a Bose-Einstein condensation?

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Bose-Einstein condensation (BEC) in two dimensions (2D) (e.g., to describe the quasi-2D cuprates) is suggested as the possible mechanism widely believed to underlie superconductivity in general. A crucial role is played by nonzero center-of-mass momentum Cooper pairs (CPs) usually neglected in BCS theory. Also vital is the unique *linear* dispersion relation appropriate to weakly-coupled "bosonic" CPs moving in the Fermi sea—rather than in vacuum where the dispersion would be quadratic but only for very strong coupling, and for which BEC is known to be impossible in 2D.

Bose-Einstein condensation (BEC) of Cooper pairs (CPs) leads to a phase transition even in 2D in any many-fermion system dynamically capable of forming CPs. This transition could be germane to superconductivity in the quasi-2D cuprates. In the weak coupling limit one finds a nearly linear dispersion relation for the CP that suggests very high, even diverging, critical temperatures T_c. On the other hand, in the strong coupling limit a nearly quadratic dispersion relation gives vanishingly small T_c's. For intermediate coupling one gets the finite T_c's appropriate for real quasi-2D superconductors.

The single-Cooper pair problem may appear academic at first but has significant consequences. The familiar BEC formula for the transition temperature $T_c \simeq 3.31\hbar^2 n_B^{2/3}/m_B k_B$, with n_B the number density of bosons of mass m_B and k_B the Boltzmann constant, is a special case of the more general expression [1] valid for any space dimensionality $d > 0$ and any boson dispersion relation $\varepsilon_K = C_s K^s$ with $s > 0$ and C_s a constant, given by

$$T_c = \frac{C_s}{k_B}\left[\frac{s\,\Gamma(d/2)\,(2\pi)^d n_B}{2\pi^{d/2}\,\Gamma(d/s) g_{d/s}(1)}\right]^{s/d}. \qquad (1)$$

If $\mu_B(T)$ is the boson chemical potential and $e^{\mu_B(T)/k_BT} \equiv z$ the fugacity, $g_\sigma(z) \equiv \sum_{l=1}^{\infty} z^l/l^\sigma$. For $z = 1$ and $\sigma \geq 1$ this is just $\zeta(\sigma)$, the Riemann Zeta-function of order σ which is finite for $\sigma > 1$ and infinite for $\sigma = 1$, while the series $g_\sigma(1)$ diverges for all $\sigma \leq 1$. For $s = 2$, $C_2 = \hbar^2/2m_B$, and since $\zeta(3/2) \simeq 2.612$, this leads to the BEC T_c-formula cited above. Since $g_{d/2}(1)$ diverges for all $d/2 \leq 1$, $T_c = 0$ for all $d \leq 2$. Eq. (1) follows from the boson number equation

$$N = N_0(T) + \sum_{K \neq 0}\left[e^{\{\varepsilon_K - \mu_B(T)\}/k_BT} - 1\right]^{-1} \qquad (2)$$

where $N_0(T)$ is the number of bosons in the $K = 0$ state. At $T = T_c$ both $N_0(T_c)$ *and* $\mu_B(T_c)$ virtually vanish so that using $\sum_k \to (L/2\pi)^d \int d^dk$ in (2) then yields (1).

The fact that a CP can have a *linear*, as opposed to the usual quadratic, dispersion relation

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was mentioned as far back as 1964 by Schrieffer [2], p. 33. We have found it to be so for weak coupling; it becomes quadratic only for extremely strong coupling. In weak coupling $\varepsilon_K \equiv \Delta_0 - \Delta_K \simeq a(d)\hbar v_F K$, where Δ_K is the (positive) binding energy of a CP of center-of-mass momenta (CMM) $\hbar K$, $v_F \equiv \hbar k_F/m$ is the Fermi velocity, m the fermion effective mass, while $a(d) \equiv 2/\pi$ and $1/2$ in 2D and 3D, respectively [3]. For linear dispersion $s = 1$, $C_1 = a(d)\hbar v_F$, another special case of (1) is

$$T_c = \frac{a(d)\hbar v_F}{k_B}\left[\frac{\pi^{(d+1)/2}\, n_B}{\Gamma[(d+1)/2]g_d(1)}\right]^{1/d}. \qquad (3)$$

Now $T_c = 0$ for all $d \leq 1$ only—and $T_c > 0$ for all $d > 1$, which is precisely the range of dimensionalities for all known superconductors if one includes the quasi-1D organo-metallic Bechgaard salts [4]. Using the interpolation $a(d) = (7/2-6/\pi)+(8/\pi-13/4)d+(3/4-2/\pi)d^2$, which reduces to 1, $2/\pi$ and $1/2$ in 1D, 2D and 3D, respectively, Fig. 1 graphs (1) and (3) *vs* d if one imagines all fermions in the many-fermion system paired into CPs of mass $m_B = 2m$. The particle number density of the original fermions is $n \equiv k_F^d/2^{d-2}\pi^{d/2}d\ \Gamma(d/2) = 2n_B$. Here $k_B T_F \equiv E_F = \hbar^2 k_F^2/2m$. These curves are an *upper bound* to a more realistic T_c where only a fraction of all fermions are actually bound.

The above holds for "unbreakable" CPs, i.e., bosons existing for all CMM so that the integrals over momenta go from 0 to ∞. However, CPs actually break up [3] into two "unpaired fermions" above a certain CMM K_0. This increases in value as coupling is increased and tends to infinity (as will be seen below) for infinite coupling. The CP breakup K_0, defined by $\Delta_{K_0} = 0$, for very weak coupling is just $K_0 \simeq \Delta_0/a(d)\hbar v_F \to 0$ as $\Delta_0 \to 0$. Eq. (2) with K_0 rather than ∞ as an upper limit eventually yields

$$T_c \simeq \frac{(d-1)[2\pi a(d)\hbar v_F]^d n_B}{A_d k_B \Delta_0^{d-1}} \underset{\Delta_0 \to 0}{\longrightarrow} \infty, \qquad (4)$$

where $A_d = 2\pi$ or $4\pi/3$ in 2D or 3D, respectively. Hence, since in that limit any remaining CPs are condensed in the $K = 0$ state at all temperatures, the critical temperature T_c must be *infinite*. Note that $T_c \equiv 0$ explicitly for $d = 1$.

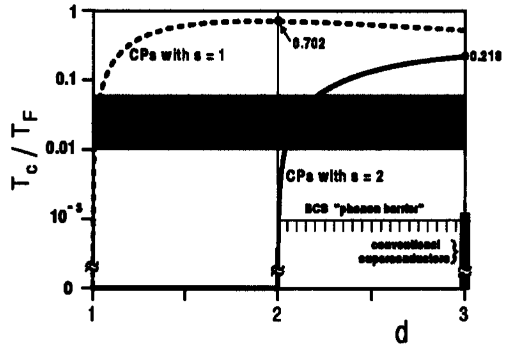

Figure 1. Upper bounds to BEC critical temperatures T_c as function of system dimensionality d, as explained in text. Shaded areas refer to empirical data [5] while BCS "phonon barrier" refers to BCS $T_c \simeq 1.13\Theta_D \exp(-1/\lambda)$ with Θ_D the Debye temperature $\simeq 300$ K and $\lambda \equiv N(0)V = 1/2$ where $N(0)$ is the density of states at the Fermi surface and V the attractive BCS coupling constant.

Indeed, if the unpaired fermions resulting from broken CPs are taken into account in a more realistic *binary boson-fermion mixture model* this artificially infinite T_c is "tamed" down [1] to a finite T_c—which remarkably enough practically coincides with that of the pure unbreakable boson gas (3). Detailed calculations using the BCS model interaction gives a T_c still almost an order of magnitude too large compared with the empirical range [5] of $T_c \approx (0.01 - 0.06)T_F$ for cuprates—even for a moderate coupling of $\lambda = 1/2$. However, the calculated T_c of about 800 K is about 17 times larger than that of the BCS theory $T_c \simeq 1.13\Theta_D \exp(-1/\lambda)$ of about 46 K. For cuprates $d \simeq 2.03$ has been suggested [6] as more realistic as it accounts for inter-layer couplings, but results would be very similar to those discussed here for $d = 2$.

A far more general interfermion interaction is the S-wave attractive separable potential [7] whose double Fourier transform is

$$V_{pq} = -(v_0/L^2)g_p g_q. \qquad (5)$$

Here L is the size of the "box" confining the many-fermion system, $v_0 \geq 0$ is the interaction strength and $g_p \equiv (1+p^2/p_0^2)^{-1/2}$ where p_0 is the inverse range of the potential. Hence, e.g., $p_0 \to \infty$ implies $g_p = 1$ and corresponds to the contact or delta potential $V(r) = -v_0\delta(\mathbf{r})$, and $p_0 = k_F$ to a range of order of the average interfermion spacing, etc. Such an interaction model may mimic a wide variety of possible dynamical mechanisms in superconductors: a force mediated by phonons, or plasmons, or excitons, or magnons, etc., or even a purely electronic interaction. In the first instance mentioned one may have, e.g., a (possibly singular) coulombic interfermion repulsion surrounded by a longer-ranged electron-phonon attraction. The former is central to the problem at hand; the latter (whether or not phonon-based) is indispensable to create the CPs detected experimentally [8] in both conventional as well as cuprate superconductors. In vacuum, a two-body bound state with (positive) binding energy $B_2 \geq 0$ is possible for any 2D potential with sufficient attraction. The vacuum t-matrix [9] associated with the Lippmann-Schwinger equation then develops a pole at an energy $E = -B_2$ so that for any dimension d (5) leads to

$$\frac{L^d}{v_0} = \sum_k \frac{g_k^2}{B_2 + \hbar^2k^2/m}. \qquad (6)$$

In 1D the integral on the rhs is exact and gives the well-known binding energy $B_2 = mv_0^2/4\hbar^2$ of the single bound state, but in 2D that integral diverges logarithmically for large k. On the other hand, the CP equation for two fermions above the Fermi surface (of energy E_F) with momenta wavevectors $\mathbf{k}_1$ and $\mathbf{k}_2$ (and CMM wavevector $\mathbf{K} \equiv \mathbf{k}_1 + \mathbf{k}_2$) is given by

$$\sum_k{}' \frac{g_k^2}{\hbar^2k^2/m + \Delta_K - 2E_F + \hbar^2K^2/4m} = \frac{L^d}{v_0} \qquad (7)$$

where $\mathbf{k} \equiv \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$ is the relative momentum wavevector, $2E_F - \Delta_K$ the total pair energy, $\Delta_K \geq 0$ as before, and the prime on the summation implies restriction to states *above* the Fermi surface, viz., $|\mathbf{k} \pm \mathbf{K}/2| > k_F$. In principle, (7) can be solved numerically for Δ_K as a function of coupling strength v_0 for all $0 \leq v_0 < +\infty$. More conveniently, however, for an interaction of the form (5) one can solve for Δ_0 (analytically if $g_k = 1$) and for Δ_K numerically, both as functions of B_2 alone, after eliminating the interaction strength v_0 by combining (6) and (7). This yields a *renormalized CP equation* employing $0 \leq B_2/E_F < \infty$ [10] as dimensionless interaction coupling parameter instead of the (possibly singular) potential strength term $1/v_0$ is now eliminated. A much greater generality for the equation with $g_k = 1$, viz., for *any* interfermion interaction with binding energy B_2, is conceivable. In 2D one has the surprising result (traceable to the fact that unlike 1D or 3D the fermionic density of states is a *constant* independent of k_F) that $\Delta_0 = B_2$ for *all* coupling, at least for an attractive delta interaction. Fig. 2 shows exact numerical results for the nonnegative *CP excitation energy* $\varepsilon_K \equiv \Delta_0 - \Delta_K$ mentioned earlier, for zero range (full curves). For very weak coupling the exact curves are virtually linear, i.e., $\varepsilon_K \to 2\hbar v_F K/\pi$, and for very large coupling tend aymptotically to the exact quadratic $\hbar^2K^2/2(2m)$ (short-dashed curves). The long-dashed loops (reminiscent of the "roton" part of the excitation spectrum of liquid ^{4}He) emerge for finite range at sufficiently strong coupling.

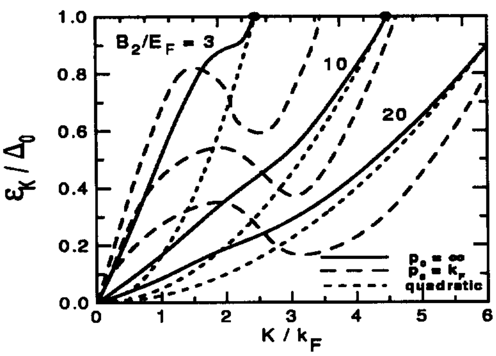

Figure 2. Dimensionless CP excitation energy ε_K/Δ_0 *vs* dimensionless CMM wavenumber K/k_F, as explained in text. Full curves are exact zero-range results; short-dashed the quadratic approximation; and long-dashed the exact finite-range result with $p_0 = k_F$. Dots mark CP breakup points.

When the zero-range results like those in Fig. 2 are used in (2) assuming $n_B = n/2$ and $m_B = 2m$, one gets Fig. 3 for the BEC T_c's of a pure gas of breakable or unbreakable CPs. Consequently, for a substantial range of intermediate couplings in 2D *finite* BEC T_c's are possible that lie within the empirical range [5] of cuprate T_c's even for a simple pure boson gas of CPs. Significantly, T_c is *no longer* zero as would be predicted in a BEC picture by a quadratic relation appropriate for "local-pair" CPs in vacuum—a result that convinced many that BEC is irrelevant for quasi-2D cuprate superconductors. More accurate BEC T_c's should include refinements such as allowing for *unpaired fermions* in a more realistic binary boson-fermion mixture model, CP-fermion interactions, non-S-wave interactions, etc.

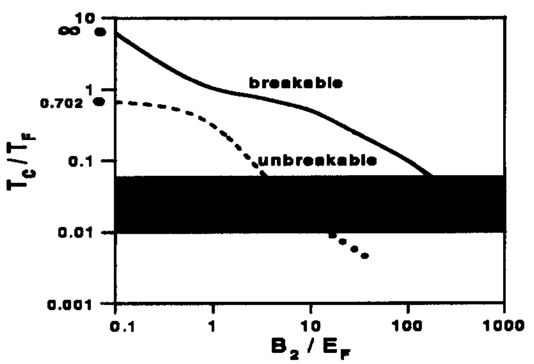

Figure 3. Critical BEC T_c (in units of T_F) calculated from (2) for a pure gas of breakable (i.e., with finite limit K_0) CPs using the exact numerical dispersion illustrated in Fig. 2, *vs* all coupling $0 \leq B_2/E_F < \infty$. The unbreakable (i.e., $K_0 = \infty$) case corresponds to the interpolation *ansatz* $\varepsilon_K = \frac{2}{\pi}\hbar v_F K[1 - \tanh(B_2/E_F)] + \frac{\hbar^2 K^2}{2(2m)}\tanh(B_2/E_F)$.

Finally, CPs are here considered "bosonic" even though they do *not* obey (Ref. [2] p. 38) Bose commutation relations. This is because for a given K they have *indefinite* occupation number as (in the thermodynamic limit) there are an indefinitely large number of allowed (relative wavevector) $\mathbf{k}$ values corresponding to an indefinitely large number of possible pairs of vectors $\mathbf{k}_1$ and $\mathbf{k}_2$. Hence, for any coupling and thus *any degree of overlap* between them, CPs do in fact obey the BE distribution (2) from which BEC is determined.

To conclude, the single CP problem with nonzero CMM (usually neglected in BCS theory) is illustrated in 2D for all coupling (and/or normal-state fermion density). BEC then suggests itself as a possible mechanism for superconductivity—in fact, for all observed superconductors from the quasi-1D organo-metallics to the more familiar 3D ones. But one must employ the correct dispersion relation in the CMM of the CPs. This relation is complicated but obtainable numerically for arbitrary coupling, and is purely linear for very weak and purely quadratic for very strong coupling.

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