Two-dimensional Bose-Einstein Condensation in Cuprate Superconductors

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Transition temperatures $T_c$ calculated using the BCS model electron-phonon interaction without any adjustable parameters agree with empirical values for quasi-2D cuprate superconductors. They follow from a two-dimensional gas of temperature-dependent Cooper pairs in chemical and thermal equilibrium with unpaired fermions in a boson-fermion (BF) statistical model as the Bose-Einstein condensation (BEC) singularity temperature is approached from above. The linear (as opposed to quadratic) boson dispersion relation due to the Fermi sea yields substantially higher $T_c$'s with the BF model than with BCS or pure-boson BEC theories.

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We provide support to a widespread conjecture (or “paradigm”) that superconductivity in general is a Bose-Einstein condensation (BEC) of the charged Cooper pairs (CPs) observed in magnetic flux quantization experiments in classical \[ \text{IFG} \] as well as cuprate \[ \text{IFG} \] superconductors. The same general conjecture is also often made regarding the superfluidity of liquid helium-3 in terms of CPs consisting of neutral-atom \[^3\text{He} \] fermions. BEC as a \textit{statistical} (as opposed to a \textit{dynamical}) mechanism of superconductivity has been entertained, among others, by Anderson \[ \text{IFG} \], by T.D. Lee \[ \text{IFG} \] and by Mott \[ \text{IFG} \] and their co-workers. But BEC normally occurs only for dimensions $d > 2$ while some modern superconductors are quasi-2D or even quasi-1D materials. We show, however, that CPs can undergo BEC for all $d > 1$. We further obtain reasonable critical temperatures $T_c$ without any adjustable parameters, thus bolstering the above mentioned conjecture even before building in full many-body self-consistency. As in BCS theory, fluctuations have also been neglected. More detailed, sophisticated treatments actually link \[ \text{IFG} \] BEC (characterized by a \textit{bosonic condensate fraction}) with the BCS theory (characterized by a \textit{fermionic gap}), but report no attempts to calculate specific $T_c$'s without adjustable parameters to compare with experiment.

A BEC picture of superconductivity is consistent with the recent discovery of the “pseudogap” in the electronic density of states \[ \text{IFG} \] above $T_c$ in certain cuprates, at least with one of its major interpretations as “pre-formed CPs” without long-range coherence or condensation, while in BCS theory CP formation and condensation occur simultaneously below the same $T_c$. We here submit that a natural candidate for such pre-formed CPs are the nonzero-center-of-mass CPs usually neglected in BCS theory.

To fix the dynamics take a 2D system of $N$ fermions of mass $m$ confined in a square of area $L^2$ interacting pairwise via the BCS model electron-phonon interaction $V_{k,k'} = -V$, with $V > 0$, whenever $\mu(T) - \hbar \omega_D < \epsilon_{k_1} = \hbar^2 k_1^2 / 2m$, $\epsilon_{k_2} < \mu(T) + \hbar \omega_D$, and zero otherwise, where $k \equiv \frac{1}{2}(k_1 - k_2)$ is the relative wavevector of the two particles; $\mu(T)$ the ideal Fermi gas (IFG) chemical potential, which at $T = 0$ becomes the Fermi energy $E_F = \hbar^2 k_F^2 / 2m$ with $k_F$ the Fermi wavenumber; and $\omega_D$ the Debye frequency. Striking direct evidence for significant electron-phonon coupling in high-temperature cuprate superconductors from angle-resolved photoemission spectroscopy (ARPES) experiments has recently been reported \[ \text{IFG} \].

If $\hbar \mathbf{K} = \hbar (\mathbf{k}_1 + \mathbf{k}_2)$ is the center-of-mass momentum (CMM) of a CP, let $E_K$ be its \textit{total} energy
(besides the CP rest-mass energy). The original CP eigenvalue equation is then

\[ 1 = V \sum_k \frac{\theta(k_1 - k_F) \theta(k_2 - k_F)}{2\epsilon_k + \hbar^2 K^2/4m - E_K} \]  

(1)

where \( \theta(x) \) is the Heaviside unit step function, and the prime on the summation sign denotes the conditions \( k_{1,2} \equiv |K/2 \pm k| < (k_F^2 + k_B^2)^{1/2} \) ensuring that the pair of particles above the Fermi “surface” cease interacting beyond the annulus of energy thickness \( 2\hbar \omega_D \equiv \hbar^2 k_B^2/m \), thereby restricting the summation over \( k \) for a given fixed \( K \). CPs obey BE statistics since there is an indefinitely large number of \( k \) values in (1) for a given value of \( K \). Setting \( E_K = 2E_F - \Delta_K \), a pair is bound if \( \Delta_K > 0 \), so that (1) becomes an equation for the (positive) pair binding energy \( \Delta_K \). Our \( \Delta_K \) and \( \Delta_0 \) follow Cooper’s notation and should not be confused with the BCS energy gap \( \Delta(T) \) at \( T = 0 \). Let \( g(\epsilon) \) be the electronic density-of-states (for each spin) in the normal (i.e., interactionless) \( N \)-fermion state; in 2D it is constant, \( g(\epsilon) = L^2 m/2\pi \hbar^2 \equiv g \). The Cooper equation (1) for the unknown quantity \( \Delta_K \) can be analyzed beyond the usual zero-CMM, \( K = 0 \), case. For \( K = 0 \) it becomes a single elementary integral, with the familiar solution \( \Delta_0 = 2\hbar \omega_D/(e^{2/\lambda} - 1) \) valid for all coupling \( \lambda \equiv gV \geq 0 \). For small \( \lambda \) one gets (2)

\[ \Delta_K \rightarrow \Delta_0 = \frac{2}{\pi} \hbar v_F K + O(K^2) \]  

(2)

where \( v_F \equiv \sqrt{2E_F/m} \) is the Fermi velocity. This linear dispersion relation is the 2D analog of the 3D result stated by Schrieffer as far back as 1964 in Ref. [23], p. 336). Although some treatments (e.g., Ref. [24]) of CPs more sophisticated than the original Cooper picture (1) numerically yield resonant pairs with a leading quadratic dispersion, linearly-dispersive resonances appear analytically from a Bethe-Salpeter equation many-body approach [25] to CPs in 3D—provided it is based on the BCS (where holes are treated on an equal footing with particles), not the IFG, ground state. In 2D, see also Refs. [26,27]. It is commonly confused with the also linearly-dispersive sound phonons of the collective excitation sometimes referred to as the Anderson-Bogulinb-Higgs mode (which for zero coupling reduces [28] to the IFG result \( \hbar v_F K/\sqrt{d} \)). The IFG sound speed \( c = v_F / \sqrt{d} \) follows trivially from the zero-temperature IFG pressure \( P = n^2 d(E/N)/dn = 2nE_F/(d + 2) \) via the familiar thermodynamic relation \( dP/dn = mc^2 \), where \( E \) is the ground-state energy and \( n \equiv N/L^d = k_F^d/2^{d-2} \pi^{d/2} d \Gamma(d/2) \) is the fermion-number density. But the simple result (2) in fact refers to actual “moving” (or “excited”) CPs in the Fermi sea, which clearly “break up” for \( K > K_0 \) as defined by \( \Delta_{K_0} \approx 0 \). Both kinds of distinct soundwave-like solutions—moving CPs and ABH phonons—appear side by side in the many-body, ladder-summation scheme of Ref. [23].

For \( N_B \) bosons of mass \( m_B \) and energy \( \varepsilon_K = C_s K^s \) with \( s > 0 \) and \( C_s \) a constant, a BEC temperature singularity occurs at \( T_c \neq 0 \) for any dimension [23,29] \( d > s \) in the number equation \( N_B = \sum_k [e^{(\varepsilon_K - \mu_B)/k_B T} - 1]^{-1} \) at vanishing bosonic chemical potential \( \mu_B \leq 0 \) when the number of \( K = 0 \) bosons just ceases to be negligible upon cooling. It is given [31] by

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

(3)

with \( n_B \equiv N_B/L^d \), and \( g_{d}(z) \) the usual Bose integrals expandable as infinite series which are \( \zeta(\sigma) \), the Riemann zeta function of order \( \sigma \), for \( \sigma > 1 \) but diverge for \( \sigma \leq 1 \). Thus \( T_c = 0 \) for all \( d \leq s \). For \( s = 2 \) and \( d = 3 \) one has \( \zeta(3/2) \approx 2.612 \), and since \( C_2 \equiv \pi^2/2m_B \) [3] then reduces to the familiar formula \( T_c \approx 3.31 \hbar^2 n_B^{2/3} / m_B k_B \) of “ordinary” BEC. But for bosons with (positive) excitation energy \( \varepsilon_K = \Delta_0 - \Delta_K \) given approximately by the linear term in (3) for all \( K \), meaning that \( s = 1 \) and \( C_1 \equiv a/d \hbar v_F \) with \( a/d = 2/\pi \) and \( 1/2 \) for \( d = 2 \) and \( 3 \), respectively, the critical temperature \( T_c \) is nonzero for all \( d > 1 \)—precisely the dimensionality range of all known superconductors down to the quasi-1D organo-metallic (Bechgaard) salts [32,34].
The number of bosons in the boson-fermion mixture to be analyzed turns out to be both coupling- and temperature-dependent and it is in conserving the fermion number that a BEC-like singularity arises. As is the case for the pure boson gas, a linear rather than a quadratic dispersion relation is needed to obtain BEC in 2D. This emerges in a statistical model for the ideal binary mixture of bosons (the CPs) and unpaired (both pairable and unpairable) fermions in chemical equilibrium [33,30] for which thermal pair-breaking into unpaired pairable fermions is explicitly allowed [37]. Assuming the BCS model interaction the total number of fermions in 2D at any \( T \) is
\[
N = L^2 k_F^2 / 2\pi = N_1 + N_2,
\]
where \( N_1 \) is the number of unpairable (i.e., non-interacting) fermions while \( N_2 \) is the number of pairable (i.e., active) ones. The unpairable fermions obey the usual Fermi-Dirac distribution with the IFG chemical potential \( \mu \) but the \( N_2 \) pairable ones are simply those in the interaction shell of energy width \( 2\hbar\omega_D \) so that, if \( \beta \equiv (k_B T)^{-1} \),
\[
N_2 = 2 \int_{\mu - \hbar\omega_D}^{\mu + \hbar\omega_D} d\epsilon \frac{g(\epsilon)}{e^\beta(\epsilon-\mu) + 1} = 2g\hbar\omega_D,
\]
which is independent of \( T \). At fixed interfermionic coupling and temperature these \( N_2 \) fermions form an ideal mixture of pairable but unpaired fermions plus CPs created near the single-fermion energy \( \mu(T) \), with binding energy \( \Delta_K(T) \geq 0 \) and total energy
\[
E_K(T) \equiv 2\mu(T) - \Delta_K(T).
\]
This generalizes the \( T = 0 \) equation \( E_K = 2E_F - \Delta_K \) introduced before.

The Helmholtz free energy \( F = E - TS \), where \( E \) is the internal energy and \( S \) the entropy, of this binary “composite boson/pairable-but-unpaired-fermion system” at temperatures \( T \leq T_c \) is then readily constructed [33] in terms of: a) the average number of unpaired but pairable fermions with fixed energy; b) \( N_{B,K}(T) \), the number of CPs with nonzero-CMM, \( 0 < K \leq K_0 \), with the CP-breakup value \( K_0 \) defined [21] by \( \Delta_{K_0} \equiv 0 \); and c) \( N_{B,0}(T) \), the number of CPs with zero CMM at temperature \( T \). The free energy \( F_2 \) of just the \( N_2 \) pairable fermions is to be minimized subject to the constraint that \( N_2 \) is conserved, i.e., one seeks the minimum of \( F_2 - \mu_2 N_2 \) with respect to (a), (b) and (c) just mentioned. The total number of pairable but unpaired fermions \( N_{20}(T) \) is then
\[
N_{20}(T) = 2g \int_{\mu - \hbar\omega_D}^{\mu + \hbar\omega_D} d\epsilon \frac{1}{e^\beta(\epsilon-\mu_2) + 1} = \frac{2g}{\beta} \ln \left[ \frac{1 + e^{-\beta(\mu-\mu_2-\hbar\omega_D)}}{1 + e^{-\beta(\mu-\mu_2+\hbar\omega_D)}} \right].
\]
The relevant number equation for the pairable fermions is thus
\[
N_2 = N_{20}(T) + 2[N_{B,0}(T) + \sum_{K>0} N_{B,K}(T)] \equiv N_{20}(T) + 2N_B(T),
\]
where \( \sum_{K>0} N_{B,K}(T) = \sum_{K>0} |\epsilon_{K}(E_K(T)-2\mu_2)|^{-1} \) is the total number of “excited” CPs (namely with CMM values \( 0 < K < K_0 \)). One can rewrite \( E_K(T) = 2\mu_2 \) here as \( \epsilon_K(T) - \mu_B(T) \), with \( \epsilon_K(T) \equiv \Delta_0(T) - \Delta_K(T) \geq 0 \) a (nonnegative) excitation energy as suggested by [33]. Hole-hole and particle-particle CPs can be shown to have the same excitation energy \( \epsilon_K(T) \). The remaining unknown \( \mu_B(T) \) is then
\[
\mu_B(T) = 2[\mu_2(T) - \mu(T)] + \Delta_0(T) = 0
\]
for \( 0 \leq T \leq T_c \) since \( N_{B,0}(T) \) is negligible for all \( T > T_c \). This is precisely the BEC condition for a pure boson gas, although one now has a binary boson-fermion mixture.

To determine \( N_B(T) \) from [33] and [30] we use [37] and see that
\[
N_{20}(T) = \frac{2g}{\beta} \ln \left[ \frac{1 + e^{-\beta(\Delta_0(T)/2-\hbar\omega_D)}}{1 + e^{-\beta(\Delta_0(T)/2+\hbar\omega_D)}} \right].
\]
for $0 \leq T \leq T_c$. Thus $2N_B(T)/N_2 \equiv 1 - N_2(T)/N_2$ is obtainable for $0 \leq T \leq T_c$ from (1) if $\Delta_0(T)$ were known. For this, $\theta(k_1 - k_F) = \theta(\epsilon_{k_1} - E_F)$ in (1) becomes $1 - n(\xi_{k_1})$ where $n(\xi_{k_1}) = (e^{\beta\xi_{k_1}} + 1)^{-1}$ with $\xi_{k_1} \equiv \epsilon_{k_1} - \mu(T)$, the IFG chemical potential $\mu(T)$ in 2D being given exactly by $\mu(T) = \beta^{-1}\ln(e^{\beta E_F} - 1) \rightarrow E_F$ as $T \rightarrow 0$. Similar arguments hold for $\theta(k_2 - k_F)$. Since for $K = 0$, $k_1 = k_2$ which implies that $\xi_{k_1} = \xi_{k_2}$, (1) then provides a simple generalization to finite-$T$ of the $K = 0$ CP equation, namely

$$1 = \lambda \int_0^{\hbar \omega_D} d\xi (e^{-\beta\xi} + 1)^{-2}[2\xi + \Delta_0(T)]^{-1}. \quad \text{(10)}$$

Its numerical solution shows $\Delta_0(T)$ to decrease monotonically with $T$ for fixed $\lambda$ and $\hbar \omega_D$, and zero only at infinite $T$. (This infinite “de-pairing” temperature is obviously spurious as the BCS model interaction loses meaning when $\mu(T)$ turns negative at large $T$.) Thus also $2N_B(T)/N_2$ decreases with $T$; it is plotted in Fig. 1 as $2n_B(T)/n_2$, since $n_B(T) \equiv N_B(T)/L^2$ and $n_2 \equiv N_2/L^2$.

Using (1) for $N_2$ the fractional number of pairable fermions that are actually paired at $T = 0$ becomes simply

$$2N_B(0)/N_2 = \frac{\Delta_0}{2\hbar \omega_D} = (e^{2/\lambda} - 1)^{-1} \xrightarrow{\lambda \rightarrow 0} e^{-2/\lambda} \quad \text{(11)}$$

for $\lambda \leq 2/\ln 2 \simeq 2.89, and \ 1 \ (\text{all pairable fermions paired into bosons}) \ \text{for} \ \lambda \geq 2.89$. This fraction is plotted against coupling $\lambda$ in Fig. 1, and contrasts sharply with the “heuristic model” of Ref. [31], Eq. (16), where $2N_B(0)/N_2 \equiv 1$ for all coupling. It is now more in line with BCS theory—which is not [38] a BEC theory—where, in any $d$, a coupling-dependent fraction is estimated (Ref. [38], p. 128) to be $(\Delta/\hbar \omega_D)^2 \equiv (\sinh 1/\lambda)^{-2} \rightarrow 4e^{-2/\lambda}$ as $\lambda \rightarrow 0$. Here $\Delta$ (again, not to be confused with the CP binding energy $\Delta_0$) is the $T = 0$ BCS energy gap for the same BCS model interaction used in this Letter. It is graphed as the thin curve in Fig. 1 and is seen to be much larger than [13] for fixed $\lambda$.

FIG. 1. Fractional number of pairable fermions that are actually paired vs. coupling $\lambda$ for the present statistical model at three different temperatures (thick curves) and estimated for BCS theory at $T = 0$ as explained below [13] (thin curve). The number of pairable fermions with the BCS model interaction used is just [13]; all of them are paired at $T = 0$ (unrealistically) in the heuristic BEC model, Ref. [3], Eq. (23).

FIG. 2. Critical BEC temperature $T_c$ in units of $T_F$ for the BCS model interaction with $\lambda = 1/2$ for varying $\nu \equiv \hbar \omega_D/\mu(T_c) \sim \Theta_D/T_F$ for: the pure unbreakable-boson gas with some and with all fermions paired, the former being the solution of [12] and the latter taken from Ref. [3], Eq. (17); for the breakable-boson gas, from Ref. [3], Eq. (18); and for the boson-fermion mixture from [13] (thick full curve labeled “binary gas”). Dashed curve is the BCS theory $T_c$, and cuprate experimental data are taken from Ref. [13].
If the background unpaired fermions are neglected one has a pure boson gas of CPs but with $T$-dependent number density $n_B(T)$. Converting the explicit $T_c$-formula (3) for $s = 1$ and $d = 2$ into an implicit one by allowing $n_B$ to be $T$-dependent leaves

$$T_c = \frac{4\sqrt{3} \hbar v_F}{\pi^{3/2} k_B} \sqrt{n_B(T_c)}, \quad (12)$$

since $g_2(1) \equiv \zeta(2) = \pi^2/6$. This requires $n_B(T) \equiv N_B(T)/L^2$ which from (7) requires (1), along with $\Delta_0(T)$ from (11). Solving these three coupled equations simultaneously for $\lambda = 1/2$ gives the remarkably constant value $T_c/T_F \approx 0.004$ over the entire range of $\nu \equiv \hbar \omega_D/E_F$ values 0.03 – 0.07 typical of cuprate superconductors. On the other hand, the BCS theory formula $T_{BCS}^B \equiv 1.13\Theta_D e^{-1/\lambda}$ with $\lambda = 1/2$ yields $T_c/T_F = 0.005 - 0.011$ over the same range of $\nu$ values. Unfortunately, both sets of predictions are well below empirical cuprate values of $T_c/T_F$ varying (4) from 0.03 – 0.09. Pure gas model results (11) for either breakable or unbreakable bosons without unpaired fermions are seen in the figure to overestimate empirical $T_c/T_F$ values by factors ranging from two to more than two orders of magnitude. All these results are wide off the mark.

To obtain the critical temperature without neglecting the background unpaired fermions, one needs the exact CP excitation energy dispersion relation $\epsilon_K(T) \equiv \Delta_0(T) - \Delta_K(T)$ which is neither precisely linear in $K$ nor independent of $T$. To determine $\Delta_K(T)$ we need a working equation that generalizes Ref. [22] for $T > 0$ via the new CP eigenvalue equation (10). For the critical temperature from the finite-temperature dispersion relation, besides solving for $\Delta_K(T)$, one requires (4), (7) and (10). At $T = T_c$, both $N_{B,0}(T_c) \simeq 0$ and $\mu_B(T_c) \simeq 0$ so that (3) leads (37) to the implicit $T_c$-equation for the binary gas

$$1 = \frac{T_c}{\nu} \ln \left[ \frac{1 + e^{-(\Delta_0(T_c)/2-\nu)/T_c}}{1 + e^{-(\Delta_0(T_c)/2+\nu)/T_c}} \right] + \frac{8(1 + \nu)}{\nu} \int_0^{\kappa_0(T_c)} \frac{\kappa dk}{e^{[\Delta_0(T_c)-\Delta_8(T_c)]/T_c} - 1}, \quad (13)$$

where quantities with tildes are in units of $\mu(T_c) \simeq E_F$ or $T_F$, while $\kappa \equiv K/2\sqrt{k_F^2 + k_B^2}$ and $\nu \equiv \Theta_D/T_F$. Four coupled equations must now be solved self-consistently for the exact $T_c$ for each $\lambda$ and $\nu$, including (10) for $\Delta_0(T)$, and Eq. (35) of Ref. [37] for both $\Delta_8(T)$ and $\kappa_0(T_c)$. Results with $\lambda = 1/2$ labeled “binary gas” in Fig. 2 show a huge enhancement of $T_c$, with respect to the self-consistent result from (12), arising from the equilibrating presence of the unpaired fermions and in spite of the very small number of bosons suggested by Fig. 1 for $\lambda = 1/2$.

For cuprates $d \simeq 2.03$ has been suggested (14) as more realistic since it reflects inter-CuO-layer couplings, but our results in that case would be very close to those for $d = 2$ since, e.g., from (3) $T_c$ for $s = 1$ (but not for $s = 2$) varies little with $d$ around $d = 2$. Indeed, if $m_B/\pi$ and $m_B$ are the boson masses perpendicular and parallel, respectively, to the cuprate planes, an “anisotropy ratio” $m_B/m_{B,\perp}$ varied from 0 to 1 allows “tuning” $d$ continuously from 2 to 3.

Other boson-fermion models (11,12,24,4,43,44) have been introduced, some even addressing (12,44) $d$-wave interaction effects as opposed to the pure $s$-wave considered here, and some also focusing (12,24) on the pseudogap. But calculating cuprate $T_c$ values in quasi-2D without adjustable parameters is not reported—and indeed predict $T_c \equiv 0$ in exactly 2D.

To conclude, a statistical model treating ordinary CPs as non-interacting bosons in thermal and chemical equilibrium with unpaired fermions yields a boson number that rises very slowly from zero with coupling, and that decreases with temperature. When the CP dispersion relation is approximately linear, it exhibits a BEC of zero-CMM pairs at precisely 2D. Transition temperatures for the boson-fermion mixture based on the exact CP dispersion relation for the BCS model electron-phonon interaction are greatly enhanced over both BCS theory as well as pure-Bose-gas BEC $T_c$’s, and are in rough agreement with empirical cuprate superconductor $T_c$’s without any adjustable parameters.
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