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Statistical model of superconductivity in a 2D binary boson–fermion mixture

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Abstract

A two-dimensional (2D) assembly of noninteracting, temperature-dependent, composite-boson Cooper pairs (CPs) in chemical and thermal equilibrium with unpaired fermions is examined in a binary boson–fermion statistical model as the superconducting singularity temperature is approached from above. The model is derived from *first principles* for the BCS model inter-fermion interaction from three extrema of the system Helmholtz free energy (subject to constant pairable-fermion number) with respect to: (a) the pairable-fermion distribution function; (b) the number of excited (bosonic) CPs, i.e., with nonzero total momenta—usually ignored in BCS theory—and with the appropriate (linear, as opposed to quadratic) dispersion relation that arises from the Fermi sea; and (c) the number of CPs with zero total momenta. Compared with the BCS theory condensate, higher singularity temperatures for the Bose–Einstein condensate are obtained in the binary boson–fermion mixture model which are in rough agreement with empirical critical temperatures for quasi-2D superconductors. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

Recent experiments [1] indicate that composite bosons in ultra-cold clouds of most alkali atoms do indeed Bose–Einstein (BE) condense. Since Cooper pairs (CPs) of fermions (electrons or holes) in a many-fermion system form composite bosons in the sense of coupling to integer angular momentum, it is natural to consider the possible BE condensation of such pairs. The belief that some such condensate is central to superconductivity is more than 50 years old [2–7]. High-T_c, as well as some organic, superconductors [8] are quasi-two-dimensional (2D). Quasi-1D superconductors have also been found [9]. BE condensation (BEC) is impossible in two or less space dimensions [10] for usual or "ordinary" bosons (i.e., with a quadratic energy-momentum, or dispersion, relation). It is however still possible to have BEC in all dimensions $d > 1$ for noninteracting bosons if they obey a *linear* dispersion relation [11]—such as CPs moving in the Fermi sea. This possibility arises because the Hohenberg theorem [10], which prohibits BEC in 2D, relies on an f-sum rule based on the quadratic dispersion relation appropriate to bosons [12] moving in a vacuum. Such a linear dispersion relation for the CPs in a binary boson–fermion mixture model was recently found [13] to be consistent, without any adjustable parameters, with the anomalous linear (quadratic) temperature-dependence above T_c in the resistivity of optimally-doped (overdoped) cuprates whether hole- or electron-doped. For the observed quadratic T-dependence in overdoped samples linear-dispersion CP charge carriers are *essential*.

Although extensive studies in the BCS-Bose "crossover" problem in superconductivity have spanned [14] a period of over thirty years, we note that BEC is distinct from the standard (i.e., zero center-of-mass momentum CPs) BCS theory condensation where only that *one* bosonic state exists.

In this paper, it is shown that in addition BEC is still possible in 2D even if the number of composite bosons (pairs of fermions) in a binary boson–fermion mixture is not fixed—as chemical/thermal equilibrium renders it coupling- and temperature-dependent—as long as the total number of fermions is fixed. This gives rise to an interesting statistical-mechanics problem irrespective of the particular mechanism for pair formation, and may have a vital application for superconductivity as well as for (neutral-atom) superfluidity such as in liquid ^{3}He [15], dilute mixtures of ^{3}He in ^{4}He [16], or in trapped Fermi gases [17]. The statistical model dealt with here may be seamlessly linked to BCS theory, via the fermionic energy gap, when boson/unpaired-fermion interactions are included as, e.g., in Refs. [18] and [19]. However, in these two papers the quadratic CP dispersion relation has been assumed. The quadratic form has recently been shown [20] to apply *only* in the zero-density or vacuum limit when the Fermi sea disappears.

In Section 2, we recall a 2D gas of fermions at $T=0$ interacting via a constant pairing interaction in an annulus about the Fermi surface—viz., the *BCS model interaction*. The binding energy of a *single* pair near the Fermi surface (CP problem) decreases practically linearly with the center-of-mass momentum (CMM) of the pair for all values of the momentum below breakup, the breakup momentum typically being only about four orders of magnitude smaller than the Fermi momentum. In Section 3 we discuss why the interacting many-fermion system can be treated as a set of independent CPs (i.e., composite bosons with fermion number two) mixed in with pairable fermions which are not bound into pairs, i.e., unpaired fermions. In Section 4 the more realistic scenario is considered of the BEC of these pairs, incorporating pair breakup beyond a certain CMM. Although the number of pairs is not fixed but rather strongly coupling- and temperature-dependent, BEC is still possible in 2D. A simple binary boson–fermion statistical model is introduced by constructing the Helmholtz free energy for an ideal mixture of pairable but unpaired fermions plus paired fermions (both zero and nonzero CMM pairs), all in chemical and thermal equilibrium. The latter results through extrema of the free energy in: (a) the pairable fermion occupation probabilities; (b) the excited boson numbers (nonzero CMM CPs) and (c) the ground boson number (zero CMM pairs). In Section 5 the coupling- and temperature-dependence of the boson number is derived. In Section 6 the critical BEC singularity temperature is obtained first by ignoring the unpaired fermions in a pure boson-gas model and then exactly for the boson–fermion binary mixture model from a T-dependent dispersion relation derived and calculated numerically, and results compared with empirical data. Finally, Section 7 gives conclusions.

2. Cooper-pair dispersion relation

Consider a 2D system of N fermions of mass m confined in a square “pen” of area L^2 and interacting pairwise via the BCS model interaction

$$V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -V & \text{if } \mu(T) - \hbar\omega_D < \varepsilon_{k_1} (\equiv \hbar^2 k_1^2/2m), \quad \varepsilon_{k_2} < \mu(T) + \hbar\omega_D \\ 0 & \text{otherwise}, \end{cases} \tag{1}$$

where $\mathbf{k} \equiv \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$ is the relative wavevector of the two particles (see Fig. 3 below); $V_{\mathbf{k},\mathbf{k}'}$ the 2D double Fourier integral of the underlying nonlocal interaction $V(\mathbf{r}, \mathbf{r}')$ in the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$; $\mu(T)$ the ideal Fermi gas chemical potential which at $T = 0$ becomes the Fermi energy $E_F \equiv \hbar^2 k_F^2/2m$ with k_F the Fermi wavenumber; $2\hbar\omega_D \equiv \hbar^2 k_D^2/m$ the width of the annulus about the Fermi circle in which the pairing interaction is nonzero, with ω_D being the Debye frequency. This model interaction mimics the net effect of an attractive electron-phonon interaction overwhelming the repulsive interfermion Coulomb repulsions, whenever $V > 0$.

If $\hbar\mathbf{K} = \hbar(\mathbf{k}_1 + \mathbf{k}_2)$ is the CMM of a pair, let E_K be its *total* energy (besides the CP rest-mass energy). The eigenvalue (CP [21]) equation for a pair of fermions at $T = 0$ immersed in a background of $N - 2$ inert, spectator fermions within a (sharp) Fermi circular perimeter of radius k_F is then

$$1 = V \sum_{\mathbf{k}}{}' \frac{\theta(k_1 - k_F)\theta(k_2 - k_F)}{2\varepsilon_k - (E_K - \hbar^2 K^2/4m)}, \tag{2}$$

where again $\varepsilon_k \equiv \hbar^2 k^2/2m$, $\theta(x)$ is the Heaviside unit step function, and the prime on the summation sign denotes the conditions

$$k_1 \equiv \left|\mathbf{k} + \frac{1}{2}\mathbf{K}\right| < (k_F^2 + k_D^2)^{1/2} \quad \text{and} \quad k_2 \equiv \left|\mathbf{k} - \frac{1}{2}\mathbf{K}\right| < (k_F^2 + k_D^2)^{1/2} \tag{3}$$

ensuring that the pair of fermions *above* the Fermi "surface" cease interacting beyond the annulus of energy thickness $\hbar\omega_D$ in accordance with (1), thereby restricting the summation over $\mathbf{k}$ for a given fixed $\mathbf{K}$. Without these restrictions (2) would just be the Schrödinger equation in momentum space for the pair. Setting $E_K \equiv 2E_F - \Delta_K$, the pair is *bound* if $\Delta_K > 0$, and (2) becomes an eigenvalue equation for the (positive) pair binding energy Δ_K. Our Δ_K and Δ_0 should *not* be confused with the BCS energy gap $\Delta(T)$.

Let $\lambda \equiv g(E_F)V \geqslant 0$ be a dimensionless coupling constant with $g(E_F)$ the electronic density-of-states (for each spin) at the Fermi surface in the normal (i.e., interactionless) state, which in 2D is constant

$$g(\varepsilon) = L^2 m/2\pi\hbar^2 \equiv g\,. \tag{4}$$

The Cooper Eq. (2) for the unknown quantity Δ_K is analyzed in Ref. [22]. For zero CMM, $K = 0$, it becomes a single elementary integral, with the familiar [21] solution

$$\Delta_0 = \frac{2\hbar\omega_D}{\mathrm{e}^{2/\lambda} - 1} \tag{5}$$

valid for *all* coupling λ. For small K, it is not too difficult to extract [22] the asymptotic result

$$\Delta_K \underset{K\to 0}{\longrightarrow} \Delta_0 - \frac{2}{\pi}\left[1 + \frac{\Delta_0}{2\hbar\omega_D}(1 + \sqrt{1+\nu})\right]\hbar v_F K$$
$$+O(K^2) \underset{\lambda\to 0}{\longrightarrow} \Delta_0 - \frac{2}{\pi}\hbar v_F K + O(K^2) \tag{6}$$

where $\nu \equiv \Theta_D/T_F$, and v_F is the Fermi velocity defined through $E_F \equiv \hbar^2 k_F^2/2m = \frac{1}{2}mv_F^2$. For weak coupling, $\lambda \to 0$, this *linear dispersion relation* gives the 2D analog of the 3D result stated as far back as 1964 in Ref. [23], p. 33 (see also, Ref. [24], p. 336) but with the 2D coefficient $2/\pi$ of the last expression of (6) replaced by $\frac{1}{2}$.

3. Justification of boson formalism

These CP boson-like structures could be called "quasi-bosons" since their creation and annihilation operators are known *not* to obey the usual boson commutation relations [23], p. 38. However, they do obey the Bose–Einstein distribution since the energy E_K of the CP is given only by the total CMM, K, but is *independent* of the relative momentum k. Thus, the possible energy states for the pair are E_K as defined in (2).

The number of pairs $N_{\mathbf{K}}$ that can occupy such a state can take on indefinite values since there exist also indefinitely many relative momenta, namely

$$N_{\mathbf{K}} \equiv \sum_{\mathbf{k}} \mathcal{N}_{\mathbf{k},\mathrm{K}} = 0, 1, 2, \ldots . \tag{7}$$

Here, $\mathcal{N}_{\mathbf{k},\mathrm{K}} = 0, 1$ is the number of pairs characterized by both $\mathbf{k}$ and $\mathbf{K}$, and is the same number as that characterized by definite $\mathbf{k}_1$ and $\mathbf{k}_2$, namely $\mathcal{N}_{\mathbf{k},\mathrm{K}} = n_{\mathbf{k}_1} n_{\mathbf{k}_2} = 0, 1$ where $n_{\mathbf{k}_i} = 0, 1$ is the occupation number for a *single* fermion, these remarks all referring to *singlet* pairing. Much of all this has been known [25] at least since 1958, albeit in somewhat different language.

This view of an *actual* Cooper *pair* should not be confused with, say, an Anderson [26] phonon-like collective *excitation* (or *modes*) with weak-coupling dispersion relation in 2D [27] given by $(1/\sqrt{2})\hbar v_F K$ in the long-wavelength limit, and which evolves into the *plasmon* when Coulomb repulsions between fermions are switched on. CPs here, like deuterons, carry fermion number two and as such are *definite* in number (although in the CP case this number is coupling- and temperature-dependent) and can thus undergo BEC. This is distinct from collective excitations which are indefinite in number. Park [28], e.g., distinguishes between "permanent" and "ephemeral" bosons, the latter sometimes being referred to as "quasiparticles" to distinguish from the former "particles".

For N_B ordinary bosons of mass m_B and energy $\varepsilon_K = \hbar^2 K^2/2m_B$ in any positive dimension, $d > 0$, a temperature singularity T_c [29] appears in the number equation $N_B = \sum_{\mathbf{K}} [\mathrm{e}^{(\varepsilon_K - \mu_B)/k_B T} - 1]^{-1}$ at vanishing bosonic chemical potential $\mu_B \leqslant 0$ when the number of $\mathbf{K} = 0$ bosons just ceases to be negligible upon cooling. It is given by

$$T_c = \frac{2\pi\hbar^2}{m_B k_B} \left[\frac{n_B}{g_{d/2}(1)} \right]^{2/d} \tag{8}$$

with n_B the boson particle density N_B/L^d, and $g_{d/2}(z)$ the usual Bose integrals

$$g_\sigma(z) \equiv \frac{1}{\Gamma(\sigma)} \int_0^\infty \mathrm{d}x \frac{x^{\sigma-1}}{z^{-1}\mathrm{e}^x - 1} = \sum_{l=1}^{\infty} \frac{z^l}{l^\sigma} \underset{z\to 1}{\longrightarrow} \zeta(\sigma) , \tag{9}$$

where $\Gamma(\sigma)$ is the gamma function and $\zeta(\sigma)$ the Riemann zeta function of order σ. The last identification in (9) holds when $\sigma > 1$ for which $\zeta(\sigma) < \infty$, while the series $g_\sigma(1)$ diverges for $\sigma \leqslant 1$, thus giving $T_c = 0$ for $d \leqslant 2$. For $d = 3$ one has $\zeta(3/2) \simeq 2.612$ so that (8) becomes the familiar formula $T_c \simeq 3.31\hbar^2 n_B^{2/3}/m_B k_B$ of "ordinary" BEC. On the other hand, for bosons with (positive) excitation energy $\varepsilon_K \equiv \Delta_0 - \Delta_K$ given approximately by the linear term in (6) for all K, the singularity that lead to (8) now yields [30], for weak coupling,

$$T_c = \frac{a(d)\hbar v_F}{k_B} \left[\frac{\pi^{\frac{d+1}{2}} n_B}{\Gamma(\frac{d+1}{2}) g_d(1)} \right]^{1/d} \tag{10}$$

where [11] $a(d)=1,\ 2/\pi$ and $1/2$ for $d=1,\ 2$ and 3, respectively. Note that now $T_c>0$ *for all* $d>1$, which is *precisely* the dimensionality range of all known superconductors including the quasi-1D organo-metallic (Bechgaard) salts [9]. This is *not* inconsistent with the Hohenberg theorem [10] that there is no broken symmetry, i.e., long-range order, in a Bose fluid for $d=1$ or 2, since this is based on an f-sum rule for bosons with a quadratic dispersion relation. Indeed, both (8) and (10) are special cases of the more general expression [31] for any space dimensionality $d>0$ and any boson dispersion relation $\varepsilon_K=C_sK^s$ with $s>0$ and C_s a constant, given by

$$T_c=\frac{C_s}{k_B}\left[\frac{s\Gamma(d/2)(2\pi)^d n_B}{2\pi^{d/2}\,\Gamma(d/s)g_{d/s}(1)}\right]^{s/d} . \tag{11}$$

In what follows the number of bosons will be temperature-dependent and it is *in conserving the fermion number* that the singularity arises. As is the case for the pure boson gas, a linear rather than a quadratic dispersion relation will be needed to obtain BEC in 2D. This emerges in a statistical model of an ideal binary *mixture* of bosons (the CPs) and unpaired (both pairable and unpairable) fermions in chemical equilibrium [4], for which thermal pair-breaking into unpaired pairable fermions is explicitly allowed.

4. First-principles statistical model

Under interaction (1) at any T the total number of fermions in 2D is $N=L^2k_F^2/2\pi=N_1+N_2$ and is just the number of noninteracting (i.e., unpairable) fermions N_1 plus the number of pairable ones N_2. The unpairable fermions obey the usual Fermi–Dirac distribution with fermionic chemical potential μ. On the other hand, the N_2 pairable fermions are simply those in the interaction shell of energy width $\hbar\omega_D$ so that

$$N_2=2\int_{\mu-\hbar\omega_D}^{\mu+\hbar\omega_D}\mathrm{d}\varepsilon\frac{g(\varepsilon)}{\mathrm{e}^{\beta(\varepsilon-\mu)}+1}=2g\hbar\omega_D\,, \tag{12}$$

since the density of electronic states (4) is constant and the remaining integral exact. At any interfermionic coupling and temperature these fermions form an ideal mixture of pairable but unpaired fermions plus CPs that are created near the single-fermion energy $\mu(T)$, with binding energy $\Delta_K(T)\geqslant 0$ and total energy

$$E_K(T)\equiv 2\mu(T)-\Delta_K(T)\,. \tag{13}$$

This generalizes the $T=0$ equation $E_K\equiv 2E_F-\Delta_K$ introduced below (3).

The Helmholtz free energy $F=E-TS$, where E is the internal energy and S the entropy, for this binary "*composite boson/pairable-but-unpaired-fermion system*" at temperatures $T \leqslant T_c$ is then [32]

$$F_2 = 2\int_{\mu-\hbar\omega_D}^{\mu+\hbar\omega_D} \mathrm{d}\varepsilon\, g(\varepsilon)\{n_2(\varepsilon)\varepsilon + k_B T[n_2(\varepsilon)\ln n_2(\varepsilon) + \{1-n_2(\varepsilon)\}\ln\{1-n_2(\varepsilon)\}]\}$$

$$+ [2\mu(T) - \Delta_0(T)]N_{B,0}(T) + \sum_{K>0}^{K_0}\{[2\mu(T) - \Delta_K(T)]N_{B,K}(T)$$

$$+ k_B T[N_{B,K}(T)\ln N_{B,K}(T) - \{1+N_{B,K}(T)\}\ln\{1+N_{B,K}(T)\}]\} . \qquad (14)$$

The integral term is the contribution from the unpaired fermions and runs over all levels in the energy shell where the BCS model interaction is nonzero, $n_2(\varepsilon)$ being the average number of unpaired but pairable fermions with energy ε; the prefactor two comes from the spin. The second term gives the free energy of the bosons with CMM $K = 0$ since their entropy is negligible in the thermodynamic limit; here $N_{B,0}(T)$ is the number of (bosonic) CPs with zero CMM at temperature T. The summation term represents the free energy of the bosons with nonzero CMM, while $N_{B,K}(T)$ is that with arbitrary nonzero CMM K, and the cutoff K_0 is defined [22] by $\Delta_{K_0} \equiv 0$. The free energy F_2 is to be minimized subject to the constraint that the total number of pairable fermions N_2 is conserved.

If $N_{20}(T)$ is the number of pairable but unpaired fermions, the relevant *number equation* for the pairable (i.e., active) fermions is then

$$N_2 = N_{20}(T) + 2[N_{B,0}(T) + N_{B,0<K<K_0}(T)] \equiv N_{20}(T) + 2N_B(T) , \qquad (15)$$

where $N_{B,\,0<K<K_0}(T)$ denotes the *total* number of "excited" bosonic pairs (namely with CMM such that $0 < K < K_0$), i.e., $N_{B,\,0<K<K_0}(T) \equiv \sum_{0<K<K_0} N_{B,K}(T)$. Minimizing the free energy, subject to the constraint that (15) be a constant, is equivalent to minimizing the grand potential

$$\Omega_2 = F_2 - \mu_2 N_2 . \qquad (16)$$

(a) Minimizing Ω_2 with respect to the *fermion occupation probabilities* $n_2(\varepsilon)$ yields the Fermi–Dirac distribution with fermion chemical potential μ_2, *not* μ, namely

$$n_2(\varepsilon) = \frac{1}{\mathrm{e}^{\beta(\varepsilon-\mu_2)}+1}; \qquad \beta \equiv (k_B T)^{-1} . \qquad (17)$$

Thus, the total number of pairable (but unpaired) fermions then becomes

$$N_{20}(T) \equiv 2\int_{\mu-\hbar\omega_D}^{\mu+\hbar\omega_D} \mathrm{d}\varepsilon\, g(\varepsilon) n_2(\varepsilon) = 2\int_{\mu-\hbar\omega_D}^{\mu+\hbar\omega_D} \mathrm{d}\varepsilon \frac{g(\varepsilon)}{\mathrm{e}^{\beta(\varepsilon-\mu_2)}+1} , \qquad (18)$$

and should be compared with (12) for N_2 which contains only μ. Since in 2D $g(\varepsilon)$ is a constant (4), (18) becomes the exact expression

$$N_{20}(T) = \frac{2g}{\beta}\ln\left[\frac{1+\mathrm{e}^{-\beta(\mu-\mu_2-\hbar\omega_D)}}{1+\mathrm{e}^{-\beta(\mu-\mu_2+\hbar\omega_D)}}\right] . \qquad (19)$$

(b) Minimizing Ω_2 with respect to the *excited boson numbers* $N_{B,K}(T)$, $K > 0$, yields the Bose–Einstein distribution summed over all $0 < K < K_0$, namely

$$N_{B,0<K<K_0}(T) \equiv \sum_{K>0}^{K_0} N_{B,\,K}(T) = \sum_{K>0}^{K_0} \left[e^{\beta\{E_K(T)-2\mu_2\}} - 1 \right]^{-1} . \qquad (20)$$

The factor multiplying β in (20) may be rewritten as $\varepsilon_K(T) - \mu_B(T)$, where $\varepsilon_K(T) \equiv \Delta_0(T) - \Delta_K(T) \geqslant 0$ is a (nonnegative) excitation energy as suggested by (6), while $\mu_B(T)$ turns out to be

$$\mu_B(T) = 2[\mu_2(T) - \mu(T)] + \Delta_0(T) . \qquad (21)$$

This allows rewriting (20) in the more meaningful *boson* form

$$N_{B,\,0<K<K_0}(T) = \sum_{K>0}^{K_0} \left[e^{\beta\{\varepsilon_K(T)-\mu_B(T)\}} - 1 \right]^{-1} \qquad (22)$$

where $\mu_B(T)$ is clearly the bosonic chemical potential associated with the entire binary mixture.

(c) Finally, minimizing Ω_2 with respect to the *number of zero CMM* (*or*, "*ground state*") *bosons* $N_{B,0}(T)$ gives

$$2[\mu_2(T) - \mu(T)] + \Delta_0(T) = 0 \quad (0 \leqslant T \leqslant T_c) , \qquad (23)$$

valid only in the stated temperature range as $N_{B,0}(T)$ is negligible for all $T > T_c$. However, in view of (21) this implies that $\mu_B(T) = 0$ for all $0 \leqslant T \leqslant T_c$—which is precisely the BEC condition for a *pure* boson gas, even though one now deals with a binary boson–fermion *mixture*.

5. Boson number

To determine $N_B(T)$ from (15) we need (19) which with (23) reduces to

$$N_{20}(T) = \frac{2g}{\beta} \ln \left[\frac{1 + e^{-\beta\{\Delta_0(T)/2 - \hbar\omega_D\}}}{1 + e^{-\beta\{\Delta_0(T)/2 + \hbar\omega_D\}}} \right] \quad (0 \leqslant T \leqslant T_c) . \qquad (24)$$

At $T = 0$ two distinct coupling regimes emerge by inspecting (24): (a) for $\Delta_0/2 < \hbar\omega_D$ or, from (5) for $\lambda \leqslant 2/\ln 2 \simeq 2.89$, we have that $N_{20}(0) = 2g(\mu)(\hbar\omega_D - \Delta_0/2)$; while (b) for $\Delta_0/2 > \hbar\omega_D$ (or $\lambda \geqslant 2.89$) $N_{20}(0)$ is identically zero. Hence, the number of bosons $N_B(0)$ at $T = 0$ from (15) is just $N_B(0) = \frac{1}{2}[N_2 - N_{20}(0)]$. Using (12) for N_2 the *fractional number of pairable fermions that are actually paired* at $T = 0$, namely $2N_B(0)/N_2 = 1 - N_{20}(0)/N_2$, becomes simply

$$2N_B(0)/N_2 = \begin{cases} \Delta_0/2\hbar\omega_D = (e^{2/\lambda} - 1)^{-1} \underset{\lambda\to 0}{\longrightarrow} e^{-2/\lambda} & (\text{for } \lambda \leqslant 2/\ln 2 \simeq 2.89) , \\ 1 & (\text{for } \lambda \geqslant 2/\ln 2 \simeq 2.89) . \end{cases} \qquad (25)$$

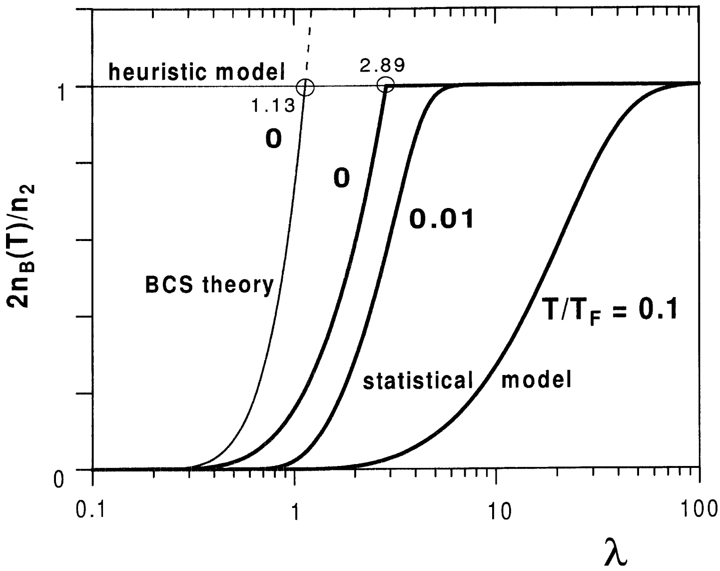

Fig. 1. Fractional number of pairable fermions that are actually paired, at three different temperatures, vs. coupling λ for the present first-principles model (25) (thick curves) and estimated for BCS theory at $T = 0$ as explained below (25) (thin curve). The number of pairable fermions with the BCS model interaction used is just (12); all of them are actually paired at $T = 0$ in the heuristic BEC model, Ref. [31] Eq. (23).

This fraction is plotted against coupling λ in Fig. 1 as $2n_B(0)/n_2$, since $n_B(T) \equiv N_B(T)/L^2$ and $n_2 \equiv N_2/L^2$. Since $N_B(0) = \frac{1}{2}g\Delta_0$ for $\lambda \leqslant 2.89$, only those fermions in an energy shell of width $\Delta_0/2$ around the Fermi surface actually pair at $T = 0$, while for $\lambda \geqslant 2.89$ *all* pairable fermions actually pair up since then $N_B(0) = g\hbar\omega_D \equiv \frac{1}{2}N_2$. This result contrasts sharply with the "heuristic model" [31], Eq. (22), where $2N_B(0)/N_2 \equiv 1$ for *all* coupling, and is more in line with BCS theory which implies, in any d, a coupling-dependent fraction estimated (Ref. [5, p. 128]; see also [33]) to be $[g(E_F)2\Delta/2g(E_F)\hbar\omega_D]^2 = (\Delta/\hbar\omega_D)^2 \equiv (\sinh 1/\lambda)^{-2} \underset{\lambda\to 0}{\longrightarrow} 4\mathrm{e}^{-2/\lambda}$, where $\Delta \equiv \hbar\omega_D/\sinh(1/\lambda)$ (again, not to be confused with the CP binding energy Δ_0) is the $T = 0$ BCS energy gap for the same BCS model interaction (1) used in this paper; this is graphed as the thin curve in Fig. 1 and is seen to be much larger than (25) for fixed λ. The breakdown of BCS theory for BCS model interaction couplings larger than $\lambda \simeq 1.13$ is clear both because: (a) the alluded fraction cannot exceed unity and (b) physically, if the fermionic energy gap $\Delta \geqslant \hbar\omega_D$ no pairable fermions are available at all. This breakdown is indicated by the dashed curve in Fig. 1. (A strong-coupling many-body model differing from that of BCS theory but based on the BCS model interaction has been solved by Thouless [34]).

Also displayed in Fig. 1 are two finite-temperature results for $2N_B(T)/N_2 = 1 - N_{20}(T)/N_2$ which are obtainable from (24) for any T provided one knows $\Delta_0(T)$ for any $T > 0$. For $T > 0$, the $\theta(k_1 - k_F) \equiv \theta(\varepsilon_{k_1} - E_F)$ in (2) becomes $1 - n(\xi_{k_1})$, where

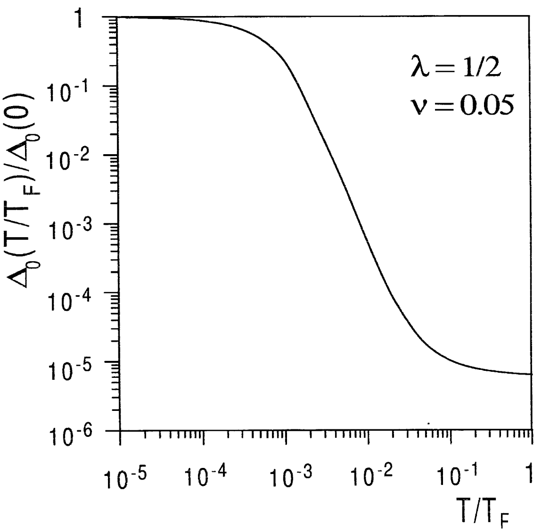

Fig. 2. Temperature dependence of $K = 0$ CP binding energy $\Delta_0(T)$ obtained numerically from (27) for $\lambda = \frac{1}{2}$ and $v = 0.05$. Note that when $T = \infty$ (27) is analytical for $\Delta_0(\infty)$; the latter then turns out to be about 10^{-8}, so that the curve saturates from above to this value at $T = \infty$.

$n(\xi_{k_1}) \equiv (e^{\beta\xi_{k_1}} + 1)^{-1}$ is the Fermi–Dirac distribution with $\xi_{k_1} \equiv \varepsilon_{k_1} - \mu(T)$, with the ideal fermion gas chemical potential $\mu(T)$ in 2D being given exactly by

$$\mu(T) = \beta^{-1} \ln(e^{\beta E_F} - 1) \underset{T \to 0}{\longrightarrow} E_F \,. \tag{26}$$

Note that $\mu(T)$ decreases monotonically with temperature from its maximum value of E_F but does not turn negative until $T = T_F/\ln 2 \simeq 1.44 T_F$ so that the BCS model interaction (1), which *requires* $\mu(T)$ to be nonnegative, will not break down (i.e., become meaningless) over the entire range of temperatures relevant in this paper, see Fig. 4 below. Similar arguments hold for $\theta(k_2 - k_F)$. Since $k_1 = k_2$ implies that $\xi_{k_1} = \xi_{k_2}$, (2) then leads to a simple generalization to finite-temperature of the $K = 0$ CP equation, namely

$$1 = \lambda \int_0^{\hbar\omega_D} d\xi (e^{-\beta\xi} + 1)^{-2} [2\xi + \Delta_0(T)]^{-1} \,. \tag{27}$$

Its numerical solution for $\Delta_0(T)$ is illustrated in Fig. 2 for $\lambda \equiv gV = \frac{1}{2}$ and $v \equiv \hbar\omega_D/E_F = 0.05$. Note that if one assumes a T^* such that $\Delta_0(T^*) = 0$, the resulting integral in (27) diverges and the equation can only be satisfied for $\lambda = 0$; thus, there is no temperature T^* at which "depairing" will occur for any fixed v and any nonzero λ.

6. Critical temperature

Neglecting the background unpaired fermions and modeling our system as a *pure boson gas* of CPs but with temperature-dependent number density $n_B(T)$, one converts the explicit T_c-formula (10) into an *implicit* one by allowing n_B to be T-dependent. For $d=2$ (10) becomes, since $g_2(1)\equiv\zeta(2)=\pi^2/6$,

$$T_c=\frac{4\sqrt{3}}{\pi^{3/2}}\frac{\hbar v_F}{k_B}\sqrt{n_B(T_c)}\,. \tag{28}$$

This requires $n_B(T)\equiv N_B(T)/L^2$ which in turn requires (24), along with $\Delta_0(T)$ as determined from (27), and is given by the expression $2N_B(T)/N_2=1-N_{20}(T)/N_2$. Solving (28) self-consistently with $\lambda=\frac{1}{2}$ gives the remarkably constant value $T_c/T_F\simeq 0.004$ over the entire range of $\nu\equiv\hbar\omega_D/E_F$ values 0.03–0.07 typical [35] of cuprate superconductors. On the other hand, the BCS formula $T_c^{BCS}\simeq 1.13\Theta_D e^{-1/\lambda}$ with $\lambda=\frac{1}{2}$ gives $T_c/T_F=0.005, 0.008$ and 0.011 for $\nu=0.03, 0.05$ and 0.07, respectively. Clearly, both sets of predictions are somewhat small compared with empirical cuprate values of T_c/T_F that range [36] from 0.01–0.1.

To obtain the exact critical temperature *without* neglecting the background unpaired fermions, one needs the exact CP excitation energy dispersion relation $\varepsilon_K(T)\equiv\Delta_0(T)-\Delta_K(T)$ which is neither exactly 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 (27). Because of symmetry, see Fig. 3, one can restrict the angle θ to the interval $(0,\pi/2)$ where $k_1\geqslant k_2$, i.e., to quadrant I. Recalling (13), in

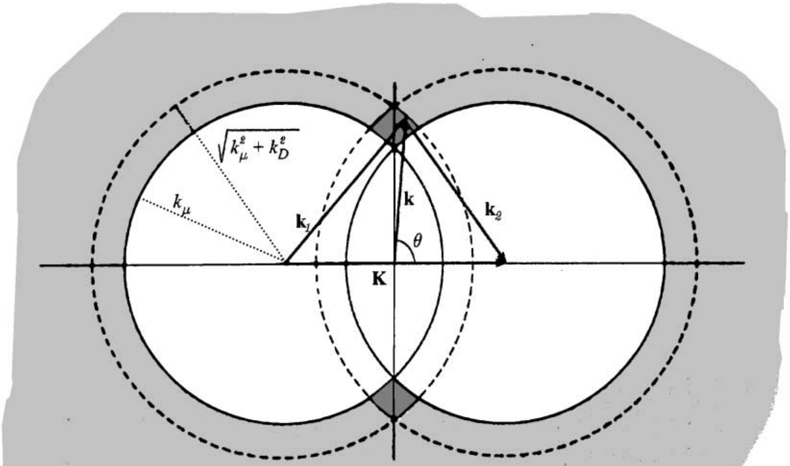

Fig. 3. Cross-section of overlap "volume" in momentum space (darkest shading) where the tip of the relative wavevector $\mathbf{k}$ (for two fermions with wavevectors $\mathbf{k}_1$ and $\mathbf{k}_2$) must point for the attractive BCS model interaction (1) between them to be nonzero and form a Cooper pair of CMM magnitude $\hbar K$.

d-dimensions (2) becomes

$$1 = V\left(\frac{L}{2\pi}\right)^d \int' \mathrm{d}\mathbf{k} \frac{[1 - n(\xi_{k_1})][1 - n(\xi_{k_2})]}{\hbar^2(k^2 - k_\mu^2)/m + \Delta_K(T) + \hbar^2 K^2/4m} . \tag{29}$$

Here k_μ is such that $\mu \equiv \hbar^2 k_\mu^2/2m$ and becomes k_F as $T \to 0$, while k_D is such that $\hbar\omega_D \equiv \hbar^2 k_D^2/2m$. The prime on the integral sign now denotes the restrictions

$$k_2^2 \equiv |\mathbf{k} - \tfrac{1}{2}\mathbf{K}|^2 = k^2 - kK\cos\theta + \tfrac{1}{4}K^2 > k_\mu^2 , \tag{30}$$

$$k_1^2 \equiv |\mathbf{k} + \tfrac{1}{2}\mathbf{K}|^2 = k^2 + kK\cos\theta + \tfrac{1}{4}K^2 < k_\mu^2 + k_D^2 . \tag{31}$$

In Fig. 3 the darkest shading corresponds to these (BCS model interaction) restrictions. The conditions (30) and (31) can be studied separately but must be satisfied simultaneously. If $K < 2\sqrt{k_\mu^2 - k_D^2}$, (30) and (31) are equivalent to

$$(k_\mu^2 - \tfrac{1}{4}K^2\sin^2\theta)^{1/2} + \tfrac{1}{2}K\cos\theta < k < [(k_\mu^2 + k_D^2) - \tfrac{1}{4}K^2\sin^2\theta]^{1/2} - \tfrac{1}{2}K\cos\theta . \tag{32}$$

Note that for $K > \sqrt{k_\mu^2 + k_D^2} - \sqrt{k_\mu^2 - k_D^2}$ there exists a minimum value $\theta_{\min}$ of θ given by

$$\cos\theta_{\min} \equiv \frac{k_D^2}{K\sqrt{2(2k_\mu^2 + k_D^2) - K^2}} , \tag{33}$$

while $\theta_{\min}=0$ for $K < \sqrt{k_\mu^2 + k_D^2} - \sqrt{k_\mu^2 - k_D^2}$. We introduce the dimensionless variables

$$\kappa \equiv \frac{K}{2(k_F^2 + k_D^2)^{1/2}} \leqslant 1, \quad \xi \equiv \frac{k}{k_F}, \quad \tilde{\Delta}_\kappa \equiv \frac{\Delta_K}{E_F}, \quad v \equiv \frac{\Theta_D}{T_F} \equiv \frac{k_D^2}{k_F^2} , \tag{34}$$

with $k_B\Theta_D \equiv \hbar\omega_D \equiv \hbar^2 k_D^2/2m$ and $k_B T_F \equiv E_F$, where k_B is Boltzmann's constant. Recall the $d = 2$ constant expression (4) for $g(\varepsilon)$, the restrictions (32), and that for $K \geqslant 0$ and $T > 0$ the step functions in (2) $\theta(k_{1,2} - k_F) \equiv \theta(|\frac{1}{2}\mathbf{K} \pm \mathbf{k}| - k_F)$ become $[\exp\{-\beta[\hbar^2(\frac{1}{2}\mathbf{K}\pm\mathbf{k})^2/2m - \mu(T)]\}+1]^{-1}$—but with $2\varepsilon_k$ in (2) replaced by $\varepsilon_{k_1} + \varepsilon_{k_2}$, E_F by $\mu(T)$ and Δ_K by $\Delta_K(T)$. One finally arrives at a *working equation* for the binding energy $\Delta_K(T)$ that generalizes Eq. (18) of Ref. [22], namely

$$\begin{aligned} 1 = \frac{4}{\pi}\lambda \int_{\theta_{\min}}^{\pi/2} \mathrm{d}\theta \\ \times \int_{\xi_{\min}(\theta)}^{\xi_{\max}(\theta)} \mathrm{d}\xi\, \xi \frac{[1 + \exp\{-\tilde{\beta}[\xi^2 + (1+v)\kappa^2 + 2\sqrt{1+v}\,\kappa\xi\cos\theta - 1]\}]^{-1}}{2\xi^2 + 2(1+v)\kappa^2 - 2 + \tilde{\Delta}_\kappa(\tilde{T})} \\ \times[1 + \exp\{-\tilde{\beta}[\xi^2 + (1+v)\kappa^2 - 2\sqrt{1+v}\,\kappa\xi\cos\theta - 1]\}]^{-1} , \end{aligned} \tag{35}$$

Table 1
Critical temperatures T_c/T_μ for $\lambda = \frac{1}{2}$ depicted in Fig. 4 according to (36). The exact result is compared with the linear-in-K approximation for both $\Delta_K(T)$ and $\Delta_K(0)$ in order to test sensitivity of a temperature-dependence of the CP binding energy for nonzero K

v	Linear approx. with $\Delta_K(T)$	Linear approx. with $\Delta_K(0)$	Exact
0.03	0.078	0.068	0.065
0.04	0.089	0.079	0.075
0.05	0.100	0.088	0.084
0.06	0.109	0.096	0.091
0.07	0.117	0.104	0.098

where $v \equiv \hbar\omega_D/\mu$, $\xi_{\min}(\theta) \equiv \sqrt{1+v}\,\kappa\cos\theta + \sqrt{1-(1+v)\,\kappa^2\sin^2\theta}$, $\xi_{\max}(\theta) \equiv -\sqrt{1+v}\,\kappa\cos\theta + \sqrt{(1+v)(1-\kappa^2\sin^2\theta)}$ and

$$\theta_{\min} = \begin{cases} 0 & \text{if } 2\kappa < 1-\sqrt{(1-v)/(1+v)}\,, \\ \cos^{-1}(v/\{4\sqrt{1+v}\,\kappa\sqrt{1+v/2-(1+v)\kappa^2}\}) & \text{otherwise}\,. \end{cases}$$

In (35) we have introduced the more general dimensionless quantities $\xi \equiv k/k_\mu$, $\tilde{\Delta}_\kappa(\tilde{T}) \equiv \Delta_K(T)/\mu$, where $\tilde{T} \equiv k_B T/\mu$ or $\tilde{\beta} \equiv \mu\beta$, and $\kappa \equiv K/2\sqrt{k_\mu^2 + k_D^2}$.

To obtain the critical temperature from the finite-temperature dispersion relation, besides solving (29) for $\Delta_K(T)$, one needs (12), (15), (22) and (26). At $T = T_c$ both $N_{B,0}(T_c) \simeq 0$ and $\mu_B(T_c) \simeq 0$ so that one gets the implicit T_c-equation for the *binary mixture gas*

$$1 = \frac{\tilde{T}_c}{v}\ln\left[\frac{1+\mathrm{e}^{-\{\tilde{\Delta}_0(\tilde{T}_c)/2-v\}/\tilde{T}_c}}{1+\mathrm{e}^{-\{\tilde{\Delta}_0(\tilde{T}_c)/2+v\}/\tilde{T}_c}}\right] + \frac{8(1+v)}{v}\int_0^{\kappa_0(\tilde{T}_c)} \mathrm{d}\kappa \frac{\kappa}{\mathrm{e}^{[\tilde{\Delta}_0(\tilde{T}_c)-\tilde{\Delta}_\kappa(\tilde{T}_c)]/\tilde{T}_c}-1}\,. \tag{36}$$

This must be solved numerically for the exact T_c for each λ and v in conjunction with (27) for $\tilde{\Delta}_0(\tilde{T})$ and (35) for both $\tilde{\Delta}_\kappa(\tilde{T})$ and $\kappa_0(\tilde{T}_c)$. Results for $\lambda = 1/2$ are shown in Table 1 and Fig. 4 for a range of v values typical [35] of cuprates.

In order to make this comparison we have taken $T_\mu/T_F \simeq 1$, a very good approximation up to the highest temperatures dealt with. For example, from Fig. 4 the highest $T_c/T_F \simeq 0.14$ already gives $T_\mu/T_F \simeq 0.9999$ from (26), while for smaller T_c/T_F the values of T_μ/T_F are even closer to 1. The T_c resulting from the exact dispersion relation for $T = 0$ (dot-dashed curve) is somewhat higher than the exact result (full curve) but lower than that using the linear approximation for $\Delta_K(T)$ (dotted curve). It is also clear that the effect of using the exact or linear (in K) cases dominates the effect of the dispersion relation T-dependence. For cuprates $d \simeq 2.03$ has been suggested [37] to be more realistic as it reflects inter-CuO-layer couplings but our results in that case would be very similar to those reported here for $d = 2$.

Thus, for $v = 0.05$ the exact T_c is seen to be about 46% lower than the heuristic result found in Ref. [31], Eqs. (15) and (23). It is curious that all results depend very

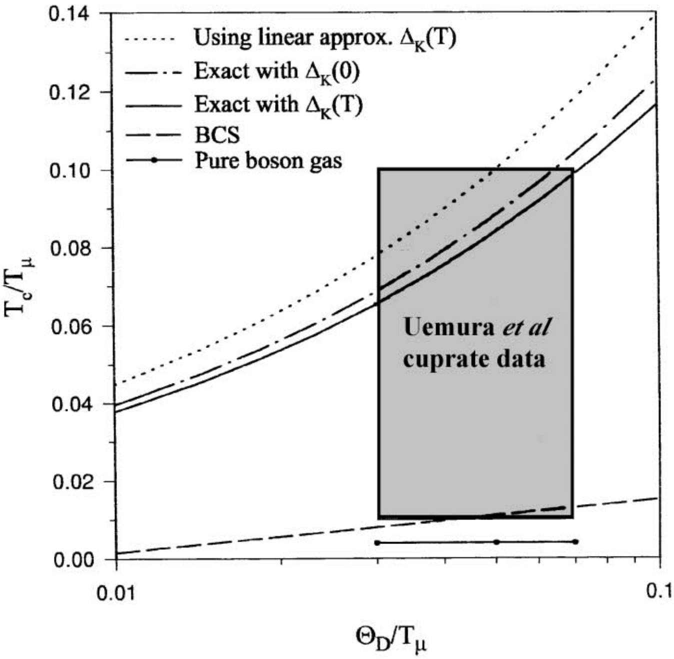

Fig. 4. Critical BEC temperature T_c in units of T_F, resulting for the boson–fermion mixture from (36) for $\lambda = \frac{1}{2}$ for varying $\nu \equiv \hbar\omega_D/\mu \simeq \Theta_D/T_F$: with no approximations (full curve); using $\Delta_K(T)$ evaluated at $T = 0$ (dot-dashed); using the linear-in-K approximation for $\Delta_K(T)$ (dotted). The dashed straight line is the BCS formula $T_c \simeq 1.13\Theta_D e^{-1/\lambda}$ for $\lambda = \frac{1}{2}$. The very lowest full horizontal line is the solution of the implicit T_c-equation (28) for the pure unbreakable-boson gas for $\nu = 0.03, 0.05$ and 0.07. A huge T_c enhancement thus follows *from the mere presence* of background unpaired fermions. Cuprate data are taken from Ref. [36].

weakly on the T-dependence of the CP binding energy $\Delta_K(T)$, in spite of its being substantial throughout the temperatures spanned in this paper, as seen in Fig. 2.

We defer study of the condensate fraction $N_{B,0}(T)/N_B(T)$ below T_c and merely surmise that it may ultimately help explain the apparent absence [38,39] in cuprates of the Hebel–Slichter peak of nuclear-spin (NMR) relaxation rates vs. temperature for $0 \leqslant T \leqslant T_c$. Such a peak, originally seen [40] in aluminum, is perhaps the most stringent and qualitatively convincing experimental test of BCS theory (Refs. [23], p. 71 and [41], p. 79 ff). Besides cuprates, it is also absent [42] in several quasi-1D Bechgaard [9] and in several quasi-2D (ET) organic salt superconductors.

7. Conclusions

A simple statistical model treating CPs as non-interacting bosons in thermal and chemical equilibrium with unpaired fermions is proposed. The model gives rise to a boson number that is strongly coupling- and temperature-dependent. Since the CP dispersion relation is approximately linear, it exhibits a Bose–Einstein condensation of zero-CMM pairs at precisely two dimensions. Exact transition temperatures for the boson–fermion mixture based upon the exact CP dispersion relation are in reasonable agreement with empirical cuprate data.

Needless to say, further corrections are yet to be included in the present simple binary mixture boson–fermion model, e.g., (i) realistic Fermi surfaces, (ii) Van Hove singularities [43] or other means of accounting for periodic-crystalline effects, as well as (iii) the all important d-wave interfermionic interaction, (iv) the boson–fermion interaction and (v) residual interbosonic interactions. As to the latter, also generally neglected in BCS theory, if the lowering [44] of T_c in liquid ^{4}He by about 29% with respect to the ideal Bose gas BEC T_c is any guide, interbosonic interactions will also lower T_c in a more realistic picture. As to the boson–fermion interaction, it is precisely this ingredient that enabled T.D. Lee and coworkers [18], and Tolmachev [19] more generally, to link BCS and BEC through a relation stating that the BE condensate fraction is proportional to the (BCS-like) fermionic gap $\Delta(T)$ squared.

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