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Bose–Einstein condensation of nonzero-center-of-mass-momentum Cooper pairs

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Abstract

Cooper pair (CP) binding with both zero and nonzero center-of-mass momenta (CMM) is studied with a set of renormalized equations assuming a short-ranged (attractive) pairwise interfermion interaction. Expanding the associated dispersion relation in 2D in powers of the CMM, in weak-to-moderate coupling a term *linear* in the CMM dominates the pair excitation energy, while the quadratic behavior usually assumed in Bose–Einstein (BE) condensation studies prevails for any coupling *only* in the limit of zero Fermi velocity when the Fermi sea disappears, i.e., in vacuum. In 3D this same behavior is observed numerically. The linear term, moreover, exhibits CP breakup beyond a threshold CMM value which vanishes with coupling. This makes all the excited (nonzero-CMM) BE levels with preformed CPs collapse into a single ground level so that a BCS condensate (where only zero CMM CPs are usually allowed) appears in zero coupling to be a special case in either 2D or 3D of the BE condensate of linear-dispersion-relation CPs.

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1. Introduction

We consider an s-wave short-range, attractive (rank one) separable interfermionic potential [1] in d-dimensional momentum space $V_{pq} = -(v_0/L^d) \times g_p g_q$, where $v_0 \geqslant 0$ is the interaction strength, L the size of the system, and the g_p's are dimensionless form factors of the type $g_p = (1 + p^2/p_0^2)^{-1/2}$ in which p_0 is the inverse range of the potential. Thus, e.g., $p_0 \to \infty$ implies $g_p = 1$ which corresponds to a contact or delta potential $-v_0\delta(\mathbf{r})$ in configuration space. In either 2D or 3D such a potential well has an infinite number of bound states. As a result a many-fermion system with this interfermion interaction will collapse in the thermodynamic limit to infinite binding per particle and infinite density. However, the potential can be "regularized", i.e., constructed [2] with v_0 infinitesimally small so that it supports a *single* bound state.

The Cooper pair (CP) equation [3] for two interacting electrons of mass m above the Fermi

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surface, with momenta wave vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ and finite, nonzero-center-of-mass-momenta (CMM) wave vector $\mathbf{K} \equiv \mathbf{k}_1 + \mathbf{k}_2$, and relative momentum wave vector $\mathbf{k} \equiv (1/2)(\mathbf{k}_1 - \mathbf{k}_2)$, gives the total pair energy $E_K \equiv 2E_F - \Delta_K$ in terms of v_0, with $E_F \equiv \hbar^2 k_F^2/2m$ the Fermi energy. Here $\Delta_K \geqslant 0$ is the CP binding energy; it should not be confused with the BCS energy gap Δ. One can eliminate the variable v_0 in favor, in 2D, of the vacuum bound-state energy $B_2 \geqslant 0$ of the potential by combining [4] the CP equation with the respective Lippmann–Schwinger one for the same interfermion interaction acting not in the Fermi sea but in vacuum. Then Δ_K can be extracted as a function of B_2 from the resulting *renormalized CP equation*

$$\sum_k \frac{g_k^2}{B_2 + \hbar^2 k^2/m} - \sum_{k,(|\mathbf{K}/2 \pm \mathbf{k}| > k_F)} \times \frac{g_k^2}{\hbar^2 k^2/m + \Delta_K - 2E_F + \hbar^2 K^2/4m} = 0. \quad (1)$$

2. Cooper pair dispersion relation

After some algebra one finds the remarkable identity, but only in 2D, that $\Delta_0 = B_2$, i.e., for an attractive delta interaction (regularized or not) the vacuum and zero-CMM CP binding energies coincide for *all* coupling. Using $E_F/k_F \equiv \hbar v_F/2$ one can expand Δ_K in powers of K for any coupling B_2 and get

$$\begin{aligned} \varepsilon_K &\equiv (\Delta_0 - \Delta_K) \\ &= \frac{2}{\pi}\hbar v_F K + \left[1 - \left\{2 - \left(\frac{4}{\pi}\right)^2\right\}\frac{E_F}{B_2}\right] \\ &\quad \times \frac{\hbar^2 K^2}{2(2m)} + O(K^3) \quad (2D) \end{aligned} \quad (2)$$

where a nonnegative *CP excitation energy* ε_K has been defined. It is this excitation energy that enters in the BE distribution function in determining the critical temperature in a picture of superconductivity as a BE condensation (BEC) of CPs. The leading term in Eq. (2) is linear in CMM, followed by a quadratic term. The latter is precisely the kinetic energy of what was originally the ordinary CP (and now is what is sometimes called a "local pair") – namely the familiar nonrelativistic energy of the composite pair of mass $2m$ in vacuum. This dispersion relation has been the starting point for virtually all BEC studies of superconductivity (see, e.g., Refs. [1,5–13], among others). However, it is clear from Eq. (2) that the quadratic term $\hbar^2 K^2/2(2m)$ will prevail for any nonzero coupling *only* when $E_F/k_F \equiv \hbar v_F/2 \to 0$, i.e., in the vacuum limit when there is no Fermi sea.

Fig. 1 shows exact numerical results (full curves) of Eq. (1) in 2D for different B_2/E_F of the CP excitation energy ε_K/Δ_0 as function of CMM K/k_F. Note that the CPs *break up* at $\varepsilon_K/\Delta_0 = 1$ where $\Delta_K = 0$, this being marked by large dots in the figure. In addition to the exact results we also exhibit the linear approximation $2\hbar v_F K/\pi$ (dot-dashed lines) for small B_2/E_F, as well as the quadratic approximation $\hbar^2 K^2/2(2m)$ (dashed parabolas) for large B_2/E_F.

In 3D one obtains [14] similar results except that the dimensionless s-wave scattering length $k_F a$ in vacuum plays the role of a coupling parameter instead of the dimensionless binding energy B_2/E_F in the 2D case. Here, the limit $\Delta_0 \to 0$ implies

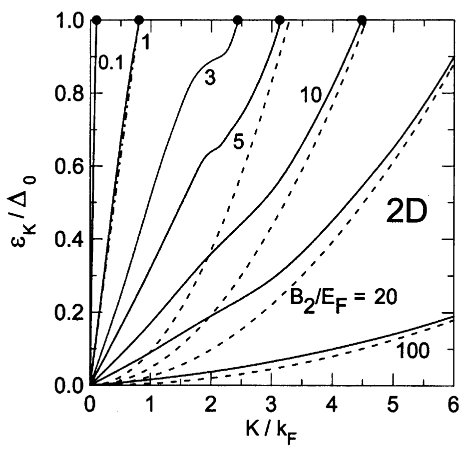

Fig. 1. Exact numerical results (full curves) for CP dispersion relation $\varepsilon_K \equiv \Delta_0 - \Delta_K$ (in units of $K = 0$ CP binding energy Δ_0) obtained from Ref. [1] when $g_k = 1$ for different coupling values B_2/E_F. CPs break up when Δ_K turns negative, as indicated by large dots. The dot-dashed line is the linear approximation (virtually coincident with the exact curve for all $B_2 \leqslant 0.1E_F$) while the quadratic approximation is shown dashed (see text for details).

$a \to 0^-$ or $1/k_F a \to -\infty$ and corresponds to weak coupling, while the limit $\Delta_0 \to \infty$ implies $a \to 0^+$ or $1/k_F a \to +\infty$ and is strong coupling. In fact, for $a = -|a| \to 0^-$ one finds $\Delta_0 \to (8E_F/e^2)\exp(-\pi/k_F|a|)$, a result first obtained by Van Hove [15]. On the other hand, $a \to 0^+$ yields $\Delta_0 \to \hbar^2/ma^2$. Repeating the expansion carried out in 2D but without explicitly determining the coefficient of the quadratic term gives

$$\varepsilon_K \equiv (\Delta_0 - \Delta_K) \to \tfrac{1}{2}\hbar v_F K + O(K^2) \quad (3D) \tag{3}$$

i.e., the same result cited in 1964 in Ref. [16] for the BCS model interaction. The linear terms in both Eqs. (2) and (3) are identical [17] for the BCS model interaction in weak coupling. In this case $g_k = \theta(\hbar^2k^2/2m - \max[0,(E_F - \hbar\omega_D)])\theta(E_F + \hbar\omega_D - \hbar^2k^2/2m)$, where $\theta(x)$ is the Heaviside step function and ω_D the Debye frequency. It becomes $g_k = 1$ as $\hbar\omega_D \to \infty$.

3. Boson number

Using a statistical model [18] guaranteeing both thermal and chemical equilibrium in an ideal boson–fermion mixture, the number of bosons $N_B(T)$ formed within the N-fermion system, valid at and below the BEC transition temperature T_c, is

$$N_B(T) \equiv \frac{1}{2}[N - N_0(T)] = \frac{N}{2}\left[1 - (T/T_F)\ln\left(1 + e^{-\beta\{\Delta_0(T)/2 - \mu(T)\}}\right)\right], \tag{4}$$

where $N_0(T)$ is the number of unpaired fermions, $\Delta_0(T)$ the appropriate finite-T generalization [18] of the CP $K = 0$ binding energy, $\beta \equiv 1/k_BT$, and the ideal Fermi gas chemical potential $\mu(T)$ in 2D is given exactly by

$$\mu(T) = \beta^{-1}\ln\left(e^{\beta E_F} - 1\right) \underset{T\to 0}{\longrightarrow} E_F. \tag{5}$$

Fig. 2 illustrates the zero CMM CP binding energy $\Delta_0(T)$ for three values of $B_2/\mu(T)$.

At $T = 0$ Eq. (4) becomes

$$N_B(0) = N\Delta_0(0)/4E_F \equiv NB_2/4E_F \quad (B_2 \leqslant 2E_F)$$
$$= N/2 \quad (B_2 \geqslant 2E_F). \tag{6}$$

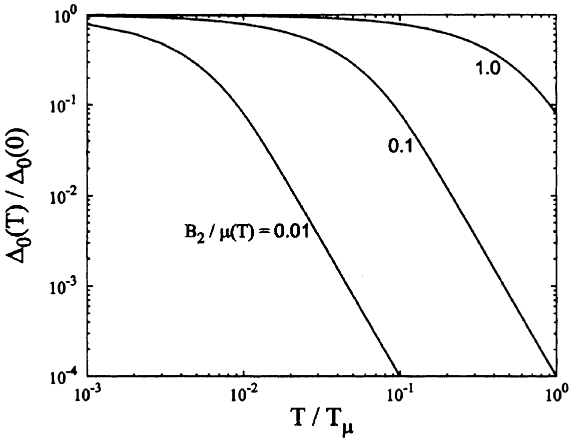

Fig. 2. Temperature dependence of 2D zero-CMM CP binding energy $\Delta_0(T)$ vs. T/T_μ for several couplings $B_2/\mu(T)$, where $k_BT_\mu \equiv \mu$.

This should be compared with the BCS theory estimate (Ref. [5], p. 128)

$$N_B(0) \sim (\Delta/E_F)^2\frac{N}{2} = N(B_2/E_F), \tag{7}$$

where here Δ is the BCS $T = 0$ energy gap, and the exact 2D result [19] $\Delta = \sqrt{2E_FB_2}$ was used in the last step. Since $N_B \leqslant N/2$, the estimate implies a breakdown for $B_2 \geqslant E_F/2$ in the BCS case.

4. Critical temperature

Neglecting the background unpaired fermions and modeling the entire system as a *pure boson gas* of unbreakable CPs but with temperature-dependent boson number density $n_B(T) \equiv N_B(T)/L^2$, the explicit BEC T_c-formula for linear dispersion bosons in 2D [20] becomes an *implicit* one by allowing n_B to be T-dependent, namely

$$T_c = \frac{4\sqrt{3}}{\pi^{3/2}}\frac{\hbar v_F}{k_B}\sqrt{n_B(T_c)}. \tag{8}$$

This differs from the familiar BEC 3D formula $T_c \simeq 3.31\hbar^2 n_B^{2/3}/m_Bk_B$ for quadratic-dispersion bosons. Both equations are special cases of the more general expression [20] of the form $T_c \propto n_B^{s/d}$ for any space dimensionality $d > 0$ and any boson dispersion relation $\varepsilon_K \propto K^s$ with $s > 0$. Solving

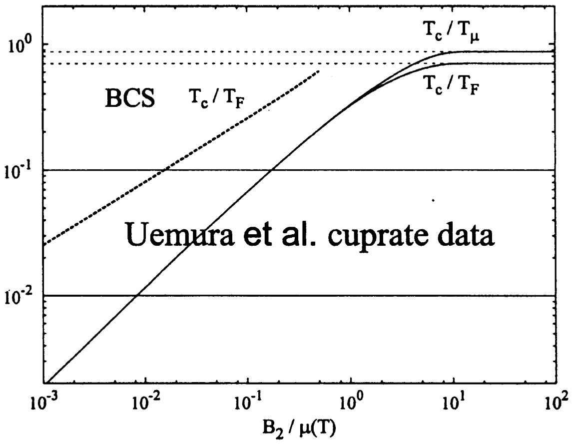

Fig. 3. Critical BEC temperatures (full curves), for the pure unbreakable-boson gas, in units either of T_F or $T_\mu \equiv \mu(T)/k_B$, compared with the BCS result (slanted dashed curve), vs. dimensionless coupling $B_2/\mu(T)$. Empirical cuprate data are taken from Ref. [21].

Eq. (8) with Eqs. (4) and (1) for $K=0$ self-consistently gives T_c/T_F vs. B_2/E_F as displayed in Fig. 3 and compared with empirical values for cuprates that range [21] from 0.01–0.1.

Also shown in the figure are the BCS theory T_c's (see also Ref. [22]) obtained by solving the single implicit equation

$$\int_0^1 \frac{dx}{x} \tanh \frac{T_F}{2T_c} x = \ln\left(\frac{\pi T_c}{e^{\gamma} B_2}\right), \tag{9}$$

where γ is the Euler constant. Note that $k_B T_c \to (e^{\gamma}/\pi)\sqrt{2B_2E_F}$ as coupling goes to zero, and also that $2\Delta/k_BT_c \to 2\pi/e^{\gamma} \simeq 3.53$.

5. BCS and Bose–Einstein condensates

Finally, Fig. 4 depicts in either 2D or 3D both condensates, the BCS one with its *single* $K=0$ pair-correlation state and the BE condensate [20] with both (ground) $K=0$ *and* several (excited) $K>0$ CP states that form a "band" (shown in the figure as a discrete spectrum for clarity) extending up to the breakup state K_0 defined by $\Delta_{K_0}=0$. For perfectly linear dispersion CPs, i.e., in 2D $\varepsilon_K \equiv \Delta_0 - \Delta_K = 2\hbar v_F K/\pi$, the breakup CMM wave number is then just $K_0 = \pi\Delta_0/2\hbar v_F$. As this vanishes with coupling all the excited boson levels collapse downwards and merge with the ground $K=0$ level, i.e., the bandshrinks to the single ground level. Thus, for zero coupling the BCS condensate appears to be a special case of the BE condensate provided that the BCS CCs are essentially CPs, as is widely believed.

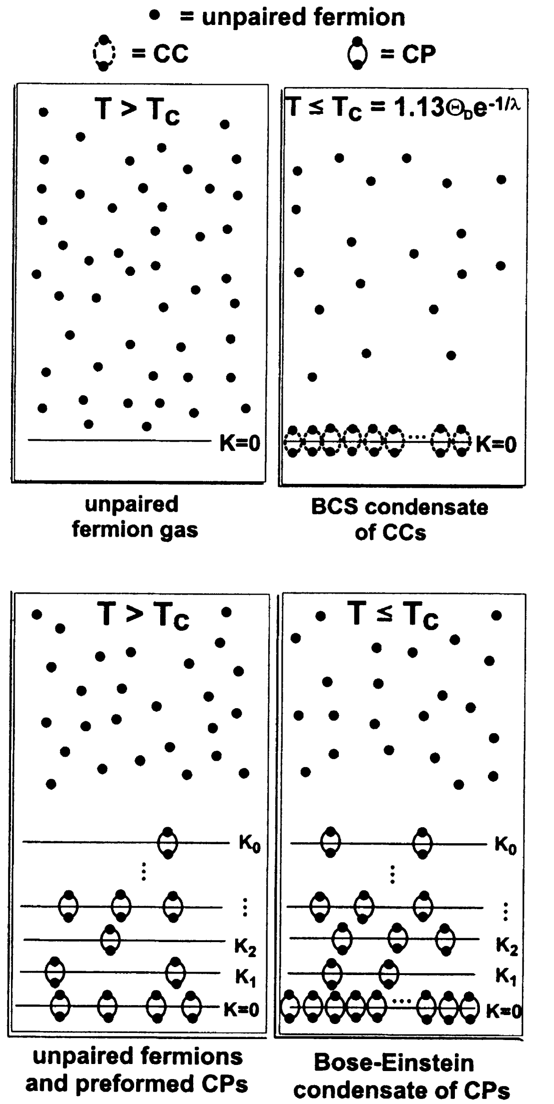

Fig. 4. BCS pair condensate of Cooper correlations (CCs) and BE condensate of CPs, both below T_c, compared as explained in text, along with their respective normal states at $T > T_c$. Horizontal *ellipsis* indicate a fractional particle occupation which is macroscopic, or significant compared with unity.

6. Discussion

Besides including the background unpaired fermions in the real *mixture* problem with our simple initial s-wave interfermion interaction, further refinements pending are: (i) realistic Fermi surfaces; (ii) Van Hove singularities or other means of accounting for periodic-crystalline effects; as well as the following interactions; (iii) the all-important d-wave; (iv) residual interbosonic ones; and (v) the crucial CP-fermion interaction vertex. It is precisely the latter ingredient that enabled Lee and coworkers [12], and Tolmachev [13] more generally, to link BCS and BEC through a relation whereby the BE condensate fraction is proportional to the (BCS-like) fermionic gap $\Delta(T)$ squared.

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