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

J. Batle, M. Casas

Departament de Física, Universitat de les Illes Balears
07071 Palma de Mallorca, Spain

M. Fortes, M.A. Solís

Instituto de Física, Universidad Nacional Autónoma de México
Apdo. Postal 20-364, 01000 México, DF, Mexico

M. de Llano, A.A. Valladares

Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México
Apdo. Postal 70-360, 04510 México, DF, Mexico

O. Rojo

PESTIC, Secretaría Académica & CINVESTAV - IPN, 04430 México, DF, Mexico

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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 attractive pairwise interfermion interaction. 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 ground level so that a BCS condensate (where only zero 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 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 \( V_{pq} = - (v_0 / L^d) g_p g_q \) where \( v_0 \geq 0 \) 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 \(- v_0 \delta(r)\) 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 CP equation 3 for two interacting electrons of mass \( m \) above the Fermi surface, with momenta wavevectors \( k_1 \) and \( k_2 \) and finite, nonzero CMM wavevector \( K \equiv k_1 + k_2 \), and relative momentum wavevector \( \mathbf{k} \equiv \mathbf{k}_1 - \mathbf{k}_2 \), gives the total pair energy \( E_K = 2E_F - \Delta_K \) in terms of \( v_0 \), with \( E_F \equiv \hbar^2 k_F^2 / 2m \) the Fermi energy. Here \( \Delta_K \geq 0 \) is the CP binding energy; it should not be confused with the BCS energy gap \( \Delta \). One can eliminate the variable \( v_0 \) in favor, in 2D, of the vacuum bound-state energy \( B_2 \geq 0 \) 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 \( \Delta_K \) can be extracted as a function of \( B_2 \) from the resulting renormalized CP equation

\[
\sum_k \frac{g_k^2}{B_2 + \hbar^2 k^2 / m} = \sum_{k,(|K/2|k_1)|>k_F)} \frac{g_k^2}{\hbar^2 k^2 / m + \Delta_K - 2E_F + \hbar^2 K^2 / 4m} = 0.
\]  

(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 attrac-
tive delta interaction (regularized or not) the vacuum and zero-CMM CP binding energies coincide for all coupling. Using $E_F/k_F = \hbar v_F/2$ one can expand $\Delta_K$ in powers of $K$ for any coupling $B_2$ and get

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

where a nonnegative CP *excitation energy* $\epsilon_K$ 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 (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., [1, 6, 8], among others). However, it is clear from (2) that the quadratic term $\hbar^2 K^2/(2m)$ will prevail for any nonzero coupling only when $E_F/k_F = \hbar v_F/2 \to 0$, i.e., in the vacuum limit when there is no Fermi sea.

Figure 1 shows exact numerical results (full curves) of (1) in 2D for different $B_2/E_F$ of the CP excitation energy $\epsilon_K/\Delta_0$ as function of CMM $K/k_F$. Note that the CPs break up at $\epsilon_K/\Delta_0 = 1$ 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 $\hbar^2 K^2/(2m)$ (dashed parabolas) for large $B_2/E_F$.

In 3D one obtains 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 $a \to 0^-$ 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 $\Delta_0 \to (8E_F/\pi^2) \exp(-\pi/|k_F a|)$, a result first obtained by Van Hove [13]. 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

$$
\epsilon_K \equiv (\Delta_0 - \Delta_K) \to \frac{1}{2} \hbar v_F K + O(K^2), \quad (3D) \quad (3)
$$

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

3. Boson number

Using a statistical model [13] 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

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

where $N_0(T)$ is the number of unpaired fermions, $\Delta_0(T)$ the appropriate finite-$T$ generalization [13] of
the CP \( K = 0 \) binding energy, \( \beta \equiv 1/k_B T \), and the ideal Fermi gas chemical potential \( \mu(T) \) in 2D is given exactly by

\[
\mu(T) = \beta^{-1} \ln(e^{\beta E_F} - 1) \xrightarrow{T \to 0} E_F. \tag{5}
\]

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

At \( T = 0 \) \cite{footnote} becomes

\[
N_B(0) = N \Delta_0(0)/4E_F \equiv NB_2/4E_F \quad (B_2 \leq 2E_F) = N/2 \quad (B_2 \geq 2E_F). \tag{6}
\]

This should be compared with the BCS theory estimate (Ref. \cite{footnote}, p. 128)

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

where here \( \Delta \) is the BCS \( T = 0 \) energy gap, and the exact 2D result \cite{footnote} \( \Delta \) \( \Delta = \sqrt{2E_FB_2} \) was used in the last step. Since \( N_B \leq N/2 \), the estimate implies a breakdown for \( B_2 \geq E_F/2 \) 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 \cite{footnote} becomes an implicit one by allowing \( n_B \) to be \( T \)-dependent, namely

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

This differs from the familiar BEC 3D formula \( T_c \simeq 3.31 \hbar^2 n_B^{2/3}/m_B k_B \) for quadratic-dispersion bosons. Both equations are special cases of the more general expression \cite{footnote} of the form \( T_c \propto n_B^{s/d} \) for any space dimensionality \( d \geq 0 \) and any boson dispersion relation \( \varepsilon_K \propto K^s \) with \( s > 0 \). Solving (\ref{footnote}) with (\ref{footnote}) and (\ref{footnote}) for \( K = 0 \) self-consistently gives \( T_c/T_F \) vs. \( B_2/E_F \) as displayed in Figure 3 and compared with empirical values for cuprates that range \cite{footnote} from 0.01 \( \sim 0.1 \).

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

Also shown in the figure are the BCS theory \( T_c \)'s (see also Ref. \cite{footnote}) obtained by solving the single implicit equation

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

where \( \gamma \) 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 \( 2\Delta/k_B T_c \to 2\pi/e^{\gamma} \simeq 3.53 \).

5. BCS and BE condensates

Finally, Figure 4 depicts in either 2D or 3D both condensates, the BCS one with its single \( K = 0 \) pair-correlation state and the BE condensate \cite{footnote} 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 $\varepsilon_K \equiv \Delta_0 - \Delta_K = 2v_F K/\pi$, the breakup CMM wavenumber is then just $K_0 = \pi \Delta_0/2v_F$. As this vanishes with coupling all the excited boson levels collapse downwards and merge with the ground $K = 0$

![Diagram](image)

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

level, i.e., the “band” shrinks 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.

### 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 T.D. Lee and coworkers [7], and Tolmachev [8] 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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