

Excited cooper pairs

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Excited Cooper pairs formed in a many-fermion system are those with nonzero total center-of-mass momentum (CMM). They are normally neglected in the standard Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity for being too few compared with zero CMM pairs. However, a Bose-Einstein condensation picture requires both zero and nonzero CMM pairs. Assuming a BCS model interaction between fermions we determine the populations for *all* CMM values of Cooper pairs by actually calculating the number of nonzero-CMM pairs relative to that of zero-CMM ones in both 2D and 3D. Although this ratio decreases rapidly with CMM, the number of Cooper pairs for any specific CMM less than the maximum (depairing or breakup) momentum turns out to be typically larger than about 95% of those with zero-CMM at zero temperature T . Even at $T \sim 100$ K this fraction in 2D is still as large as about 70% for typical quasi-2D cuprate superconductor parameters.

Keywords: Excited Cooper pairs; BCS theory; Bose-Einstein condensation

Los pares de Cooper excitados formados en un sistema de muchos electrones, son aquellos con momentos de centro de masa (CMM) diferente de cero. Normalmente éstos no son tomados en cuenta en la teoría estandar de la superconductividad de Bardeen-Cooper-Schrieffer (BCS) al suponer que su número es muy pequeño comparados con los pares de centro de masa igual a cero. Sin embargo, un esquema de condensación Bose-Einstein requiere de ambos pares, con CMM cero y diferente de cero. Asumiendo una interacción modelo BCS entre los fermiones, determinamos la población de pares Cooper con cada uno de todos los posibles valores del CMM calculando el número de pares con momentos de centro de masa diferente de cero relativo a los pares de CMM igual a cero, en 2D y 3D. Aunque esta razón decrece rápidamente con el CMM, el número de pares de Cooper para cualquier CMM específico menor que el momento máximo (o rompimiento del par) es típicamente más grande que el 95% de aquellos con CMM cero. Aún a $T \sim 100$ K esta fracción en 2D es alrededor del 70% para parámetros típicos de cupratos superconductores cuasi-bidimensionales.

Descripciones: Pares de Cooper excitados; teoría BCS; condensación Bose-Einstein

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1. Introduction

Pairing of fermions in superconductivity theories is commonly considered to be only among partners of equal and opposite linear momenta, thus forming pairs with *zero* net center-of-mass momentum (CMM). Although it is recognized [1] that pairs with total momentum different from zero are present in a superconductor, these are generally neglected by arguing that they are much less numerous than pairs with zero total momentum. To our knowledge, this has never before been explicitly calculated.

Since it was generally accepted that BCS theory is at best hard-pressed to explain the new high-critical-temperature superconductors, many new and original microscopic paradigms have been proposed [2]. However, there still lacks both a dynamical mechanism as well as a many-body theory able to account for such high transition-temperatures and, better still, capable of predicting the existence of new materials with even higher (hopefully room) critical temperatures.

Into this host of new theories of superconductivity has been reintroduced [3] the Bose-Einstein condensation of fermion (electron or hole) pairs considered as bosons, in

which an *appreciable* fraction of them occupies the lowest energy level of the system when it is cooled below a certain critical temperature. This idea is not new since Blatt, Schrafroth and others [4] used it even before the BCS theory appeared. Cooper pairs can at worst be considered "quasi-bosons" even though their creation/annihilation operators do not exactly satisfy the well-known Bose commutation relations since for definite CMM (but *not* definite *relative* momentum) they obey [3] Bose-Einstein statistics. Specifically, an indefinite number of pairs with fixed $(\mathbf{k}_1, \mathbf{k}_2)$ can vectorially add up to the *same* CMM $\hbar\mathbf{K}$, zero or not—the Pauli principle for each pair of fermions being strictly obeyed.

On the other hand, collective modes (or phonon-like excitations) in a superconductor have indeed been recognized since the late 1950's by Bogoliubov, Tolmachev, Shirkov, Nambu, Anderson, Rickayzen, and Bardasis and Schrieffer. A review of the early work by Martin is available [5], as is a more recent note by Belkhir and Randeria [6]. However, we do *not* deal here with "collective-mode phonons" but rather with (nonzero CMM) "Cooper pairs" which can Bose-Einstein-condense while phonons cannot. Cooper pairs

re entities distinct from collective modes such as zero-sound phonons or plasmons since they: a) are bounded in number before the thermodynamic limit is taken, and b) are fixed in number as they carry a fixed constituent-fermion-number (namely two)—while phonons or plasmons, say, *do not* share either property.

Although extensive studies in the BCS-Bose “crossover” problem have been reported [7] for over thirty years, we note that BEC within the standard (*i.e.*, $K = 0$ Cooper-pair) BCS picture is strictly impossible as only *one* boson state is allowed to exist, namely, $K = 0$. The significantly novel ingredient in Ref. 3 is to take account of the electron pairs with *linear*, as opposed to a *quadratic*, dispersion relation.

If bosons satisfy a quadratic dispersion relation, *i.e.*, their kinetic energies are $\epsilon_k = \hbar^2 k^2 / 2m$, then the critical temperature in d -dimensions [8, 9] valid for any dimension $d > 0$ is

$$T_c = \frac{2\pi\hbar^2}{mk_b} \left[\frac{n_b}{g_{d/2}(1)} \right]^{2/d},$$

where m is the boson mass, n_b the number density of bosons, k_b the Boltzmann constant, and $g_{d/2}(1)$ the Bose function $g_\sigma(z) = \sum_{l=1}^{\infty} z^l / l^\sigma$. For $z = 1$ and $\sigma \geq 1$, $g_\sigma(z) = \zeta(\sigma)$, the Riemann Zeta function of order σ . Thus, if $0 < d \leq 2$ then $T_c = 0$ because the function $g_\sigma(1) \rightarrow \infty$ for $\sigma \leq 1$. $d = 2$, $g_1(1) = \zeta(1) = 1 + \frac{1}{2} + \frac{1}{3} + \dots$, the harmonic series which diverges. If $d = 1$ we have the series $g_{1/2}(1) = 1 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \dots$, which plainly diverges faster than $g_1(1)$. In particular, if $d = 3$ the critical temperature is the familiar result

$$T_c = \frac{2\pi\hbar^2 n^{2/3}}{mk_b [\zeta(3/2)]^{2/3}} \simeq \frac{3.31\hbar^2}{mk_b} n^{2/3},$$

since $\zeta(3/2) \simeq 2.612$. Superconductivity for quasi-2D materials could *in principle* be explained as a BE condensation of such bosons, but *not* for quasi-1D materials like the organometallic Bechgaard-salt superconductors consisting of parallel molecular chains [10].

However, Cooper pairs by definition move not in a vacuum but rather in a Fermi sea. Thus, they need not possess a quadratic dispersion relation. The correct [11] dispersion relation for Cooper pairs is *linear* in the long wavelength limit, specifically, for weak coupling

$$\epsilon_K = a(d)v_f \hbar K \quad \text{when } K \rightarrow 0,$$

where $\hbar K$ is the CMM of the pair, $a(d)$ a dimensionless coefficient of order one, d the system dimension, and v_f the Fermi velocity of the underlying fermion gas. Cooper pairs with $K > 0$ move in every possible direction; they are *not* to be confused with those moving with a nonzero *drift-velocity* in a given direction, and which participate in a supercurrent with $K = 0$ pairs belonging to the BE condensate. The critical temperature associated with these bosons in the weak-coupling limit is [9]

$$T_c = \frac{a(d)\hbar v_f}{k_b} \left[\frac{\pi^{(d/2+1/2)} n_b}{\Gamma(d/2 + 1/2) g_d(1)} \right]^{1/d},$$

where $\Gamma(x) \equiv (x-1)!$ is the gamma function. Note that now $T_c > 0$ for all $d > 1$, *i.e.*, the bosons can BE condense if the system dimension is greater than one.

It would be more realistic to visualize a model not of a *pure boson gas* but a chemical-equilibrium *mixture* [12] of unpaired fermions and bosons composed of two fermions paired by, say, the BCS model interaction [see (2) below]. This model of an ideal boson-fermion mixture at zero absolute temperature is *precisely* that described [13] by the BCS theory “condensation energy” in the ground state by assuming only that *all* pairable fermions are actually paired. As no interaction between Cooper pairs is included, this assumption would appear to be tacit in BCS theory.

In this paper we calculate and exhibit in detail the fraction of fermion pairs with a CMM wavenumber $K > 0$ relative to that of pairs with $K = 0$, in both 3D and in 2D. This fraction as a function of K and for different materials (or different $\nu \equiv \Theta_D/T_F$, where Θ_D and T_F are the Debye and Fermi temperatures of the superconductor, respectively) is *found to be substantial*, thus justifying their inclusion in a theory of superconductivity viewed as a Bose-Einstein condensation. Section 2 recalls the BCS model interaction between carrier electrons, along with the general multiple integral required to determine the number of Cooper pairs of any K ; in Sec. 3 those integrations are performed to calculate the ratio of the number of electron pairs with a given nonzero CMM to those with $K = 0$ in 3D, relegating the 2D results to the Appendix; Section 4 exhibits the number of Cooper pairs in 2D for any nonzero temperature; Section 5 contains results and discussion; and Sec. 6 conclusions.

2. Cooper pairing

Classical superconductivity has been reasonably explained by the Bardeen, Cooper and Schrieffer (BCS) theory where the central idea consists in electrons correlating to form (Cooper) pairs which then move in coherence throughout the superconductor volume. These Cooper pairs can in principle possess zero or nonzero CMM, but only the former are retained in standard BCS theory. The number of Cooper pairs, relative to the total electron number, is determined by the number of electrons which can pair up to actually bind.

With the *BCS model interaction* these lie in a narrow energy (or momentum) interval about the Fermi surface. The BCS model interaction between a pair of electrons encompasses, however imperfectly, the sum of two crucial dynamical effects: the Coulomb repulsion between electrons and an electron-phonon attraction that results from the attractive distortions produced by an electron of the background positive-ionic lattice. Some attraction, of course, is vital to bind the Cooper pairs. This particular dynamical mechanism is sufficient to explain the vanishing resistance in a superconductor, where a phonon of maximum energy $\hbar\omega_D$ is transferred be-

tween the partner electrons that form a Cooper pair. The maximum energy of a vibrating-ionic-lattice phonon is $\hbar\omega_D \equiv \hbar^2 k_D^2 / 2m^*$, where k_D is some defined wavenumber thusly associated with the Debye frequency ω_D , and m^* is the effective electron mass. If \mathbf{r}_1 and \mathbf{r}_2 are the position vectors of two electrons their relative and center-of-mass coordinates are $\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2$ and $\mathbf{R} \equiv \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$, respectively. The relevant wave vectors are related through

$$\mathbf{K} \equiv \mathbf{k}_1 + \mathbf{k}_2, \quad \mathbf{k} \equiv \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$$

or

$$\mathbf{k}_1 = \frac{\mathbf{K}}{2} + \mathbf{k}, \quad \mathbf{k}_2 = \frac{\mathbf{K}}{2} - \mathbf{k}, \quad (1)$$

with $\hbar\mathbf{K}$ the total momentum of the pair, and $\hbar\mathbf{k}$ its relative momentum, see Fig. 1. The BCS model interaction to be used here is then represented in momentum space simply by the double Fourier transform

$$V_{\mathbf{k},\mathbf{k}'}^{\mathbf{K}} = \begin{cases} -V \theta(2\sqrt{k_F^2 + k_D^2} - K) & \text{if } k_F < |\mathbf{k} \pm \frac{1}{2}\mathbf{K}|, |\mathbf{k}' \pm \frac{1}{2}\mathbf{K}| < \sqrt{k_F^2 + k_D^2}, \\ 0 & \text{otherwise,} \end{cases} \quad (2)$$

where $V > 0$ measures the intensity of the net attractive potential between the pair whose electrons have energies $\varepsilon_{\mathbf{k}_1}$, $\varepsilon_{\mathbf{k}_2}$ and $\varepsilon_{\mathbf{k}'_1}$, $\varepsilon_{\mathbf{k}'_2}$, before and after the interaction, respectively. The positive coupling constant V represents the net attractive effect of the electron-phonon attraction which overwhelms the repulsive Coulomb interaction so as to insure bound pairs. To interact, two electrons must each be within an energy interval $\hbar\omega_D$ above [14] the Fermi surface of energy E_F . Since $K \geq 0$, the step function $\theta(x)$ ensures that the interaction is nonzero only if $0 \leq K \leq 2\sqrt{k_F^2 + k_D^2}$. This means that two fermions suffer a constant attraction $-V$ when the tip of their relative-momentum wavevector \mathbf{k} points

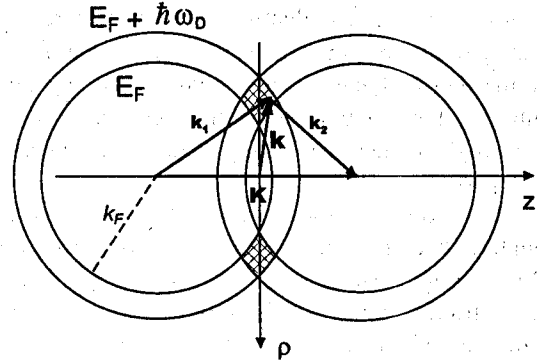


FIGURE 1. Cross section of the overlap volume of two identical spherical shells in k -space of energy thickness $\hbar\omega_D$, whose centers are separated by the magnitude of the total (CMM) wavevector $\mathbf{K} \equiv \mathbf{k}_1 + \mathbf{k}_2$ of the bound pair of fermions with wavevectors \mathbf{k}_1 and \mathbf{k}_2 formed via the BCS model interaction (2). Here $\mathbf{k} \equiv \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$ is the relative wavevector of the pair.

anywhere inside the overlap volume in k -space of the two spherical shells shown in the Fig. 1. For the particular case illustrated in the figure, this overlap volume is "ring" shaped.

The number N_K of pairs with a given K is proportional to the probability of finding one electron with wavevector \mathbf{k}_1 and a second electron with wavevector \mathbf{k}_2 which combine to give a resultant CMM wavenumber K . At $T = 0$ this probability is just the volume V_K in k -space as this consists of a simple-cubic lattice (of lattice spacing $2\pi/L$ with L the size of the box containing the system) of points each of which represents an electron state with either spin. Specifically

$$N_K \propto \int' d\mathbf{k} (1 - n_{\mathbf{k}_1})(1 - n_{\mathbf{k}_2}) \xrightarrow{T \rightarrow 0} V_K = \int' d\mathbf{k} \theta(k_1 - k_F) \theta(k_2 - k_F), \quad (3)$$

where $n_{\mathbf{k}_i}$ is the average number of electrons with wavevector of magnitude k_i , $i = 1, 2$, and where the prime means integration only over the overlapping volume allowed by (2). As in the original Cooper-pair problem [14] we restrict ourselves to $T = 0$. In this way, the magnitudes of the vectors \mathbf{k}_1 and \mathbf{k}_2 must be inside the interval $[k_F, k_F + \hbar\omega_D]$ which form shells of energy thickness $\hbar\omega_D$ about the Fermi energy. Actually bound pairs will be formed only if they suffer the attractive interaction (2), *i.e.*, we stress again, only if the tip of their relative momentum \mathbf{k} is within the overlap volume of both shells, the center-to-center distance of these spherical shells being equal to the magnitude of \mathbf{K} . For example, bound pairs with a total momentum $\hbar\mathbf{K} = 0$ are those formed by all the electrons that lie in the energy shell of magnitude $\hbar\omega_D$ about the Fermi energy. Further, the primed integral sign in

(3) requires the following factors in the integrand

$$\begin{aligned} & 1 \quad \text{if } \varepsilon_{\mathbf{k}_i} < E_F + \hbar\omega_D \\ \text{and} & \\ & 0 \quad \text{if } \varepsilon_{\mathbf{k}_i} > E_F + \hbar\omega_D, \end{aligned} \quad (4)$$

for $i = 1$ and 2 , in keeping with the upper limit to k_1 and k_2 in the BCS model interaction (2).

Strictly speaking, at $T = 0$ only $K = 0$ pairs are present [3], whereas at $T > 0$ there are both zero- and nonzero- K pairs. At $T > 0$ the step-function-sharp Fermi surface smooths out into the Fermi-Dirac distribution $n_{\mathbf{k}_i} = [\exp\{\beta[\hbar^2 k_i^2 / 2m^* - \mu(T)]\} + 1]^{-1}$ where the chemical potential $\mu(T) \xrightarrow{T \rightarrow 0} E_F$.

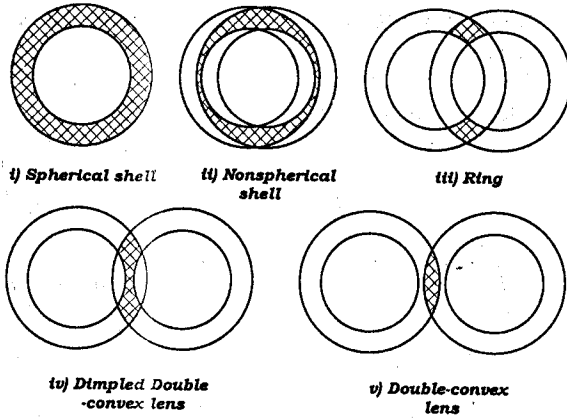


FIGURE 2. Distinct topologies associated with the overlapping volume of two spherical shells in k -space as the magnitude of \mathbf{K} , their center-to-center distance, is increased.

3. Nonzero vs. zero CMM pairs

To calculate the number of pairs with $K > 0$ relative to those with $K = 0$, we combine conditions (4) into the primed integral (3) which, recalling (1), then becomes the overlap volume in k -space

$$V_K \equiv \int dk \theta \left(\left| \frac{K}{2} + \mathbf{k} \right| - k_F \right) \theta \left(\left| \frac{K}{2} - \mathbf{k} \right| - k_F \right) \times \theta \left(\sqrt{k_F^2 + k_D^2} - \left| \frac{K}{2} + \mathbf{k} \right| \right) \times \theta \left(\sqrt{k_F^2 + k_D^2} - \left| \frac{K}{2} - \mathbf{k} \right| \right). \quad (5)$$

Though tedious, this is a straightforward multiple integration, and yields the overlapping volume of the two shells of thickness $\hbar\omega_D \equiv \hbar^2 k_D^2 / 2m^*$. Note that the overlap volume of two spheres is well-known [16] and corresponds to the particular case $k_D^2 / k_F^2 \rightarrow \infty$ above. As the number of pairs for any $K \geq 0$ is proportional to the overlap volume of the corresponding shells, the ratio required is just V_K / V_0 . There are five distinct topologies associated with the overlap volumes generated by separating the two perfectly coincident shells, depending on the magnitude K of vector \mathbf{K} which is center-to-center separation of the shell centers, Fig. 1. These topologies are shown in Fig. 2, with shaded (overlap) areas designated as follows: *i*) Spherical shell; *ii*) Non-spherical shell; *iii*) Ring; *iv*) Dimpled double-convex lens; and *v*) Double-convex lens. Although only cases *i*) and *ii*) will be physically relevant here, the rest are reported for completeness. Next we calculate the fraction of the bound pairs of electrons with $K > 0$ to those with $K = 0$, as a ratio of overlapping volumes, and as a function of K for 3D. The analogous results for 2D are summarized in the Appendix.

Consider a pair of spherical shells in k -space of identical widths $\sqrt{k_F^2 + k_D^2} - k_F$, whose centers are separated by a distance $K \equiv |\mathbf{k}_1 + \mathbf{k}_2|$. Due to axial symmetry of the resulting overlap volumes, it is convenient to use cylindrical

TABLE I. Values of different-topology boundary points κ_1 , κ_2 and κ_3 , for several values of $\nu \equiv \hbar\omega_D / E_F$. Typically, $\nu \simeq 10^{-3}$ for conventional, and $\simeq 0.05$, for cuprate superconductors.

ν	κ_1	κ_2	κ_3
1	0.1464	0.7071	0.8535
10^{-1}	0.0233	0.9535	0.9767
10^{-2}	0.0025	0.9950	0.9975
10^{-3}	0.0002	0.9995	0.9997

coordinates (ρ, φ, z) with the z axis along the vector \mathbf{K} . In these coordinates the volume element $dk = \rho d\rho d\varphi dz$ is substituted into (5). We further introduce the dimensionless variables

$$\kappa \equiv \frac{K}{2\sqrt{k_F^2 + k_D^2}}$$

and

$$\nu \equiv \frac{k_D^2}{k_F^2} = \frac{\hbar\omega_D}{E_F}, \quad (6)$$

where κ is the CMM wavenumber in terms of the maximum value it can acquire with nonzero interaction according to (2), and ν is clearly the ratio of the Debye-to-Fermi energies. The values κ_1 , κ_2 and κ_3 mark the boundaries within the interval $0 < \kappa < 1$ between different topologies; this can be deduced through simple geometry to be

$$\kappa_1 = \frac{1}{2} \left(1 - \frac{1}{\sqrt{1+\nu}} \right), \quad \kappa_2 = \frac{1}{\sqrt{1+\nu}}$$

and

$$\kappa_3 = \frac{1}{2} \left(1 + \frac{1}{\sqrt{1+\nu}} \right). \quad (7)$$

Explicitly, topology (i) above corresponds to $\kappa = 0$; (ii) to $0 < \kappa < \kappa_1$; (iii) to $\kappa_1 < \kappa < \kappa_2$; (iv) to $\kappa_2 < \kappa < \kappa_3$; and (v) to $\kappa = 1$. Table I lists actual values of these boundaries for several values of ν , including the typical ν values of conventional ($\nu \simeq 10^{-3}$) and cuprate ($0.03 \lesssim \nu \lesssim 0.07$) superconductors.

Consider now the ratio V_K / V_0 defined before, corresponding to the five distinct overlap topologies mentioned.

3.1. Spherical-shell-shaped overlap, $\kappa = 0$

When the CMM wavenumber K of pair is zero, or $\kappa = 0$, the wavevectors of the individual electrons satisfy $\mathbf{k}_1 = -\mathbf{k}_2$ so that the electrons of the pair lie in an spherical shell of internal radius k_F and external radius $\sqrt{k_F^2 + k_D^2}$, at the same distance from the center and diametrically opposite the each other. The centers of the two spherical shells of width $\hbar\omega_D$ are fixed at the origin, and the overlap volume defined by integral (5) is just

$$V_0 \equiv V_i = \left(\frac{4\pi}{3} \right) k_F^3 \left[(1 + \nu)^{3/2} - 1 \right]. \quad (8)$$

On the other hand, when $K > 0$ the tip of wavevector k_1 must lie, say, in the shell centered at the left while the tail of wavevector k_2 must lie in the shell centered at the right, both shell centers being separated by a distance K . As K is increased from zero the overlap volume of the two shells then acquires the four shapes mentioned above. These four distinct cases are labeled (ii) through (v).

3.2. Non-spherical-shell-shaped overlap, $0 < \kappa < \kappa_1$

The overlap volume is

$$V_{ii}(K) = 2 \int_0^{k_F+K/2} dz \int_{\sqrt{k_F^2-(z-K/2)^2}}^{\sqrt{(k_F^2+k_D^2)-(z+K/2)^2}} \rho d\rho \int_0^{2\pi} d\varphi \\ + 2 \int_{k_F+K/2}^{\sqrt{(k_F^2+k_D^2)-K/2}} dz \int_0^{\sqrt{(k_F^2+k_D^2)-(z+K/2)^2}} \rho d\rho \int_0^{2\pi} d\varphi,$$

or

$$V_{ii}(\kappa) = \left(\frac{4\pi}{3}\right) k_F^3 (1+\nu)^{3/2} \left[1 - (1+\nu)^{-3/2} - \left(\frac{3}{2}\right) \kappa \frac{(2+\nu)}{(1+\nu)} + \kappa^3 \right],$$

so that dividing by (8) leaves

$$\frac{V_{ii}(\kappa)}{V_0} = 1 - \left[\left(\frac{3}{2}\right) \frac{\sqrt{1+\nu}(2+\nu)}{(1+\nu)^{3/2}-1} \right] \kappa + \left[\frac{(1+\nu)^{3/2}}{(1+\nu)^{3/2}-1} \right] \kappa^3, \quad (9)$$

which goes smoothly to 1 when $\kappa \rightarrow 0$, as expected.

3.3. Ring shaped overlap, $\kappa_1 < \kappa < \kappa_2$

The overlap volumes is now

$$V_{iii}(K) = 2 \int_0^{\nu k_F/4\kappa\sqrt{1+\nu}} dz \times \int_{\sqrt{k_F^2-(z-K/2)^2}}^{\sqrt{(k_F^2+k_D^2)-(z+K/2)^2}} \rho d\rho \int_0^{2\pi} d\varphi,$$

or

$$V_{iii}(\kappa) = 2\pi k_F^3 (1+\nu) \left[\frac{3\nu^2}{(16\kappa(1+\nu)^{3/2})} \right],$$

so that dividing by (8) leaves

$$\frac{V_{iii}(\kappa)}{V_0} = \left(\frac{3}{2}\right) \frac{(1+\nu)}{(1+\nu)^{3/2}-1} \left[\frac{3\nu^2}{16\kappa(1+\nu)^{3/2}} \right]. \quad (10)$$

3.4. "Dimpled-double-convex-lens"-shaped overlap,

$$\kappa_2 < \kappa < \kappa_3$$

The overlap volume is

$$V_{iv}(K) = 2 \int_0^{K/2-k_F} dz \int_0^{\sqrt{(k_F^2+k_D^2)-(z+K/2)^2}} \rho d\rho \int_0^{2\pi} d\varphi \\ + 2 \int_{K/2-k_F}^{\nu k_F/4\kappa\sqrt{1+\nu}} dz \int_{\sqrt{k_F^2-(z-K/2)^2}}^{\sqrt{(k_F^2+k_D^2)-(z+K/2)^2}} \rho d\rho \int_0^{2\pi} d\varphi,$$

or

$$V_{iv}(\kappa) = \left(\frac{4\pi}{3}\right) k_F^3 \left[-1 + \left(\frac{3}{16}\right) \frac{\nu^2}{\kappa\sqrt{1+\nu}} + \left(\frac{3}{2}\right) \kappa\sqrt{1+\nu} - \left(\frac{1}{2}\right) (1+\nu)^{3/2} \kappa^3 \right],$$

so that dividing by (8) gives

$$\frac{V_{iv}(\kappa)}{V_0} = \frac{1}{(1+\nu)^{3/2}-1} \left[-1 + \left(\frac{3}{16}\right) \frac{\nu^2}{(\kappa\sqrt{1+\nu})} + \left(\frac{3}{2}\right) \kappa\sqrt{1+\nu} - \left(\frac{1}{2}\right) (1+\nu)^{3/2} \kappa^3 \right]. \quad (11)$$

3.5. "Double-convex-lens"-shaped overlap, $\kappa_3 < \kappa < 1$

Finally, we have

$$V_v(K) = 2 \int_0^{\sqrt{k_F^2+k_D^2}-K/2} dz \times \int_0^{\sqrt{(k_F^2+k_D^2)-(z+K/2)^2}} \rho d\rho \int_0^{2\pi} d\varphi,$$

or

$$V_v(\kappa) = \left(\frac{4\pi}{3}\right) k_F^3 (1+\nu)^{3/2} \left[1 - \left(\frac{3}{2}\right) \kappa + \left(\frac{1}{2}\right) \kappa^3 \right],$$

so that dividing by (8) leaves

$$\frac{V_v(\kappa)}{V_0} = \frac{(1+\nu)^{3/2}}{(1+\nu)^{3/2}-1} \left[1 - \left(\frac{3}{2}\right) \kappa + \left(\frac{1}{2}\right) \kappa^3 \right]. \quad (12)$$

Note that $V_v(\kappa)/V_0$ vanishes for $\kappa = 1^-$ as it should, and must be implicitly made to vanish for all $\kappa > 1$, in accordance with (2).

4. Finite temperature

The above zero-temperature results are qualitatively unchanged at higher temperatures T , up to values of T of physical interest, and to illustrate this we focus on 2D only. The number of up-spin electrons that pair up under the BCS model interaction in 2D at $T = 0$ into a CMM $\hbar K$ Cooper pair is by inspection

$$A(K, 0) = \sum_{\mathbf{k}} \theta \left(\left| \frac{\mathbf{K}}{2} + \mathbf{k} \right| - k_F \right) \theta \left(\left| \frac{\mathbf{K}}{2} - \mathbf{k} \right| - k_F \right) \theta \left(\sqrt{k_F^2 + k_D^2} - \left| \frac{\mathbf{K}}{2} + \mathbf{k} \right| \right) \theta \left(\sqrt{k_F^2 + k_D^2} - \left| \frac{\mathbf{K}}{2} - \mathbf{k} \right| \right), \quad (13)$$

where $\Theta_D \equiv \hbar^2 k_D^2 / 2mk_B$ is the Debye, and $T_F \equiv E_F / k_B \equiv \hbar^2 k_F^2 / 2mk_B$ the Fermi, temperatures. Defining $\nu \equiv \Theta_D / T_F$, and since $k_D = \sqrt{\nu} k_F$, $\mathbf{k} \equiv \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$ and $\mathbf{K} \equiv \mathbf{k}_1 + \mathbf{k}_2$, for $T \geq 0$ this above number is more generally

$$A(K, T) = \sum_{\mathbf{k}} \left(1 - n_{|\frac{\mathbf{K}}{2} + \mathbf{k}|} \right) \left(1 - n_{|\frac{\mathbf{K}}{2} - \mathbf{k}|} \right) \theta \left(\left| \frac{\mathbf{K}}{2} + \mathbf{k} \right| - k_\mu \right) \theta \left(\left| \frac{\mathbf{K}}{2} - \mathbf{k} \right| - k_\mu \right) \\ \times \theta \left(\sqrt{k_\mu^2 + k_D^2} - \left| \frac{\mathbf{K}}{2} + \mathbf{k} \right| \right) \theta \left(\sqrt{k_\mu^2 + k_D^2} - \left| \frac{\mathbf{K}}{2} - \mathbf{k} \right| \right), \quad (14)$$

where

$$k_\mu \equiv \sqrt{2m\mu(T)/\hbar^2},$$

$$\mu(T) = \beta^{-1} \ln(e^{\beta E_F} - 1) \xrightarrow{T \rightarrow 0} E_F \quad \text{in 2D,}$$

$$\varepsilon_{k_i} \equiv \hbar^2 k_i^2 / 2m$$

and

$$1 - n_{k_i} \equiv \left(e^{-[\varepsilon_{k_i} - \mu(T)]/k_B T} + 1 \right)^{-1} \\ \xrightarrow{T \rightarrow 0} \theta(\varepsilon_{k_i} - k_F) \quad (i = 1, 2).$$

Defining $\kappa \equiv K/2k_F\sqrt{1+\nu}$ and $\tilde{\mu} \equiv \mu/E_F$, Fig. 3 displays (14) relative to $A(0, 0)$ vs. \tilde{T} and κ . However, κ varies from 0 to only $\kappa_0 \simeq 0.0007$, which is the value of κ beyond which Cooper pairs (with $\lambda = 1/2$ and $\nu = 0.05$, as in this example) break up. Note that even for temperatures T as high as ~ 100 K and $T_F \sim 10^4$ K as is typical of quasi-2D cuprates, there is a reduction of only about 25% with respect to the zero-temperature result in the *relative numbers of nonzero CMM Cooper pairs in each state K* all the way up to breakup.

5. Results and discussion

The number of Cooper pairs with a specific $K > 0$ relative to those with $K = 0$, namely the ratio of k -space volumes V_K/V_0 , as a function of $\kappa \equiv K/(2\sqrt{k_F^2 + k_D^2})$ for the four distinct cases in Secs. 3.2–3.5 just mentioned, are graphed in Fig. 4 for different ν values. Fortuitously, and as expected, the resulting curves are smoothly continuous, even though they arise from the *analytically distinct* expressions (9), (10), (11) and (12) in the variable κ . The limit $\nu = \infty$ of (12), though physically irrelevant here, correctly reduces to the well-known analytic expression for the overlap volume of two solid spheres [16] of radii k_F and separated by a center-to-center distance K . Indeed, as stressed in Ref. 1, the fraction V_K/V_0 decreases rapidly from unity to zero as K increases from $K = 0$ (to its maximum possible

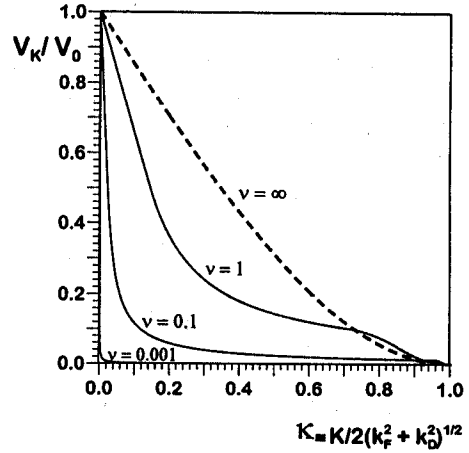


FIGURE 3. Fraction of bound pairs with nonzero CMM, $\hbar\mathbf{K} > 0$, to that of bound pairs with zero CMM, in 3D, for several values of $\nu = k_D^2/k_F^2$. Typically, $\nu = 10^{-3}$ for conventional, while $0.03 \leq \nu \leq 0.07$ for cuprate, superconductors. The limit $\nu = \infty$ refers to the well-known [16] overlap volume in k -space of two solid spheres of radii k_F and center-to-center distance equal to K , and follows correctly from (12).

value $K = 2\sqrt{k_F^2 + k_D^2} = 2k_F\sqrt{1+\nu}$, or $\kappa = 1$). This decrease is more pronounced for smaller ν . For cuprates [17] $0.03 \leq \nu \leq 0.07$ while for conventional superconductors $\nu \simeq 0.001$.

From Ref. 11 Cooper-pair binding energies satisfy an almost *linear* dispersion relation in K , and break up (in the linear approximation) for $\kappa \geq 1.4 \times 10^{-4}$ in 2D and for $\kappa \geq 1.8 \times 10^{-4}$ in 3D, for $\nu = 0.01$ and for a coupling of $\lambda = 1/2$. In Fig. 5 we plot V_K/V_0 as a function of κ , in the interval $10^{-7} < \kappa \equiv K/(2\sqrt{k_F^2 + k_D^2}) < 10^{-3}$ for 3D (full curves) and for 2D (dashed curves). The small “flags” mark the Cooper-pair breakup points, according to Ref. 11. Clearly, the number of pairs with $K > 0$ in the interval $0 < \kappa \equiv K/(2\sqrt{k_F^2 + k_D^2}) < 10^{-4}$ before Cooper-pair breakup roughly occurs is larger than about 95% of those with $K = 0$.

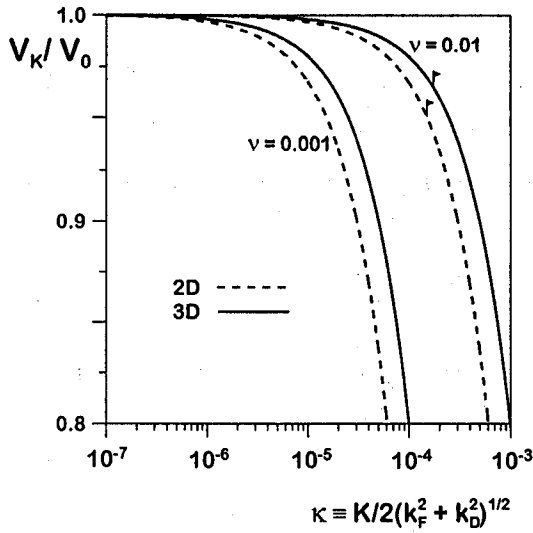


FIGURE 4. Enlargement of Fig. 3 over the interval $10^{-7} \leq K/(2\sqrt{k_F^2 + k_D^2}) \leq 10^{-3}$, except that dashed curves refer here to 2D results. Tiny "flags" mark Cooper-pair breakup total momenta values in the linear approximation of Ref. 11.

6. Conclusions

In conclusion, for a many-fermion system at $T = 0$ interacting via the familiar BCS model interaction we have calculated and graphed the fraction of Cooper pairs of electrons with a given nonzero total momentum, with respect to pairs with zero total momentum. It was found that the number of pairs with a nonzero total momentum smaller than the maximum (breakup) momentum is larger than about 95% of the number of pairs with total momentum $K = 0$, for 2D and 3D, $\nu \equiv \Theta_D/T_F > 0.01$ and $\lambda = 1/2$, where ν is the Debye-to-Fermi-temperature ratio and λ the usual dimensionless coupling constant of the BCS model interaction.

Finally, the effect of temperature on the number of nonzero K pairs (relative to that with $K = 0$) does not change in order of magnitude. For example, in 2D this fraction at the highest possible (breakup) value of K is reduced from about 0.95 at zero temperature to about 0.70 for T_c and T_F values typical of quasi-2D cuprate superconductors.

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Appendix

Nonzero CMM Cooper-pair fraction in 2D

Here we report results in 2D for the fraction A_K/A_0 of bound pairs with a given total momentum $\hbar\mathbf{K}$ different from zero

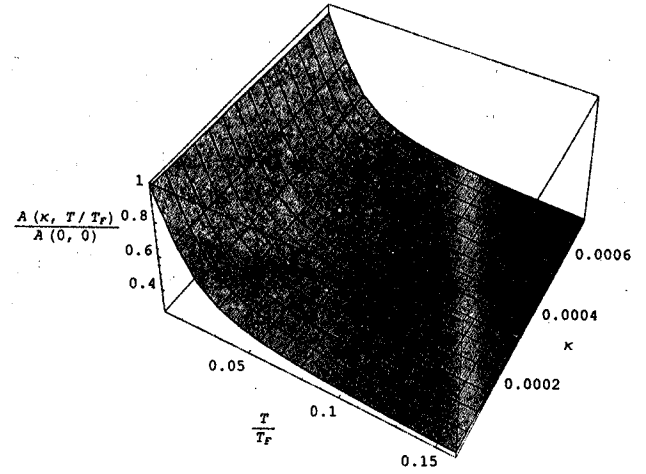


FIGURE 5. Number of Cooper pairs in 2D with nonzero CMM K , relative to that with zero CMM, as function both of reduced temperature T/T_F and Cooper-pair reduced CMM $\kappa \equiv K/2k_F\sqrt{1+\nu}$ (up to the breakup value K_0 as discussed in text).

relative to that of pairs with zero total momentum, in terms of the overlapping area of two identical circular tapes of inner radius k_F and width $\sqrt{k_F^2 + k_D^2} - k_F$, whose centers are separated by a distance K . As in 3D let $\kappa \equiv K/(2\sqrt{k_F^2 + k_D^2})$ and $\nu \equiv k_D^2/k_F^2$. In terms of these dimensionless variables the boundaries separating topologically different overlapping areas as the magnitude of \mathbf{K} is increased from zero, are given by (7). Five distinct shapes (topologies) of overlapping areas can be identified:

i) *Single-circular-tape-shape*, $\kappa = 0$

Both circular tapes merge into a single one of area

$$A_0 \equiv A_i = \pi k_F^2 \nu.$$

For $K > 0$ one distinguishes four cases:

a) *Non-circular-tape-shaped*, $0 < \kappa < \kappa_1$

The result is

$$\begin{aligned} \frac{A_{ii}(\kappa)}{A_0} &= \frac{(1+\nu)}{\nu} \left[1 - \left(\frac{2}{\pi}\right) \sin^{-1}(\kappa) - \left(\frac{2}{\pi}\right) \kappa \sqrt{1-\kappa^2} \right. \\ &\quad \left. - (1+\nu)^{-1} - \left(\frac{2}{\pi}\right) \kappa (1+\nu)^{-1/2} \sqrt{1-(\kappa\sqrt{1+\nu})^2} \right. \\ &\quad \left. - \left(\frac{2}{\pi}\right) (1+\nu)^{-1} \sin^{-1}(\kappa\sqrt{1+\nu}) \right] \\ &\simeq 1 - \left[\frac{4(1+\nu) + 2\pi\sqrt{1+\nu}}{\pi\nu} \right] \kappa \quad \text{for } \kappa \ll 1, \quad (15) \end{aligned}$$

which, as expected, goes smoothly to 1 as $\kappa \rightarrow 0$.

b) Two-identical-“areas”-shaped, $\kappa_1 < \kappa < \kappa_2$

$$\begin{aligned} \frac{A_{iii}(\kappa)}{A_0} = & \frac{(1+\nu)}{\nu} \left(\frac{2}{\pi}\right) \left\{ \sin^{-1} \left[\frac{\nu}{4\kappa(1+\nu)} + \kappa \right] - \kappa\sqrt{1-\kappa^2} + \left[\frac{\nu}{4\kappa(1+\nu)} + \kappa \right] \sqrt{1 - \left[\frac{\nu}{4\kappa(1+\nu)} + \kappa \right]^2} - \sin^{-1}(\kappa) \right. \\ & - \left[\frac{\nu}{4\kappa(1+\nu)} - \kappa \right] (1+\nu)^{-1/2} \sqrt{1 - \left[\frac{\nu}{4\kappa\sqrt{1+\nu}} - \kappa\sqrt{1+\nu} \right]^2} \\ & \left. - \kappa(1+\nu)^{-1/2} \sqrt{1 - (\kappa\sqrt{1+\nu})^2} - (1+\nu)^{-1} \sin^{-1}(\kappa\sqrt{1+\nu}) - (1+\nu)^{-1} \sin^{-1} \left(\frac{\nu}{4\kappa\sqrt{1+\nu}} - \kappa\sqrt{1+\nu} \right) \right\}. \end{aligned}$$

c) “Double-dagger”-shaped, $\kappa_2 < \kappa < \kappa_3$

$$\begin{aligned} \frac{A_{iv}(\kappa)}{A_0} = & \frac{(1+\nu)}{\nu} \left(\frac{2}{\pi}\right) \left\{ -\kappa\sqrt{1-\kappa^2} - \sin^{-1}(\kappa) + \left[\frac{\nu}{4\kappa(1+\nu)} + \kappa \right] \sqrt{1 - \left[\frac{\nu}{4\kappa(1+\nu)} + \kappa \right]^2} \right. \\ & + \sin^{-1} \left[\frac{\nu}{4\kappa(1+\nu)} + \kappa \right] - \left(\frac{\pi}{2}\right) (1+\nu)^{-1} - \left[\frac{\nu}{4\kappa(1+\nu)} - \kappa \right] (1+\nu)^{-1/2} \sqrt{1 - \left[\frac{\nu}{4\kappa\sqrt{1+\nu}} - \kappa\sqrt{1+\nu} \right]^2} \\ & \left. - (1+\nu)^{-1} \sin^{-1} \left[\frac{\nu}{4\kappa\sqrt{1+\nu}} - \kappa\sqrt{1+\nu} \right] \right\}. \end{aligned}$$

d) Two-convex-curves-shaped, $\kappa_3 < \kappa < 1$

$$\frac{A_v(\kappa)}{A_0} = \frac{(1+\nu)}{\nu} \left[1 - \left(\frac{2}{\pi}\right) \kappa\sqrt{1-\kappa^2} - \left(\frac{2}{\pi}\right) \sin^{-1}(\kappa) \right]. \quad (16)$$

As expected, this gives $A(\kappa)/A_0 \rightarrow 0$ as $\kappa \rightarrow 1^-$, and must be made to vanish for all $\kappa > 1$, as in the 3D case (12).

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