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The Cooper pair problem for generalized Fermi surfaces

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Abstract. The Fröhlich second-order perturbative treatment of the electron–phonon system with a generalized Fermi sea is extended to infinite order by solving the Cooper electron-pair problem in that sea. Substantially tighter-bound pairs follow for fixed coupling no matter how weak.

1. Introduction

Multiply-connected Fermi surfaces are the rule rather than the exception even in simple monoatomic metals [1]. In a complex compound material like $YBa_2Cu_3O_7$, very recent work [2] reveals a four-sheeted Fermi surface, one of which is shaped like a hollow cylinder. We suggest how one might surmount the theoretical restriction to low T_c ($\leqslant$40 K—popularly referred to as the 'phonon barrier'—characteristic of the BCS-Eliashberg formalism with phonons (and traceable to the dominant role played by the Debye temperature in the Cooper pair problem [3]). A multiply-connected but generalized Fermi sea with a weak attractive interaction leads to tighter-bound Cooper pairs and suggests T_c values which scale as the Fermi temperature, in qualitative agreement with recent muon-spin-relaxation measurements [4] performed on a large class of copper-oxide superconductors.

The well-known eigenvalue equation for the Cooper pair energy E_0, for the BCS model interaction [5], is

$$1 = V \sum_k{}' \frac{(1-n_k^0)}{2E_k - E_0} \rightarrow V \int_{E_F}^{E_F+\hbar\omega_D} \mathrm{d}\mathscr{E}\, \frac{g(\mathscr{E})}{2\mathscr{E} - E_0} \tag{1}$$

where E_k are the unperturbed single-particle energies, $V > 0$ is the strength of the effective attractive electron–electron interaction induced by coulombic as well as electron–phonon coupling, and $n_k^0 \equiv \theta(k_F - k)$, with $\theta(x) \equiv \frac{1}{2}[1 + \mathrm{sgn}(x)]$ the unit step function. The constant V is non-zero only within a very thin shell of thickness $\hbar\omega_D$ above the Fermi surface of energy $E_F = \hbar^2 k_F^2/2m$, k_F being the Fermi sphere radius. The prime over the summation sign means restriction to those (unoccupied) states such that $E_F < E_k < E_F + \hbar\omega_D$. The integral involves the electronic density of states $g(\mathscr{E})$ which can in turn be factored out from the integral as a constant $g(\mathscr{E}_F)$ due to the smallness of

$\hbar\omega_D/E_F$. This leaves an elementary integral to be performed that gives a logarithm, and solving for E_0 yields

$$E_0 = 2E_F - \frac{2\hbar\omega_D}{\exp(2/g(E_F)V) - 1}$$

$$\equiv 2E_F - \Delta_0 \xrightarrow[V\to 0]{} 2E_F - 2\hbar\omega_D \exp(-2g(E_F)V). \tag{2}$$

Putting $\varepsilon_0 \equiv E_0/2E_F$, $\nu \equiv \hbar\omega_D/2E_F$ and $\lambda \equiv g(E_F)V/2$, it will be convenient for later to rearrange the first equation to read

$$e^{-1/\lambda} = (\varepsilon_0 - 1)/(\varepsilon_0 - 1 - 2\nu) \tag{3}$$

which is easily solved graphically for any fixed λ. Because 2ν is typically on 10^{-3} to 10^{-2}, the value of ε_0 differs *very little* from unity (and hence $\Delta_0/2E_F$ is very close to zero) for all but the largest values of λ.

In the BCS many-electron formalism a temperature-dependent energy gap parameter $\Delta(T)$ emerges, which for $T = 0$ is [6]

$$\Delta(0) = \frac{\hbar\omega_D}{\sinh(1/\lambda)} \xrightarrow[\lambda\to 0]{} 2\hbar\omega_D\, e^{-1/\lambda} \tag{4}$$

i.e., a quantity asymptotically identical to the weak-coupling limit of the Cooper pair binding energy Δ_0 defined in (2). The transition temperature T_c is then determined by the solution of $\Delta(T_c) = 0$, and gives [7] (for $kT_c \ll \hbar\omega_D$)

$$\Delta(0) = \pi\, e^{-\gamma} k_B T_c \simeq 1.76 k_B T_c \tag{5}$$

where $\gamma \simeq 0.577$ is the Euler constant. Combining (4) and (5) leaves

$$T_c \simeq 1.13\, \Theta_D\, e^{-1/\lambda} \tag{6}$$

where $\Theta_D \equiv \hbar\omega_D/k_B$ is the Debye temperature. Since $\Theta_D \sim 10^2$ K, (6) with acceptable values of λ severely limits T_c to a few Kelvin. More refined T_c formulae [8], beginning with the MacMillan [9] formula based on strong-coupling Migdal–Eliashberg theory [10] with phonons, in principle allow values of T_c as high as around 35 K. But this formula, recently used [11] with electron–phonon coupling constants extracted from high-temperature resistivity measurements, carried out on both the lanthanum and yttrium cuprates, predicts a vanishingly small value of T_c in either substance. A recent realistic tight-binding band-structure calculation inputted into the Eliashberg equations gave Weber [12] T_c values between 30 and 40 K for the copper-oxide superconductors $La_{2-x}(Ba, Sr)_xCuO_4$ having empirical T_c values in the range 30–36 K. But for $YBa_2Cu_3O_7$ with an observed $T_c \simeq 95$ K, Weber and Mattheiss [13], using similar techniques, were not able to extract a T_c larger than about 30 K. Consequently, $T_c \simeq 40$ K has come to be known as the 'phonon barrier' for transition temperatures, and its smallness has prompted speculation of mechanisms *other than phononic*, such as exchange of excitons, plasmons, magnons, etc.

We stress again that the BCS formula (6) is valid not only for weak-coupling ($\lambda \ll 1$) *but also* for small T_c, specifically $Z = \Theta_D/2T_c \gg 1$. This latter restriction can readily be lifted [14], and we merely quote the result which is now a transcendental equation in T_c, namely

$$T_c \simeq C(\Theta_D/2T_c)\Theta_D(e^{-1/\lambda})^{\coth(\Theta_D/2T_c)}. \tag{7a}$$

The dimensionless coefficient $C(\Theta_D/2T_c)$ is given by

$$C(Z) = \frac{1}{2}\left[\exp\left(-\int_0^Z dx\,(\ln x)\,\mathrm{sech}^2\,x\right)\right]^{\coth Z} \xrightarrow[Z\to\infty]{} \frac{2}{\pi}e^{\gamma} \simeq 1.13 \tag{7b}$$

where $\gamma \simeq 0.577$ is Euler's constant. The function $C(Z)$ can be seen [14] to be monotonic decreasing in Z; it is a number of order unity for most cases of interest and the same holds for the exponent coth Z in (7*b*). Thus, the T_c-dependence *on the* RHS of (7*a*), which generalizes the BCS formula (6), is comparatively weak.

2. Abnormal occupancy in neutral fluids

The all-important Fermi sea assumed in the Cooper and BCS theories is strictly appropriate to the perfect Fermi gas Slater determinant ground state wave function for N particles enclosed in a volume Ω, namely

$$\Phi = (N!)^{-1/2}\,\det_{n_k^0}(\Omega^{-1/2}\,e^{ik_i\cdot r_j}) \qquad n_k^0 \equiv \theta(k_F - k)$$

with $i, j = 1, 2, \ldots, N$. For an interacting system in the Hartree–Fock (HF) approximation the most general occupancy consistent with the Pauli principle, however, is

$$n_k = 0 \text{ or } 1 \qquad \sum_k n_k = N. \tag{8}$$

We have raised the general question [15] of what the optimum occupancy might be for an *imperfect*, fully-interacting many-fermion fluid in the non-linear (HF) approximation with plane wave (PW) solutions in any dimension. In real solids, of course, Fermi surfaces can contrast drastically with the familiar Fermi sphere. Overhauser [16] has explicitly considered multiply-connected Fermi seas associated with both charge- and spin-density-wave states. The HF equations also admit Bloch wave solutions with *lower* total HF energy than with PW solutions, as seen from the calculations performed by Harris and Monkhorst two decades ago [17] in H, H_2, Li and Be crystals. However, we will not be concerned with translation-symmetry-breaking (i.e., non-PW) orbitals as they would not alter the Cooper result (2), save in renormalizing the value of $g(E_F)$ at most. With PW solutions as early as 1950 Fröhlich [18] already contemplated a departure from the Fermi sphere in the electron–phonon system, within second-order perturbation theory. He found a lower energy state *if* the electron–phonon coupling exceeded a certain critical value, a result now seen to be inconsistent with the empirical fact that actual superconducting critical temperatures can be immeasurably small. This difficulty disappears by viewing the problem in *infinite* order, which amounts to solving the Cooper problem in *any* Fermi sea.

In the PWHF approximation with a many-fermion Hamiltonian H for a simple 1D fluid under a sufficiently attractive (but non-collapsing in the thermodynamic limit), short-ranged, two-body interaction v_{12}, HF total energies $\mathscr{E}_{\mathrm{PWHF}}(n_k)$ were found [15], over a range of particle densities $N/\Omega = k_F^3/3\pi^2$, which are *lower* than $\mathscr{E}_{\mathrm{PWHF}}(n_k^0)$. In general,

$$\begin{aligned}\mathscr{E}_{\mathrm{PWHF}}(n_k) &\equiv \langle\Phi|H|\Phi\rangle = \langle\Phi|t+v|\Phi\rangle \\ &= \sum_k t_k n_k + \tfrac{1}{2}\sum_{k_1k_2}(\langle k_1k_2|v_{12}|k_1k_2\rangle - \langle k_1k_2|v_{12}|k_2k_1\rangle)n_{k_1}n_{k_2} \\ &= \tfrac{1}{2}\sum_k (t_k + E_k(n_\ell))n_k \end{aligned} \tag{9}$$

where $t_k \equiv \hbar^2k^2/2m$, and $E_k(n_\ell)$ is the self-consistent HF single-particle spectrum *which itself depends on the occupancy* n_ℓ. The Fröhlich Fermi sea, which satisfies (8), is

$$\begin{aligned} &n_k = \theta(\alpha k_F - k) + \theta(k - \beta k_F)\theta(\gamma k_F - k) \qquad \alpha^3 - \beta^3 + \gamma^3 \equiv 1 \\ &0 \leqslant \alpha \leqslant \beta \leqslant \gamma \qquad \alpha \leqslant 1 \qquad \gamma \geqslant 1, \end{aligned} \tag{10}$$

and becomes the normal sea n_k^0 when $\alpha = \beta = \gamma = 1$. The result that $\mathscr{E}_{\mathrm{PWHF}}(n_k)$ can be below $\mathscr{E}_{\mathrm{PWHF}}(n_k^0)$ over a range of densities was reminiscent [15] of a (first-order) gas–liquid phase transition. This conforms with the appearance, as coupling is increased, of 2- or more-particle clusterings of some kind, since emptying *smaller-k* states means suppression of particle orbits with *larger* relative spatial extensions. ((These correlations, however, *exclude* Cooper pairs at the HF level of approximation since the BCS model interaction (cf. equation (11) below) produces no effect whatsoever within HF.) The search for lower-energy, abnormally-occupied Slater PW determinants for a wide variety of pair-interaction cases was subsequently extended [19] to 3D, and to a much larger class of distributions n_k. In still further work [20] it was shown for example, that a repulsive-core plus square-well two-body potential can favour abnormal occupancy. Since this potential models [21] the He–He interaction semi-realistically rather well, and n_k is *not* infinitesimally related to n_k^0, the result suggests, e.g., that liquid-^{3}He is non-Fermi-liquid-like (in the sense of Landau), in agreement with other more general studies [22] using a more realistic pair potential. Several many-boson fluids were also found [23] which prefer abnormal occupancy. More recently, two such examples have surfaced in nuclear physics:

(i) in a relativistic HF theory [24] of an infinite meson–nucleon system, where an energy-lowering shift, at high density, to the distribution (10) with $\alpha \equiv 0$ might be interpreted [25] as indicating a nuclear–quark-matter phase transition, and

(ii) in constrained (good total spin) HF calculations [26] of the finite nucleus ^{24}Mg with realistic two-nucleon potentials.

Clearly, even at the PWHF level of approximation, Fermi seas more general than the familiar spherical sea are favoured, usually for sufficiently strong interparticle coupling.

3. Tighter-bound Cooper pairs

We have reconsidered the Fröhlich abnormal occupancy (10) scheme [18]—though not in and of itself as a superconducting state—using the BCS model interaction,

$$\langle kl|v_{12}|kl\rangle = \begin{cases} -V & \text{if } E_F < E_k, E_l < E_F + \hbar\omega_D \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

Two novel results emerge:

(i) the Fröhlich problem can be solved to *infinite* (instead of only second) order, and
(ii) precisely because of (i), it is vastly simpler than the treatment of [18].

Robustly tighter-bound Cooper pairs emerge, for *any* coupling strength, in the equivalent Bethe–Goldstone approximation implied by the Cooper treatment. The approximation is clearly more 'highly-summed' than HF. It is proposed that when these new electron pairs are suitably incorporated into the BCS–Bogoliubov [27]–Anderson [28]–Gor'kov [29]–Nambu [30]–Migdal–Eliashberg [10] formalisms, a comprehensive understanding of *both* low- and high-T_c superconductivity may be attained, *perhaps* solely in terms of the phonon mechanism.

The model distribution (10) is very crude and is employed merely as a specific illustration of a *generalized* Fermi surface: namely that boundary in k-space separating occupied from unoccupied orbitals—but which does *not* necessarily correspond to a single, fixed energy value, say E_F, as in the usual definition of a *metallic* Fermi surface. We are not aware of any experimental method to map out such a generalized Fermi surface. The occupancy (10) is a definite step beyond the perfect Fermi gas picture and suffices to uncover an instability in the Fermi-sphere-induced Cooper pair. If the E_k in (1) are the HF single-particle energies, the three surfaces in (10) together constitute the boundary separating occupied from unoccupied orbitals, but are situated at distinct energies $E_0 = \alpha^2 E_F$, $E_1 \equiv \beta^2 E_F$ and $E_2 = \gamma^2 E_F$, with the parameters α, β and γ presumably characteristic of the material electronic band structure in the normal and/or superconducting phases. In HF, E_k for the BCS model Hamiltonian is just $\hbar^2 k^2/2m$ since the HF mean-field is a sum over *occupied* orbitals and the BCS interaction is non-zero only in *unoccupied* ones. The sum in (1) then becomes three sums, one for each surface in k-space, so that we now have

$$1 \simeq V\left(g(E_0)\int_{E_0}^{E_0+\hbar\omega_D}\frac{d\mathscr{E}}{2\mathscr{E}-E} + g(E_1)\int_{E_1-\hbar\omega_D}^{E_1}\frac{d\mathscr{E}}{2\mathscr{E}-E} + g(E_2)\int_{E_2}^{E_2+\hbar\omega_D}\frac{d\mathscr{E}}{2\mathscr{E}-E}\right) \tag{12}$$

provided that E_0 is not too close to zero so as to ensure that $g(E_0)$ can still approximately be considered constant over the interval $\hbar\omega_D$. Scattering now occurs via the BCS model interaction in the vicinity of all three surfaces in k-space. (Note that (12) is exact in 2D, when $g(\mathscr{E})$ is rigorously constant.) Performing the integrals and solving for $\exp(-2/g(E_F)V) \equiv \exp(-1/\lambda)$, with $E/2E_F \equiv \varepsilon$, and $\hbar\omega_D/2E_F \equiv \nu$ as before, leads to a transcendental equation for ε given by

$$e^{-1/\lambda} = \left(\frac{\varepsilon-\alpha^2}{\varepsilon-\alpha^2-2\nu}\right)^{\alpha}\left(\frac{\varepsilon-\beta^2+2\nu}{\varepsilon-\beta^2}\right)^{\beta}\left(\frac{\varepsilon-\gamma^2}{\varepsilon-\gamma^2-2\nu}\right)^{\gamma} \tag{13}$$

which generalizes (3), and becomes that equation when $\alpha = \beta = \gamma = 1$, as it should. Figure 1 shows a plot of both members of (13) for the typical values $\hbar\omega_D/E_F \equiv 2\nu = 10^{-3}$, $\lambda = 0.5$, and for $\alpha = 0.5$, $\gamma = 1.2$ (and thus by (10), $\beta = 0.948\ldots$). Non-simple zeros and poles occur at α^2, $\beta^2 - 2\nu$, γ^2 and $\alpha^2 + 2\nu$, β^2, $\gamma^2 + 2\nu$, respectively. Zeros are marked off on the abscissa as dots, and pole asymptotes run vertically through the crosses. The full square marks the bound-state solution to the Cooper-pair equation (3), while the open circles correspond to two bound states in the abnormal occupancy case. The open triangle is an unbound level in the pair continuum $\varepsilon > 1$. As in the normal-occupancy Cooper-pair case, the new, tighter-bound Cooper-pair solutions *will survive*,

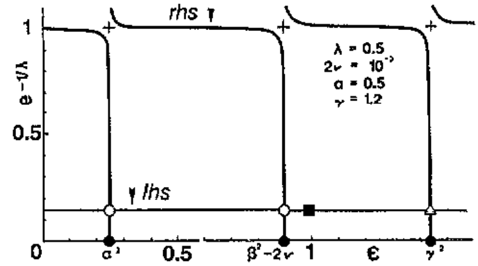

Figure 1. Typical case illustrating a graphical solution of equation (12).

no matter how weak the coupling V, since smaller coupling merely lowers the horizontal line marked '*lhs*'.

4. Higher-T_c BCS superconductivity

More interesting, however, is the possibility that these tighter-bound Cooper pairs might lead to transition temperatures T_c which can scale *both as* T_F ($\sim 10^4$–10^5 K) *and* as Θ_D ($\sim 10^2$ K). The figure suggests that the lowest ε solution may be written as

$$1 - \Delta/2E_F \equiv \varepsilon = \alpha^2 - \eta \tag{14}$$

with $0 \leqslant \eta \ll 1$ in the weak-coupling ($\lambda \ll 1$) limit. Inserting this value of ε into (13) and expanding about $\eta = 0$ yields $\eta \simeq 2\nu\, e^{-1/\alpha\lambda}$. We have not attempted to solve the BCS gap equation for the tighter-bound Cooper pairs. This should ideally be done using a Bloch (plane)-wave-filled Fermi sea. However, identifying Δ in (14) with $\Delta(0)$ in (5) leads to a T_c formula whereby T_c scales with T_F.

5. Conclusions

We conclude that tighter-bound Cooper pairs arise by generalizing the assumed spherical Fermi sea for the occupied background electrons, *without* invoking either stronger electron–phonon coupling nor unconventional interaction mechanisms. Generalized Fermi topologies might conceivably lead to the T_c scaling not only as the Debye temperature Θ_D as in normal-occupancy BCS theory, but as both Θ_D and the much larger Fermi temperature T_F. A full-fledged Bloch wave HF calculation [17] in search of abnormal occupancy in solids is probably difficult for any but the simplest crystals. The present simple extension of the Cooper-pair model might suggest, however, that experimental detection of generalized Fermi surfaces might teach us how to chemically manipulate them, namely, by doping, and accordingly design compound materials to drive higher T_c values.

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