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Bound States, Cooper Pairing, and Bose Condensation in Two Dimensions

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For a dilute gas of fermions interacting via an arbitrary pair potential in $d=2$ dimensions, we show that the many-body ground state is unstable to s-wave pairing if and *only if* a two-body bound state exists. We further obtain, within a variational pairing *Ansatz*, a smooth crossover from a Cooper-paired state ($\xi_0 k_F \gg 1$) to a Bose condensed state of tightly bound pairs ($\xi_0 k_F \ll 1$). We briefly discuss non-s-wave superconductors. Insofar as this model is applicable to the high-T_c materials, they are in the interesting regime with the coherence length ξ_0 comparable to the interparticle spacing k_F^{-1}.

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There has been a resurgence[1] of interest in superconductivity with the discovery of the high-transition-temperature (T_c) copper-oxide superconductors. Quite apart from the highly controversial issue of the pairing mechanism, the high-T_c materials have several characteristics which are strikingly different from the traditional superconductors. In this Letter we shall focus on two questions motivated by the high-T_c superconductors: (1) the conditions for a superconducting instability in $d=2$ dimensions, and (2) the nature of the superconducting ground state when the coherence length is of the order of the interparticle spacing.

We analyze these questions within a simple continuum model of a gas of fermions at $T=0$ interacting via a given two-body potential. We find that the existence of a s-wave bound state in the two-body problem is a *necessary* and sufficient condition for a many-body (s-wave) instability for a $d=2$ dilute gas (defined below). This is in marked contrast with the $d=3$ result. We also show that the corresponding necessary condition is not true for pairing in higher angular momentum channels. We study next the many-body ground state within a variational *Ansatz* and find a smooth crossover from a state with large, overlapping Cooper pairs (for a weakly attractive pair potential) to a Bose condensate of composite bosons formed out of tightly bound pairs of fermions. This crossover has been studied in three dimensions by Leggett,[2] and by Nozieres and Schmitt-Rink.[3] (See also the early work by Eagles.[4]) The distinguishing feature of the $d=2$ analysis presented here is that the s-wave mean-field equations can be solved exactly over the whole parameter range, from Cooper pairing to Bose condensation,[5] to obtain a very simple and transparent result. Some interesting features of the p-wave calculations are noted.

Consider a Fermi gas with an arbitrary static two-body potential $V(r)$, perhaps with a strongly repulsive core at short distances and a longer range attraction with a finite range of action R. Since we are interested in getting results which are independent of the detailed shape of the potential, we restrict our attention to a dilute gas, where the average interparticle spacing (or inverse Fermi momentum k_F^{-1}) is much larger than the range R, so that $k_F R \ll 1$, and the two-body interaction is completely characterized by the low-energy T matrix.

In order to investigate a possible instability[6] of the noninteracting ground state (filled Fermi sea) we look at the two-particle propagator $L \equiv \langle k'+p, -k' | L | k+p, -k\rangle$. Within the ladder approximation (see Fig. 1), it is given by $L = V + V\mathcal{K}L$, where we suppress the momentum labels and summation, with the kernel

$$[\mathcal{K}(\omega)]_{\mathbf{kk}'} = \mathrm{sgn}(\epsilon_k - \epsilon_F)[\omega - 2(\epsilon_k - \epsilon_F)]^{-1}\delta_{\mathbf{k},\mathbf{k}'}.$$

Now, unlike the usual Bardeen-Cooper-Schrieffer (BCS)

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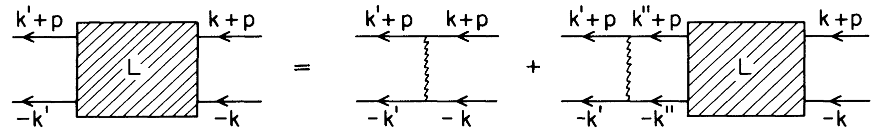

FIG. 1. The two-particle propagator L used in the instability analysis. All labels are four vectors; $k=(\mathbf{k},k_0)$, etc. In our analysis we have taken the pair momentum $\mathbf{p}=0$ and used the notation $p_0=\omega$.

assumption, the Fourier transform $V_{\mathbf{kk}'}$ may not even be defined because of the hard core in $V(r)$. We will thus rewrite our equations in terms of the well-defined T matrix $T=V+V\mathcal{G}_0T$. Here $\mathcal{G}_0$ is the free Green's function for the two-body problem

$$[\mathcal{G}_0(2E)]_{\mathbf{kk}'}=[2(E-\epsilon_k+i\eta)]^{-1}\delta_{\mathbf{k},\mathbf{k}'},$$

where E is the energy variable[7] and $\eta\to 0^+$. Formally eliminating $V_{\mathbf{kk}'}$ between the equations for L and T, we obtain $L=T+T(\mathcal{K}-\mathcal{G}_0)L$.

In $d=2$ dimensions, the low-energy T matrix, $T_{\mathbf{k},\mathbf{k}'}(2E)\simeq\tau_0(2E)$, expressed in terms of the s-wave scattering phase shift, is given by[8]

$$\tau_0(2E)=(4\hbar^2/m)[-\cot\delta_0(2E)+i]^{-1}. \tag{1}$$

Further, it can be shown that for $d=2$ the low-energy phase shift is of the form

$$\pi\cot\delta_0(2E)=\ln(2E/E_a)+\mathcal{O}(E/\epsilon_R), \tag{2}$$

where $\epsilon_R=\hbar^2/2mR^2$, and E_a is a parameter with the dimensions of energy (whose physical significance will become clear below). Note the low-energy logarithmic divergence in the T matrix, which is related to the discontinuity in the $d=2$ density of states at $E=0$.

Using the T matrix of (1) and (2) we solve for the two-particle propagator L, and look for a pole of L in the upper half of the complex ω plane—the usual signature of an instability. This is given by the solution $\omega=i\alpha$ of the form

$$\frac{1}{\tau_0(2E)}=\frac{m}{2\pi\hbar^2}\int_0^{\epsilon_\Lambda}d\epsilon[\mathcal{K}(i\alpha)-\mathcal{G}_0(2E)], \tag{3}$$

where the integral is manifestly finite in the limit $\epsilon_\Lambda\to\infty$, and the dependence on the energy variable E cancels out. Since we are interested in the onset of the instability as the attractive part of $V(r)$ is increased, we are looking for solutions with $\alpha/\epsilon_F\ll 1$, i.e., poles which have just split off from the real axis on to the complex plane. We find such a solution $\alpha\simeq(2\epsilon_FE_a)^{1/2}$ provided that $E_a\ll\epsilon_F\ll\epsilon_R$, where the last inequality follows from the diluteness condition $k_FR\ll 1$. Now, from (1) and (2), it is clear that when $E_a\ll\epsilon_R$, there is a pole in the T matrix corresponding to a bound state in the two-body problem with binding energy E_a. Thus we find that for a $d=2$ dilute Fermi gas the existence of a two-body bound state is a *necessary* condition for a many-body pairing instability. (The more obvious sufficiency condition emerges from the variational calculation below.)

A few remarks are in order. First, this result is obvious for a potential which is attractive everywhere in $d=2$, since then a two-body bound state exists for an arbitrarily weak attraction. However, for a potential with strong repulsion at short distances [or, more generally, when $\int d^2r\,V(r)$ does not converge], a two-body bound state will exist, in $d=2$, only if the attraction crosses a certain threshold, and our result is nontrivial. Second, our result is in striking contrast to the three-dimensional case. In $d=3$, the low-energy T matrix is characterized[9] by the s-wave scattering length a_s, and we obtain a pole at

$$\omega=i\alpha=i\epsilon_F 8e^{-2}\exp(-\pi/k_F|a_s|),$$

provided that $a_s<0$ and the system is dilute enough that $(k_F|a_s|)^{-1}\to\infty$. Thus for $d=3$ the onset of the many-body instability requires only that $a_s<0$, and not the existence of a two-body bound state (the threshold for which corresponds to $a_s\to-\infty$).

A simple way to restate our $d=2$ result is that an attractive phase shift at finite energies $\delta_0(\epsilon_F)>0$ (Cooper instability) implies $\delta_0(0)>0$ (a two-body bound state). However, it can be shown[10] that, even for $d=2$, this necessary connection does *not* hold[11] for higher angular momentum ($l\neq 0$) channels; attraction at the Fermi level $\delta_l(\epsilon_F)>0$ does not necessarily imply $\delta_l(0)>0$.

We now turn to the question of what effect, if any, the existence of a two-body bound state has on the pairing in the many-body ground state in two dimensions. To proceed, we make an *Ansatz*, following BCS, for the many-body ground-state wave function:

$$\Psi(1,\ldots,N)=\mathcal{A}[\phi(1,2)\phi(3,4)\ldots\phi(N-1,N)],$$

where $\mathcal{A}$ is an antisymmetrization operator. The variational freedom is in the choice of the pair wave function ϕ. The subsequent analysis proceeds along the standard BCS route,[6] except that the chemical potential for the fermions is not, in general, fixed at the Fermi energy, and must be determined self-consistently along with the gap function.

The usual gap equation is $\Delta_{\mathbf{k}}=-\sum_{\mathbf{k}'}V_{\mathbf{kk}'}\Delta_{\mathbf{k}'}/2E_{\mathbf{k}'}$, with $E_{\mathbf{k}}=[(\epsilon_k-\mu)^2+|\Delta_{\mathbf{k}}|^2]^{1/2}$. As before, we would like to eliminate the possibly ill-defined $V_{\mathbf{kk}'}$ in favor of the T matrix for the two-body problem. To this end we use a renormalization procedure[12] in which we introduce a momentum cutoff $\Lambda>\mathcal{O}(R^{-1})$, and integrate out the high momentum ($k > \Lambda$) contributions to the gap equation, to obtain an effective interaction Γ in place of V. We thus obtain

$$\Delta_{\mathbf{k}} = -\sum_{k<\Lambda} \Gamma_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}}, \text{ and } \Gamma = T - T\mathcal{G}_0 P^{<} \Gamma , \tag{4}$$

where the projection operator $P^{<} = \sum_{k<\Lambda} |\mathbf{k}\rangle\langle\mathbf{k}|$. Finally we wish to obtain finite results in the limit $\Lambda \to \infty$.

We shall first focus on s-wave pairing where the two fermions in a pair are in a spin singlet and the gap function $\Delta_{\mathbf{k}}$ has no angular dependence. We then find that the kernel of the renormalized gap equation (4) is given by

$$\Gamma_{kk'} \simeq \tau_0(2E) \left[1 + \tau_0(2E) \int_0^{\Lambda} \frac{dp}{2\pi} \frac{p}{2(E - \epsilon_p + i\eta)} \right]^{-1} , \tag{5}$$

provided $kR \ll 1$ and $k'R \ll 1$. It follows that the gap function is constant, i.e., $\Delta_{\mathbf{k}} \simeq \Delta$, in the low-energy limit $kR \ll 1$, and is determined by

$$\frac{4\pi\hbar^2}{m\tau_0(2E)} = \int_0^{\epsilon_\Lambda} d\epsilon_k \left[\mathcal{G}_0(2E) - E_k^{-1} \right] , \tag{6}$$

where the cutoff $\epsilon_\Lambda = \hbar^2\Lambda^2/2m$.

The second equation which will be used to determine Δ and μ self-consistently is the number equation

$$\int_0^{\infty} d\epsilon_k \left[1 - (\epsilon_k - \mu)/E_k \right] = 2\epsilon_F , \tag{7}$$

where we have used the $d=2$ relationship between the Fermi energy and the number density $\epsilon_F = \pi\hbar^2 n/m$. Solving (6) and (7) we obtain the result

$$\Delta = (2\epsilon_F E_a)^{1/2}, \text{ and } \mu = \epsilon_F - E_a/2 , \tag{8}$$

where we recall that E_a is the binding energy in the two-body problem.

These remarkably simple results have a direct physical significance. Just beyond the threshold for instability $E_a \ll \epsilon_F$, and we find that we recover the BCS result.[13] The chemical potential $\mu \simeq \epsilon_F$, the Fermi energy, and $\Delta/\epsilon_F \sim (\xi_0 k_F)^{-1} \ll 1$, so that the pair size ξ_0 is much larger than the interparticle spacing k_F^{-1}.

In the opposite limit of very strong attraction (or, of very low density), we have a deep two-particle bound state $E_a \gg \epsilon_F$, and we find Bose condensation of essentially noninteracting composite bosons, each made up of a tightly bound pair of fermions. The chemical potential for the fermions $\mu \simeq -E_a/2$, which is one half of the energy to break a pair, and the pair size is much smaller than the interparticle spacing $(\xi_0 k_F)^{-1} \gg 1$.

In between these two limits, and in particular when $\xi_0 k_F \sim 1$, the pairing *Ansatz* has variational significance. The usual calculation of the condensation energy gives the result $\Delta E = -\frac{1}{2} n E_a$, for arbitrary E_a/ϵ_F. It is interesting to note that this is just the energy of $N/2$ noninteracting pairs each with a binding energy E_a. Our results above suggest that there is a smooth crossover from the BCS limit to Bose condensation, since there is no singularity in (8) as a function of the parameter E_a/ϵ_F that interpolates between these two limits. If one looks at the excitation spectrum, however, there is a point, $\mu = 0$, or equivalently $E_a/\epsilon_F = 2$, at which a weak singularity exists. This may be seen from the gap to single-particle excitations $E_{\text{gap}} \equiv \min E_{\mathbf{k}}$ which is Δ for $\mu > 0$ and $(\mu^2 + \Delta^2)^{1/2}$ for $\mu < 0$. The point $\mu = 0$ could be argued to mark the transition between the BCS-type regime ($\mu > 0$) and the Bose condensed regime ($\mu < 0$).

We have also analyzed this crossover for the case of $d=2$ p-wave pairing. The calculations[10] in this case are considerably complicated by the appearance of ultraviolet divergences in the gap and chemical potential equations, which we regulate by using corresponding results from the two-body problem. The main results are the following. In the two extreme limits the solution reproduces the BCS result (without the existence of a two-body bound state) and Bose condensation of tightly bound pairs. In between these two limits the ground-state solution is continuous, but has a weak singularity at $\mu = 0$. Interestingly, the gap to single-particle excitations does not necessarily have the same symmetry as the pairing amplitude Δ. For $\Delta \sim \cos\theta$, while E_{gap} has the expected $\cos\theta$ dependence in the BCS limit, it changes to the isotropic $E_{\text{gap}} = |\mu|$ for all $\mu < 0$. The details of these results will be published separately.[10]

Rough estimates[14] of the parameter $k_F \xi_0$ for the high-T_c materials lead to values of about 5–10 for $YBa_2Cu_3O_7$, and about 10–20 for $La_{1.85}Sr_{0.15}CuO_4$. This suggests that the copper-oxide superconductors are neither in the Cooper-pairing limit ($k_F \xi_0 \gg 1$) nor in the Bose limit ($k_F \xi_0 \ll 1$), but are in the interesting intermediate regime.

Finally, the pairing *Ansatz* has obvious limitations in the "intermediate coupling" regime where $\xi_0 k_F \sim 1$. While the results above give a qualitatively reasonable description in this regime, a definitive analysis would involve going beyond the mean-field level. A finite temperature analysis of the intermediate coupling regime remains an open problem. If the transition temperature $T_c < E_a$, which is possible even away from the extreme Bose limit, there will be a regime between these two temperatures where some bound pairs exist above T_c, leading to anomalous "normal" state properties.

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[1]See, e.g., *Proceedings of the International Conference on*

High-T_c Superconductors and Materials and Mechanisms of Superconductivity, Interlaken, Switzerland, edited by J. Müller and J. L. Olsen, [Physica (Amsterdam) **153–155C**, Pts. I and II (1988)].

[2]A. J. Leggett, in *Modern Trends in the Theory of Condensed Matter,* edited by A. Pekalski and J. Przystawa (Springer-Verlag, Berlin, 1980).

[3]P. Nozieres and S. Schmitt-Rink, J. Low Temp. Phys. **59**, 195 (1985).

[4]D. M. Eagles, Phys. Rev. **186**, 456 (1969).

[5]We shall see that the $d=2$ ground state has off-diagonal long-range order (ODLRO) over the whole parameter range. Note that in two dimensions Hohenberg's theorem [P. C. Hohenberg, Phys. Rev. **158**, 383 (1967)] does not preclude ODLRO at $T=0$. At finite temperatures, a Josephson coupling between the two-dimensional planes in a copper-oxide superconductor will presumably stabilize the phase fluctuations, which would otherwise have destroyed ODLRO in a single plane.

[6]See, e.g., J. R. Schrieffer, *Theory of Superconductivity* (Benjamin-Cummings, Menlo Park, 1964).

[7]The unusual factor of 2 is introduced for later convenience. With this convention the energy variable $2E$ is related to the relative momentum $\mathbf{q}$ by $2E=\hbar^2q^2/2m_0$, where $m_0=m/2$ is the reduced mass, so that $E=\hbar^2q^2/2m$.

[8]For a discussion of scattering theory in two dimensions see, e.g., S. K. Adhikari, Am. J. Phys. **54**, 362 (1986).

[9]In $d=3$ dimensions the low-energy s-wave phase shift is given by $q\cot\delta_0(q)=-1/a_s+\mathcal{O}(qR)^2$, where a_s is the scattering length.

[10]M. Randeria, J.-M. Duan, and L.-Y. Shieh (to be published).

[11]The low-energy expansion for $\cot\delta_l(E)$ has a leading singularity A_l/E^l for $l>0$. The sign of $\delta_l(0)$ then depends upon that of A_l, and is not necessarily fixed by the sign of $\delta_l(\epsilon_F)$. (See Ref. 10.)

[12]This renormalization procedure is a simple variant of the one used by P. W. Anderson and P. Morel, Phys. Rev. **123**, 1911 (1961).

[13]The BCS essential singularity is hidden inside the two-body binding energy E_a. Quite generally one can show that for $d=2$, E_a is ϵ_R times an exponentially small term, just beyond the threshold.

[14]These rather crude estimates are insensitive to whether we use the three-dimensional electronic density to determine k_F, or use formal valence arguments to estimate the electronic density in the copper-oxide planes. This suggests that even if we were to consider the high-T_c superconductors as three-dimensional systems, they would still be in the intermediate coupling regime.