Superconductivity in a two-dimensional Fermi gas: Evolution from Cooper pairing to Bose condensation

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We study a two-dimensional continuum model of a dilute gas of fermions at T=0 interacting via a given two-body potential, with an aim to investigate superconductors with coherence length of the order of the interparticle spacing $[k_F\xi_0 \sim O(1)]$, a striking feature of the high- T_c materials. We find that a two-body bound state in vacuum is a necessary and sufficient condition for an s-wave pairing instability. We also find that the existence of such a bound state in a higher-angular-momentum (l > 0) channel is not a necessary condition for an *l*-wave pairing instability. We further investigate using a variational *ansatz* the evolution from a state with large overlapping Cooper pairs $(k_F\xi_0 >> 1)$ to one with Bose condensation of composite bosons $(k_F\xi_0 << 1)$. For the *s*-wave case an exact solution of the variational equations shows a smooth crossover from one regime to the other at T=0. The *p*-wave solution has a weak singularity when the chemical potential goes through zero, which is the bottom of the band. We show, quite generally, independent of the dimensionality and of model details, that the gap-to-single-particle excitations is nodeless, even if the anisotropic pair wave function has nodes, when the coupling is strong enough that the chemical potential is negative.

I. INTRODUCTION

There has been renewed interest,¹ both theoretical and experimental, in superconductivity with the discovery of the high-transition-temperature (T_c) copper oxide superconductors. In spite of vigorous activity, there is still no agreement on many of the basic issues: for example, the appropriate microscopic Hamiltonian, the pairing mechanism, and the symmetry of the order parameter. On the other hand, there are certain characteristics of the new high- T_c materials that are strikingly different from the traditional superconductors and can, we believe, be fruitfully studied independently of these controversial issues.

One of the most striking characteristics of the high- T_c materials is their extremely short coherence length, or pair size, ξ_0 . Rough estimates of the parameter $k_F\xi_0$ for the high- T_c materials lead to values of about 10–20 for La_{1.85}Sr_{0.15}CuO₄, approximately 5–10 for YBa₂Cu₃O₇, and possibly even smaller for the thallium compounds. In contrast, the traditional Bardeen-Cooper-Schreiffer (BCS) superconductors have $k_F\xi_0 \sim 10^3 - 10^4$. These rather crude estimates for the new materials are not very sensitive to whether we use the in-plane coherence lengths or the cube root of the coherence volume for ξ_0 , or 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.

We shall argue further that superconductors with a pair size ξ_0 comparable to the average interparticle spacing k_F^{-1} , are in an interesting *intermediate regime* between the limit of large, overlapping Cooper pairs $(k_F\xi_0 \gg 1)$ and that of Bose condensation of composite bosons $(k_F\xi_0 \ll 1)$ consisting of tightly bound fermion pairs. The Cooper pair limit is, of course, described by

the standard BCS pairing theory.² Aspects of the "Bose limit" have been studied in the specific context of strong electron-phonon coupling, under the name of bipolaronic superconductivity.³ While both of the extreme limits are well understood, the intermediate regime is only beginning to be explored.

In this paper we shall study two-dimensional (2D) superconductivity⁴ at T=0 in a simple continuum model of a Fermi gas with a given two-body interaction. Motivated by the high- T_c superconductors, we shall focus on two questions: (1) the conditions for a pairing instability in two dimensions, and (2) the evolution of the superconducting ground state from the Cooper pair to the Bose condensation limit, with a view to understand the intermediate regime where the pair size is of the order of the interparticle spacing. Some of the results were first reported in an earlier paper.⁵

In the remainder of this section we briefly summarize our approach and our main results, and conclude with an outline of the rest of the paper. The first question that we address is what are the conditions under which a pairing instability takes place in this 2D Fermi gas. We show that, in the presence of hard-core repulsion, a nontrivial threshold in the attraction must be crossed before the gas undergoes an s-wave Cooper instability, and this coincides with the threshold for the formation of a two-body bound state in vacuum. In other words, a two-body bound state in vacuum is a necessary and sufficient condition for the many-body instability. The necessary condition is in marked contrast with the three-dimensional result. We also find that the existence of such a bound state in a higher-angular-momentum (l > 0) channel is not a necessary condition for an *l*-wave pairing instability. These results, which were first obtained⁵ diagrammatically, are derived here from a simpler analysis of the energy dependence of the scattering phase shifts, starting with the Cooper problem.

We next study the many-body ground state within a variational approach to examine the evolution from a state with large, overlapping Cooper pairs to a Bose condensate of composite bosons formed out of tightly bound pairs of fermions, as the attraction in the pair potential is increased. This crossover has been studied earlier by many authors (see Refs. 6-11); our analysis is based on the approach of Leggett.⁷

We make a variational pairing ansatz for the ground state of the many-body system. There are two main differences from the standard BCS procedure in the subsequent calculation. First, as the attraction gets stronger there is a significant rearrangement of the occupation probability in momentum space, which then no longer resembles a Fermi function with slight rounding. As a result the chemical potential μ is no longer fixed at ε_F and must^{6,7} be determined self-consistently together with Δ . Second, a renormalization of the nonlinear gap equation for Δ is required to handle a possible hard core in the interaction.

We find that the resulting coupled integral equations for the gap and chemical potential can be solved *exactly* for the 2Ds-wave case to obtain a surprisingly simple and transparent result.⁵ We obtain a smooth crossover in the ground state from the Cooper pair regime to the Bose condensation limit, as a function of the attractive potential. Some of the results of this 2D crossover were also obtained by Miyake⁹ in the context of dilute ³He in ⁴He films.

The analysis of the evolution of non-s-wave pairing from the BCS regime to the Bose limit is of great interest for a number of reasons. First, for the high- T_c materials there are some experiments which may be interpreted as indicating non-s-state pairing, 12-14 however, the situation is highly controversial since there are other experiments¹⁵ that suggest s-wave pairing, or at least, the absence of nodes in the gap. Second, many analyses¹⁶ of microscopic models for the high- T_c systems, e.g., the Hubbard model, seem to favor d-wave pairing. And finally, independent of its possible relevance to the high- T_c systems, the question is of interest in its own right, as emphasized by Leggett⁷ and by Anderson.¹⁷ Other than a preliminary 3D calculation by McClure,⁸ the crossover analysis for anisotropic superconductors has not been done to the best of the authors' knowledge. The twodimensional equations are much simpler than in 3D, and therefore offer the possibility of making more progress.

The analysis of pairing in higher-angular-momentum states is considerably more complicated than the s-wave case due to the appearance of apparent ultraviolet divergences in the integral equations for the gap function Δ and the chemical potential μ . For the p-wave case we have solved this problem by regulating these divergences using corresponding results from the two-body problem in vacuum. The results for the superconducting ground state provide a continuous interpolation between the expected answers in the Cooper pair and the Bose limits. The ground-state solution, though continuous, has a weak singularity as the chemical potential goes through zero.

An interesting consequence of the analysis given later, that does not depend upon either two dimensionality or on the specific model under consideration, is that E_{gap} , the gap to single-particle excitations, is not the same as the order parameter or "gap function" Δ , provided the attraction is strong enough to cause the chemical potential to be reduced below the bottom of the band $(\mu < 0)$. For non-s-wave superconductors, especially those with nodes in their pair wave functions, this has important consequences: Quite generally, we find that the gap to single-particle excitations is nodeless, for negative values of the chemical potential, even when the anisotropic pair wave function has nodes. We give an explicit example in which the gap and the order parameter do not even have the same symmetry once the coupling is sufficiently strong. Thus, from the point of view of experiments that measure the gap-to-single-particle excitations, strongly coupled superconductors with anisotropic pairs will appear to be s wave.

The rest of this paper is organized as follows. In Sec. II we introduce our model, a dilute 2D Fermi gas, and describe the two-body T matrix and phase shifts which will be used in the rest of the paper. (Details of 2D scattering theory are discussed in Appendix A). In Sec. III we investigate the connection between the onset of the Cooper instability and the existence of bound states in the two-body problem. In Sec. III we use a pairing ansatz for the many-body ground state and derive a renormalized gap equation. We study s-wave pairing in Sec. V, and show that the gap and chemical potential equations can be solved exactly to obtain a smooth crossover from a Cooper paired state to one with tightly bound pairs. In Sec. VI we turn to the case of *p*-wave pairing. The gap and chemical potential equations have apparent ultraviolet divergences that are regularized by appealing to the two-body problem. (The details of the rather lengthy algebra associated with this regularization are relegated to Appendixes B and C). We discuss the evolution of the anisotropic pairs from the Cooper to the Bose limit. In Sec. VII we discuss a general feature of strong coupling, which makes it essential to distinguish between the gap-to-single-particle excitations and the order parameter, or pair wave function. We list some open problems in Sec. VIII, and summarize our conclusions in Sec. IX.

II. PRELIMINARIES

We will study a 2D Fermi gas of N particles in a unit volume, each of mass m, with Fermi energy $\varepsilon_F = \pi \hbar^2 N/m$. As stated in the Introduction, the fermions interact via a given two-body static potential V(r)which, for example, may be strongly repulsive at short distances in addition to having a longer-range attractive part; see Fig. 1. Note that we are not asking for the microscopic origin of this attraction but are simply assuming that such an nonretarded "effective" potential exists.¹⁸ We restrict our attention to a *dilute* gas, where the average interparticle spacing k_F^{-1} is much larger than R,



FIG. 1. Example of a two-body potential V(r) with a repulsive core and an attractive tail of finite range R. As explained in the text, our results will be expressed in terms of quantities that are independent of the detailed shape of the potential.

the range of attraction in V(r). The diluteness condition $k_F R \ll 1$ will allow us to obtain analytical results that are *independent of the detailed shape of the potential* V(r). The two-body potential will enter the final results only through a few parameters that characterize the low-energy scattering phase shifts.

Since we are interested in a V(r) which may have strong repulsion at short distances, its Fourier transform $V_{kk'}$ is not necessarily well defined. To avoid problems due to the hard core we use, as usual, the two-body T matrix which is given by the sum of the Born series:

$$T(E) = V + V\mathcal{G}_0(E)T(E) . \qquad (2.1)$$

Even in the absence of a hard core, the T matrix and the scattering phase shifts (to be introduced later) provide the most economical description of the two-body interaction in the low-energy limit of a dilute gas.

In the equation above \mathcal{G}_0 is the free Green function for the two-body problem

$$(\mathcal{G}_0(2E))_{\mathbf{k}\mathbf{k}'} = [2(E - \varepsilon_{\mathbf{k}} + i\eta)]^{-1} \delta_{\mathbf{k},\mathbf{k}'}, \qquad (2.2)$$

where E is the energy variable, $\varepsilon_k = \hbar^2 k^2 / 2m$ and $\eta \to 0^+$. The unusual factor of 2 is introduced for later convenience. With this convention the energy variable 2E is related to the relative momentum **q** by $2E = \hbar^2 q^2 / 2m_0$, where $m_0 = m/2$ is the reduced mass, so that $E = \hbar^2 q^2 / 2m$. We thus never need to use the reduced mass m_0 in the subsequent analysis.

We will find it useful to expand the various matrix elements in terms of angular momentum eigenfunctions. We start with the expansion of a plane wave in two dimensions in a Fourier series:

$$\exp(i\mathbf{k}\cdot\mathbf{r}) = \sum_{l=-\infty}^{\infty} i^{l} J_{l}(kr) \exp(il\phi) , \qquad (2.3)$$

where $\phi = \cos^{-1}(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}})$ and $J_l(z)$ is a Bessel function of order *l*. Using this we obtain

$$V_{\mathbf{k}\mathbf{k}'} = \langle \mathbf{k} | V | \mathbf{k}' \rangle = \sum_{l=-\infty}^{\infty} \exp(il\theta) V_{kk'}^{(l)}$$
(2.4)

where
$$\theta = \cos^{-1}(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}')$$
 and
 $V_{kk'}^{(l)} = 2\pi \int_0^\infty dr \, r J_l(kr) J_l(k'r) V(r)$. (2.5)

A similar expansion of the *T*-matrix $T_{\mathbf{k}\mathbf{k}'}$ may be used to write the components of (2.1) as

$$T_{kk'}^{(l)}(2E) = V_{kk'}^{(l)} + \int \frac{dq}{2\pi} q V_{kq}^{(l)}(\mathcal{G}_0(2E))_{qq} T_{qk'}^{(l)}(2E) . \quad (2.6)$$

We conclude this section by writing down explicit results for the s-wave (l=0) and p-wave (l=1) cases, which will be used in the following sections. Details of 2D scattering theory may be found in Ref. 19 and in Appendix A.

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

$$\frac{1}{\tau_0(E)} = (m/4\hbar^2) [-\cot\delta_0(E) + i] .$$
 (2.7)

Further, it can be shown that the low-energy phase shift in 2D is of the form

$$\cot \delta_0(E) = \frac{1}{\pi} \ln(E/E_a) + O(E/\varepsilon_R) , \qquad (2.8)$$

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

In Fig. 2 we sketch the qualitative behavior of the parameter E_a as a function of the attractive potential, e.g., the well depth V_0 in a "hard core plus square well" potential. Beyond the threshold V_B , the T matrix has a pole on the negative real axis at $E = -E_a$, indicating a two-body bound state. Thus E_a is the binding energy of that bound state. In Fig. 3 we sketch the low-energy phase shift $\delta_0(E)$.

We now turn to the *p*-wave case. From (2.5) we find that $V_{kk'}^{(1)} \simeq kf(k')$ for $kR \ll 1$ and arbitrary k', and consequently [using (2.6)] the low-energy T matrix has the



FIG. 2. Schematic variation of the parameter E_a characterizing the low-energy s-wave phase shift in 2D as a function of the attraction. E_a is measured in units of $\varepsilon_R = \hbar^2/2mR^2$ and V_0 is, for example, the well depth in a "hard-core plus square-well" potential. V_B corresponds to the threshold for the formation of a two-body bound state; for a purely attractive potential the region to the left of V_B does not exist since $V_B = 0$.



FIG. 3. Schematic variation of the low-energy s-wave scattering phase shift in 2D as function of energy. The lower curve corresponds to a potential whose attraction lies between 0 and V_B in Fig. 2, so that no bound state exists. The upper curve corresponds to an attraction large enough to ensure a bound state. Notice that $\delta_0(2\varepsilon_F) > 0$ implies that $\delta_0(0) > 0$.

form

$$T_{kk'}^{(1)}(E) \simeq kk' \tau_1(E)$$
 for $kR \ll 1$, $k'R \ll 1$. (2.9)

It can be shown that $\tau_1(E)$ is related to the *p*-wave phase shift via

$$\frac{1}{\tau_1(E)} \simeq \frac{1}{2} \left[\frac{m}{\hbar^2} \right]^2 E\left[-\cot\delta_1(E) + i \right].$$
 (2.10)

Finally, the low-energy phase shift is given by

$$\cot\delta_{1}(E) = \frac{E_{b}}{E} + \frac{1}{\pi} \ln \left[\frac{E}{E_{c}} \right] + O(E/\varepsilon_{R}) , \qquad (2.11)$$

where E_b and E_c have unit of energy, and are determined by the two-body interaction. Note that the leading divergence at low energies is a simple pole.

III. PAIRING INSTABILITY

In this section we study the condition for the onset of a pairing instability in the many-body system, and its connection with the existence of bound states in vacuum. We have earlier⁵ addressed this question by calculating the two-particle propagator in the particle-particle channel and looking for the appearance of a pole in the upper-half plane. Here we shall take a simpler approach following the original Cooper² calculation. Although this approach has well-known deficiencies (which we discuss later), it provides a more intuitive understanding of the results of Ref. 5.

Consider then the problem of two fermions, interacting with the given pair potential V(r), above the surface of free Fermi sea. The Fermi sea affects the pair by forbidding the occupancy of the states below k_F . The Schrödinger equation for the pair wave function ψ_k (in the center-of-mass frame) is

$$\frac{\hbar^2 k^2}{m} \psi_{\mathbf{k}} + \sum_{k' \leq k_F} V_{\mathbf{k}\mathbf{k}'} \psi_{\mathbf{k}'} = (\Delta E + 2\varepsilon_F) \psi_{\mathbf{k}} , \qquad (3.1)$$

with $\psi_{\mathbf{k}} = 0$ for $k < k_F$.

Introducing the projection operator $Q = \sum_{k>k_F} |\mathbf{k}\rangle \langle \mathbf{k}|$, and using (2.2), we may rewrite (3.1) as

$$\mathcal{G}_0^{-1}Q\psi = QVQ\psi , \qquad (3.2)$$

where we have suppressed the momentum labels and summations for simplicity. We may formally eliminate the potential V in (3.2), in favor of the T matrix using (2.1) rewritten as $V = (1 + T\mathcal{G}_0)^{-1}T$. We then sum the resulting equation over **k** and cancel $\sum_k Q\psi$ from both sides. Finally using the low-energy ($kR \ll 1$, $k'R \ll 1$) s-wave T-matrix $T_{kk'}^{(0)} \simeq \tau_0$, the result may be simplified to

$$\frac{1}{\tau_0(2E)} = \frac{1}{2} \sum_{\mathbf{k} < \mathbf{k}_F} \frac{1}{\varepsilon_k - E} , \qquad (3.3)$$

where $2E = \Delta E + 2\varepsilon_F$.

We are interested in the onset of a pairing instability as the attractive part of V(r) is increased. This corresponds to a solution $\Delta E < 0$ of (3.3) such that $|\Delta E|/\varepsilon_F \ll 1$. In the 2D s-wave case, using the low-energy T-matrix (2.7) and (2.8), we can solve (3.3) to obtain a solution $\Delta E = -E_a$ satisfying these conditions only if $E_a \ll \varepsilon_F$ $\ll \varepsilon_R$ (where the last inequality follows from the diluteness condition). Now it is clear from (2.7) and (2.8) that whenever $E_a \ll \varepsilon_R$ there is a pole in the two-body T matrix at E_a , corresponding to a bound state with binding energy E_a . Thus we obtain the result⁵ that the existence of a two-body bound state in vacuum is a *necessary* condition for a pairing instability. The (more obvious) sufficiency condition wil emerge from the variational calculation in Sec. V.

A few remarks are in order. First, this result is obvious for a potential which is everywhere attractive in 2D, since then a two-body bound state exists²⁰ 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 threshold must be crossed before a two-body bound state will exist even in 2D, and our result is nontrivial. Second, our result is in striking contrast to the three dimensional (3D) case. In 3D the low-energy s-wave phase shift is given by

$$q \cot \delta_0(q) = -1/a_s + O(qR)^2$$

where a_s is the scattering length. A pairing instability requires only that $a_s < 0$ and not the existence of a twobody bound state, the threshold for which is $a_s \rightarrow -\infty$.

We now make a few remarks on the Cooper calculation before returning to a further discussion of the above result. Note that the "binding energy" $|\Delta E|$ in the presence of the Fermi sea is found to coincide with the binding energy in vacuum. However, we will find below (in Sec. V) that the "gap" (or the growth rate of the two particle propagator; see Ref. 5) is given by $\Delta = \sqrt{2\epsilon_F E_a}$, which differs from $|\Delta E| = E_a$ by a factor of 2 in the exponent; in particular $|\Delta E| \ll \Delta$. The reason for this difference is the simple way in which the Fermi sphere is put in by hand in the Cooper calculation. A similar factor of 2 "error" is well known in three dimensions. For an arbitrary static pair potential in 3D the solution of the Cooper problem (3.3) is

$$|\Delta E| = 8\varepsilon_F e^{-2} \exp(-2\pi/k_F |a_s|)$$

provided that $a_s < 0$ and $(k_F a_s)^{-1} \rightarrow -\infty$. On the other hand, the gap for the many-body problem is larger by a factor of 2 in the exponent, and is given by⁵

$$\Delta = 8\varepsilon_F e^{-2} \exp(-\pi/k_F |a_s|) .$$

Returning to our result connecting pairing and binding, another way to understand it is the following. The standard relationship between the T matrix and the scattering phase shift [Eq. (2.7) in 2D, or its analogue in 3D] can be used to show that the condition for obtaining a solution to the Cooper problem (3.3) with $\Delta E < 0$ is that the phase shift at the Fermi surface be attractive: $\delta_0(2\varepsilon_F) > 0$. On the other hand, the condition for a twobody bound state in vacuum is $\delta_0(0) > 0$; in fact, from Levinson's theorem $\delta_0(0)(\mod \pi)$ counts the number of bound states.

The s-wave phase shifts as a function of energy are calculated as outlined in Appendix A. From Figs. 2 and 3 for the 2D case, it is easy to see that $\delta_0(2\varepsilon_F) > 0$ (Cooper instability) implies $\delta_0(0) > 0$ (a two-body bound state). In contrast, the 3D case (see Figs. 4 and 5) can have $\delta_0(2\varepsilon_F) > 0$ without necessarily having $\delta_0(0) > 0$, when the scattering length a_s is negative.

It is perhaps worthwhile to emphasize again the conditions under which the "necessary" result was obtained. First, it is a strictly two-dimensional result due to the logarithmic singularity in the 2D T matrix, or the corresponding nonzero density of states at $E=0^+$. Second, it requires the same two-body potential for the two-body



FIG. 4. Schematic variation of the s-wave scattering length a_s as a function of attraction in *three* dimensions. For a purely repulsive potential $(V_0=0)$, $a_s > 0$ and decreases with increasing attraction. For attraction greater than V_C , a_s is negative and diverages at V_B , the threshold for a bound state. For $V_0 > V_B$, the (positive) a_s is the spatial extent of that state.



FIG. 5. Schematic variation of the *three*-dimensional lowenergy s-wave scattering phase shift as function of energy. The bottom curve corresponds to $0 < V_0 < V_c$, i.e., an essentially repulsive interaction, for which there is neither a two-body bound state nor a Cooper instability. The middle curve corresponds to a potential with $a_s < 0$ (see Fig. 4), for which the many-body system undergoes a Cooper instability even though the two-body problem in vacuum does not have a bound state. Finally the top curve represents a deep attractive potential for which there is both a bound state and a pairing instability.

and many-body problems, i.e., the "effective potential" V(r) must be independent of the density of the system. Third, one can construct counterexamples that violate the diluteness condition and thereby have phase shifts at zero and at $2\varepsilon_F$ whose signs are not related.

Finally, even in two dimensions this necessary connection does not hold for higher-angular-momentum $(l \neq 0)$ channels. Attraction at the Fermi level $\delta_l(2\varepsilon_f) > 0$, which can be shown to be the condition for a Cooper instability in the *l* channel, does not necessarily imply $\delta_l(0) > 0$. From Appendix A, one can see that the lowenergy expansion for $\cot \delta_l(E)$ has a leading singularity A_l/E^l for l > 0. The sign of $\delta_1(0)$ then depends upon that of A_l , and is not necessarily fixed by the sign of $\delta_l(2\varepsilon_F)$. In Sec. VI we shall study the *p*-wave case in detail, and show explicitly the existence of *p*-state Cooper pairing in the absence of a corresponding bound state in vacuum.

IV. PAIRING ANSATZ: GAP AND CHEMICAL POTENTIAL EQUATIONS

We now turn to an analysis of the many-body ground state. Within a model of the sort that we are considering, one can imagine increasing the attractive part of the potential to the point that the two-body solution looks like a tightly bound pair, or "composite boson." We will show later that the many-body ground state in this limit is a Bose condensate of essentially noninteracting composite bosons. The two-dimensional dilute-gas case is especially interesting because the coupled integral equations resulting from the variational analysis given later can be solved *exactly* over the entire range from Cooper pairing to the Bose limit.

Before proceding with the analysis, it may be useful to ask what kind of instabilities might be expected as the attraction in the two-body potential is increased. If a twobody bound state exists, might it not be possible to have a four-body bound state, or, for that matter, a gas-liquid transition. We know of no general results on conditions that the two-body potential V(r) must satisfy in order that these other possibilities *not* occur. For the problem of phase separation, one must necessarily leave the dilute-gas regime, and then it is unlikely that general results, independent of the detailed shape of the potential, can be obtained; however, some results are known²¹ for specific forms of the interaction. For the remainder of this paper we shall simply assume that the only instability taking place in the system is pairing.

Following BCS we make a pairing ansatz for the many-body ground-state wave function:

$$\Psi(1,...,N) = \mathcal{A}[\phi(1,2)\phi(3,4)\cdots\phi(N-1,N)], \quad (4.1)$$

where \mathcal{A} is an antisymmetrization operator. While this form for the ground-state wave function clearly makes explicit the macroscopic occupation of the pair state ϕ , it is not very useful for the purpose of calculations. To determine the optimal pair wave function ϕ variationally, we must use the BCS trick of working with a particlenonconserving wave function.

The subsequent analysis proceeds along the standard BCS route (see, e.g., Ref. 2) with two exceptions. First, the potential $V_{kk'}$ may be ill defined, as discussed earlier, and thus it has to be replaced by a low-energy pseudopotential in the gap equation; the details of this renormalization will be given later. Second, and more important, as emphasized by Leggett,⁷ the chemical potential μ for the fermions is not, in general, fixed at the Fermi energy, and must be determined self-consistently along with the gap function Δ_k . We will find that the occupation probability in momentum space

$$n_{\mathbf{k}} = \frac{1}{2} \left[1 - \frac{\varepsilon_k - \mu}{E_{\mathbf{k}}} \right] , \qquad (4.2)$$

with

$$E_{\mathbf{k}} \equiv [(\varepsilon_{k} - \mu)^{2} + |\Delta_{\mathbf{k}}|^{2}]^{1/2}, \qquad (4.3)$$

will no longer resemble a Fermi function slightly rounded near ε_F , as the two-body attraction is increased. The chemical potential is then determined by demanding that

$$2\sum_{\mathbf{k}} n_{\mathbf{k}} = N , \qquad (4.4)$$

where N is the total number of particles, taking the volume of the system to be unity, and the 2 is for spin.

The gap function Δ_k is determined, as usual, from

$$\Delta_{k} = -\sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}} .$$
 (4.5)

A more useful gap equation would be in terms of the T matrix, since $V_{\mathbf{k}\mathbf{k}'}$ may not even be well defined, possibly due to a strongly repulsive core. To this end we use a

simple variant of the pseudopotential technique used by Anderson and Morel²² for ³He. Since, in a weak-coupling problem, only fermions near the Fermi surface are significantly affected by pairing, they calculated an effective kernel for a thin shell around ε_F , integrating out the contributions outside the shell. As indicated earlier, in our problem *all* the fermions are affected as the attraction grows stronger, and thus we use a renormalization procedure in which we integrate out the high momentum contributions in (4.5) and obtain an effective low-energy kernel in place of $V_{kk'}$.

We begin by introducing a momentum cutoff $\Lambda > O(R^{-1})$, where R is the range of V(r); at the end, we will show that the results are independent of the cutoff and we may take $\Lambda \rightarrow \infty$. For $k > \Lambda$, we may approximate $E_k \simeq \varepsilon_k$, provided μ and $|\Delta_k|$ are sufficiently small, as we will find at the end of the calculation. This allows the gap equation to be written as

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} \langle V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} - \sum_{\mathbf{k}'} \langle V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2\varepsilon_{\mathbf{k}'}} , \qquad (4.6)$$

where we use the superscripts $\langle \rangle$ to restrict the summation over $k < \Lambda$ ($k > \Lambda$). The second term is the linear part of the integral equation, which can then be iterated as usual. This leads to

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} \langle \Gamma_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} , \qquad (4.7)$$

with the kernel Γ defined by

$$\Gamma_{\mathbf{k}\mathbf{k}'} = V_{\mathbf{k}\mathbf{k}'} - \sum_{\mathbf{k}''} {}^{>} V_{\mathbf{k}\mathbf{k}''} \frac{1}{2\varepsilon_{\mathbf{k}''}} \Gamma_{\mathbf{k}''\mathbf{k}'} .$$
(4.8)

Introducing projection operators $P^{>}$ and $P^{<}$ defined by

$$P^{>} = \sum_{\mathbf{k}} {}^{>} |\mathbf{k}\rangle \langle \mathbf{k}|, \quad P^{<} = 1 - P^{>}, \quad (4.9)$$

and using (2.2) we can rewrite (4.8) in a more compact notation as

$$\Gamma = V + V \mathcal{G}_0(0) P^{>} \Gamma . \tag{4.10}$$

We may now eliminate the potential V between the definition of the T matrix and (4.10) thus obtaining

$$\Gamma = T(E) - T(E) [\mathcal{G}_0(E) - \mathcal{G}_0(0)P^>]\Gamma . \qquad (4.11)$$

The second term can be further simplified by recognizing that $\langle \mathbf{k} | [\mathcal{G}_0(E) - \mathcal{G}_0(0)] | \mathbf{k} \rangle$, with $E = \hbar^2 q^2 / 2m$, is at most of $O(q^2 R^2 / \varepsilon_k)$ for $q \ge \Lambda$, and thus may be ignored in the low-energy limit $qR \ll 1$. Thus (4.11) reduces to

$$\Gamma + T(E) - T(E)\mathcal{G}_0(E)P < \Gamma , \qquad (4.12)$$

which when written in terms of the angular momentum components of the kernel Γ yields

$$\Gamma_{\mathbf{k}\mathbf{k}'}^{(l)} = T_{\mathbf{k}\mathbf{k}'}^{(l)}(E) - \int_{q < \Lambda} \frac{dq}{2\pi} q T_{\mathbf{k}q}^{(l)}(E) (\mathcal{G}_0(E))_{qq} \Gamma_{q\mathbf{k}'}^{(l)}(E) . \quad (4.13)$$

Finally, let us summarize the results of the renormal-

ization of the gap equation. Given the two-body interaction in terms of its T matrix, we can use (4.12), or (4.13), to obtain the pseudopotential Γ , which in turn will determine the gap function Δ_k from the "renormalized" gap equation (4.7).

V. s-WAVE PAIRING

First consider the case of s-wave pairing: the two fermions in a pair are in a spin singlet and the gap function Δ_k has no angular dependence. We thus keep only the l=0 piece of the equations derived in the previous sections. Using the low-energy form of the s-wave T matrix, $T_{kk'}^{(0)}(2E) \simeq \tau_0(2E)$, in (4.13) we find that the equation is separable and may be solved to obtain

$$\Gamma_{kk'}^{(0)} \simeq \tau_0(2E) \left[1 + \tau_0(2E) \int_0^{\Lambda} \frac{dq}{2\pi} \frac{q}{2(E - \varepsilon_q + i\eta)} \right]^{-1},$$
(5.1)

for $kR \ll 1$ and $k'R \ll 1$. Note that the *E* dependence of the right-hand side of (5.1) is illusory, and Γ is, in fact, independent of *E*, as it must be; thus our final results will also turn out to be independent of the energy parameter *E*.

Using the kernel (5.1) in the l=0 part of the gap equation (4.7), we find that the gap function is constant, i.e., $\Delta_{\mathbf{k}} \simeq \Delta$, in the low-energy limit $kR \ll 1$. Further, Δ is determined by

$$\frac{4\pi\hbar^2}{m\tau_0(2E)} = \int_0^\infty d\varepsilon_k \left[\frac{1}{\varepsilon_k - E - i\eta} - \frac{1}{\left[(\varepsilon_k - \mu)^2 + \Delta^2 \right]^{1/2}} \right], \quad (5.2)$$

where we have set the upper limit of integration $\varepsilon_{\Lambda} = \hbar^2 \Lambda^2 / 2m \rightarrow \infty$, since the integral is manifestly finite. The integral above is elementary, and using the expression (2.7) for the *T* matrix in terms of the low-energy scattering phase shift (2.8) on the left-hand side of (5.2), we find the result²³

$$(\mu^2 + \Delta^2)^{1/2} - \mu = E_a \quad . \tag{5.3}$$

The second equation, which will be used to determine Δ and μ self-consistently, is the number equation [see (4.2) and (4.4)]

$$\int_0^\infty d\varepsilon_k \left[1 - \frac{\varepsilon_k - \mu}{\left[(\varepsilon_k - \mu)^2 + \Delta^2 \right]^{1/2}} \right] = 2\varepsilon_F , \qquad (5.4)$$

where the Fermi energy is related via $m\varepsilon_F/\pi\hbar^2 = N$ to the number density in two dimensions. This gives

$$(\mu^2 + \Delta^2)^{1/2} + \mu = 2\varepsilon_F , \qquad (5.5)$$

which, together with (5.3), leads to the final results. The gap function $\Delta_k \simeq \Delta$ for $kR \ll 1$ is given by

$$\Delta = (2\varepsilon_F E_a)^{1/2} , \qquad (5.6)$$

and the chemical potential for the fermions is

$$\mu = \varepsilon_F - \frac{E_a}{2} \quad . \tag{5.7}$$

Notice that the interaction V(r) enters the many-body solution only through E_a , the binding energy of the twobody bound state in vacuum. We should note that the 2D dilute Fermi gas is very special in that the coupled integral equations for Δ and μ could be solved exactly. The diluteness condition effectively results in separable integral equations, and the two dimensionality, with its constant density of states, led to integrals which could be computed analytically.

It is also useful to calculate the pair size ξ_0 defined by

$$\xi_0^2 = \frac{\langle \psi_k | r^2 | \psi_k \rangle}{\langle \psi_k | \psi_k \rangle} , \qquad (5.8)$$

where the "pair wave function"²⁴ is given by $\psi_k = \Delta_k / 2E_k$. The matrix elements in (5.8) can be explicitly evaluated (using $r^2 \rightarrow \nabla_k^2$) to obtain

$$\xi_0^2 = \frac{\hbar^2}{4m} \frac{1}{\Delta} \left[\frac{\mu}{\Delta} + \frac{\mu^2 + 2\Delta^2}{\mu^2 + \Delta^2} \left[\frac{\pi}{2} + \tan^{-1} \frac{\mu}{\Delta} \right]^{-1} \right].$$
 (5.9)

To understand the physical significance of these remarkably simple results we look at two extreme limits of the solutions. For very weak attraction just beyond the threshold for instability, the two-particle binding energy is extremely small, i.e., $E_a \ll \varepsilon_F$, and we find that we recover the BCS results with large, overlapping Cooper pairs. The chemical potential $\mu \simeq \varepsilon_F$, and the gap function $\Delta \ll \varepsilon_F$ has the usual essential singularity in the coupling, although this is not apparent from the form of (5.6). This essential singularity is hidden inside the twobody binding energy E_a ; as shown in Appendix A, one can show quite generally that in two dimensions, E_a is ε_R times an exponentially small term,²⁵ just beyond the threshold. Finally, from (5.9) we find that $\xi_0 \sim \hbar v_F / \Delta$ so that $\xi_0 k_F \sim \epsilon_F / \Delta \gg 1$. Thus the pair size ξ_0 is much larger than the interparticle spacing.

In the opposite limit of very strong attraction, or of very low density, we have a deep two-body bound state $E_a \gg \varepsilon_F$, and we find that we are in a regime in which we have Bose condensation of essentially noninteracting composite bosons or "diatomic molecules". The chemical potential $\mu \simeq -\frac{1}{2}E_a$, which is one half the energy to dissociate a tightly bound pair. The pair size $\xi_0^2 \sim \hbar^2/mE_a$ is much smaller than the interparticle spacing, since $\xi_0 k_F \ll 1$. If the preceding calculation is viewed as a mean-field theory, then it is somewhat surprising that it should have given sensible results in the limit of tightly bound pairs. However, viewed as a variational calculation it is easy to see that the ansatz (4.1) can describe a Bose condensed state of composite bosons in a dilute system.

In between the two extreme limits, i.e., for arbitrary values of E_a / ε_F , the pairing ansatz (4.1) has variational significance. We postpone discussion of the limitations of such a trial wave function to Sec. VIII. The condensation energy can be calculated in the usual way to obtain

$$\Delta \mathcal{E} = \mathcal{E}_{sup} - \mathcal{E}_{nor} = -\frac{1}{2}NE_a \tag{5.10}$$

for all values of E_a/ε_F . It is amusing to note that this is just the energy of N/2 noninteracting pairs. Alternatively, we may use the 2D density of states per spin $N(0) = m/2\pi\hbar^2$, and (5.6), to rewrite the aforementioned result as $\Delta \mathcal{E} = -N(0)\Delta^2/2$. This is the familiar BCS result which is, in fact, valid for all E_a/ε_F , not just in the BCS limit. Finally, we note in passing that the difference in the thermodynamic potential $(\Omega = \mathcal{E} - \mu N, \text{ at } T = 0)$ between the normal and paired states is exactly zero: $\Delta \Omega = 0$.

Our results for the many-body ground state suggest that there is a smooth crossover from the BCS limit to Bose condensation, since there is no singularity in the solutions (5.6) and (5.7) of the gap equation and the number equation as a function of the parameter E_a/ϵ_F that interpolates between these two limits. However, there is a weak singularity if one looks at the excited states, as we show next.

The gap-to-single-particle excitations are given by the minimum of the Bogoliubov quasiparticle energy

$$E_{gap} \equiv \min_{\epsilon_k \ge 0} \left[(\epsilon_k - \mu)^2 + |\Delta_k|^2 \right]^{1/2} .$$
 (5.11)

So long as μ is positive, the minimum occurs at $\varepsilon_k = \mu$ and the energy gap coincides with the gap parameter Δ ; see Fig. 6(a). However, when the attraction is sufficiently strong to cause the chemical potential to go below the bottom of the band ($\varepsilon_k = 0$) the minimum in (5.11) is at $\varepsilon_k = 0$ and the energy gap is no longer Δ ; see Fig. 6(b). (The latter distinction will turn out to be especially important in the non-s-wave case treated in the following section). The gap-to-single-particle excitations for the s-wave case are thus found to be

$$E_{gap} = \begin{cases} \Delta & \text{for } \mu > 0, \\ (\mu^2 + \Delta^2)^{1/2} & \text{for } \mu < 0, \end{cases}$$
(5.12)

and has a weak singularity at $\mu = 0$, or equivalently at $E_a / \varepsilon_F = 2$. The point $\mu = 0$ could be argued to mark the transition between the BCS-type regime ($\mu > 0$) and the Bose condensed regime ($\mu < 0$).

VI. p-WAVE PAIRING

It is interesting to study the evolution from Cooper pairing to Bose condensation for anisotropic pairing for the reasons discussed in the Introduction. We now consider the simplest case of anisotropic pairing, where the two fermions in the pair are in a spin triplet state, and the gap function has the angular dependence $\Delta_k \sim e^{i\theta}$. (The analysis for a sin θ angular dependence is similar, but more involved²⁶).

We do not address the question of the relative stability of various pairing solutions. For a spin-independent potential V(r), the lowest-energy solution in the tightly bound (Bose) limit is necessarily the s state one. If V(r)



FIG. 6. The quasiparticle energy E_k plotted as a function of ε_k . In the top figure (a) the chemical potential μ is positive and the minimum of E_k occurs at $\varepsilon_k = \mu$, and the energy gap $E_{gap} = \Delta$, the "gap parameter". The lower figure (b) is for $\mu < 0$, i.e., below the bottom of the band. The minimum now occurs at the bottom of the band $\varepsilon_k = 0$, and E_{gap} is no longer the same as Δ .

has a hard core, for instance, then in the BCS limit the lowest-energy solution is non s-wave. Thus there will likely be a first-order phase transition (crossing of free energy surfaces) between an anisotropic and an s-state solution as the attraction is increased. On the other hand, for a spin-dependent potential it is possible to have anisotropic pairing all the way into the Bose regime. In this section we shall simply confine ourselves to the l=1 or p-wave channel.

The analysis of the *p*-wave equations is more complicated than the *s*-wave case due to the appearance of apparent ultraviolet divergences in the gap and number equations. We divide this section into three parts. First, we describe the regularization of the gap equation by using our knowledge of the two-body Schrödinger equation, to which the nonlinear gap equation reduces in the short-distance limit. Second, we regularize the divergence in the number equation using a strategy analogous to the one in the first part. Finally, we solve the manifestly finite gap and number equations, and discuss the evolution of the ground-state solution from Cooper pairing to Bose condensation.

A. Gap equation

We use the l=1 (*p*-wave) components of the equations derived in Secs. II and IV. Using the *T* matrix of (2.9) in (4.13), we obtain the low-energy ($kR \ll 1$, $k'R \ll 1$) kernel of the gap equation

$$\Gamma_{kk'}^{(1)} \simeq kk' \tau_1 (2E_0 \left[1 + \tau_1 (2E_0) \int_0^{\Lambda} \frac{dq}{2\pi} \frac{q^3}{2(E_0 - \varepsilon_q + i\eta)} \right]^{-1} .$$
(6.1)

We make the usual approximation (following Anderson and $Morel^{22}$) that the solution of the nonlinear gap equation has

the same angular behavior as that of its kernel. We then find from the l = 1 piece of the gap equation (4.7) that the gap function is of the form

$$\Delta_{\mathbf{k}} \simeq k \Delta_1 e^{i\theta} \quad \text{for } kR \ll 1 . \tag{6.2}$$

The coefficient Δ_1 of the gap function, or equivalently, the more convenient variable G defined by

$$G \equiv m \Delta_1^2 / \hbar^2 , \qquad (6.3)$$

is determined by the p-wave gap equation

$$2\pi \left[\frac{\hbar^2}{m}\right]^2 \frac{1}{\tau_1(2E)} = \int_0^{\varepsilon_A} d\varepsilon_k \varepsilon_k \left[\frac{1}{\varepsilon_k - E - i\eta} - \frac{1}{\left[(\varepsilon_k - \mu)^2 + 2G\varepsilon_k\right]^{1/2}}\right],$$
(6.4)

where the cutoff $\varepsilon_{\Lambda} = \hbar^2 \Lambda^2 / 2m$.

It is easy to see that the gap equation has a logarithmic ultraviolet divergence which comes from using the lowenergy form of the kernel and the gap function, and simply taking the cutoff to infinity. The gap function (6.2) clearly will not rise linearly with k for arbitrarily large momentum, and thus the divergence encountered earlier is unphysical, arising from the improper use of an approximation outside its domain of validity. (Fortunately no such problems were encountered in the *s*-wave analysis, where just naively taking the cutoff to infinity yielded finite, cutoff independent answers.)

One way of regulating this divergence is to notice that the divergent term, $(\mu - G - E)\ln\varepsilon_{\Lambda}$, has a coefficient which involves an arbitrary parameter *E*, the argument of the free Green's function and the *T* matrix (restricted only by the low energy condition $E \ll \varepsilon_R$). Thus by a proper choice of its value, namely

$$E = E_0 \equiv \mu - G \quad , \tag{6.5}$$

we are able to eliminate the logarithmic divergence and obtain a finite answer from (6.4) in the limit $\varepsilon_{\Lambda} \rightarrow \infty$. While this trick clearly works, it would be satisfying to know why. Some insight into this may be obtained by recognizing that the nonlinear gap equation (4.5) rewritten as

$$2E_k\psi_k = \sum_{k'} V_{\mathbf{k}\mathbf{k}'}\psi_{k'}; \quad \psi_k = \Delta_k/2E_k \tag{6.6}$$

reduces, in the short-distance limit $(kR \gg 1)$, to the linear, two-body Schrödinger equation

$$2(\varepsilon_k - E')\psi_k = \sum_{k'} V_{\mathbf{k}\mathbf{k}'}\psi_{k'} . \qquad (6.7)$$

Relating the "eigenvalue" E' of this Schrödinger equation to the *p*-wave gap equation parameters, we find $E' = E_0$, which is the same result as (6.5).

We introduce dimensionless variables $\tilde{G} = G/\epsilon_F$, $\tilde{\mu} = \mu/\epsilon_F$, etc., and express the left-hand side of (6.4) in terms of the *p*-wave phase shift for the two-body problem using (2.10). With the choice (6.5) the regularized gap equation can be written as

$$\begin{aligned} |\tilde{\mu}| + \tilde{\mu} - \tilde{G} + (\tilde{\mu} - \tilde{G}) \ln(|\tilde{\mu}| - \tilde{\mu} + \tilde{G}) - (\tilde{\mu} - \tilde{G}) \ln(\tilde{\mu} - \tilde{G}) \\ = -\pi(\tilde{\mu} - \tilde{G}) \cot\delta_1(2E_0) . \end{aligned}$$
(6.8)

Note the appearance of $|\tilde{\mu}|$ in the equation above which signals a singularity at $\mu = 0$ (see below).

B. Number equation

The second equation needed to determine the gap and the chemical potential self-consistently is the number equation

$$\int \frac{dk \ k}{2\pi} \left[1 - \frac{\varepsilon_k - \mu}{\left[(\varepsilon_k - \mu)^2 + 2G\varepsilon_k \right]^{1/2}} \right] = N , \qquad (6.9)$$

where $N = m \varepsilon_F / \pi \hbar^2$ is the number density of fermions. The above integral cutoff at an energy ε_{Λ} , and expressed in dimensionless variables, is given by

$$\frac{m}{2\pi\hbar^2} \{ |\tilde{\mu}| + \tilde{\mu} + \tilde{G} - \tilde{G} \ln[(|\tilde{\mu}| - \tilde{\mu} + \tilde{G})/2] + \tilde{G} \ln\tilde{\epsilon}_{\Lambda} \} .$$
(6.10)

We thus find a logarithmic divergence if we simply take the cutoff to infinity, which again arises due to the use of the low-energy form of the gap function in (6.9) for large Λ .

The regularization of the divergence that we previously encountered was related to the fact that in the shortdistance limit the gap equation reduced to a two-body Schrödinger equation. Similarly, the number equation of the many-body problem is analogous to the wavefunction normalization integral in the two-body problem. Thus the normalization should have the same shortdistance behavior as the integral in the number equation. We will use this analogy to regularize the divergence in (6.9), following Ref. 8.

Now the wave function $|\psi_{\mathbf{k}_0}\rangle$ of the two-body problem is, in general, not normalizable. For positive-energy solutions (scattering states), this problem can be avoided by formally giving the energy a small imaginary part. For negative energies also the normalization is well defined *only* for certain discrete values of the energy (bound states), and not for arbitrary $E_0 < 0$. However, let us define the "scattered part" $|\chi_{\mathbf{k}_0}\rangle$ of the wave function, where

$$|\psi_{\mathbf{k}_0}\rangle = |\mathbf{k}_0\rangle + |\chi_{\mathbf{k}_0}\rangle$$

with

$$|\chi_{\mathbf{k}_{0}}\rangle = \sum_{\mathbf{k}} |\mathbf{k}\rangle (\mathcal{G}_{0}(2E_{0}))_{\mathbf{k}\mathbf{k}} T_{\mathbf{k}\mathbf{k}_{0}}(2E_{0}) .$$
(6.11)

The normalization integral for χ given by

$$\mathcal{N} = \sum_{\mathbf{k}} |\chi_{\mathbf{k}}|^2 = \int d^2 \mathbf{r} |\chi(\mathbf{r})|^2 .$$
 (6.12)

can be shown to be well defined (see Appendixes B and C).

Our strategy will now be to subtract \mathcal{N} from either side of (6.9), thus obtaining

$$\sum_{k < \Lambda} \left[1 - \frac{\varepsilon_k - \mu}{\left[(\varepsilon_k - \mu)^2 + 2G\varepsilon_k \right]^{1/2}} \right] - \lambda \sum_{k < \Lambda} |\chi_k|^2$$
$$= N - 2\pi\lambda \int drr |\chi(r)|^2 , \quad (6.13)$$

where λ is, for the moment, an arbitrary free parameter (with dimensions of L^{-4}). The aim is to choose λ such that the left-hand side above has a finite limit as the cutoff $\Lambda \rightarrow \infty$.

We first compute (in Appendix B) the normalization in momentum space, making the usual low-energy approximation for the T matrix, and find that it has, as expected, the same logarithmic singularity as the number equation. The ultraviolet singular part of $\sum_{k < \Lambda} |\chi_k|^2$ is given by

$$\frac{1}{4\pi} \left[\frac{m}{\hbar^2} \right]^2 k_0^2 |\tau_1(2E_0)|^2 \ln \tilde{\epsilon}_{\Lambda}$$
(6.14)

for both positive and negative E_0 [see Eqs. (B4) and (B5)]. Using (6.10) and (6.14), we can now choose

$$\lambda = \left[\frac{\hbar^2}{m}\right]^2 \frac{\tilde{G}}{\tilde{E}_0 |\tau_1(2E_0)|^2} \tag{6.15}$$

to ensure that a finite, cutoff independent result is obtained on the left-hand side of (6.13) in the limit $\tilde{\epsilon}_{A} \rightarrow \infty$.

On the right-hand side of (6.13), we use a manifestly finite result for \mathcal{N} calculated in position space [see Appendix C; especially Eqs. (C19) and (C23)]. Although the expressions for \mathcal{N} are naturally different for $E_0 > 0$ and $E_0 < 0$, we find, as expected the same regularized number equation to be valid for both signs of E_0 . After some straightforward algebra we find the regularized number equation to be

$$\begin{aligned} |\tilde{\mu}| + \tilde{\mu} - \tilde{G} \ln[(|\tilde{\mu}| - \tilde{\mu} + \tilde{G})/2] + \tilde{G} \ln(\tilde{\mu} - \tilde{G}) \\ = 2 + \pi \tilde{G} \left[\cot\delta_1(2E_0) + \tilde{E}_0 \frac{d}{d\tilde{E}_0} \cot\delta_1(2E_0) \right], \end{aligned}$$
(6.16)

where $\tilde{E}_0 = \tilde{\mu} - \tilde{G}$.

C. Solution of *p*-wave equations

We will now consider the solution of the many-body gap equation (6.8) and the number equation (6.16) as functions of the scattering phase shift which describes the two-body interaction. As shown earlier [see (2.11)],

$$\cot \delta_1(2E_0) = \tilde{E}_b / 2\tilde{E}_0 + (1/\pi) \ln(2\tilde{E}_0 / \tilde{E}_c) + O(E_0 / \epsilon_R) ,$$

where $\tilde{E}_b = E_b / \varepsilon_F$ and $\tilde{E}_c = E_c / \varepsilon_F$ are parameters that characterize the low-energy $(k_0 R \ll 1)p$ -wave phase shift. Using this in (6.8) and (6.16), we obtain the two equations that determine \tilde{G} and $\tilde{\mu}$:

$$\begin{split} |\tilde{\mu}| + \tilde{\mu} - \tilde{G} + (\tilde{\mu} - \tilde{G}) \ln(|\tilde{\mu}| - \tilde{\mu} + \tilde{G}) \\ = (\tilde{\mu} - \tilde{G}) \ln \tilde{E}_c - \pi \tilde{E}_{b/2} , \quad (6.17) \end{split}$$

and

$$|\tilde{\mu}| + \tilde{\mu} - \tilde{G} - \tilde{G} \ln(|\tilde{\mu}| - \tilde{\mu} + \tilde{G}) = 2 - \tilde{G} \ln \tilde{E}_c . \quad (6.18)$$

A numerical solution of these equations will be given later, after we obtain analytical results in various limits and analyze the singularties of the solution.

First, consider the case of a very weakly attractive interaction. It is easy to show that this corresponds to $\tilde{E}_c \ll 1$ and $\tilde{E}_b \gg 1$. In this situation there is no *p*-wave bound state in the two-body problem in vacuum, as there is a finite threshold for the appearance of such a state. We find a self-consistent solution of (6.17) and (6.18) with $\tilde{G} \ll 1$ and $\tilde{\mu} \simeq 1$. In terms of our original variables [using (6.2) and (6.3)], we find the chemical potential and coefficient of the gap function to be

$$\mu \simeq \varepsilon_F$$
, and $\Delta_1 \simeq \left[\frac{\hbar^2 E_c}{m}\right]^{1/2} \exp\left[-\frac{\pi E_b}{4\varepsilon_F}\right]$. (6.19)

This is clearly the BCS limit in which the pair size can be shown to be much larger than the interparticle spacing.

Next, consider the opposite limit where the two-body attraction is sufficiently strong to give a *p*-wave bound state whch is deep on the scale of ε_F . (The threshold for the existence of a bound state is the vanishing of E_b , so that we must have $E_b < 0$). We expect that in this extreme Bose limit the chemical potential is negative ($\mu < 0$) and, further, that $|\tilde{\mu}| \gg \tilde{G}$ and $|\tilde{\mu}| \gg 1$. From (6.18) and (6.17) we then find that μ and G are given by

$$2|\mu|\ln(2|\mu|/E_c) \simeq -\pi|E_b|$$
 (6.20)

and

$$G \simeq \frac{2}{1 + \ln(E_c/2|\mu|)}$$
 (6.21)

In Appendix A we show that the binding energy ε_1 of a *p*-wave bound state is given by [see Eq. (A8)]

$$\varepsilon_1 \ln(\varepsilon_1/E_c) \simeq -\pi |E_b|$$
.

Thus, in the extreme Bose limit, the chemical potential of the fermions is exactly one-half the pair binding energy:

$$\mu = -\frac{1}{2}\varepsilon_1 , \qquad (6.22)$$

as might have been expected. The many-body solution thus describes the Bose condensed state of composite bosons consisting of tightly bound pairs in this limit.

In between these two extreme limits, let us look for possible singularities of the solutions of (6.17) and (6.18); see Fig. 7. First notice that the many-body equations do not have any singularity at $E_b = 0$, which is the threshold





"Bose Limit"

FIG. 7. "Phase diagram" for 2D p-wave $exp(i\theta)$ pairing, where E_a and E_b are the two parameters which characterize the low-energy p-wave phase shift. The upper left-hand corner corresponds to the extreme BCS limit with large overlapping pairs, $\mu = \epsilon_F$, and a small gap with an essential singularity. The extreme Bose limit is in the lower right-hand corner, with pairs smaller than the interparticle spacing and $|\mu|$ one half the pair binding energy. The line $E_b = 0$ is the threshold for binding in the two-body problem. The chemical potential vanishes on the dashed line $E_b / \varepsilon_F = -4/\pi$, and the ground-state solution shows a weak singularity along this line. The dotted lines represent curves of constant phase shift $\delta_1(2\varepsilon_F)$. The phase shift increases from 0 to π as we move from the BCS to the Bose limit.

for the formation of a two-body bound state in vacuum. (For E_b small and positive, there are *p*-wave resonances in the two-body problem; these also appear not to have any effect on the many-body solution). However, there is a singularity at $\mu = 0$, or equivalently at $\tilde{E}_{b} = -4/\pi$. The existence of this singularity is obvious from the appearance of $|\mu|$ in the equations. A straightforward analysis of (6.17) and (6.18) shows that the singularity is rather weak; both $\tilde{G}(\tilde{E}_b, \tilde{E}_c)$ and $\tilde{\mu}(\tilde{E}_b, \tilde{E}_c)$ are continuous, but their second derivatives are discontinuous at $(\tilde{E}_b = -4/\pi, \tilde{E}_c)$. We have also numerically solved the p-wave gap and number equations for a particular "hard-core plus square-well" potential; the results of this analysis are plotted in Figs. 8 and 9.

Note that the appearance of a singularity in the *p*-wave ground-state solution is to be contrasted with the s-wave results of Secs. V. In the s-wave case the ground state evolved smoothly from the BCS to the Bose limits, and it was only in the gap to excited states that a singularity appeared. We should, of course, emphasize that the singularity obtained above is within a variational calculation, and thus need not necessarily correspond to a physical singularity in the true ground state. However, we believe that the point $\mu = 0$, where the chemical potential for the

FIG. 8. Numerical solution of the 2D p-wave $exp(i\theta)$ gap and number equations. $G = m \Delta_1^2 / \hbar^2$ is plotted as a function of the attraction V_0 . The potential used has a hard core of radius 0.1R and a "square well" of depth V_0 from 0.1R to R; $\varepsilon_R = \hbar^2/2mR^2 = 100$ in units in which $\varepsilon_F = 1$. Note the change in the sign of the curvature of G at the point where μ goes through zero (see Fig. 9). Also note the exponential behavior of G in the inset, which is in agreement with the asymptotic solution in the BCS limit (see text).

fermions goes below the bottom of the band does, in fact, have a real physical significance. As we shall show in the next section there is a qualitative change in the excitation spectrum for non-s-state superconductors when μ goes through zero.

VII. GAP VERSUS ORDER PARAMETER

In the usual weak coupling BCS theory, the energy gap-to-single-particle excitations E_{gap} turns out to be Δ , which was originally introduced as a variational parameter for the pair wave function in the BCS ground state. An interesting consequence of the preceding calculations is that E_{gap} , the gap-to-single-particle excitations, can



FIG. 9. Numerical solution of the 2D p-wave $exp(i\theta)$ gap and number equations. The chemical potential μ is plotted as a function of the attraction for the "hard-core plus square-well" potential described in the caption for Fig. 8. The dashed line is the asymptotic solution in the extreme Bose limit (see text).

We will show further, that as a result of this, strong coupling anisotropic superconductors with nodes in their pair wave functions will appear s wavelike insofar as their excitation spectrum is conecerned. As discussed in the Introduction, there are some experiments that suggest s-state pairing, or no nodes in the gap, in the high- T_c materials, whereas others indicate "unconventional" pairing. While, it is not clear at the present time if the high- T_c superconductors are sufficiently strongly coupled to have $\mu < 0$, our observation offers the possibility of reconciling some of the apparently contradictory experimental signals. For example, the fluctuation specific-heat experiment probes the order parameter¹² (which may have nodes), while the penetration depth¹⁵ experiments are probing the excitation spectrum (which will be nodeless, provided the coupling is sufficiently strong).

Let us consider a non-s-state "gap function" Δ_k of the general form

$$\Delta_{\mathbf{k}} = g(k) f(\widehat{\mathbf{k}}) , \qquad (7.1)$$

where g and f are functions whose form is determined by that of the interaction in the gap equation, with $f(\hat{\mathbf{k}})$ representing the angular dependence. The gap to singleparticle excitations is given by the minimum of the Bogoliubov quasiparticle energy

$$E_{\text{gap}}(\hat{\mathbf{k}}) \equiv \min_{\varepsilon_k \ge 0} [(\varepsilon_k - \mu)^2 + |\Delta_k|^2]^{1/2} .$$
 (7.2)

In the BCS limit $\mu \simeq \varepsilon_F$, and we find, as expected, that the minimum in (7.2) is at $\varepsilon_k = \mu$, and $E_{gap}(\hat{\mathbf{k}}) \simeq g(k_F) f(\hat{\mathbf{k}})$. Thus nodes of the anisotropic pair wave function (zeroes of f) are also nodes of the excitation spectrum in the BCS limit.

However, the situation in strong coupling is quite different, the first hint of which was already seen at the end of Sec. V (see Fig. 6). When the coupling (i.e., the two-body attraction in our model) is sufficiently strong to cause the chemical potential to go below the bottom of the band ($\mu < 0$), the minimum in (7.2) shifts to $\varepsilon_k = 0$, and the energy gap is no longer just Δ_k . From (7.1) and (7.2) we find

$$E_{\rm gap}(\hat{\mathbf{k}}) = [|\mu|^2 + |g(0)|^2 |f(\hat{\mathbf{k}})|^2]^{1/2}, \qquad (7.3)$$

thus $E_{gap} \ge |\mu|$. For superconductors with nodes in their pair wave functions this has important consequences: quite generally, we find that the gap-to-single-particle excitations is nodeless, for negative values of the chemical potential, even when the anisotropic pair wave function, or order parameter, has nodes.

In the extreme Bose limit, this result is easy to understand. The energy gap is then just the "ionization potential" for the composite boson, which is clearly an isotropic quantity. The preceding argument shows that this absence of nodes is not just true in the Bose limit, but



FIG. 10. The energy gap for the 2D sin θ solution. Figure (a), valid for $\mu > G'$, shows an angle-dependent E_{gap} over the entire Fermi surface (see text). For $G' > \mu > 0$ the energy gap has angular dependence only in a wedge around the poles, but is angle-independent outside this wedge, as shown in (b). The case $\mu < 0$ is shown in (c) and has an isotropic gap: $E_{gap} = |\mu|$.

persists all the way up to $\mu < 0$.

We conclude this section with a calculation of the energy gap for the specific case of 2D *p*-wave solution with $\Delta_k \simeq k \Delta_2 \sin \theta$. As in the previous section one can solve the coupled integral equations for μ and $G' = m \Delta_2^2 / \hbar^2$, the details of which we omit.²⁶

The energy gap for the $\sin\theta$ solution is obtained from (7.2) and sketched in Fig. 10. In the extreme BCS limit, where $\mu \simeq \varepsilon_F \gg G'$, the energy gap has the expected $\sin\theta$ dependence. More generally, for $\mu > G'$, we find

$$E_{\rm gap} = (2\mu G' \sin^2\theta - G'^2 \sin^4\theta)^{1/2}$$

For $G > \mu > 0$ the energy gap has the above angular dependence in a wedge around the poles, but is angle independent, and equal to μ outside these wedges, as shown in Fig. 10(b). The angle ϕ of the wedge is given by

 $\sin^2(\phi/2) = \mu/G'$. As the chemical potential μ decreases, so does the angle of the wedge, and the overall magnitude of the gap. Finally, for $\mu < 0$, the gap is nodeless, as we had argued on general ground earlier. In fact, it is also isotropic, and given by $E_{gap} = |\mu|$.

VIII. OPEN PROBLEMS

We describe some open problems related to superconductors with pair size comparable to the interparticle spacing.

The pairing ansatz (4.1), which has been the basis for most of our conclusions, has obvious limitations in the "intermediate coupling" regime, where $\xi_0 k_F \sim 1$. While the results obtained from it have variational significance, and presumably give a qualitatively reasonable description in the intermediate regime, a definite analysis would involve going beyond this ansatz. Since we have only taken pair correlations into account in our variational ansatz, we see that, e.g., in the extreme Bose limit, the composite bosons are noninteracting. Thus in order to make a virial expansion about this limit, we would need to include three- and four-body correlations between the constituent fermions.

All our results have been restricted to T=0. A finitetemperature analysis of the intermediate regime remains an open problem, although some progress has been made.¹⁰ In the BCS limit the formation and condensation of pairs occurs together. In the Bose limit, the formation of pairs is a very high-energy (\approx binding energy E_a) crossover phenomena, while the Bose condensation occurs at a lower temperature which is determined by the density, independent of the interactions. A physical picture for the transition in the intermediate regime is lacking at the present time.

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 , perhaps leading to anomalous "normal"-state properties. However, since the bound pairs are being probed on the scale of their compositeness $(k_F\xi_0 \sim 1)$ they cannot be simply treated as point bosons, thus making the problem difficult.

IX. CONCLUSIONS

We conclude by summarizing our results. We have studied a two-dimensional Fermi gas with a given twobody interaction. (1) We find that the existence of an swave bound state in vacuum is a necessary and sufficient condition for an s-wave pairing instability. (2) This necessary condition is not true for higher-angularmomentum channels, i.e., it is possible to have *l*-wave Cooper pairing without a corresponding bound state in the two-body problem. (3) Within a variational ansatz, consisting of an antisymmetrized product of pair wave functions, we studied the evolution of the many-body ground state as a function of the attraction. For the swave case we find a smooth crossover from large overlapping Cooper pairs $(k_F \xi_0 \gg 1)$ to a condensate of composite bosons $(k_F \xi_0 \ll 1)$. (4) For the *p*-wave case we find a continuous evolution from the BCS limit to the Bose limit, with a weak singularity as the chemical potential goes below the bottom of the band. (5) The energy gap to single-particle excitations is, in general, distinct from the "gap function" or order parameter. We show that, independent of dimensionality and of details of the model, the energy gap is nodeless, even if the order parameter is not, once the coupling is strong enough to cause the chemical potential to go below the bottom of the band.

The high-temperature superconductors, with pair sizes comparable to the average interparticle spacing $(k_F\xi_0 \simeq 1-10)$, appear to be in the interesting intermediate regime between cooperative BCS pairing and condensation of independent pairs. The use of these ideas in understanding experiments on the high- T_c materials must await a finite temperature theory of the intermediate regime.

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APPENDIX A: PHASE SHIFTS AND BOUND STATES IN TWO DIMENSIONS

In this appendix, we briefly review some elementary results of 2D scattering theory—phase shifts, bound states, etc.,—which are used in this paper. Reference 19 provides useful background information.

Consider a potential of finite range: V(r)=0 for $r \ge R$; see, e.g., Fig. 1. The radial wave function, for energy $E = \hbar^2 k^2 / 2m$ and angular momentum l, is of the form

$$\psi_l(r; E) = A \left[\cot \delta_l(E) J_l(kr) - N_l(kr) \right], \quad r > R$$
(A1)

outside the range of the potential. Here J_l and N_l are the Bessel and Neumann functions of order l and $\delta_l(E)$ is the phase shift of the *l*th partial wave. Next define the logarithmic derivative of the wave function inside the range of the potential (i.e., r < R)

$$\beta_l(E) = \frac{1}{R} \left[\frac{1}{\psi_l} \frac{d\psi_l}{dr} \right]_{r=R^-}, \qquad (A2)$$

where β_l is a functional of the potential V(r), in addition to being a function of the energy. Matching logarithmic derivatives at R we obtain

$$\cot \delta_{l}(E) = \frac{x N_{l}'(x) - \beta_{l} N_{l}(x)}{x J_{l}'(x) - \beta_{l} J_{l}(x)}; \quad x = kR , \quad (A3)$$

where primes denote derivatives.

1. s-wave channel

First consider the l=0 or s-wave case. From an asymptotic expansion of (A3) we obtain the low-energy



$$\pi \cot \delta_0(E) = \ln(E/E_a) + O(E/\varepsilon_R)$$
(A4)

with E_a given by

$$E_a = 4\varepsilon_R \exp\left[-2\gamma + \frac{2}{\beta_0}\right], \qquad (A5)$$

where γ is Euler's constant and β_0 is the logarithmic derivative evaluated at E = 0.

In three dimensions it is conventional to express the low-energy s-wave phase shift in terms of the scattering length. For our purposes it is best to use the parameter E_a , with units of energy, to characterize the low-energy phase shift in 2D. As shown further this parameter has a simple physical interpretation of binding energy in the regime of our interest (in much the same way as the 3D scattering length is related to the size of the bound state once such a state exists). Thus we are able to avoid the apparently controversial question²⁷ of the definition of a "scattering length" in 2D.

Let us now see how E_a varies as a function of the potential. For a purely repulsive potential β_0 can be shown to be positive, and thus $E_a \sim O(\varepsilon_R)$. Imagine turning on an attractive tail to the potential (e.g., hard core plus square well). As a function of the attraction β_0 decreases leading to an increase in E_a ; see Fig. 2. With increasing attraction β_0 goes through zero and thus from (A5) we find that E_a shows discontinuous behavior; E_a first diverges as $\beta_0 \rightarrow 0+$, and then increases from zero with an essential singularity $\exp(2/\beta_0)$ for small negative β_0 .

The connection between the s-wave T matrix and the phase shift is given by Eq. (2.7); see Ref. 19. It is easy to see from (2.7) and (A4) that for $E_a \ll \varepsilon_R$ there is a pole in the T matrix at $E = -E_a$ that signals the existence of an s-wave bound state. Thus $\beta_0=0$ is the threshold for the formation of a two-body bound state in vacuum, and E_a is just the binding energy of this state beyond the threshold.

For a *purely attractive* potential in 2D there is no threshold to binding. In this case the essential singularity discussed earlier can be seen explicitly from the result²⁰

$$E_a \simeq 2\varepsilon_R \exp\left[\left(-\frac{m^2}{m}\right) \middle/ \left|\int dr \ rV(r)\right|\right] . \tag{A6}$$

2. p-wave channel

An asymptotic expansion of (A3), for l = 1, gives the low-energy *p*-wave phase shift of Eq. (2.11):

$$\cot\delta_1(E) = \frac{1}{\pi} \ln \left[\frac{E}{E_c} \right] + \frac{E_b}{E} + O(E/\varepsilon_R) . \tag{A7}$$

The parameters E_b and E_c characterize the low-energy *p*-wave phase shift, and can be straightforwardly calculated from β_1 and its derivative with respect to the energy, both evaluated at E = 0. Note that the leading singularity in (A7) is a pole, and in addition there is the logarithm characteristic of 2D. [We mention in passing, that it can be shown from (A3) that for arbitrary *l* the leading singularity in (A3) that for arbitrary *l* the leading singularity in (A3) that for arbitrary *l* the leading singularity in (A3) that for arbitrary *l* the leading singularity is a pole.

larity in a low-energy expansion of $\cot \delta_l(E)$ is an *l*th order pole].

From Ref. 19 we can show that the connection between the *p*-wave *T* matrix and the δ_1 is given by Eq. (2.10). Now, a *p*-wave bound state corresponds to a pole on the negative real axis of the l=1 *T* matrix. From this we find that the threshold for the formation of a *p*-wave bound state is $E_b=0$, (i.e., no bound state exists for $E_b > 0$). For $E_b < 0$, the binding energy ε_1 of this state is given by the solution of the equation

$$\varepsilon_1 \ln(\varepsilon_1 / E_c) = -\pi |E_b| \quad . \tag{A8}$$

APPENDIX B: NORMALIZATION INTEGRAL IN MOMENTUM SPACE

Using Eq. (6.11) we obtain

$$\sum_{\mathbf{k}} |\chi_{\mathbf{k}}|^2 = \int_0^{2\pi} \frac{d\theta}{2\pi} \int_0^\infty \frac{dkk}{2\pi} \left| \frac{1}{2(E_0 - \varepsilon_k + i\eta)} T_{\mathbf{k}\mathbf{k}_0}(2E_0) \right|^2.$$
(B1)

We retain only the l = 1 piece from the Fourier decomposition of T_{kk_0} and take its low-energy limit, namely

$$T_{\mathbf{kk}_{0}}(2E_{0}) = e^{i\theta}T_{kk_{0}}^{(1)}(2E_{0}) \simeq e^{i\theta}kk_{0}\tau_{1}(2E_{0}) , \qquad (\mathbf{B}2)$$

where $E_0 = \hbar^2 k_0^2 / 2m$, and the final form is valid for $kR \ll 1$ and $k_0R \ll 1$, and from (2.10) and (2.11) τ_1 is given by

$$\tau_1(2E_0) = \frac{-4\hbar^2}{mk_0^2} \sin\delta_1(k_0) e^{i\delta_1(k_0)} .$$
 (B3)

If we use this low-energy form of the T matrix in (B1), we need to introduce an ultraviolet cutoff Λ in the momentum integral, since there is a logarithmic divergence at high momenta. The normalization integral, with the cutoff, is given by

$$\sum_{k < \Lambda} |\chi_k|^2 = \frac{1}{4\pi} \left[\frac{m}{\hbar^2} \right]^2 k_0^2 |\tau_1(2E_0)|^2 \mathcal{J}(E_0) , \qquad (B4)$$

with

$$\mathcal{J}(E_0) \equiv \int_0^{\varepsilon_{\Lambda}} \frac{\varepsilon d\varepsilon}{(E_0 - \varepsilon)^2 + \eta^2} \\ = \begin{cases} \ln|\varepsilon_{\Lambda}/E_0| - 1 + \pi E_0/\eta & \text{for } E_0 > 0\\ \ln|\varepsilon_{\Lambda}/E_0| - 1 & \text{for } E_0 < 0, \end{cases}$$
(B5)

where $\varepsilon_{\Lambda} = \hbar^2 \Lambda^2 / 2m$ and $\eta \rightarrow 0+$. Notice that in addition to the expected $\log \varepsilon_{\Lambda}$ divergence (for all E_0), there is an additional $1/\eta$ divergence for the positive-energy eigenfunctions (scattering states), since they are, of course, non-normalizable. This, as we shall see, will be compensated by an identical contributon from the position-space normalization integral.

APPENDIX C: NORMALIZATION INTEGRAL IN POSITION SPACE

This calculation is somewhat more involved than the momentum-space calculation given earlier. The main

trick, following McClure,⁸ is to generalize a result in Landau and Lifshitz,²⁰ which relates the wave function normalization integral to the scattering phase shifts; [see Eq. (128.10) and problem 4, Sec. 134 in Ref. 20]. The chief complication comes from the fact that we want this result for the normalization of the only the *scattered* part $\chi(r)$ of the radial wave function R(r).

1. Case I: $E_0 > 0$

We shall first evaluate the normalization for $E_0 = \hbar^2 k_0^2 / 2m > 0$. From the l=1 component of (6.11) we have $R(r;k_0) = iJ_1(k_0r) + \chi(r;k_0)$, where $J_1(z)$ is the first-order Bessel function. We define $f(r) = \sqrt{k_0r}R(r)$, $f_0(r) = i\sqrt{k_0r}J_1(k_0r)$, and $X(r) = \sqrt{k_0r}\chi(r)$. f(r) and $f_0(r)$ satisfy the Schrödinger equations

$$f''(r) + [(k_0 + i\alpha)^2 - U_1(r)]f(r) = 0, \qquad (C1)$$

and

$$f_0''(r) + [(k_0 + i\alpha)^2 - U_1(r)]f_0(r) = -U(r)f_0(r) .$$
 (C2)

Here $(k_0+i\alpha)^2 = 2m(E_0+i\eta)/\hbar^2$, so that $\alpha = m\eta/\hbar^2 k_0$ $\rightarrow 0+$, and $U_l(r) = U(r) + (l^2 - \frac{1}{4})(1/r^2)$, with U(r) $= mV(r)/\hbar^2$ since the reduced mass is $m_0 = m/2$. X(r) then satisfies the inhomogeneous equation

$$X''(r) + [(k_0 + i\alpha)^2 - U_1(r)]X(r) = U(r)f_0(r) .$$
 (C3)

We differentiate (C3) with respect to k_0 and eliminate the U_1 term between the resulting expression and the complex conjugate of (C3). We then obtain the normalization integral as the sum of three terms:

$$2(k_0 + i\alpha) \int_0^r dr |X|^2 = Q_1 + Q_2 + Q_3 , \qquad (C4)$$

where

$$Q_1 = Q(r) - Q(0)$$
 with $Q = \frac{\partial X}{\partial k_0} \frac{\partial X^*}{\partial r} - X^* \frac{\partial}{\partial k_0} \frac{\partial X}{\partial r}$, (C5)

$$Q_2 = -4ik_0 \alpha \int_0^r dr X^* \frac{\partial X}{\partial k_0} , \qquad (C6)$$

and

$$Q_3 = \int_0^r dr \ U(r) \left[X^* \frac{\partial f_0}{\partial k_0} - \frac{\partial X}{\partial k_0} f_0^* \right] . \tag{C7}$$

For $E_0 > 0$, we have to first take the limit $r \to \infty$, and then $\alpha \to 0+$. In this limit Q_1 can be shown to vanish. To evaluate Q_2 , notice that it can be rewritten as

$$Q_2 = -4ik_0 \alpha \int_R^r dr \, X^* \frac{\partial X}{\partial k_0} \,, \tag{C8}$$

where we have dropped the (finite) contribution to the integral from 0 to R, the range of the potential, since we have a vanishing prefactor α . We thus only have to compute the divergent part of the integral in (C8) for which it suffices to use the asymptotic form of the scattered wave function X(r). This is given by

$$X(\mathbf{r}) \simeq \frac{1}{\sqrt{2\pi}} \exp(-\alpha \mathbf{r} + ik_0 \mathbf{r} - i\pi/4) S_1(k_0)$$
$$\times \left[1 + \frac{3i}{8k_0 \mathbf{r}} + \cdots\right], \qquad (C9)$$

for $E_0 > 0$, with $S_1(k_0) = \exp[i2\delta_1(k_0)] - 1$. The subleading terms in (C9) lead to integrals of the form

$$\alpha \int_{R}^{\infty} dr \exp(-2\alpha r) r^{-n} \quad n \ge 1 , \qquad (C10)$$

all of which vanish, in the limit $\alpha \rightarrow 0+$, as α for n > 1, and as $\alpha \log \alpha$ for n = 1. The nonvanishing contributions to (C8) give

$$Q_2 = \frac{E_0 |S_1(k_0)|^2}{\pi \eta} - \frac{ik_0 S_1^*(k_0)}{\pi} \frac{dS_1(k_0)}{dk_0} , \qquad (C11)$$

where we have used $\eta = \hbar^2 k_0 \alpha / m \rightarrow 0+$ and have dropped terms of order $k_0 R \ll 1$.

The imaginary part of the left-hand side of (C4) is handled in exactly the same way as Q_2 , and we obtain, as $\alpha \rightarrow 0+$

$$2i\alpha \int_0^\infty dr |X|^2 = \frac{i}{2\pi} |S_1(k_0)|^2 .$$
 (C12)

Finally we want to evaluate Q_3 . Substituting $X(r) = f(r) - f_0(r)$ in (C7), and using the definitions used in (C1) and (C2), we obtain

$$Q_{3} = \frac{im}{\hbar^{2}} \int_{0}^{\infty} drr \ V(r) \left[R^{*}(r) \left[\frac{1}{2} J_{1}(k_{0}r) + k_{0} \frac{\partial J_{1}(k_{0}r)}{\partial k_{0}} \right] + J_{1}(k_{0}r) \left[\frac{1}{2} R(r) + k_{0} \frac{\partial R(r)}{\partial k_{0}} \right] \right].$$
(C13)

To make progress we must recall the identity

$$\langle \mathbf{k} | V | \psi_{\mathbf{k}_0} \rangle = \langle \mathbf{k} | T(2E_0) | \mathbf{k}_0 \rangle , \qquad (C14)$$

where the argument of the T matrix is $2E_0$ due to our (unusual) convention [see Eq. (2.2)]. Using the l=1 Fourier component of (C14), and (B3) rewritten as

$$\tau_1(2E_0) \simeq 2i\hbar^2 S_1(k_0) / mk_0^2 , \qquad (C15)$$

we obtain

$$\frac{m}{\hbar^2} \int_0^\infty dr r \ V(r) J_1(kr) R(r;k_0) = -\frac{k}{k_0} \frac{S_1(k_0)}{\pi} , \quad (C16)$$

for $kR \ll 1$, $k_0R \ll 1$. This result, together with its derivatives, allows us to express all the integrals in (C13) in terms of the phase shift. We find

$$Q_{3} = \frac{-i}{2\pi} [S_{1}^{*}(k_{0}) + S_{1}(k_{0})] - \frac{i}{\pi} [S_{1}^{*}(k_{0}) - S_{1}(k_{0})] - \frac{ik_{0}}{\pi} \frac{dS_{1}(k_{0})}{dk_{0}} .$$
 (C17)

We can now obtain the wave function normalization integral using (C4) and



The final result, valid for $E_0 > 0$, is

$$\mathcal{N} = \frac{2\hbar^2}{m} \sin^2 \delta_1(k_0) \frac{1}{\eta} - \frac{2}{k_0^2} \sin 2\delta_1(k_0) + \frac{2}{k_0} \frac{d\delta_1(k_0)}{dk_0} ,$$
(C19)

where $\eta \rightarrow 0+$. Note (1) that although the intermediate quantities Q_i were complex, \mathcal{N} is real as it must be, and (2) that the $1/\eta$ divergence in the position-space evaluation of \mathcal{N} is identical to the one obtained in the momentum-space result. Both these serve as nontrivial checks on the algebra.

Finally, we may rewrite λ of Eq. (6.15) in terms of the phase shift, using (B3),

$$\lambda = \frac{mk_0^2 G}{8\hbar^2 \sin^2 \delta_1(k_0)} .$$
 (C20)

This expression is useful, in conjunction with (C19), to evaluate the right-hand side of (6.13).

2. case II: $E_0 < 0$

The calculation proceeds in much the same way as for E_0 positive, and is in fact simpler because the wave functions are all real, the T matrix is real, and η (or α) can be set equal to zero at the very outset.

For $E_0 = -\hbar^2 q_0^2 / 2m$ the l = 1 wave function may be obtained from the analytic continuation of the $E_0 > 0$ re-

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sult with $k_0 = iq_0$. Then

$$R(r;iq_0) = -I_1(q_0r) + \chi(r;iq_0)$$

where $I_1(z)$ is the first-order modified Bessel function. Following the logic of the previous computation, we find [the analogue of Eq. (C4)]

$$2\int_{0}^{\infty} dr X^{2}(r) = \int_{0}^{\infty} dr r U(r) \left[R(r) \frac{\partial I_{1}(q_{0}r)}{\partial q_{0}} - I_{1}(q_{0}r) \frac{\partial R}{\partial q_{0}} \right], \quad (C21)$$

where $X(r) = \sqrt{q_0 r} \chi(r)$. To evaluate the integrals on the right-hand side, we use a result similar to (C16)

$$\int_{0}^{\infty} dr r \ U(r) I_{1}(qr) R(r; iq_{0}) = -\frac{m}{2\pi\hbar^{2}} qq_{0}\tau_{1}(2E_{0}) ,$$
(C22)

and its derivatives with respect to q and q_0 . The final result for the normalization integral for $E_0 < 0$ is then found to be

$$\mathcal{N} \equiv 2\pi \int_0^\infty dr r \, \chi^2(r) = -\frac{m}{\hbar^2} E_0 \frac{d\tau_1(2E_0)}{dE_0} \,. \tag{C23}$$

Note that it is simpler to write this result in terms of τ_1 rather than the phase shift $\delta_1(k_0)$, as we had done for the $E_0 > 0$ in (C19). This is because the $E_0 < 0$ phase shift is complex with $\text{Im}[\cot \delta_1(k_0)]=1$ as can be seen from (2.10) and the fact that $\tau_1(2E_0)$ is real.

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- ²¹For Lennard-Jones potentials, see M. D. Miller and L. H. Nosanow, J. Low Temp. Phys. **32**, 145 (1978). For the lattice model with a negative Hubbard U, the pairing instability always wins over a gas-liquid transition as shown by Nozieres and Schmitt-Rink (Ref. 10). This is due to the on-site nature of the attraction, so that once a tightly bound pair is formed no other fermion can make use of the attraction. On the other hand, depending upon filling, the negative-U model can also have a charge-density-wave instability.
- ²²P. W. Anderson and P. Morel, Phys. Rev. 123, 1911 (1961).
- ²³Note that the dependence on E has canceled out as anticipated, as have the imaginary parts (for E > 0) on the two sides of Eq. (5.2). For E < 0, one can set $\eta = 0$ and the T matrix is real.
- ²⁴This pair wave function $\psi_k = \Delta_k / 2E_k$ is related to the Fourier

transform ϕ_k of the function $\phi(1,2)$ in Eq. (4.1) as follows. Using the standard BCS notation u_k and v_k (see Ref. 2), $\psi_k = v_k u_k$, whereas $\phi_k = v_k / u_k$. In the extreme Bose limit $v_k \ll 1$ and hence $\psi_k \simeq \phi_k$.

- ²⁵Notice that the density of the system only enters in the prefactor of Δ and not in the exponential, because in two dimensions the density of states is a constant independent of k_F . Thus unlike in the three-dimensional version of this model, where the BCS limit is obtained only for a dilute gas, here it is valid for a gas that is dense on the scale of the pair size $\xi_0 k_F \gg 1$, provided of course $k_F R \gg 1$, where R is the range of the potential.
- ²⁶M. Randeria, J.-M. Duan, and L.-Y. Shieh (unpublished).
- ²⁷See, e.g., S. K. Adhikari, W. G. Gibson, and T. K. Lim, J. Chem. Phys. 85, 5580 (1986), and references therein.