Phase Separation and an Upper Bound for a Generalized Superfluid Gap for Cold Fermi Fluids in the Unitary Regime

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(Received 5 January 2005; revised manuscript received 29 April 2005; published 14 September 2005)

An upper bound is derived for Δ for a cold dilute fluid of equal amounts of two species of fermion in the unitary limit $k_f a \to \infty$ (where k_f is the Fermi momentum, a is the scattering length, and Δ is a pairing energy: the difference in energy per particle between adding to the system a macroscopic number (but infinitesimal fraction) of particles of one species compared to adding equal numbers of both. The bound is $\delta \leq \frac{5}{3}[2(2\xi)^{2/5} - (2\xi)]$ where $\xi = \epsilon/\epsilon_{\rm FG}$, $\delta = 2\Delta/\epsilon_{\rm FG}$; ϵ is the energy per particle and $\epsilon_{\rm FG}$ is the energy per particle of a noninteracting Fermi gas. If the bound is saturated, then systems with unequal densities of the two species will separate spatially into a superfluid phase with equal numbers of the two species and a normal phase with the excess. If the bound is not saturated, then Δ is the usual superfluid gap. If the superfluid gap exceeds the maximum allowed by the inequality, phase separation occurs.

DOI: 10.1103/PhysRevLett.95.120403 PACS numbers: 05.30.Fk, 21.65.+f

During the past several years there has been considerable theoretical interest in studies of cold, dilute, Fermi systems with equal densities of two strongly coupled species [1–10]. In this context, "species" refers both to spin states and to internal quantum numbers. There is an idealized version of this problem in which the following conditions are met: the particles of each species are of equal mass, and $1/a \ll n^{1/3} \ll 1/r_0$ and $T \ll n^{1/3}$ where r_0 is the typical distance scale of the interaction, a is the scattering length for free particle scattering *between* the two species, n is the density of each species, T is the temperature, and units have been chosen with $\hbar = 1$. In the extreme limit of this situation where $n^{1/3} a \to \infty$, $\Lambda a \to \infty$, $n^{1/3}/\Lambda \to 0$, and $T n^{-1/3} \to 0$ (where Λ is the typical momentum scale characterizing the interaction), there is only a single momentum scale in the problem, namely, $n^{1/3}$. This is sometimes called the unitary regime. It is convenient to reexpress this in terms of a nominal Fermi momentum $k_f \equiv (6\pi^2 n)^{1/3}$. Thus all physical observables in the problem can be expressed as appropriate powers of this scale times appropriate constants. For example, the average energy per particle can be written as $\epsilon = \xi \frac{3}{5} \times \frac{k_f^2}{2m} = \xi \epsilon_{\rm FG}$ where ξ is a universal constant ($\epsilon_{\rm FG}$ is the energy density on a noninteracting Fermi gas). A pairing energy parameter that gives the difference in energy per particle between adding a macroscopic number (but infinitesimal fraction) of particles of one species as compared to adding equal numbers of both to the system with equal particle numbers can similarly by given as $2\Delta = \delta \frac{3}{5} \times \frac{k_f^2}{2m} = \delta \epsilon_{\rm FG}$. The connection between Δ and the usual superfluid gap is somewhat subtle and is discussed below.

This problem is of interest in part due to the universality of the behavior. The coefficients such as ξ and δ apply to *all* problems in this regime regardless of the microscopic details of the problem. The problem also is of theoretical interest in that it represents the exact intermediate limit between two weakly coupled regimes with $|k_f a| \ll 1$. The true weak-coupling regime between fermions has $k_f a < 0$ and is a BCS superfluid; the regime with $k_f a$ small and positive corresponds to weakly coupled molecules in a Bose-Einstein condensate (BEC) [11]. The problem is also challenging: there appears to be no simple analytical method to compute the universal coefficients.

The problem is relevant to physical systems of interest. In nuclear physics the problem of low density neutron matter can be caricatured by such a system: the two species are the two spin states of the neutron; the s-wave scattering length between spin up and spin down neutrons is much larger than the characteristic range of the nucleon-nucleon force [3,12,13]. The problem has become of importance at the interface between atomic and condensed matter physics since the scattering length between atoms, in particular m states, can be tuned via altering an external magnetic field. The scattering length diverges at a Feshbach resonance. There has been intense experimental work on pairing in fluids of trapped fermionic atoms and the transition from the BCS to the BEC regime [14]. Of course, the trap itself can play an important dynamical role in the problem and significant theoretical effort has gone into describing the role of the trap, which adds a spatial dependence to the problem [15]. This Letter focuses on the ideal case where the particles are visualized as being contained in a large box.

The fact that no direct analytical computations of the relevant dimensionless parameters exists means other methods must be found to learn something about these dimensionless parameters. One strategy is to attempt to extract them numerically [5–8]. A possible difficulty with such an approach is that *a priori* estimates of the errors may be difficult to obtain in a reliable way. Thus, a constraint based on reliable analytical methods is potentially quite useful. One possible idea is to see whether the coefficients ξ and δ can be related to each other analytically. This is also a formidable challenge for which no rigorous answer is known. However, as is discussed in this Letter, it is possible to give a rigorous upper bound on δ for any assumed value for ξ:

$$\delta \leq \tfrac{5}{3}[2(2\xi)^{2/5} - (2\xi)]. \tag{1}$$

As is discussed below, Δ need not be the superfluid gap, and the superfluid gap can exceed this bound; if it does, one predicts an interesting phenomenon in the case where the densities of the two species are unequal.

To derive this bound, consider a generalization of the problem to the case where the two species (denoted a and b) have different numbers of densities: the only relevant quantities with dimensions of inverse lengths $n_a^{1/3}$ are $n_b^{1/3}$. One completely general way to parametrize the ground state energy density of this system subject to the constraint of fixed density of the two species consistent with the correct dimensional scaling is

$$\mathcal{E}(n_a, n_b) = \alpha n_a^{5/3} f(n_b/n_a), \tag{2}$$

where f is a universal function that depends only on the ratio of the number densities and α is a constant with dimension of mass^{-1}. At the point $n_b = 0$, the system is a noninteracting Fermi gas of species a (by hypothesis the only relevant interactions are for species a and b to interact with each other). Without loss of generality one can fix $f(0)$ to be unity, and this in turn fixes α to its Fermi gas value. The parametrization in Eq. (2) is very natural if one envisions starting with a Fermi gas of species a and slowly adding in particles of species b. Comparing Eq. (2) with the definition of ξ, one sees that $\xi = f(1)/2$. The factor of $1/2$ in this relation reflects the fact that at $x = 1$ the two species contribute equally; where the noninteracting $f(1) = 2$ and ξ is defined as the fraction relative to the noninteracting case.

The key thermodynamic consideration to derive a bound is the possibility of phase separation. This constrains the energy density as a function of the densities. In particular, if we consider the energy density $\mathcal{E}(n_a, n_b)$ at two different pairs of number densities for the two species, $(n_a^{(1)}, n_b^{(1)})$ and $(n_a^{(2)}, n_b^{(2)})$, then the average of the energy densities at these two number densities cannot exceed the energy density at the average number density:

$$\frac{\mathcal{E}(n_a^{(1)}, n_b^{(1)}) + \mathcal{E}(n_a^{(2)}, n_b^{(2)})}{2} \geq \mathcal{E}\left(\frac{n_a^{(1)} + n_a^{(2)}}{2}, \frac{n_b^{(1)} + n_b^{(2)}}{2}\right); \tag{3}$$

if Eq. (3) were false, it would be possible for a system with a fixed but large volume and number densities $(\frac{n_a^{(1)}+n_a^{(2)}}{2}, \frac{n_b^{(1)}+n_b^{(2)}}{2})$ to lower its energy by dividing the volume into two equal regions with different phases: one with number densities $(n_a^{(1)}, n_b^{(1)})$ and the other with $(n_a^{(2)}, n_b^{(2)})$.

Equation (3) implies that in regions where $\mathcal{E}(n_a, n_b)$ is continuous its curvature in any direction in the n_a, n_b plane is positive:

$$\hat{n}_i \frac{\partial^2 \mathcal{E}}{\partial n_i, \partial n_j} \hat{n}_j \geq 0 \tag{4}$$

for all unit vectors $\hat{n}$ where i, j can assume the value of a or b and summation of over i and j is implicit.

In order for Eq. (4) to hold for any unit vector $\hat{n}$, the matrix

$$\mathbf{K}(n_a, n_b) \equiv \begin{pmatrix} \frac{\partial^2 \mathcal{E}}{\partial n_a^2} & \frac{\partial^2 \mathcal{E}}{\partial n_a \partial n_b} \\ \frac{\partial^2 \mathcal{E}}{\partial n_b \partial n_a} & \frac{\partial^2 \mathcal{E}}{\partial n_b^2} \end{pmatrix} \tag{5}$$

must have only non-negative eigenvalues; thus det($\mathbf{K}$) ≥ 0. Inserting the parametrization of Eq. (2) into the definition of $\mathbf{K}$ and imposing a positive determinant yields a constraint on the curvature of the function f

$$f''(x) \geq \frac{2f'^2(x)}{5f(x)}. \tag{6}$$

We know $f(0) = 1$ and $f(1) = 2\xi$ and that f continuously connects these with its curvature constrained by Eq. (6). Consider the curve that obeys these boundary conditions and saturates inequality (6) at all points in between. Define that curve as $f_{\max}$:

$$f''_{\max}(x) = \frac{2f'_{\max}(x)}{5f_{\max}(x)} \quad \text{where } f_{\max}(1) = 2\xi; \quad \text{with} \quad f_{\max}(0) = 1. \tag{7}$$

The differential equation in Eq. (7) can easily be solved subject to the boundary conditions. There is only one real solution:

$$f_{\max}(x) = \{1 + [(2\xi)^{3/5} - 1]x\}^{5/3}. \tag{8}$$

The differential equation for $f_{\max}$ was derived by considering a path associated with varying the densities n_a and n_b, which always is in the direction where the second derivative of $\mathcal{E}$ is zero: thus the derivatives of $\mathcal{E}$ with respect to n_a (or n_b) (i.e., the chemical potentials) are constants along the path. Therefore $f_{\max}$ represents a situation in which the system for $x = 0$ and 1 and at all points in between are at the same chemical potential (but different total density). This is precisely the condition for phase separation: at $0 < x < 1$ a fraction r of the particles is in the superfluid phase with a density of n_s and a fraction $1 - r$ is in the normal phase with a density n_n. It is a simple exercise of matching chemical potentials and densities to show that in such a phase separated system

$$n_n = n_a\{1 + x[(2\xi)^{3/5} - 1]\}, \qquad n_s = \frac{n_n}{(2\xi)^{3/5}}, \qquad r = \frac{x(2\xi)^{3/5}}{1 + x[(2\xi)^{3/5} - 1]}, \tag{9}$$

where n_a is the *average* density of type a over the entire system. Note that Eqs. (8) and (9) can also be derived by assuming at the outset two phases and then varying their densities and fractions subject to the constraints of fixed average density and fixed ratio of the total number of the two species.

The phase separated configuration with fixed x and n_a has a known energy. The actual minimum energy configuration is either this energy or below it so $f_{\max}$ serves as an upper bound for f:

$$f(x) \leq f_{\max}(x); \tag{10}$$

a homogeneous phase violating this condition is energetically unstable against phase separation, and thus the ground state is phase separated; the upper bound is saturated if phase separation occurs.

It is worth observing that the preceding analysis is valid only for $n_b/n_a \leq 1$. However, the regime $x > 1$ can easily be studied as it corresponds to more of species b than a. For $n_b > n_a$ one can use the previous analysis with b and a switched:

$$\mathcal{E}(n_a, n_b) = \alpha n_b^{5/3} f(n_a/n_b) \tag{11}$$

with f the same function as above.

One can determine Δ from $f(x)$. For an ordinary superfluid Δ is the gap. The gap represents the amount of energy saved by pairing: Δ is the difference in energy per particle gained by adding particles of one species type (say, type a) to a system of equal particle number as compared to the energy of adding equal numbers of a or b:

$$2\Delta = \frac{[E(N+2M, N) - E(N,N)] - [E(N+M, N+M) - E(N,N)]}{M}, \tag{12}$$

where $E(N_a, N_b)$ is the total energy and N_a (N_b) is the total number of particles of species a (b) and $M \ll N$ is the number of particles of each type added. Going to the thermodynamic limit gives Δ as the discontinuity of the derivative of $\mathcal{E}$ with respect to the density of one of the species:

$$2\Delta = \lim_{\epsilon \to 0}\left(\frac{\partial \mathcal{E}}{\partial n_b}\bigg|_{(nb=na+\epsilon)} - \frac{\partial \mathcal{E}}{\partial n_b}\bigg|_{(nb=na-\epsilon)}\right). \tag{13}$$

Using the general parametrizations of $\mathcal{E}$ of Eqs. (2) and (11) yields

$$2\Delta = \frac{k_f^2}{2m}\xi\left(2 - \frac{6f'(1)}{5\xi}\right)\delta = \xi\frac{5}{3}\left(2 - \frac{6f'(1)}{5\xi}\right), \tag{14}$$

where the second form follows since $\delta \equiv \Delta/(\frac{3}{5}\frac{k_f^2}{2m})$.

Equation (14) provides the basis for inequality (1). Note that $f \leq f_{\max}$ in the interval from zero to unity and that by construction $f(1) = f_{\max}(1)$. This is possible only if $f'(1) > f'_{\max}(1)$. Thus, $\delta \leq \xi[\frac{10}{3} - 2f'_{\max}(1)/\xi]$. Using the explicit form of $f_{\max}$ from Eq. (8) immediately yields inequality (1).

The interpretation of inequality (1) is subtle. Δ is the usual superfluid gap $\Delta_{\rm SF}$ in the case where the system does not phase separate for unequal numbers (i.e., the inequality is not saturated). If there is only one possible phase when particles are added, then 2Δ must simply represent the pairing energy for this phase. In the case where inequality is saturated, however, this is not the case. Although Δ retains the definition given above, it should not be interpreted as $\Delta_{\rm SF}$; if a mixed phase is energetically preferred, Δ represents the amount of energy per particle to add particles of one species into a normal phase that forms in equilibrium with the superfluid phase [16]. The distinction is the following: $\Delta_{\rm SF}$ is the energy per particle to a single particle to a system with equal numbers of the two species; Δ represents the energy cost per particle when adding a large number (but infinitesimal fraction) of particles of one species. Clearly, $\Delta_{\rm SF} \geq \Delta$; either phase separation does not happen and the two are equal or it does not and it is energetically cheaper to add unpaired particles in a new phase.

To summarize, inequality (1) always holds with Δ defined as above. If, in addition, the system is known not to phase separate at unequal particle numbers, then (i) the inequality is not as such saturated and (ii) $\Delta = \Delta_{\rm SF}$.

An important corollary of this analysis is that if $\delta_{\rm SF} > \frac{5}{3}[2(2\xi)^{2/5} - (2\xi)]$ (where $\delta_{\rm SF}$ is the analog of δ for the superfluid gap) phase separation must occur for $x < 1$ and if $\delta_{\rm SF} < \frac{5}{3}[2(2\xi)^{2/5} - (2\xi)]$ then the type of phase separation considered here (into fully paired and fully unpaired phases) does not occur.

Given one nontrivial physical assumption, it is possible to make a much stronger connection between ξ and δ than inequality (1). The dynamical assumption is that for $n_a \neq n_b$, the system does separate spatially into two phases: a superfluid phase (which prefers to have equal numbers of the two species) and a normal phase with the remainder. This possibility was explored in an intriguing recent paper by Bedaque, Caldas, and Rupak (BCR) [17]. The BCR paper argued on the basis of a generalized BCS ansatz that such phase separation occurs. The analysis of BCR was aimed at a broader class of problems than the strongly coupled limit of $k_f a \gg 1$; indeed, the detailed analysis is only strictly legitimate in the case of small BCS gaps and hence weak coupling. Thus, it is an open question as to whether such phase separation occurs at strong coupling and asymmetric systems. However, BCR argued that it was plausible that their conclusion holds even away from the weak-coupling limit.

Note that if there is phase separation as suggested by BCR, the inequalities in (1) and (10) must be saturated. Since the chemical potentials for both species are constant at all points along the path, a region with $n_b = 0$ is in chemical equilibrium a region with $n_b = n_a$; this is necessary and sufficient for phase separation of the BCR type. Thus, the BCR assumption implies that for $0 > x > 1$, $f(x) = \{1 + [(2\xi)^{3/5} - 1]x\}^{5/3}$ and thus

$$\delta = \frac{5}{3}[2(2\xi)^{2/5} - (2\xi)]. \quad (15)$$

Clearly it is important to establish whether phase separation occurs for $x \neq 1$. As discussed above, this can be immediately answered if one knows ξ and δ_{SF} (the analog of δ for the superfluid gap). Estimates of ξ and δ_{SF} have been obtained numerically using Monte Carlo methods for finite but large systems [5–8]. The most recent extracted value [7] of ξ is approximately 0.42 ± 0.01, which implies that the dividing line between whether phase separation occurs or not is approximately $\delta_{SF} = 1.70$ with fairly small numerical uncertainty. The extracted value for δ_{SF} is 1.68 ± 0.1. Unfortunately this is not accurate enough to determine whether phase separation occurs. The numerical simulations in Ref. [7] for $x < 1$, are energetically consistent with phase separation. The present analysis implies that if these numerical simulations are reliable, then either δ_{SF} does exceed $\frac{5}{3}[2(2\xi)^{2/5} - (2\xi)]$ (presumably by a small amount) or phase separation does not occur for $x < 1$ with the energy just slightly below the phase separated energy. Thus, the analysis here provides a highly nontrivial constraint on the numerics. Finally, it is worth noting that it is surprising just how close δ_{SF} is to the critical value for phase separation: present numerical simulations do not rule out the intriguing possibility that they are exactly equal.

The author acknowledges Shmuel Nussinov and Boris Gelman for introducing him to the problem. Sanjay Reddy is gratefully acknowledged for making an insightful critique about aspects of a previous version of this paper. This critique clarified an important point about the nature of the gap. This work was supported by the U.S. Department of Energy through Grant No. DE-FG02-93ER-40762.

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