Superfluid stability in the BEC-BCS crossover

C.-H. Pao and Shin-Tza Wu
Department of Physics, National Chung Cheng University, Chiayi 621, Taiwan

S.-K. Yip
Institute of Physics, Academia Sinica, Nankang, Taipei 115, Taiwan
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We consider a dilute atomic gas of two species of fermions with unequal concentrations under a Feshbach resonance. We find that the system can have distinct properties due to the unbound fermions. The uniform state is stable only when either (a) beyond a critical coupling strength, where it is a gapless superfluid, or (b) when the coupling strength is sufficiently weak, where it is a normal Fermi gas mixture. Phase transition(s) must therefore occur when the resonance is crossed, in contrast to the equal population case where a smooth crossover takes place.

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Feshbach resonance[1] has opened up a new playground for the field of cold trapped atoms. Using this resonance, the effective interaction between the atoms can be varied over a wide range. In particular, for two fermion species with a Feshbach resonance between them, the ground state can be tuned from a weak-coupling Bardeen-Cooper-Schrieffer (BCS) superfluid to a strong-coupling regime where the fermions pair up to form bosons which in turn undergo Bose Einstein condensation (BEC).[2,3]

Though this problem has been under intense theoretical[4] and experimental[5] investigations, almost all works thus far are restricted to the case where the concentrations of the two fermionic species are equal. We here generalize this study to the case of unequal populations of the two species, and investigate in detail the thermodynamic stability of this system, in particular the question when the uniform state can be stable.

Studies of fermions with unequal populations or mismatched Fermi surfaces and a pairing interaction have a long history. It was studied by Fulde and Ferrell[6] and Larkin and Ovchinnikov[6] (FFLO) in the 1960s in relation to superconductivity in materials with ferromagnetically coupled paramagnetic impurities. It was found that in this case the system is likely to have an inhomogeneous gapless superconducting phase. Advances in the techniques of manipulating dilute ultracold atoms have revived interests in the related problems.[7] These studies, in our present language, are still restricted to the weak-coupling regime. We, however, would extend our analysis to all coupling strengths.

In the "canonical" problem of two species of fermions with equal mass (say, spin up and spin down electrons) and equal concentrations (thus a single Fermi surface), if the cross-species interaction is varied from weak to strong coupling, at low temperatures the system would undergo a *smooth crossover* from a superfluid with loosely bound Cooper pairs (the "BCS" limit) to one with condensation of tightly bound bosonic molecules (the "BEC" limit).[2] The situation, however, can be very different if one considers two species of fermions with *unequal concentrations* (i.e., *mismatched* Fermi surfaces), even if they have identical mass. This can be anticipated because, on the one hand, far into the BCS side, the system is basically in the FFLO regime[7] and therefore must go into a spatially inhomogeneous phase. On the other hand, in the far end of the BEC side, the system is expected to behave like an ordinary (weakly interacting) Bose-Fermi mixture and thus has a stable homogeneous phase. Here the bosons are the fermion pairs and the fermions are the "leftover" unpaired atoms of the majority species. Deep into the BEC regime, the size of the Fermion pairs is small and the interaction between the bosons and the leftover unpaired fermions is expected to be weak. It is therefore a very interesting question as to what happens in between. This is the question we want to address in this paper.

For simplicity, we shall assume that the resonance is sufficiently wide so that the physics reduces effectively to a single channel regime. This is probably valid[8] for many Feshbach resonances under current experimental investigations. Thus, in our calculations, we would not invoke explicitly the presence of the "closed channel" which leads to this Feshbach resonance. We simply model the fermions as interacting through a short-range, s-wave effective interaction (dependent on the external magnetic field) characterized by the corresponding scattering length a. $1/a$ varies from ∞ for large negative detuning (closed channel bound state energy much below the continuum threshold) to $-\infty$ for large positive detuning.

Now we proceed to the details of our calculation and results. We consider two fermion species, denoted as "spin" $\uparrow$ and $\downarrow$, of equal mass m. Because of the unequal concentrations of the two species and the possible existence of pairing, it is useful to introduce three fields: the chemical potentials μ_σ ($\sigma=\uparrow$ or $\downarrow$) and the pairing field Δ. We shall confine ourselves to zero temperature and generalize the BCS mean field approach of Ref. 3. The excitation spectrum for each spin is (see, e.g., Ref. 11 for details)

$$E_\sigma(\mathbf{k}) = \frac{\xi_\sigma(\mathbf{k}) - \xi_{-\sigma}(\mathbf{k})}{2} + \sqrt{\left(\frac{\xi_\sigma(\mathbf{k}) + \xi_{-\sigma}(\mathbf{k})}{2}\right)^2 + \Delta^2}, \tag{1}$$

where $\xi_\sigma(\mathbf{k})=\hbar^2k^2/2m-\mu_\sigma$ are the quasiparticle excitation energies for normal fermions, and $-\uparrow\equiv\downarrow$. The density of each spin species is then

$$n_\sigma = \int \frac{d^3k}{(2\pi)^3}[u_{\mathbf{k}}^2 f(E_\sigma) + v_{\mathbf{k}}^2 f(-E_{-\sigma})], \quad (2)$$

with the coherence factors

$$u_{\mathbf{k}}^2 = 1 - v_{\mathbf{k}}^2 = \frac{E_\uparrow(\mathbf{k}) + \xi_\downarrow(\mathbf{k})}{E_\uparrow(\mathbf{k}) + E_\downarrow(\mathbf{k})}.$$

Here f is the Fermi function. The equation for the order parameter Δ reads

$$-\frac{m}{4\pi a}\Delta = \Delta \int \frac{d^3k}{(2\pi)^3}\left[\frac{1 - f(E_\uparrow) - f(E_\downarrow)}{E_\uparrow + E_\downarrow} - \frac{m}{\hbar^2 k^2}\right]. \quad (3)$$

We solve equations (2) and (3) self-consistently for fixed total density $n \equiv n_\uparrow + n_\downarrow$ and density difference $n_d \equiv n_\uparrow - n_\downarrow$. We shall always take $\uparrow$ to be the majority species so that $n_d \geqslant 0$.

It is convenient to introduce the average chemical potential $\mu \equiv (\mu_\uparrow + \mu_\downarrow)/2$ and the difference $h \equiv (\mu_\uparrow - \mu_\downarrow)/2 \geqslant 0$. Then we have

$$E_{\uparrow,\downarrow}(\mathbf{k}) = \sqrt{\xi(\mathbf{k})^2 + \Delta^2} \mp h \quad (4)$$

where $\xi(\mathbf{k}) \equiv \hbar^2 k^2/2m - \mu$. Hence $E_\downarrow(\mathbf{k}) > 0$ always. From Eq. (2) we get

$$n_d = \int \frac{d^3k}{(2\pi)^3} f(E_\uparrow(\mathbf{k})) \quad (5)$$

and so the integration is only over the region where $E_\uparrow(\mathbf{k}) < 0$. In the following, it is useful to note that the minimum (or most negative) $E_\uparrow(\mathbf{k})$ occurs at $\xi(\mathbf{k})=0$ for $\mu>0$, where it is $\Delta - h$, and at $k=0$ for $\mu<0$, where it is $\sqrt{\mu^2+\Delta^2}-h$.

As in the case of equal concentrations, it is convenient to express our results in dimensionless variables. We shall define an inverse length scale k_F through the total density n via $k_F \equiv (3\pi^2 n)^{1/3}$, and an energy scale $\epsilon_F \equiv \hbar^2 k_F^2/2m$. We thus write $\tilde{\mu} \equiv \mu/\epsilon_F$, $\tilde{h} \equiv h/\epsilon_F$, $\tilde{\Delta} \equiv \Delta/\epsilon_F$, $\tilde{n}_d \equiv n_d/n$, and define the dimensionless coupling constant $g \equiv 1/(k_F a)$, which varies from ∞ for large negative detuning to $-\infty$ for large positive detuning.

We now describe the results of our calculations. We first make contact with the BCS-BEC crossover for equal concentrations. The inset of Fig. 1 shows the typical behaviors of $\tilde{\mu}$, $\tilde{\Delta}$, and $\tilde{h}$ as functions of g for a given density difference $\tilde{n}_d$. The behavior of $\tilde{\mu}$ or $\tilde{\Delta}$ is similar to that in the case of equal concentrations.[3] For example, $\tilde{\mu}$ is large and negative in the BEC limit whereas it is of order 1 in the BCS regime. Unlike that case, however, g has to be larger than a minimum coupling g_c in order for a finite order parameter Δ to exist. This critical coupling strength g_c increases with increasing n_d. Note that $n_d \neq 0$ requires a finite h, which is equivalent to, for superconductors, a Zeeman magnetic field, which is pair breaking.[9] For $g<g_c$, Eq. (3) requires that $\Delta=0$ and the system is in the normal state. (For clarity of this inset, we plot only the $\Delta \neq 0$ solutions.) The main part of Fig. 1 shows $\tilde{h}$ as a function of g in the intermediate regime ($|g| \lesssim 1$) for three different $\tilde{n}_d$ (0.2, 0.5, and 0.8). The horizontal dotted lines indicate the normal state in which the gap function Δ is zero (described above).

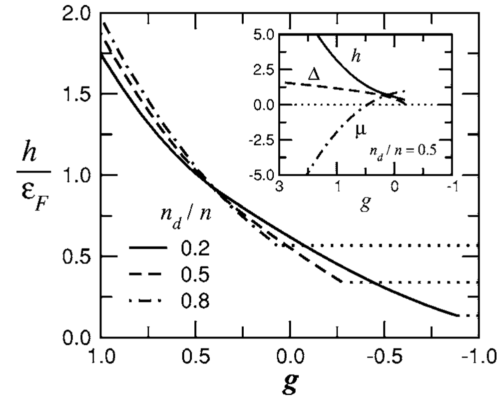

FIG. 1. Main figure: scaled chemical potential difference $h/\epsilon_F = \tilde{h}$ versus the coupling constant g for three different values of $n_d/n = \tilde{n}_d$. The inset includes also the results for $\tilde{\Delta}$ and $\tilde{\mu}$ for $n_d/n = 0.5$.

The behavior for $g<g_c$ is easy to understand. There is no pairing and the system reduces to a Fermi gas. In this case, the chemical potentials are given by $\mu_\sigma = (6\pi^2 n_\sigma)^{2/3}/(2m)$ which implies $\mu = [(6\pi^2)^{2/3}/4m](n_\uparrow^{2/3} + n_\downarrow^{2/3})$ and $h = [(6\pi^2)^{2/3}/(4m)](n_\uparrow^{2/3} - n_\downarrow^{2/3})$ (both independent of g). On the other hand, for large and positive g (the strong-coupling BEC limit), one can show from Eqs. (2), (3), and (5), that both h and $|\mu|$ are large and to leading order given by $\hbar^2/(2ma^2)$. However, $(\mu+h)/2 = \mu_\uparrow = (6\pi^2 n_d)^{2/3}/(2m) \ll |\mu|$ or h. These expressions simply reflect that the system becomes a Bose-Fermi mixture with boson concentration $n_\downarrow$ and free fermion concentration n_d.

Notice that the lines (for $\Delta \neq 0$) of $\tilde{h}$ versus g cross each other from small to large $\tilde{n}_d$ near $g \sim 0.45$. For $g \gtrsim 0.5$, $\tilde{h}$ increases with $\tilde{n}_d$ for fixed g. For $g \lesssim 0.45$, $\tilde{h}$ decreases as $\tilde{n}_d$ increases when the coupling strength is fixed. We shall return to these features again below.

Now we make contact with the superconductivity literature. It is helpful here to note that h plays the role of an effective external Zeeman field. We plot in Fig. 2 $\tilde{\Delta}$ as a function of $\tilde{h}$ for various coupling strengths g. The horizontal portion of each curve corresponds to $n_d=0$. In this region, $h<\Delta$ and so that $E_\uparrow(\mathbf{k})>0$ for all $\mathbf{k}$ [see Eq. (4)]. The other part of the curve corresponds to $n_d>0$, and exists only in the region $h>\Delta$. (More precisely, for larger g where μ becomes negative, this condition should read $h>\sqrt{\mu^2+\Delta^2}$.) For small g ($\lesssim 0.3$), $\tilde{\Delta}$ decreases with decreasing $\tilde{h}$. This solution is the generalization of that first discovered by Sarma.[10] We find that this superfluid state corresponds to one where $\tilde{n}_d$ increases with decreasing $\tilde{h}$, and hence unstable (to be discussed again below). For sufficiently large coupling ($g \gtrsim 0.5$), $\tilde{\Delta}$ decreases with increasing $\tilde{h}$. This state has $\tilde{n}_d$ increases with $\tilde{h}$, and satisfies one of the stability conditions to be discussed below.

In Fig. 3 the chemical potential difference $\tilde{h}$ is plotted as

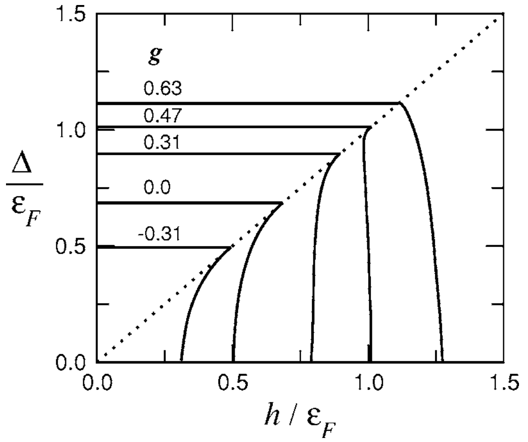

FIG. 2. Scaled pair order parameter $\Delta/\varepsilon_F=\tilde{\Delta}$ versus $h/\varepsilon_F=\tilde{h}$ for the given coupling constants g.

a function of $\tilde{n}_d$. These results correspond to those of Fig. 1 presented in a different manner. Let us explain how this graph should be read, with $g=-0.31$ as an example. For $\tilde{n}_d=0$, $\tilde{h}$ can take any value up to $\tilde{h}_1\approx 0.5$ given by the intersection of the line labeled by $g=-0.31$ with the $\tilde{n}_d=0$ axis. This portion corresponds to the line with Δ being a constant in Fig. 2 For $0<\tilde{n}_d<0.46$ the dependence of $\tilde{h}$ on $\tilde{n}_d$ is given by the solid line labeled by $g=-0.31$. This line corresponds to the state with $\Delta\neq 0$ but $\Delta<h$ in Fig. 2 discussed above. For $\tilde{n}_d>0.46$, the system enters into the normal state with the $(\tilde{h},\tilde{n}_d)$ relation represented by the dotted lines, given by $\tilde{h}=0.5[(1+\tilde{n}_d)^{2/3}-(1-\tilde{n}_d)^{2/3}]$ (see the discussion on Fig. 1 above). Lastly, for $\tilde{n}_d=1$, $\tilde{h}$ can take any value larger than $\tilde{h}_2\equiv 0.5\times 2^{2/3}\approx 0.79$. This is because this line corresponds simply to a Fermi gas with only $\uparrow$ particles, and h can take any value larger than μ so that $\mu_\downarrow=(\mu-h)/2<0$. For $g\gtrsim 0.3$, the graph can be read in a similar manner except that the dotted line representing the normal state is not involved.

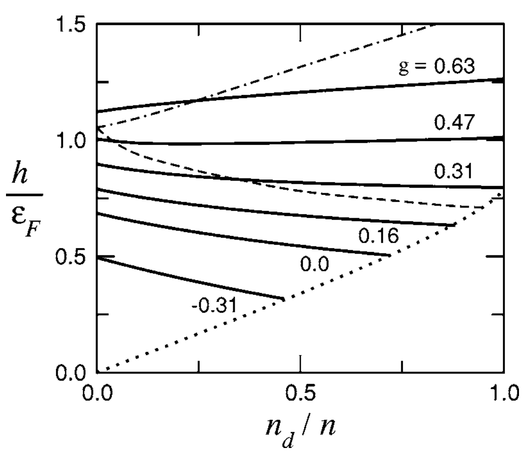

FIG. 3. $h/\varepsilon_F=\tilde{h}$ versus $n_d/n=\tilde{n}_d$ for constant g's. Full lines are for $\Delta\neq 0$ and the dotted lines are for $\Delta=0$. The dashed line indicates (for the $\Delta\neq 0$ states with n_d neither 0 nor 1) where ρ_s changes sign, with $\rho_s>0$ (above) or, $\rho_s<0$ (below). The dot-dash line indicates $\mu=0$, with $\mu<0$ above this line.

For the uniform superfluid to be stable, two criterions must be fulfilled.[11,12] First, the susceptibilities matrix $\partial n_\sigma/\partial\mu_{\sigma'}$ can have only positive eigenvalues. One can show that this requires that $\partial\tilde{n}_d/\partial\tilde{h}$, evaluated at constant g, must be positive.[13] That is, the plot of $\tilde{h}$ versus $\tilde{n}_d$ must have positive slope. From Fig. 3, we see that for small g ($\lesssim 0.3$), the slope of each curve is always negative which indicates the superfluid state is unstable. For g greater than about 0.3, the slope of these curves change sign at some $\tilde{n}_d$ between 0 and 1. In this case a stable superfluid state may occur for sufficiently large $\tilde{n}_d$. After $g\gtrsim 0.5$, the slopes of these curves are positive for all $n_d\geqslant 0$ and the above stability criterion is satisfied for all n_d.

The second stability criterion is that the superfluid density ρ_s must be positive.[11] ρ_s can be evaluated as discussed in Ref. 11. $\rho_s=n$ for $n_d=0$. For $n_d\neq 0$,

$$\frac{\rho_s}{n}=\left[1-\frac{\theta(\sqrt{\mu^2+\Delta^2}-h)\tilde{k}_1^3+\tilde{k}_2^3}{2\sqrt{1-(\Delta/h)^2}}\right], \tag{6}$$

with $\tilde{k}_{1,2}=[(\tilde{\mu}\mp\sqrt{\tilde{h}^2-\tilde{\Delta}^2})]^{1/2}$ and $\theta(x)$ is the step function. The line $\rho_s=0$ is plotted as the dashed lines in Fig. 3, with $\rho_s>0$ above and $\rho_s<0$ below (for $n_d\neq 0$). Thus the states correspond to $n_d\neq 0$ and $\Delta\neq 0$ below this dashed line are all unstable. $\rho_s<0$ indicates that the system is unstable towards a state with spatially varying Δ and hence a state such as FFLO can be more preferable. From our results, it turns out that the condition for $\rho_s>0$ is actually a slightly weaker requirement than the positive susceptibility discussed in the last paragraph (though we are not aware of any reason why it must be so).

We here note that, for $\tilde{n}_d\to 0^+$, the location where ρ_s changes sign is exactly at $\mu=0$. Though this can be seen from Eq. (6), it is more instructive to return to the more basic equation for the superfluid density: $\rho_s=n+\rho_p$. Here ρ_p, the paramagnetic response, is related to the backflow of quasiparticles and is given by[11] $\rho_p=-1\big/(6\pi^2m)\int_0^\infty dkk^4\delta(E_\uparrow(\mathbf{k}))$. For $\mu<0$, the solution to $E_\uparrow(\mathbf{k})=0$ exists only when $h>\sqrt{\mu^2+\Delta^2}$ and takes place at $k=k_2$ with $\hbar^2k_2^2/2m=\sqrt{h^2-\Delta^2}+\mu$. For $n_d\to 0^+$, h is just slightly larger than $\sqrt{\mu^2+\Delta^2}$ [see Eq. (5)]. k_2 is small and hence $\rho_p\to 0^+$ and $\rho_s\approx n>0$. For $\mu>0$, $E_\uparrow(\mathbf{k})=0$ happens when $h>\Delta$ and take place at two k values: $k=k_2$ as already given in the $\mu<0$ case above and $k=k_1$ with $\hbar^2k_1^2/2m=-\sqrt{h^2-\Delta^2}+\mu$. For $n_d\to 0^+$, h is just slightly larger than Δ and the $E_\uparrow(\mathbf{k})=0$ points occur near $\xi(\mathbf{k})\approx 0$ hence $\partial E_\uparrow(\mathbf{k})/\partial k\to 0$. Since k_1 and k_2 are finite, $\rho_p\to-\infty$ and $\rho_s<0$.

Finally we show our phase diagram in Fig. 4 covering the entire BEC to BCS regimes. On the BEC side, with $g\gtrsim 0.5$, the superfluid state is stable in which both the slope of $\tilde{h}(\tilde{n}_d)$ and the superfluid density are positive (see Fig. 3). On the upper right of Fig. 4, the pairing order parameter Δ is zero and the system is in the normal state. The uniform state is unstable in the shaded region.[14]

Lastly we discuss the "breached gap" state.[15] This state is characterized by $E_\uparrow(\mathbf{k})<0$ for a region of k that lies between $k_1<k<k_2$ where k_1 is finite (>0). We searched for but do

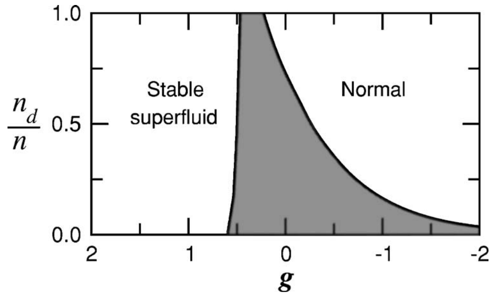

FIG. 4. Phase diagram for the two fermion species with interspecies coupling g with the stable uniform phases (white regions) shown. No uniform phases are stable in the shaded region (except when $n_d/n=0$ or 1).

not find this state to be stable. For all the region with a stable uniform superfluid, we found that $E_\uparrow(\mathbf{k})<0$ for all k such that k less than k_2 (including $k=0$). Thus there is always just one "Fermi surface" for the excess unpaired Fermions.

In conclusion, we have investigated the stability of a fermion mixture with unequal concentrations under a Feshbach resonance. We show that, in contrast to the case of equal concentrations, there is *no* smooth BCS-BEC crossover. The system is a uniform stable superfluid Bose-Fermi mixture only for sufficiently large coupling. For weak interactions the normal state is the only stable uniform state. The uniform state is unstable for intermediate coupling strengths. Phase transitions must occur when the Feshbach resonance is varied between large positive detuning and large negative detuning.

Note added. Recently, several other theoretical papers treating the same subject appeared.[16,17] Another two groups[18] also have reported important experiments on this imbalanced density system with trap potential. In these experiments, when the interaction strength is varied across the Feshbach resonance, signatures of quantum phase transitions have indeed been observed.

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[13] We have evaluated the full susceptibility matrix and checked that the eigenvalues are indeed all positive when $\partial\tilde{n}_d/\partial\tilde{h}$ is positive.

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