Phase Separation in Mixtures of Repulsive Fermi Gases Driven by Mass Difference

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We show that phase separation must occur in a mixture of fermions with repulsive interaction if their mass difference is sufficiently large. This phenomenon is highly dimension-dependent. Consequently, the density profiles of phase separated 3$d$ mixtures are very different from those in 1$d$. Noting that the ferromagnetic transition of a spin-1/2 repulsive Fermi gas is the equal mass limit of the phase separation in mixtures, we show from the Bethe Ansatz solution that a ferromagnetic transition will take place in the scattering states when the interaction passes through the strongly repulsive regime and becomes attractive.

In the last few years, there have been considerable interests in strongly repulsive Fermi gases. Many of these studies were stimulated by the initial report of ferromagnetism in the Fermi gas of $^6$Li$^1$. The possibility of itinerant ferromagnetism was first proposed by Stoner for electron gas$^2$. The idea is that if Coulomb repulsion increases faster than kinetic energy with increasing density, as indicated by Hartree-Fock calculation, the system will turn ferromagnetic at sufficiently high densities to avoid repulsion at the expense of increasing kinetic energy. However, Hartree-Fock approximation overestimates repulsion energy. So far, itinerant ferromagnetism has not been found in metals.

Itinerant ferromagnetism had also been predicted for strongly repulsive Fermi gas based on perturbative and mean field calculations$^3$ prior to the MIT experiment$^1$. However, such approaches are known to be unreliable in strongly interacting regime. In fact, later experiment has not observed ferromagnetism in strongly interacting $^6$Li Fermi gas$^3$. It is hard to determine whether it is due to the absence of Stoner ferromagnetism or that ferromagnetism is supersedes by severe atom loss. Still, Stoner’s idea of avoiding repulsion by tuning ferromagnetic remains sound, and should apply to systems such as Fermi-Fermi mixtures, where the analog of ferromagnetic transition in spin-1/2 systems is the equal mass limit.

First, let us introduce some definitions. The energy density $\mathcal{E}_{nm}$ of the ground state of a homogenous mixture of light and heavy fermions with masses ($m_L$, $m_H$) and densities ($n_L$, $n_H$) is

$$\mathcal{E}_{nm} = \mathcal{E}_L + \mathcal{E}_H + \mathcal{E}_LG \left( \frac{m_L}{m_H}, n_L^{1/d}, n_H^{1/d}, \frac{a}{n_L}, \frac{a}{n_H} \right), \quad (1)$$

where $\mathcal{E}_L$ and $\mathcal{E}_H$ are the interaction energies in units of $\mathcal{E}_L$, and $G$ is a dimensionless function of the variables displayed. “$a$” is the length scale associated with the interaction. In 3$d$, $a$ is the s-wave scattering length $a_s$ in the pseudo-potential $\hat{U} = 2\pi a_s/m \sum_{i>j} \delta(r_i - r_j) \left( \frac{\partial}{\partial r_{ij}} r_{ij} \right)$, where $r_{ij} = |r_i - r_j|$ for two interacting atoms at $r_i$ and $r_j$, $m^{-1} = m_L^{-1} + m_H^{-1}$, and we have set $\hbar = 1$. By applying harmonic confinement along the axial (with frequency $\omega_z$) or the transverse ($\omega_z$) direction, the system can be reduced to a quasi 2$d$ or a quasi 1$d$ system. For quasi 2$d$ systems, $a$ is related to the binding energy as $\epsilon_b = 1/(2m\omega^2)$, where $\epsilon_b = \frac{\hbar^2}{2m_a^2}$, $a_s = \sqrt{\hbar^2/(m\omega_z)}$ is the confinement length and $A \approx 0.915$.$^8$. For quasi 1$d$
systems, \( a = -\frac{\alpha}{2}(\frac{\pi}{n \mu} - B) \) where \( \alpha \) is \( \sqrt{1/(m_\perp \omega)} \) and \( B \approx 1.46 \). In all dimensions, the energy satisfies the adiabatic theorem, \( \partial E_{hm}/\partial \zeta = C/m > 0 \), where \( C \) is the contact. \( \zeta \) is \(-1/(2\pi a)\), \( \ln(k_0)/\pi \) and \( a/4 \) respectively for 3d, 2d and 1d systems and \( k_0 \) is an arbitrary momentum scale\[10\] [13]. That we parametrize the interaction in terms of \( \zeta \) because it is proportional to the magnetic field in experiments that tunes the system across the strongly interacting regime.

\[
E_{hm} = V\mathcal{E}_L(n_L)(1 + \gamma^\alpha x + G), \quad \alpha = 1 + 2/d. \tag{3}
\]

Next, we consider the fully phase separated state. Let \( V_H \) and \( V_L \) be the volumes of the heavy and light fermions, \( V_H + V_L = V \). The ratio \( V_H/V_L \) is determined by equating the pressure \( P \) of these two separated gases. Since the pressure of an ideal gas is proportional to its energy density, \( P = 2E/d \), we have \( \mathcal{E}_L(n'_L) = \mathcal{E}_H(n'_H) \), where \( n'_H/L = N_H/L/V_H/L \). This gives \( V_H/V_L = \gamma x^{1/\alpha} \). The total energy of the phase separated state is \( E_{PS} = V_H\mathcal{E}_H(n'_H) + V_L\mathcal{E}_L(n'_L) = V\mathcal{E}_L(n_L)(V/V_L)^{(2+d)/d}, \) or

\[
E_{PS} = V\mathcal{E}(n_L) \left(1 + \gamma x^{1/\alpha}\right)^\alpha. \tag{4}
\]

The phase separated state will have lower energy if \( E_{hm} - E_{PS} > 0 \), or

\[
I(x) = G(x) - \left[(1 + \gamma x^{1/\alpha})^\alpha - 1 - \gamma^\alpha x\right] > 0. \tag{5}
\]

When the mass ratio is sufficiently small such that

**Proof of the Theorem:** Consider a system with \( N_L \) and \( N_H \) fermions in a volume \( V \), we define

\[
m_L/m_H \equiv x, \quad N_H/N_L \equiv \gamma, \tag{2}
\]

the total energy of the homogenous mixture is

\[
E_{hm} = V\mathcal{E}_L(n_L)(1 + \gamma^\alpha x + G), \quad \alpha = 1 + 2/d. \tag{3}
\]

FIG. 1. Figure 1A, 1B, and 1C are the phase diagrams for a 3d, 2d, and 1d Fermi-Fermi mixture with \( N_L = N_H \) in a volume \( V \). \( k_F = (6\pi/n)^{1/3} \) and \( \pi n \) respectively for 3d and 1d, with \( n = N_L/V = N_H/V \). To the right of the vertical blue line, the mean-field interaction energy is less than half of total kinetic energy for a homogenous mixture (L,H), and the system is weakly interacting deeper in that region. The gray dashed-dot lines indicate the case of a Li-K mixture with \( m_L/m_H = 6/40 \). Figure 1D, 1E, and 1F are the phase diagrams of a 3d, 2d, and 1d Li-K mixture in chemical potential plane for weak interactions. \( \mu_H, \mu_L \) are scaled by \( (\pi\mu_g^d)^{1/(2-d)} \) in 3d and 1d, and \( 1/\pi \) in 2d. The red dashed-dot lines in 1D and 1F represent trajectories for the density profiles of a trapped system, corresponding to (a-d) in Fig.2, with the squares denoting the chemical potentials at the trap center. From Figure 1A to 1F, the black (orange) solid lines represent the 1st (2nd)-order boundaries with (without) density discontinuity. In Figure 1B, the boundary is given by the function \( g_c(m_L/m_H) = 2\pi/\sqrt{\mu_H\mu_L} \). In 1E, the two solid orange lines are the boundaries for interaction \( g < g_c \), with two slopes \( (g/g_c)\sqrt{m_H/m_L} \) and \( (g_c/g)\sqrt{m_H/m_L} \) respectively. When \( g \geq g_c \), the two boundaries merge into one (shown by dashed line) with slope \( \sqrt{m_H/m_L} \).
homogeneous mixtures with different densities (denoted as (L) in the fully phase separated state (PS), denoted as (H).

Corollary: Because of the adiabatic theorem, if a mixture with mass ratio $m_L/m_H$ phase separates at a given interaction parameter $\zeta$, it will continue to phase separate at stronger interactions, i.e. at a larger $\zeta$.

(B). Phase diagram: To demonstrate the effect of mass-imbalance on phase separation, we shall construct the phase diagram as a function of interaction and mass ratio. To obtain results with certainty, we consider a homogeneous Fermi-Fermi mixture of weakly repulsion. To this end, there are two classes of eigenstates: one where all quasi-momenta are real, i.e., all particles are in scattering states, (denoted as class (i)), and one that contains at least one pair complex conjugate quasi-momenta, i.e. with at least one fermion bound pair, (denoted as class (ii)).

Refractive transition of 1d spin-1/2 Fermi gas: The phase diagram for 1d Fermi-Fermi mixture is not only constraint by the results in the weakly interacting regime, but also by the exact Bethe Ansatz solution along the line $m_L/m_H = 1$ [17], which is a spin-1/2 repulsive Fermi gas with interaction $g \sum_{ij} \delta(x_i - x_j)$, where $g = -4(\overline{m})^{-1}$. Because of the integrability of this system, there are two classes of eigenstates: one where all quasi-momenta are real, i.e., all particles are in scattering states, (denoted as class (i)), and one that contains at least one pair complex conjugate quasi-momenta, i.e. with at least one fermion bound pair, (denoted as class (ii)). Repulsive Fermi gas, which falls into class (i), is referred to as in the “upper branch”: since it is a many-body eigenstate, it will not decay into class (ii) [13].

Experimentally, one can tune the system from weak to strong repulsion ($\zeta = 0^-$, $g^+ = 0^+$), and then to strongly attraction ($\zeta = 0^+$, $g^- = 0^-$). The regime where $g^- = 0^+$ will be referred to as the Tonk-Girardeau (TG) regime. The ground state of a repulsive ($\zeta < 0$ ) spin-1/2 Fermi gas with equal spin population is a spin-singlet according to the Lieb-Mattis theorem [19]. In the TG limit, the spatial wavefunction of the ground state is identical to that of a fully spin polarized Fermi gas up to a sign (which changes in various regions in configuration space). As a result, its energy $E(0)$ is given by that of a fully spin polarized state with huge spin degeneracy [17] – all spin configurations including the spin configurations (a) to (c) mentioned above are degenerate, with $H$ and $L$ now labeling the two spin species. This means that the two phase boundaries in Fig.1C will converge to the equal mass point $m_L/m_H = 1$ at resonance. Crossing the TG limit to the attractive side, the energies of all spin states continue to increase according to the adiabatic theorem, hence $E(\zeta > 0) > E(0)$; except for the largest spin state which remains at $E(0)$ regardless of interaction. As a result, the system will make transition to this maximum
spin state. In practice, such transition can be facilitated by the presence of small magnetic field gradients that destroy spin conservation. It is useful to note that atom loss in the TG regime is vanishing small \[22\], and therefore will not affect the observation of ferromagnetism.

\[ P_L(\mu_L) = P_H(\mu_H), \quad \mu_H/\mu_L = \beta, \quad \beta = (m_L/m_H)^{d/(d+2)}. \]  

The phase boundary between the mixture \((L, H)\) and \(L\) (or \((H)\)) is obtained by equating \(P_{hm}(\mu_L, \mu_H) = P_{L(H)}(\mu_{L(H)})\). The phase boundaries for the 3d, 2d, and 1d mixtures are shown in Figure 1D, 1E, and 1F respectively. Within the region of homogenous mixture, the inversion of Eq.[8] may yield several solutions of densities \((n'_L, n'_H)\), \((n''_L, n''_H)\) for given chemical potentials \((\mu_L, \mu_H)\). The thermodynamic state is given by the one with highest pressure. In the 3d case, the homogeneous mixture is contained within the “bubble” in Figure 1D. Within this region, the thermodynamic state is unique except on the line that is an extension of the boundary Eq.[10] where two states \((n'_L, n'_H)\), \((n''_L, n''_H)\) have identical chemical potential and pressure. This is a line of first order transition. Furthermore, the densities of these two phases are related as \(n'_L = \beta n''_L\), \(n'_H = \beta^{-1} n''_H\), since Eq.[7] to [9] are invariant under this change. The density discontinuities across this line \(\Delta n_L = \beta n_H - n_L, \Delta n_H = \beta^{-1} n_L - n_H\) then has the ratio \(\Delta n_L/\Delta n_H = -\beta\).

In Fig.2a to 2d, we show the density profiles of the 3d and 1d mixtures in a trap obtained by applying \(\Delta\) to the equation of state \(n_{L(H)}(\mu_L) = n_{L(H)}(\mu_L - V_i(\mathbf{r}), \mu_H - V_H(\mathbf{r})), \) where \(V_i(\mathbf{r}) = m_{L(H)}(\omega_{L(H)}^2 r^2/2\) are the harmonic potentials experienced by the light(H) and heavy(H) particles. Moving from the center of the trap to the surface of the cloud corresponds to following the trajectories indicated in Fig.1D and 1F. Fig.2a and 2b show the density profiles of a 3d mixture at different interaction strengths. The discontinuities in the densities obey the related mentioned above. Fig.2c and 2d show a 1d mixture under different trapping potentials.

Two features of the density profiles should be emphasized. Firstly, the density profiles of a 3d mixture differ significantly from that of the 1d mixture, (see Fig.1D and 1F). Phase separation takes place in the outer part of the atom cloud in 1d but in the inner part in 3d. This is because the strongly interacting regime occurs in the low (high) density region in 1d (3d). Secondly, in Fig. 2a-2d, we note that \(n_{L(H)}\) can increase with \(r\). This is different from the single component case, where \(dn/dr < 0\), due to the fact that \(dn/d\mu > 0\) as demanded by thermodynamic stability. In the mixture case, stability against density fluctuation requires \(\text{Det}(M) > 0\), where \(M_{ij} = \partial \mu_i / \partial n_j\), and \(i, j = L\) and \(H\). We then have \(dn_i/dr = (M^{-1})_{ij} d\mu_j/dr\), where \(M^{-1} = \text{Det}^{-1}(M) (\begin{pmatrix} A_H & -g \\ -g & A_L \end{pmatrix})\), \(A_{L(H)} = \partial^2 \mu_{L(H)} / \partial n_{L(H)}^2 > 0\).

That \(dn_{L(H)}/dr\) can be positive or negative is because it is made up of two terms. If \(dn_i/dr > 0\), it is easily shown from stability condition \((A_L A_H > g^2)\) that \(dn_H/dr < 0\). Thus one can have at most one species with a positive density derivative.
Conclusion. We have shown that the Stoner instability (phase separation) can be driven by large mass difference of Fermi-Fermi mixtures, but not necessarily by strong repulsions. In all dimensions, phase separation will occur for sufficiently large mass difference even in the weak interacting regime. Furthermore, we point out that the Bethe Ansatz solution implies a Stoner instability of the 1d spin-1/2 fermions across the TG limit, which in turn allows one to constrain the phase diagram of 1d Fermi-Fermi mixtures. In the cases we consider, atom loss would be suppressed and will not affect observation of Stoner ferromagnetism in experiments.

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