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Phase separation in fermion droplets

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Recent experiments on trapping cold Fermion droplets ^{40}K, in a harmonic well use a mixture of these atoms in two different hyperfine states. Depending on the density and the strength of the interaction, we have investigated the possibility of phase separation between these two components by using the density functional theory and the Monte Carlo technique. The static analysis reveals a second order phase transition as the density or the coupling is increased. Also, by using the Monte Carlo method, the total density functional energy has been minimized and the structure of the droplet has been obtained as a function of the dimensionless coupling strength. For large couplings the system displays a clear phase separation, whereas for intermediate ones, still above the instability point, we see a spinodal decomposition of the droplet.
Keywords: Fermion droplets, instability, phase separation, spinodal decomposition

1. INTRODUCTION

Recent realizations of two[1,2] component alkali Bose-Einstein condensates (BEC's) in a trap provide us with new systems to explore the physics in otherwise unachievable parameter regimes[3,4,5]. Dramatic results were recently observed in the phase segregation dynamics of mixtures of Rb[1,2] gases. Periodic spatial structures were found at intermediate times which then recombine at a later time.

Phase segregation phenomena have been much studied in materials science and these can be understood using classical mechanics. These were explained in terms of a concept called spinodal decomposition[6]. When a system is quenched from the homogeneous phase into a broken-symmetry phase, the ordered phase does not order instantaneously. Instead, different length scales set in as the domains form and grow with time. It has been shown for trapped bosons[7] that it is possible to have an analogous spinodal decomposition, which manifests some of the phenomenology including a periodic spatial structure at an intermediate time that is now determined by quantum mechanics. The time scale provides for a self-consistent check of the theory and is consistent with the experimental results[2]. The growth of domains at later times is determined by quantum tunneling and not by classical diffusion. Recently, it became possible[8] to cool a single component system of about a million ^{40}K fermionic atoms in a magnetic trap below the Fermi temperature, T_F leading to the realization of a spin-polarized fermion gas of atoms. Similar to electrons in a solid, the dilute gas of atoms fills all the lowest energy states below the Fermi energy, E_F. The transition to this quantum degenerate state is gradual as compared to the abrupt phase transition into a Bose condensate. For single component fermionic systems, however, the equilibrium is difficult to achieve as the s-wave elastic collisions are prohibited due to Pauli exclusion principle. In the experiments of DeMarco and Jin[8], this was circumvented by using a mixture of two nuclear spin states of ^{40}K atoms for which s-wave collisions are allowed. One of the manifestations of quantum mechanics was the nature of momentum distribution which differed from the well known classical gaussian distribution. This system corresponds to what we called the weak coupling limit in that the physical properties are close to that of a non-interacting fermion gas. The other system which is being explored[9] is the gas of ^{6}Li atoms. From theoretical point of view, the thermodynamic properties and the density and momentum distributions of a spin-polarized Fermi gas in a harmonic trap have been studied[10,11,12]. Butts and Rokhsar[10] have obtained universal forms of the spatial and momentum distributions for a single component spin-polarized non-interacting fermion gas using the Thomas-Fermi (TF) approximation. Bruun and Burnett[12] have studied an interacting fermion gas of ^{6}Li atoms which have a large negative scattering length which could also lead to the possibility of superfluidity. In the present paper, we consider mixtures of finite systems of ultracold fermionic atoms with a positive scattering length in both weak and strong coupling limits and explore its ground state using the TF approximation, and Monte Carlo simulations.

2. MODEL AND CALCULATION METHOD

We first start with the statics of a two component fermion gas of atoms with masses m1 and m2 and particle numbers N1 and N2. This is assumed to be confined in an azimuthally symmetric harmonic trap with radial and axial frequencies ω and λω, respectively which are considered to be the same for both the components. Unlike the electron gas in matter, the fermion gas of atoms is neutral and dilute. The significant interactions between atoms are, therefore, only short-ranged and these would be responsible for any phase segregation in the system. In the long wavelength limit, the system can be well described by density functional theory and the total energy can be written as:

$$E = \int [\sum_{\sigma} E_{0\sigma}(\rho_\sigma) + g\rho_1\rho_2]\, dr$$ Here

$$E_{0\sigma} = \frac{\hbar^2}{2m_\sigma}\tau_\sigma(r) + \frac{1}{2}m_\sigma\omega^2(x^2 + y^2 + \lambda^2 z^2)\rho_\sigma(r)$$

is the non-interacting part of the energy density and $\rho_\sigma(r)$ is the particle density of the component σ=1,2 with $\int \rho_\sigma(r)\, dr = N_\sigma$. The interaction term has been approximated by the contact potential g δ(r-r'). g is related to the scattering length a by $g = 2\pi\hbar^2 a/m$, with $m = m_1 m_2/m_1 + m_2$. In accordance with the experiments, we take a to be positive and consider here only the s-wave scattering. Therefore, the contribution to the interaction term is non-zero only when the species are different or are in different hyperfine states as in experiments. From the exclusion principle, there is no contact interaction between particles of the same species(spin). For the kinetic energy density τ_σ, we use a local approximation including the first and second derivatives of the particle density,

$$\tau_\sigma(r) = \frac{3}{5}(6\pi^2)^{2/3}\rho_\sigma{}^{5/3}(r) + \frac{1}{36}\frac{|\nabla\rho_\sigma|^2}{\rho_\sigma}$$

The first term represents the Thomas-Fermi (TF) approximation to the kinetic energy. The second term represents the gradient correction to the kinetic energy. Monte-Carlo results confirm that the gradient term is at least 2 orders of magnitude smaller than the TF term, but this term is important in that it can break the symmetry of the ground state and lead to lower energy asymmetric states. Without the interaction term (g), the system behaves in the same fashion as the one component system. In this case, Butts and Rokhsar[10] obtained E_F to be related to the total particle number N by $E_F = \hbar\omega(6\lambda N)^{1/3}$ and the density profile at T=0 is given by $\rho_{non-interacting}(r) = \rho_0[1 - (\bar{r}/R_F)^2]^{3/2}$ with $\bar{r}^2 = x^2 + y^2 + \lambda^2 z^2$, $R_F = [2E_F/m\omega^2]^{1/2}$,

$$K_F = \sqrt{2mE_F}/\hbar, \rho_0 = K_F^3/6\pi^2 = 8N\lambda/\pi^2 R_F^3$$

R_F gives the characteristic size of the gas. In the TF approximation, the trapping potential can be treated to be locally constant and we can define a local Fermi wavevector, $k_F(r)$, and the density at T = 0 can be written as $\rho_{non\text{-}interacting}(r) = k_F^3(r)/6\pi^2$.

We now examine the properties of the mixed (two-component) system in the presence of interactions. The strength of the coupling, which controls the phase segregation, depends on the dimensionless parameter which is the ratio between the interaction and the kinetic energies, namely $m\, g\, \rho^{1/3}/\hbar^2$ or simply $c = k_F a/\pi$. For a general two-component system with chemical potentials μ1 and μ2, the ground state is obtained by minimizing the new potential

$$\Omega = E - \int \mu_1\rho_1 + \mu_2\rho_2\, dr.$$

Similar to the one-component case, one can rewrite the results of the minimization in a dimensionless form by introducing for each of the species s, the following quantities: $R_\sigma = [2\mu_\sigma/m_\sigma\omega^2]^{1/2}$, $K_{F\sigma} = (6\pi^2\rho_\sigma)^{1/3}$, $g_\sigma = g\rho_{\sigma'0}/\mu_\sigma$, and $n_\sigma(r) = \rho_\sigma(r)/\rho_{\sigma 0}$. Here $\rho_{\sigma 0}$ is the density of the component σ in the absence of interactions, and σ' =3- σ. If one neglects the smaller terms containing derivatives of the density (the TF limit), one obtains the following algebraic equations satisfied by the dimensionless densities n1 and n2 for any coupling strength g_σ:

$$n_1^{2/3} = 1 - (\bar{r}/R_1)^2 - g_1 n_2;\quad n_2^{2/3} = 1 - (\bar{r}/R_2)^2 - g_2 n_1$$

The effect of the additional $g_\sigma\, n_{\sigma'}$ term is to deplete regions of large $n_{\sigma'}$ (without necessarily leading to a phase segregation). When there is phase segregation, the interface energy is proportional to the square root of the coefficient of the gradient term, and it often serves to distinguish different configurations. In that case, their effect cannot be neglected and these are included in the Monte Carlo simulations. We next discuss some special cases in the TF limit.

TF Limit: μ1=μ2=μ For Any Coupling

In this case $g_1 = g_2 = g$. The above equations are cubic and therefore admit 3 roots, one is equal densities (n1=n2). If a solution n2=f(n1) exists, by symmetry, the other one is necessarily n1=f(n2). The real solutions are plotted in Fig. 1, where the physical n1=n2 solution is referred to as "Sym", and the other conjugate (asymmetric) solutions are referred to as "A1" and "A2". Below we discuss these solutions in the weak and strong coupling limits.

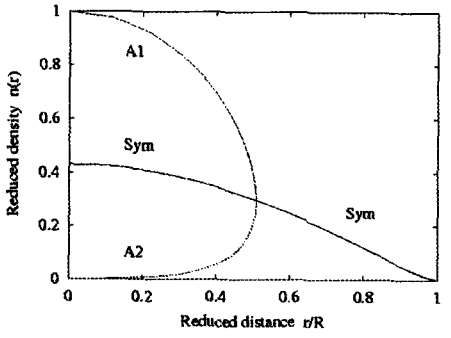

Figure 1. Dimensionless density versus dimensionless radius r/R for g=1. One of the asymmetric solutions (A2) is depleted at the center while the other one has a large concentration. For r/R larger than 0.51 both asymmetric solutions join the symmetric density profile. The sharp features around this point are due to the neglect of the gradient terms.

The solutions will all be axially symmetric in that they are functions of r only. In actuality, the axial symmetry can also be broken, but we do not find it here since we neglected the terms in gradient of the particle density in the kinetic energy. The broken symmetry solutions will be discussed in the
results from the Monte Carlo simulations where these terms were kept. In Fig. 1, the bifurcation point where the asymmetric solutions start to occur corresponds to = $n\, g^3 = 0.296$, which separate the strong coupling regime from the weak one. At the bifurcation point, we have $gn^{1/3} = 2/3$. Since $g=(K_F a)4/3\pi$, we find a critical dimensionless coupling $c=(K_F a/\pi)_c=0.646$. We shall come back and compare this value with that obtained with a different approach below.

TF Limit: Linear Instability Analysis

We next study the fluctuations of the system about its equilibrium configuration in the TF limit by expanding the thermodynamic potential Ω up to second order in the particle density variation $\delta\rho$ about its minimum which was computed above. The sign of the second derivative of Ω will decide the stability of the symmetric phase. A phase segregation occurs when the second derivative ceases to be positive definite. If the transition is first order, it would have already occurred before reaching a negative second derivative. In this case, the second derivatives of Ω lead just to a 2x2 matrix. The phase instability criterion is o have a zero eigenvalue. In the symmetric case ($\mu1=\mu2$; $\rho1=\rho2$), the instability will first occur locally at the point where the relation $g\, n^{1/3} = 2/3$ is satisfied. This implies that $n=0.296$. This is exactly the critical n_c obtained earlier from the minimization of the potential Ω. These two instabilities occuring at the same point suggest that, within the adopted model (TF), the transition might be of second order.

General Case: Monte Carlo Results

The density dirstibution that extremizes the energy functional Ω can be obtained by a Monte Carlo simulation with a weighting factor exp(-E/T) for a parameter T that is sufficiently low. This is basically the simulated annealing method and has been exploited successfully in earlier treatment[7] of the corresponding Bose system described by a Gross-Pitaevski functional. The derivative term is approximated by a finite difference calculated on a cubic mesh. For simplicity, we show here results for the case when the two components have the same mass. We first show in Fig. 2 the density profile of component 2 as a function of x and y for z=0 for the weak coupling case with no phase segregation. The values of different parameters were chosen to be $\omega=135x2\pi$ rad/sec, $a=135\ a_{Bohr}$, $\lambda=0.14$, and $N1=N2=10^6$ ($\mu1=\mu2=1.626\ 10^{-29}$ J); roughly corresponding to the experimental parameters of the ^{40}K system\cite{demarko}. In these experiments, we estimate $K_F a/\pi=0.032$. The density profile for the other component is the same and hence is not shown.

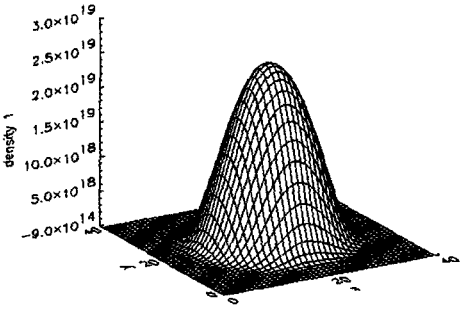

Figure 2: density profile in the weak coupling limit (c=0.032)

In the limit of strong interaction, phase segregation starts and as mentioned earlier, the system can now also break cylindrical symmetry. This happens when c is large enough, which in turn can be achieved with only large K_F, only large a, or both. To illustrate this, we show in Fig. 3 the density profiles for components 1 and 2 for the case of $a=30000\ a_B$, $\mu1=\mu2=1.86\ 10^{-30}$ J, and $\omega=300$ rad/sec. In this case, $c= K_F a/\pi=2.39$.

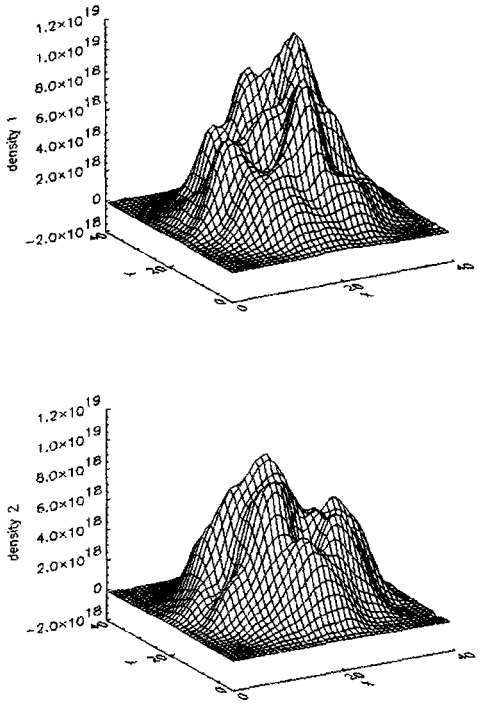

Figure 3: density profiles of the two components in the large coupling limit (c=2.39). There is clearly a phase separation.

The difference in the densities of the two components shows that the largest change occurs near the center where the density is maximum. It is to be further noted that for this case, the density distribution is still quite cylindrical but there is a slight asymmetry, as we have noticed in the graph of the difference. This asymmetry becomes more pronounced as the interaction is increased further.

3. CONCLUSION

In conclusion we have investigated the statics of the spatial phase segregation process of a mixture of fermion atoms in a harmonic trap using the density functional theory. As the coupling starts to increase, even with the same chemical potential, equilibrium distribution with unequal densities starts to appear, which quite often does not exhibit axially symmetric correlations.

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