Shell Effects and Phase Separation

in a Trapped Multi-Component Fermi System

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Abstract

Shell effects in the coordinate space can be seen with degenerate Fermi vapors in non-uniform trapping potentials. In particular, below the Fermi temperature, the density profile of a Fermi gas in a confining harmonic potential is characterized by several local maxima. This effect is enhanced for "magic numbers" of particles and in quasi-1D (cigar-shaped) configurations. In the case of a multi-component Fermi vapor, the separation of Fermi components in different spatial shells (phase-separation) depends on temperature, number of particles and scattering length. We derive analytical formulas, based on bifurcation theory, for the critical density of Fermions and the critical chemical potential, which give rise to the phase-separation.
I. INTRODUCTION

The Fermi quantum degeneracy with trapped dilute vapors of $^{40}\text{K}$ atoms has been experimentally achieved in 1999. The s-wave scattering between Fermions in the same hyperfine state is inhibited due the Pauli principle. Moreover, for $^{40}\text{K}$ atoms the p-wave scattering length becomes negligible in the limit of zero temperature. It follows that at very-low temperatures the dilute Fermi gas, in a fixed hyperfine state, is practically ideal. Nevertheless, the effect of interaction could be very effective for a Fermi vapor with two or more hyperfine states. In this paper we consider a Fermi vapor confined in a harmonic potential that models the trap of recent experiment. These trapped Fermi gases are quite interesting because the quantum degeneracy shows up not only in momentum space, as in uniform systems, but also in coordinate space.

II. IDEAL FERMI GAS AT FINITE TEMPERATURE

Let us consider an ideal Fermi gas in external potential described by the non-relativistic field

$$\hat{\psi}(r) = \sum_{\alpha} \phi_{\alpha}(r) \hat{a}_{\alpha},$$

where $\phi_{\alpha}(r) = \langle r | \alpha \rangle$ is the single-particle eigenfunction with eigenvalue $\epsilon_{\alpha}$ and $\hat{a}_{\alpha}$ is the lowering Fermi operator of the single-particle eigenstate $|\alpha\rangle$. The grand canonical thermal average of the Fermi spatial density $\hat{\psi}^+(r)\hat{\psi}(r)$ is given by

$$n(r) = \langle \langle \hat{\psi}^+(r)\hat{\psi}(r) \rangle \rangle = \sum_{\alpha} \frac{|\phi_{\alpha}(r)|^2}{e^{\beta(\epsilon_{\alpha} - \mu)} + 1},$$

where $\mu$ is the chemical potential and $\beta = 1/(kT)$ with $k$ the Boltzmann constant and $T$ the absolute temperature. Note that the thermal average of a generic operator $\hat{A}$ is defined as

$$\langle \langle \hat{A} \rangle \rangle = \frac{Tr[\hat{A}e^{-\beta(\hat{H} - \mu\hat{N})}]}{Tr[e^{-\beta(\hat{H} - \mu\hat{N})}]},$$
where $\hat{H} = \sum_\alpha \epsilon_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha$ is the Hamiltonian of the system and $\hat{N} = \sum_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha$ is the number operator. The average number $N$ of particles of the system, given by

$$N = \sum_\alpha \langle \langle a_\alpha^\dagger a_\alpha \rangle \rangle = \sum_\alpha \frac{1}{e^{\beta (\epsilon_\alpha - \mu)} + 1},$$

(4)

fixes the chemical potential. \[2\]

In the case of a harmonic external potential $U(r) = (m/2)(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2)$, one finds the Fermi density profile by using the Eq. (2) and the eigenfunctions $\phi_{n_1 n_2 n_3}(r)$ of the harmonic oscillator

$$n(r) = \sum_{n_1 n_2 n_3=0}^\infty \frac{|\phi_{n_1 n_2 n_3}(r)|^2}{e^{\beta h (\omega_1 (n_1 + 1/2) + \omega_2 (n_2 + 1/2) + \omega_3 (n_3 + 1/2) - \mu)} + 1}. \quad (5)$$

Because the Fermi gas is ideal, one has $\phi_{n_1 n_2 n_3}(r) = \phi_{n_1}(x) \phi_{n_2}(y) \phi_{n_3}(z)$, where $\phi_n(x)$ is the eigenfunction of a 1D harmonic oscillator with frequency $\omega$ and quantum number $n$. This eigenfunction can be found by means of the recursion relation \[3\]

$$\phi_n(x) = \frac{1}{\sqrt{n}} \left[ \sqrt{2} \sigma x \phi_{n-1}(x) - \sqrt{n-1} \phi_{n-2}(x) \right], \quad (6)$$

where $\phi_0(x) = \sigma^{1/2} \pi^{1/4} e^{-\sigma^2 x^2/2}$ and $\phi_1(x) = \sqrt{2} \sigma x \phi_0(x)$, with $\sigma = (m\omega/h)^{1/2}$. 

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FIG. 1. Density profiles for an ideal Fermi gas in a 1D harmonic trap. Temperature: $kT/h\omega = 10^{-3}$; at this temperature the results coincide with zero-temperature ones. $N$ is the number of Fermions. Lengths in units $a_H = (\hbar/m\bar{\omega})^{1/2}$ and densities in units $a_H^{-3}$.

The Eq. (5) and (6) are used to numerically calculate the exact density profile. Such exact density profile can be compared with the semiclassical one, that is given by [1]

$$n(r) = \frac{1}{\lambda^3} f_{3/2} \left( e^{\beta(\mu - U(r))} \right),$$

where $\lambda = (2\pi\hbar^2\beta/m)^{1/2}$ is the thermal length and

$$f_n(z) = \frac{1}{\Gamma(n)} \int_0^\infty dx \frac{x^{n-1}}{z^{-1}e^x + 1},$$

with $\Gamma(x)$ the factorial function.
FIG. 2. Density profiles for an ideal Fermi gas in a 1D harmonic trap at finite temperature, with $N = 20$ and 50. $N$ is the number of Fermions. a) $kT/\hbar \omega = 1/10$; b) $kT/\hbar \omega = 1/2$; c) $kT/\hbar \omega = 1$; d) $kT/\hbar \omega = 5$. Units as in Figure 1.

In the limit of zero temperature, with $\mu = E_F$ the Fermi energy, the semiclassical spatial distribution is given by the Thomas-Fermi approximation $n(r) = (2m)^{3/2}/(6\pi^2 \hbar^3) (E_F - U(r))^{3/2} \Theta (E_F - U(r))$, where $\Theta$ is the Heaviside step function. The Eq. (7) is the generalization of well-known formula for an ideal Fermi gas in a box that is exact in the thermodynamic limit. Note that for $|z| < 1$ one has $f_n(z) = \sum_{i=1}^{\infty} (-1)^{i+1} z^i / i^n$. Moreover, by using $g_n(z) = -f_n(-z)$ instead of $f_n(z)$, one finds the spatial distribution of the ideal Bose gas in external potential. The Fermi energy $E_F$ and the Fermi temperature $T_F$ are easily obtained by imposing the normalization condition to the Thomas-Fermi distribution. For a D-dimensional harmonic oscillator with a geometric average $\bar{\omega} = (\omega_1 \omega_2 \omega_3)^{1/3}$ of the $D$ frequencies, one finds the semiclassical result

$$E_F = kT_F = (D!N)^{1/D} \hbar \bar{\omega} .$$

For $D = 3$ one recovers the familiar result $E_F = 6^{1/3} N^{1/3} \hbar \bar{\omega}$.

In a recent paper we have performed a comparison between exact and semiclassical results. We have found that when $(kT/\hbar \bar{\omega}) > 1$, where $\bar{\omega} = (\omega_1 \omega_2 \omega_3)^{1/3}$, there are no appreciable deviations between exact and semiclassical results. Instead, for an isotropic
harmonic potential, when \((kT/\hbar\omega) < 1\) some differences are observable, in particular for 
"magic" numbers of particles \((N = (p+1)(p+2)(p+3)/6, \text{where } p \text{ is a natural number})\) that correspond to a complete shell occupation of single-particle energy levels. The differences are reduced by increasing \(N\) showing that semiclassical approximation provides an excellent representation of Fermi distribution for a wide range of parameters. In correspondence of the "magic numbers", the exact spatial density profile shows local maxima, which suggest a spatial shell structure. The magic numbers are particularly stable; in fact, for small variations of the chemical potential \(\mu\) the magic number \(N\) remains unchanged. The shell structure in the density profile is washed out by increasing the number of particles and is completely absent in the semiclassical approximation.

In the quasi-1D case, namely a cigar-shaped gas where \(\omega_1 = \omega_2 >> \omega_3\), the shell effects are strongly enhanced. This can be shown by investigating the one-dimensional problem, as recently done by Kolomeiski et al \([8]\) at \(T = 0\). We extend the calculations of Kolomeiski at finite temperature. In Fig. 1 we plot the density profile of a 1D ideal Fermi gas in harmonic potential as a function of the number \(N\) of particles at \(kT/\hbar\omega = 10^{-3}\). We have verified that at this temperature the density profiles coincide with the zero-temperature ones. The results are obtained by numerically evaluating expressions (5) and (6) in the 1D case. The local maxima, whose number grows with \(N\), are clearly visible for a small number of particles. In Fig. 2 we show the density profiles with 20 and 50 particles as a function of temperature. Remarkably, the local peaks are no more distinguishable for temperatures well below the Fermi temperature \(T_F = N\hbar\omega/k\). Thus, to see spatial shell effect on the 1D density profile, the system should be at temperatures lower than \(T_F\) by one or two orders of magnitude.

III. PHASE SEPARATION WITH TWO FERMI COMPONENTS

In the recent experiment with dilute \(^{40}\text{K}\) atoms, \([9]\) to favor the evaporative cooling, a \(^{40}\text{K}\) Fermi vapor in two hyperfine states (\(|9/2, 9/2\rangle\) and \(|9/2, 7/2\rangle\)) has been used. The problem of a dilute Fermi vapor with two hyperfine states (components) can be studied by using the
s-wave scattering approximation, the mean-field approach and semiclassical formulas. The spatial density profiles of the two components of a Fermi vapor can be written as

\[
n_1(r) = \frac{1}{\lambda^3} f_{3/2} \left( e^{\beta(\mu_1 - U(r) - gn_2(r))} \right),
\]

\[
n_2(r) = \frac{1}{\lambda^3} f_{3/2} \left( e^{\beta(\mu_2 - U(r) - gn_1(r))} \right),
\]

(10)

where \( \mu_i \) is the chemical potential of the \( i \)-th component, and \( g = 4\pi\hbar^2 a_{12}/m \), with \( a_{12} \) the s-wave scattering length between first and second component \( (a_{11} = a_{22} = 0) \). Thus, the effect of the second Fermi component on the first component is the appearance of a mean-field effective potential.

When two components have the same number of particles, the onset of phase-separation is also an example of spontaneous symmetry breaking. In fact, if the chemical potentials \( \mu_i \) of the two components are equal, Eq. (10) always admits a symmetric solution \( n(r) = n_1(r) = n_2(r) \). However, for particle number \( N \) larger than a threshold \( N_c \) the solution bifurcates and a pair of symmetry breaking solutions appears. Just beyond threshold the asymptotic solutions begin to differ from the symmetric one in a neighborhood of the origin \( r = 0 \), i.e. at the point of higher density. An analytic formula for the critical chemical potential \( \mu_c \) can be obtained by using the bifurcation theory. The system (10) can be re-written at the origin as

\[
F^\mu(x) = 0,
\]

(11)

where

\[
x = (x_1, x_2) = (n_1(0), n_2(0))
\]

\[
F^\mu(x) = \left( F_1^\mu(x), F_2^\mu(x) \right) = \left( x_1 - \frac{1}{\lambda^3} f_{3/2}(e^{\beta(\mu_1 - gx_2)}), x_2 - \frac{1}{\lambda^3} f_{3/2}(e^{\beta(\mu_1 - gx_2)}) \right).
\]

For \( \mu < \mu_c \) there exist only one symmetric solution of the previous equation, given by \( x^* = (x^*, x^*) \). At \( \mu = \mu_c \) there are two solutions and the Jacobian of the function \( F^\mu(x) \) must have the determinant equal to zero, i.e.
\[ \det \left[ \frac{\partial F^\mu}{\partial x}(x^*) \right] = \begin{vmatrix} 1 & \frac{1}{\lambda^3} \frac{\partial}{\partial x_2} f_{3/2}(e^{\beta(\mu-gx_2)}) \\ \frac{1}{\lambda^3} \frac{\partial}{\partial x_1} f_{3/2}(e^{\beta(\mu-gx_1)}) & 1 \end{vmatrix}_{x^*} = 0 . \] (12)

By imposing this condition on Eq. (10) and (11) and setting \( x^* = n(0) \), one finds

\[ \frac{g\beta}{\lambda^3} e^{\beta(\mu-gn(0))} f_{3/2}'(e^{\beta(\mu-gn(0))}) = 1 . \] (13)

At \( T = 0 \), by the use of the first term of the large \( z \) expansion of \( f_{3/2}(z) \), given by

\[ f_{3/2}(z) = \frac{4}{3\pi^{1/2}} \left[ (\ln z)^{3/2} + \frac{\pi^2}{8} (\ln z)^{-1/2} + ... \right] , \] (14)

one finds analytical expressions for the critical density \( n_c(0) \) and the critical chemical potential \( \mu_c \):

\[ n_c(0) = \frac{\pi}{48a^3} , \quad \mu_c = \frac{5\pi^2}{24} \hbar \omega \left( \frac{a_H}{a} \right)^2 . \] (15)

These remarkably simple formulas can be very useful to determine the onset of phase-separation in future experiments. Moreover, by knowing the critical chemical potential one numerically finds the number of particles. The conclusion is that by increasing the interaction between the two components one can use lower number of particles to obtain the phase-separation. At finite temperature one can use the first two terms of the large \( z \) expansion of \( f_{3/2}(z) \), i.e. Eq. (14). The analytical formulas at zero and finite temperature are in good agreement with the numerical calculations. [4]

IV. PHASE SEPARATION WITH MANY FERMI COMPONENTS

Phase-separation also appears in a Fermi vapor with three or more components. In Ref. 4 we have numerically solved the three-component extension of Eq. (10) with \( a_{12} = a_{13} = a_{23} = a \). Also for three components the spontaneous symmetry breaking and the phase-separation are controlled by scattering length, temperature and total number of particles. In particular, one finds that by increasing the scattering length at first one of the components separates from the others, which remain still mixed. The separation begins at the center of
the trap and, as the scattering length is further increased, also the other two components separate (this second phase-separation begins at the interface with the previously separated component) and one eventually sees complete phase-separation and the formation of 4 or 5 shells.

The Eqs. (15) can be extended to a M-component Fermi vapor with the same number of particles in each component. The critical density \( n_c(0) \) does not depend on the number \( M \) of Fermi components and one gets the same result of Eq. (15). Instead, the critical chemical potential reads \( \mu_c = (2M + 1)\pi^2\hbar\bar{\omega}(a_H/a)^2/24 \).

V. CONCLUSIONS

We have analyzed a degenerate Fermi gas in a harmonic external potential. Below the Fermi temperature \( T_F \) and for a small number of particles, shell effects, like local maxima in the spatial density profile for ”magic numbers”, are clearly visible. Such effects are strongly enhanced in the 1D case, but they are visible only for temperatures which are at least one order lower than \( T_F \), i.e. far from the semiclassical limit.

We have also considered a Fermi vapor with many hyperfine states. By using the bifurcation theory, we have shown that the onset of phase-separation appears by increasing the scattering length or, for a fixed scattering length, by increasing the number of particles. By raising the temperature, a larger scattering length or a larger number of particles is needed to obtain the phase-separation. A Fermi vapor with three or more components has the same behavior but at first only one of the components separates from the others, which remain still mixed. The critical density of Fermions at the origin, which gives rise to the phase-separation, satisfies the equation \( n_c(0) = \pi/(48a^3) \), where \( a \) is the s-wave scattering length.
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