Abstract: Using numerical simulation based on a density-functional equation for a trapped Fermi super-fluid valid along the BCS-unitarity crossover, we establish robust scaling over many orders of magnitude in the observables of the system as a function of fermion number. This scaling allows to predict the static properties of the system, such as energy, chemical potential, etc., for a large number of fermions, over the crossover, from the knowledge of those for a small number (∼4–10) of fermions.

Energy ($E$) and chemical potential ($\mu$) of a trapped Fermi super-fluid as a function of number $N$ of atoms

Universal scaling in a trapped Fermi super-fluid in the BCS-unitarity crossover

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1. Introduction

The Pauli principle among identical fermions leads to an effective repulsion which avoids the collapse of the hadronic universe. A many-fermion system dominated by Pauli repulsion exhibits universal behavior with the physical attraction playing a minor role. Such universal behavior manifests in correlation and scaling in the observables of few- and many-fermion systems [1]. This universality is prominent in the limit of zero Fermi-Fermi interaction in the Bardeen-Cooper-Schrieffer (BCS) theory of superfluid (SF) fermions leading to universal properties of low-temperature superconductors [2], of cold neutron matter and neutron star [3], and of a trapped Fermi SF [4] at zero temperature. This universality also manifests at unitarity [5,6], when the atomic scattering length $a$ tends to infinity ($a \to \infty$). Both at the BCS limit ($a \to -0$) and unitarity, the scattering length ceases to be a scale of length, and the only length scale of the problem in these limits is $k_F^{-1}$ where $h k_F$ is the Fermi momentum. Consequently, all energies are universal functions of Fermi momentum $h k_F$ (or of Fermi energy $E_F = h^2 k_F^2 / 2m$, where $m$ is the atomic mass, and the system acquires universal behavior with robust scaling involving the stationary observables, such as energy, chemical potential, etc., as a function of number of fermions.

How the above scaling appears in a fully paired $N$-fermion SF with equal number of spin up and down atoms confined in a spherically-symmetric trap $U(r)$ can be seen in the local-density approximation (LDA) [4,7,8], where the system obeys

$$U(r) = \frac{h^2}{2m} \left[ 3 \pi^2 n(r) \right]^{2/3} \xi = \mu_0,$$  

(1)

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where $\xi = 1$ in the BCS limit and $=0.44$ (obtained [9] from Monte Carlo calculations on a uniform Fermi SF at unitarity, $n(r)$ is the SF density, $\mu_0$ is the chemical potential, and $U(r) = m\omega^2 r^2/2$ is the harmonic trap with $\omega$ the trap frequency and normalization $\int n(r)dr = N$. The second term on the left-hand side of Eq. (1) is the chemical potential of a uniform SF Fermi gas. The total chemical potential $\mu = \mu_0 N$ and energy $E$ of the trapped system are given by

$$\mu = N \int dr \left[ U(r) + \frac{\hbar^2}{2m}(3\pi^2n)^{2/3}\xi \right] n(r),$$  \hspace{1cm} (2)

$$E = N \int dr \left[ U(r) + \frac{3\hbar^2}{5m}(3\pi^2n)^{2/3}\xi \right] n(r).$$  \hspace{1cm} (3)

It is useful to work in terms of dimensionless variables in harmonic oscillators units, obtained by setting $\hbar = m = \omega = 1$, where lengths are expressed in units of $l = \sqrt{\hbar/(m\omega)}$ and energy in $\hbar \omega$. The normalization condition for the density $n$ leads to

$$\sqrt{n(r)} = \frac{[2(3N)^{1/3}\sqrt{\xi} - r^2]^{3/2}}{3\pi^{2/3}}$$

for $2(3N)^{1/3}\sqrt{\xi} > r^2$ and 0 otherwise. Using this expression in Eq. (2) and Eq. (3) we get

$$\mu = \frac{(3N)^{4/3}\sqrt{\xi}}{3}, \quad E = \frac{(3N)^{4/3}\sqrt{\xi}}{4}.$$

An extended LDA (ELDA) was suggested [8] for this energy to include corrections for small $N$:

$$E = \frac{1}{4}(3N)^{4/3}\sqrt{\xi} \left(1 + \frac{\alpha}{N^{2/3}}\right),$$

$\alpha = 0.5$ ($\alpha$ chosen to agree with Monte Carlo data [5, 6] for trapped Fermi SF).

The energy $E = (3N)^{4/3}/4$ in the BCS limit ($\xi = 1$) also follows from a consideration of the $N$-fermion system in a spherical harmonic trap at zero temperature. The degeneracy of the $i$-th state of harmonic oscillator of energy $h\omega(i+3/2)$ is $(i+1)(i+2)/2$. If we consider many paired states up to $i = I$ ($I \gg 1$) completely fully, then $E_P = I$ (in units of $h\omega$) and the total number of fermions, considering two (spin up and down) fermions in each state, is

$$N = \sum_{i=0}^{I} (i+1)(i+2) \approx \frac{I(I+1)(I+2)(I+3)}{3} \approx \frac{I^3}{3}.$$

The total energy in oscillator units is

$$E = \sum_{i=0}^{I} i(i+1)(i+2) \approx \frac{I(I+1)(I+2)(I+3)}{4} \approx \frac{I^4}{4}.$$

Consequently, $E_P = (3N)^{1/3}$, $k_F = \sqrt{2(3N)^{1/6}}$, and $E = (3N)^{4/3}/4$, consistent with the LDA above. The energy at unitarity $E = (3N)^{4/3}\sqrt{\xi}/4$ differs from this energy at the BCS limit by a numerical factor to take into account the atomic attraction. The chemical potential, with dimension of energy, differs from energy by only a numerical factor consistent with the universal behavior.

The $E$ and $\mu$ vs. $N$ scalings valid in the BCS and unitarity limits are useful in predicting $E$ and $\mu$ for a large $N$ from a knowledge of those for a small $N$. In this paper we address two interesting questions related to these scalings.

(a) Are the scalings dependent on the LDA?

(b) Can these scalings valid at the BCS and unitarity limits be extended along the BCS-unitarity crossover [10]?

The LDA, lacking a gradient term, does not include properly the variation of the SF density near the surface. This can be remedied by, following a suggestion of von Weizsäcker [11], including a gradient term (the unitarity [10] has been an active area of research [5, 9, 13]). The crossover from the weak-coupling BCS limit to unitarity [10] is characterized by a numerical factor consistent with the universal behavior.

To study the universality along the crossover, we use a Galilei-invariant DF formulation of the trapped Fermi SF [12, 15, 16], equivalent to a hydrodynamical model with the correct phase-velocity relation [4].

$$\mathbf{v} = \frac{\hbar \nabla \theta}{2m},$$

where $\mathbf{v}$ is the SF velocity, and $\theta$ the phase of the order parameter at position $r$.

$$\left[ -\frac{\hbar^2}{8m} \nabla^2 + U + \mu(n,a) \right] \sqrt{n(r)} = \mu_0 \sqrt{n(r)},$$  \hspace{1cm} (4)

$$\mu(n,a) = \frac{\hbar^2}{2m} (3\pi^2n)^{2/3} g(n^{1/3}a),$$  \hspace{1cm} (5)

$$g(x) = 1 + \frac{\chi_1 x - \chi_2 x^2}{1 - \beta_1 x + \beta_2 x^2},$$  \hspace{1cm} (6)

$$\mu = N \int dr \left[ \frac{\hbar^2}{8m} \nabla \sqrt{n_1}^2 + U(n + \mu(n,a)n) \right],$$  \hspace{1cm} (7)

$$E = N \int dr \left[ \frac{\hbar^2}{8m} \nabla \sqrt{n_1}^2 + U(n + \int_0^n \mu(n',a)dn') \right],$$  \hspace{1cm} (8)

where $\chi_1$, $\chi_2$, $\beta_1$, and $\beta_2$ are parameters. If we choose $\chi_1 = 4\pi/(3\pi^2)^{2/3}$, $\chi_2 = 300$, $\beta_1 = 40$, $\beta_2 = \chi_2/(1 - \xi)$, the DF Eq. (4)
produces energies that agree with the fixed-node Monte Carlo (FNMC) [5] and Green-function Monte Carlo (GFMC) [6] results for the energies of a trapped Fermi SF at unitarity (for $N \leq 30$), and over the crossover [15,17] for $N = 4$ and 8; (ii) provides a smooth interpolation between the energies of a SF at the BCS and unitarity limits [12,17]; (iii) Moreover, the bulk chemical potential $\mu(n, a)$ of Eq. (4) is exact at unitarity and satisfies [12,15] the weak-coupling BCS limit [18]

$$\lim_{x \to 0} g(x) = 1 + \frac{4\pi x}{(3\pi^2)^{2/3}}.$$  

The gradient term in Eq. (4) corresponds [12] to a quantum pressure in the equivalent hydrodynamical equations and provides a correction to the LDA [7]. LDA is a good approximation for a large $N$, when the bulk chemical potential $\mu(n, a)$ – a positive term responsible for Pauli repulsion in the system even for attractive (negative), $a$ – is very large. The gradient term is consistent with the hydrodynamic flow of paired fermions of mass $2m$ [4,12].

### 3. Numerical results of scaling

We solve the DF Eq. (4) by the split-step Crank-Nicolson method by transforming it into a time-dependent equation and using the FORTRAN programs provided in [19]. The space and time steps used in discretization of the equation were 0.05 and 0.001, respectively.

The calculated energy and chemical potential of the trapped Fermi SF as a function of the number of Fermi atoms are exhibited in Fig. 1. We also compare the results for energy with those obtained by the FNMC [5] and GFMC [6] calculations as well as LDA and ELDA calculations. It is found that the DF and ELDA results for energy are in better agreement with the Monte Carlo simulations than the LDA results.

An analysis of the DF results for energy and chemical potential of Fig. 1 reveals that these functions maintain the following quantities

$$\delta(N) \equiv \left[ \frac{E(N)}{N^{2/3}} - 0.37 \right] \frac{1}{N^{2/3}},$$  

$$\kappa(N) \equiv \left[ \frac{\mu(N)}{N^{2/3}} - 0.27 \right] \frac{1}{N^{2/3}},$$  

fixed at constant values independent of $N$. This is a consequence of scalings $E(N)/N^{2/3}$ and $\mu(N)/N^{2/3}$ vs. $N^{2/3}$ as shown in Fig. 1. If the functions $\delta(N)$ and $\kappa(N)$ were really universal, then they should maintain approximate constant values along the BCS-unitarity crossover independent of $N$, although weakly dependent on the atomic scattering length $a$. To demonstrate it, we plot in Fig. 2 $E(N)/N^{2/3}$ and $\mu(N)/N^{2/3}$ vs. $N^{2/3}$ as obtained from the DF Eq. (4) along the BCS-unitarity crossover for three values of $a$ representing the BCS limit, unitarity and one in the crossover. Fig. 2 clearly illustrates the robust scaling.

To take the full advantage of the above scalings at unitarity, as shown in Fig. 1 and Fig. 2, along the full BCS-unitarity crossover we plot

$$\delta(N, k_F a) = \left[ \frac{E(N, k_F a)}{N^{2/3}} - 0.37 \right] \frac{1}{N^{2/3}},$$  

and

$$\kappa(N, k_F a) = \left[ \frac{\mu(N, k_F a)}{N^{2/3}} - 0.27 \right] \frac{1}{N^{2/3}}.$$  

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Figure 3 (online color at www.lphys.org) (a) $\delta(N,k_Fa) = \sqrt{\frac{2}{3}}(3N)^{1/6}$ vs. $|k_Fa|$ for different $N$ from the solution of DF Eq. (4) (lines) and from FNMC calculations [17] (points). (b) $\kappa(N,k_Fa) = \kappa(N,k_Fa)/N^{2/3} - 0.27|\mu(N,k_Fa)|/N^{2/3}$ vs. $|k_Fa|$ for different $N$ from the solution of DF Eq. (4) (lines)

where we display energy $E$ of the trapped Fermi SF along the crossover for different $N$ and $a$. We also calculated the energies for $N = 10^5$ atoms using the energies for $N' = 4$ and $10$. The predictions so obtained listed in Table 1, compare well with the calculated results. This demonstrates the usefulness of the scaling (11) for energy. A similar scaling holds for the chemical potential.

4. Summary and discussion

From a numerical study of the static properties of a trapped Fermi SF using a Galilei-invariant DF formulation [12], equivalent to a generalized hydrodynamic formulation with the correct phase-velocity relation [4], we establish that, because of the dominance of the Pauli repulsion, the trapped Fermi SF has a universal behavior not only in the BCS and unitarity limits but also along the BCS-unitarity crossover. This allows a prediction of the static properties of a large Fermi SF in the crossover region from a knowledge of the same with 4 (10) atoms from a knowledge of the same with 4 (10) atoms is found to have an error of less than 3%. Although we used a DF equation in our study, the observed scaling(s) should be independent of the use of the DF equation and also of the LDA. The scaling(s) is a consequence of the dominance of the Pauli principle leading to a repulsive interaction, where the actual physical attraction plays a minor passive role.

In a Bose-Einstein condensate (BEC), there is no Pauli repulsion, and the physical interaction plays a major active role. Consequently, in a BEC, the stationary observables are very sensitive to the atomic interaction and no scaling should exist in a stationary observable as a function of $N$ from weak-coupling to unitarity crossover. Nevertheless, there have been systematic studies of static properties of a BEC as a function of $N$ [20], Fermi-Bose mapping, fermionization, and other considerations of a strongly-interacting one-dimensional Bose gas are taken up in [21].
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