The Trapped Polarized Fermi Gas at Unitarity

D. Blume

Department of Physics and Astronomy, Washington State University, Pullman, Washington 99164-2814, USA

(Dated: May 14, 2008)

We consider population-imbalanced two-component Fermi gases under external harmonic confinement interacting through short-range two-body potentials with diverging s-wave scattering length. Using the fixed-node diffusion Monte Carlo method, the energies of the “normal state” are determined as functions of the population-imbalance and the number of particles. The energies of the trapped system follow, to a good approximation, a universal curve even for fairly small systems. A simple parameterization of the universal curve is presented and related to the equation of state of the bulk system.

PACS numbers: 03.75.Ss, 05.30.Fk, 34.10.+x

Strongly-correlated few- and many-body systems play an important role in atomic, nuclear and condensed matter physics (see, e.g., Refs. [1, 2, 3, 4]). These systems are characterized by intricate particle-particle correlations, which can be difficult to capture by mean-field frameworks. Furthermore, the development of effective beyond mean-field approaches is complicated by the fact that a small parameter can typically not be identified. Thus, the most promising avenues for the theoretical description of strongly-correlated systems start with a microscopic many-body Hamiltonian. In a few fortuitous cases, such as strongly-correlated one-dimensional systems [2], exact analytical solutions can be found for certain classes of model Hamiltonian. In other cases, however, a quantitative description of strongly-correlated systems relies on numerical approaches.

This paper treats strongly-correlated two-component Fermi gases under external harmonic confinement with diverging s-wave scattering length $a_s$ at zero temperature using a numerical Monte Carlo approach. The masses of the two species are assumed to be the same, and the properties of the system are determined as a function of the population difference between the two components.

The interest in population-imbalanced atomic Fermi systems [3, 4, 5, 6, 7, 8, 9, 10, 11, 12] is inherently linked to the mismatch of the Fermi surfaces of the two components, which has, e.g., been predicted to lead under certain circumstances to pairing with non-zero momentum, i.e., to the formation of so-called FFLO states [13, 14]. So far, the experimental search for FFLO states has, however, not been met with success.

Population-imbalanced Fermi systems have been realized using ultracold atom samples, and a rich behavior as functions of population-imbalance and temperature has been observed [11, 12]. In these experiments, composite fermionic atoms such as $^6\text{Li}$ are trapped in two different internal hyperfine states, referred to as spin-up and spin-down atoms in the following. The population-imbalance or polarization can be adjusted straightforwardly, and the interspecies scattering length $a_s$ between the spin-up and spin-down fermions can be varied by applying an external magnetic field in the vicinity of a so-called Fano-Feshbach resonance. To date, all experiments on population-imbalanced Fermi gases have been performed with comparatively large atom samples. Here, we consider the properties of small systems, which can be realized using present-day technology by loading a degenerate Fermi gas into a deep optical lattice, for which the tunneling between neighboring sites is negligible.

We determine the energetics of small trapped two-component Fermi gases at unitarity with varying population-imbalance using the fixed-node diffusion Monte Carlo (FN-DMC) method [15]. Two different parameterizations of the many-body nodal surface are considered: The nodal surface of the non-interacting trapped gas, and a nodal surface that is constructed by antisymmetrizing a set of pair functions. Not surprisingly, the trapped gas described by the former nodal surface can be related to the normal state of the homogeneous system. We find that the energies of the “trapped normal gas” with varying population-imbalance and number of particles fall on a universal curve that can be parameterized quite well by three parameters. Remarkably, the energies for systems with as few as $N = 5$ fermions fall on the same universal curve as those for larger systems (the largest $N$ considered in this work is 55). The relationship between the trapped and homogeneous systems is also analyzed by considering structural properties. For small $N$, we find that the energies of the trapped normal system are lower than those obtained for a nodal surface that accounts for pairing physics. For larger $N$, in contrast, the nodal surface that accounts for pairing physics results in a lower energy for small $|N_1 - N_2|$, where $N_1$ and $N_2$ denote the number of spin-up and spin-down fermions, respectively. Our \textit{ab initio} results for trapped population-imbalanced Fermi gases may serve as benchmarks for other numerically less involved techniques and aid in testing phenomenological models.

Our model Hamiltonian for the trapped two-component Fermi gas with $N$ mass $m$ fermions, where $N = N_1 + N_2$ and $N_1 \geq N_2$, reads

$$H = \sum_{i=1}^{N} \left( \frac{-\hbar^2}{2m} \nabla_{\vec{r}_i}^2 + \frac{m \omega^2}{2} r_i^2 \right) + \sum_{i=1}^{N_1} \sum_{j=N_1+1}^{N} V_{ib}(r_{ij}) \tag{1}$$

Here, $\vec{r}_i$ denotes the position vector of the $i$th atom and
the angular trapping frequency. The interaction potential $V_{\parallel}$ between spin-up and spin-down atoms depends on the interparticle distance $r_{ij} = |\vec{r}_i - \vec{r}_j|$, and is characterized by the interspecies s-wave scattering length $a_s$.

We model $V_{\parallel}$ by a square well potential with range $R_0$ and depth $V_0$ ($V_0 > 0$), $V_{\parallel}(r) = -V_0$ for $r < R_0$ and 0 for $r > R_0$. To describe the unitary regime, we fix $R_0 = 0.01a_{ho}$, where $a_{ho}$ denotes the harmonic oscillator length, and adjust the depth $V_0$ so that the free-space two-particle system supports a single zero-energy s-wave bound state. We consider regimes away from an intra-species $p$-wave Feshbach resonance, and treat like atoms as non-interacting.

The ground state wave function for fermions is, as a consequence of the Pauli exclusion principle, characterized by a complicated nodal surface, i.e., the many-body wave function changes sign when either two spin-up atoms or two spin-down atoms are exchanged. This sign change often times leads to inefficient sampling schemes, a phenomenon commonly referred to as “fermionic sign problem”. To avoid the sign problem, we adopt the FN-DMC method [15], which determines the eigenenergy of a state that has the same nodal structure as $\psi_T$ but that may differ from $\psi_T$ in other regions of configuration space. In most applications of the FN-DMC method, great effort is placed on optimizing $\psi_T$ so as to obtain a tighter upper bound to the true eigenenergy. Our calculations that utilize a pairing function fall into this category. Our study of the trapped normal state, in contrast, considers the properties of the many-body system for a fixed, non-optimized nodal structure.

The guiding function $\psi_{T1}$ of the trapped normal gas is written in terms of the ground state wave function $\psi_{NI}$ of the non-interacting trapped Fermi gas and three Jastrow factors $J_{kk'}$, $\psi_{T1} = \psi_{NI}J_{11}J_{22}J_{12}$. The positive definite Jastrow factors $J_{kk'}$ account for correlations between atoms from component $k$ and atoms from component $k'$; they reduce the statistical uncertainties but do not alter the nodal surface of $\psi_{T1}$. The function $\psi_{NI}$ can be written as a product of two Slater determinants, $\psi_{NI} = \text{Det}(M_1) \times \text{Det}(M_2)$, where the $ij$th element of the matrix $M_k$, $k = 1$ or 2, is given by the single particle harmonic oscillator function $\phi_i(\vec{r}_j)$ with $i, j = 1, \cdots, N_k$. The subscript $i$ labels the excitations: $i = 1$ corresponds to the ground state, $i = 2$ to the first excited state, and so on. For closed shells, i.e., for $N_k = 1, 4, 10, 20, 35, \cdots$, the Slater determinant $\text{Det}(M_k)$ is uniquely defined. For open shells, in contrast, degenerate states exist and $\psi_{NI}$ is not uniquely defined. In this case, we consider determinants build from different sets of harmonic oscillator orbitals and report the lowest energy. For $N_k = 5$, e.g., we fill the first two shells and place the remaining particle in either a $l = 0$ or $l = 2$ orbital ($l$ denotes the orbital angular momentum of $\phi_i$).

Tables I and II summarize our FN-DMC energies for the guiding function $\psi_{T1}$. In addition to the FN-DMC energy, we calculate the expectation value $E_{VMC}$, $E_{VMC} = \langle \psi_T|H|\psi_T\rangle/\langle \psi_T|\psi_T\rangle$, of the many-body Hamiltonian using the variational Monte Carlo (VMC) method [13]. For all systems considered in Table I [as well as for the $(N_1, N_2) = (20, 1), (35, 1), (20, 4)$, and $(35, 4)$ systems], $E_{VMC}$ is, for the simulation times employed, positive and less than about 15 % higher than the corresponding FN-DMC energy. For the systems with $(N_1, N_2) = (20, 10), (20, 20), (35, 10)$ and (35, 20), in contrast, the VMC energy becomes negative after a fairly small number of sampling steps despite the fact that the initial configurations correspond to a gas-like system. To obtain the FN-DMC energies for these systems, we start the FN-DMC calculations from non-equilibrated gas-like configurations and not, as done for the smaller systems, from configurations that are distributed according to $\psi_{T1}^2$. The resulting FN-DMC energies correspond to a gas-like state and appear converged. For the $(20, 10)$ system, e.g., we have checked that different initial configurations result, within errorbars, in the same FN-DMC energy. The existence of many-body bound states with negative energy for large systems interacting through finite-range two-body potentials is not surprising (see, e.g., Ref. [13]). In fact, even some of the smaller systems with $N \geq N_{cr}$ may possess a tightly-bound molecular-like ground state that is not sampled in our simulations. For systems with $N_1 = N_2$, it has been found previously that the critical number $N_{cr}$ is larger than 6 [16]; for systems with $N_1 - N_2 = 1$, it is larger than 5 [16].

Figure I shows the FN-DMC energies $E$ from Tables I and II scaled by the total energy $E_{NI}$ of the corresponding non-interacting gas, as a function of the concentration $x$, where $x = N_2/N_1$. A fully polarized, single-

| $N_1$ | $N_2$ | $N_1 - N_2$ | $N_{cr}$ |
|-------|-------|-------------|---------|
| 20    | 10    | 10          | 6       |
| 20    | 20    | 20          | 6       |
| 35    | 10    | 35          | 6       |
| 35    | 20    | 35          | 6       |

$N_{cr}$ is the critical number of fermions for which a molecular-like ground state is observed.
component Fermi gas corresponds to $x = 0$ while a Fermi gas with equal number of particles in the two components corresponds to $x = 1$. Notably, the scaled energies $E/E_{NI}$ fall to a good approximation on a universal curve. Applying the local density approximation (LDA) to the equation of state of the population-balanced homogeneous normal system at unitarity, the energy of the trapped unitary system with homogeneous normal system at unitarity, the energy of the trapped normal Fermi gas at unitarity, shown as a function of the non-interacting single-component Fermi gas with non-interacting, the quantity $E/E_{NI}$, $E/E_{NI}$, denotes the energy whose nodal surface coincides with that of the population-balanced unitary gas, described by a wave function whose nodal surface coincides with that of the non-interacting gas, can be described quite accurately by applying the LDA to the normal state of the homogeneous system.

To analyze the energies of trapped polarized unitary Fermi gases further, we consider the energy of a single down-fermion or impurity immersed in a cloud of up-fermions. Symbols in the inset of Fig. 2 show the scaled energy $E/E_{NI}$ as a function of $1/N_1$ ($N_1 = 5 - 20$). The fact that $E/E_{NI}$ is close to 0.75 suggests that the trapped population-balanced unitary gas, described by a wave function whose nodal surface coincides with that of the non-interacting gas, can be described quite accurately by applying the LDA to the normal state of the homogeneous system.

A linear fit to the FN-DMC energies, shown by a dashed line in the inset of Fig. 2 gives $A_\star = 0.72(1)$. The analysis performed here for the trapped system is similar to that performed for the homogeneous system. However, while we fix the impurity mass at its “bare” value, work on the homogeneous system treats the impurity as a quasi-particle with effective mass $m_{\text{eff}}$ and finds $m_{\text{eff}} = 1.09(2)m$ at unitarity.

Symbols in the main part of Fig. 2 show the scaled energy $(E - E_{NI})/E_{NI,1}$ as a function of $x$ (the plot includes all energies reported in Tables I and II). A dashed line shows the quantity $-A_\star x$. For larger $x$, the scaled energies lie above the dashed line, indicating a shielding of the attractive up-down interaction, or equivalently, the presence of an effective repulsion between the down-fermions. A simple expression for the energy of the normal state of trapped two-component systems with arbitrary $x$ ($x \geq 1/N_1$) reads

$$(E - E_{NI})/E_{NI,1} = -A_\star x + C_\star x^D. \tag{3}$$

Using $A_\star = 0.72$, a fit to our data gives $C_\star = 0.16(1)$ and $D_\star = 1.7(1)$. This fit (solid line in Fig. 2) provides a good description of our numerically determined energies. Note that our $D_\star$ value would be somewhat larger if we enforced Eq. (3) to reproduce the LDA value of 0.75 at $x = 1$.

In addition to the energies, we analyze the structural properties of population-imbalance Fermi gases. The LDA predicts to leading order in $x$ that the density of the up-fermions is unchanged while the down-fermions feel a modified trapping potential with effective angular frequency $\omega_{\text{eff}} = \omega(1 + 3A_{\text{hom}}/3)m/m_{\text{eff}} \mp 10^9$, where $A_{\text{hom}} = 0.99(1)$. The single down-fermion immersed
In a cloud of up-fermions is thus predicted to be described by the ground state harmonic oscillator function with width $a_{ho,eff}$, where $a_{ho,eff} = \sqrt{\hbar/(m_{ho} \omega_{ho})}$. A fit of the square of the harmonic oscillator function to the density profiles of the down-fermion for the $(10,1)$ and $(20,1)$ systems, calculated using the mixed estimator [13], provides a good description of the density profiles and gives $a_{ho,eff} = 0.86a_{ho}$ and $0.86a_{ho,eff}$, respectively, compared with the LDA prediction of $a_{ho,eff} = 0.87a_{ho}$. The good agreement suggests that the LDA provides a valid description even of fairly small trapped systems.

In addition to the guiding function $\psi_{T1}$, we consider the guiding $\psi_{T2}$, which is constructed by anti-symmetrizing a set of $N_2$ pair functions $\psi$ and $N_1 - N_2$ mutually orthogonal harmonic oscillator functions $\phi_i$ (recall, $N_1 \geq N_2$) [17, 19]. It has been shown previously [18, 17] that $\psi_{T2}$ results in a lower FN-DMC energy than $\psi_{T1}$ for population-balanced systems with $N \geq 6$ and for odd $N$ systems with $|N_1 - N_2| = 1$ and $N \geq 13$. Here, we extend the analysis to systems with larger $N_1 - N_2$. For the $(7,5)$ system, $\psi_{T2}$ and $\psi_{T1}$ result, within errorbars, in the same energy. For the next larger systems with $N_1 - N_2 = 2$, the guiding function $\psi_{T2}$ results in lower FN-DMC energies than $\psi_{T1}$ [$E = 28.6$, 33.7, and 38.9$\hbar\omega$ for the $(8,6)$, $(9,7)$ and $(10,8)$ systems, respectively]. For $N_1 - N_2 \geq 3$ and $N \leq 20$, in contrast, we find that the guiding function $\psi_{T1}$ results in lower FN-DMC energies than $\psi_{T2}$.

In summary, this paper treats trapped polarized two-component Fermi gases interacting through short-range two-body potentials at unitarity. This strongly-correlated regime has attracted a great deal of attention since the only meaningful length scale is the system’s size (see, e.g., Ref. [20]); consequently, the properties of the gas are governed by a few universal parameters. Using the FN-DMC method, we have determined the energies of the trapped normal gas as functions of $N$ and $\omega$. Our energies fall on a universal curve that is well described by three parameters. Guiding functions that account for pairing physics are also considered and found to result in lower energies than those obtained for the trapped normal state when $N$ is sufficiently large and $N_1 - N_2$ sufficiently small. Our results may aid in assessing the accuracy of other numerical approaches such as density functional theory approaches [21]. Furthermore, they may guide optical lattice experiments on ultracold fermionic gases.

DB gratefully acknowledges support by the NSF through grant PHY-0555316.

[1] G. Tanner, K. Richter, and J.-M. Rost, Rev. Mod. Phys. 72, 497 (2000).
[2] S. Giorgini, L. P. Pitaevskii, and S. Stringari, arXiv:cond-mat/0706.3360 (to be published in Rev. Mod. Phys.).
[3] J. Carlson and R. Schiavilla, Rev. Mod. Phys. 70, 743 (1998).
[4] G. Kotliar et al., Rev. Mod. Phys. 78, 865 (2006).
[5] D. C. Mattis, The Many-Body Problem: An Encyclopedia of Exactly Solved Models in One Dimension (World Scientific Publishing Co. Pte. Ltd., Singapore, 1993).
[6] P. F. Bedaque, H. Caldas, and G. Rupak, Phys. Rev. Lett. 91, 247002 (2003). J. Carlson and S. Reddy, Phys. Rev. Lett. 95, 060401 (2005). D. E. Sheehy and L. Radzihovsky, Phys. Rev. Lett. 96, 060401 (2006). C.-H. Pao, S.-T. Wu, and S.-K. Yip, Phys. Rev. B 73, 132506 (2006). W. Yi and L.-M. Duan, Phys. Rev. A 74, 013610 (2006). M. Haque and H. T. C. Stoof, Phys. Rev. A 74, 011602(R) (2006). K. B. Gubbels, M. W. J. Romans, and H. T. C. Stoof, Phys. Rev. Lett. 97, 210402 (2006). F. Chevy, Phys. Rev. A 74, 063628 (2006). T. N. De Silva and E. J. Mueller, Phys. Rev. Lett. 97, 070402 (2006). M. Iskin and C. A. R. Sá de Melo, Phys. Rev. Lett. 97, 100404 (2006). C.-C. Chien, Q. Chen, Y. He, and K. Levin, Phys. Rev. Lett. 98, 110404 (2007). M. M. Parish, F. M. Marchetti, A. Lamacraft, and B. D. Simons, Nature Physics 3, 124 (2007). A. Bulgac and M. M. Forbes, Phys. Rev. A 75, 031605(R) (2007). R. Combescot, A. Recati, C. Lobo, and F. Chevy, Phys. Rev. Lett. 98, 180402 (2007).
[7] C. Lobo, A. Recati, S. Giorgini, and S. Stringari, Phys. Rev. Lett. 97, 200403 (2006).
[8] N. Prokof’ev and B. Svistunov, Phys. Rev. B 77, 020408(R) (2008). N. V. Prokof’ev and B. V. Svistunov, Phys. Rev. B 77, 125101 (2008).
[9] S. Pilati and S. Giorgini, Phys. Rev. Lett. 100, 030401 (2008).
[10] A. Recati, C. Lobo, and S. Stringari, arXiv:0803.4419.
[11] M. W. Zwierlein, C. H. Schunck, A. Schro Zhukov, and W. Ketterle, Nature 442, 54 (2006). M. W. Zwierlein, A. Schro Zhukov, C. H. Schunck, and W. Ketterle, Science 311, 492 (2006). Y. Shin et al., Phys. Rev. Lett. 97, 030401 (2006). Y. Shin, C. H. Schunck, A. Schro Zhukov, and W. Ketterle, Nature 451, 689 (2008). C. H. Schunck et al., Science 316, 867 (2007). Y. Shin, Phys. Rev. A 77, 041603(R) (2008).
[12] G. P. Partridge et al., Science 311, 503 (2006). G. P. Partridge et al., Phys. Rev. Lett. 97, 190407 (2006).
[13] P. Fulde and R. A. Ferrell, Phys. Rev. 135, A550 (1964).
[14] A. I. Larkin and Y. N. Ovchinnikov, Sov. Phys. JETP 20, 762 (1965).
[15] B. L. Hammond, W. A. Lester, Jr., and P. J. Reynolds, Monte Carlo Methods in Ab Initio Quantum Chemistry (World Scientific, Singapore, 1994).
[16] D. Blume, J. von Stecher, and C. H. Greene, Phys. Rev. Lett. 99, 232301 (2007).
[17] J. von Stecher, C. H. Greene, and D. Blume, Phys. Rev. A 77, 043619 (2008).
[18] S. Y. Chang, V. R. Pandharipande, J. Carlson, and K. E. Schmidt, Phys. Rev. A 70, 043602 (2004).
[19] J. Carlson, S. Y. Chang, V. R. Pandharipande, and K. E. Schmidt, Phys. Rev. Lett. 91, 050401 (2003).
[20] T.-L. Ho, Phys. Rev. Lett. 92, 090402 (2004). F. Werner and Y. Castin, Phys. Rev. A 74, 053604 (2006).
[21] A. Bulgac, Phys. Rev. A 76, 040502(R) (2007).