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Resonantly Interacting Fermions In a Box

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We use two fundamental theoretical frameworks to study the finite-size (shell) properties of the unitary gas in a periodic box: 1) an *ab initio* Quantum Monte Carlo (QMC) calculation for boxes containing 4 to 130 particles provides a precise and complete characterization of these finite-size effects, and 2) a new Density Functional Theory (DFT) fully encapsulates these effects. The DFT predicts vanishing shell structure for systems comprising more than 50 particles, and allows us to extrapolate the QMC results to the thermodynamic limit, providing the tightest bound to date on the ground-state energy of the unitary gas: $\xi_S \leq 0.383(1)$. We also apply the new functional to few-particle harmonically trapped systems, comparing with previous calculations.

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THE FERMION MANY-BODY PROBLEM plays a fundamental role in a vast array of physical systems, from dilute gases of cold atoms, to nuclear physics in nuclei and neutron stars. The universal character of this problem – each system is governed by a similar microscopic theory, coupled with direct experimental access in cold atoms – has led to an explosion of recent interest (see Refs. [1, 2] for a review). Despite this broad applicability, we are far from fully understanding even the simplest system: the "unitary gas" comprising equal numbers of two fermionic species interacting with a resonant s-wave interaction of infinite scattering length $a \to \infty$. Lacking any scale beyond the total density $n_+ = n_a + n_b$, the unitary gas eschews perturbative expansion and requires experimental measurement or accurate numerical simulation for a quantitative description – the latter is presently more precise. Simulation is costly, however, and typical Quantum Monte Carlo (QMC) calculations can access at most a few hundred particles. Density Functional Theory (DFT) provides a complementary approach through which one may extrapolate these results to large systems beyond the reach of direct simulation.

In this Letter, we present the most precise QMC calculations to date of the unitary gas in a periodic box, studying from 4 to 130 particles, and thereby providing a benchmark for many-body theories. We use this to calibrate a local DFT, then use this DFT to study the finite-size effects ("shell" effects in nuclear physics), and extrapolate the QMC results to the thermodynamic limit. We provide the most precise bound to date of the universal Bertch parameter [3] $\xi_S = \mathcal{E}/\mathcal{E}_{FG} \leq 0.383(1)$. ($\mathcal{E}_{FG} = 3/5 n_+ E_F$ is the energy density of a free Fermi gas with the same total density $n_+ = k_F^3/(3\pi^2)$, and $E_F = \hbar^2 k_F^2/(2m)$ is the Fermi energy.) We also explore the finite-size properties of the DFT – a crucial element in the program to calculate properties of finite nuclei with a universal DFT [4]. We find that a carefully crafted local DFT can capture the finite-size effects in these systems, even down to 2 particles, without the need for particle number projection or similar complications. We limit our discussion to strictly symmetric systems ($n_a = n_b$), leaving odd-even staggering and quasiparticle dispersions to future work: both break the $n_a = n_b$ symmetry, introducing a new dimensionless variable to the functional characterizing the asymmetry. We thus only extract accurately the thermodynamic energy parameter ξ_S.

The QMC results presented here are directly applicable to cold ^{6}Li or ^{40}K atoms, and constrain dilute neutron matter in neutron stars [5]; likewise, the general DFT approach has myriads of applications throughout cold-atom and nuclear physics (see Ref. [6] for a review). Our calculation of ξ_S is consistent with previous results, but an order of magnitude more precise. QMC methods using either continuum [5, 7–11] or lattice formulations [12] compute $\xi_S \approx 0.40 - 0.44$ with an uncertainty no better than the last digit. Experimental groups found qualitative agreement [13], which led to precision measurements: notably with Duke [14] and Paris [15] quoting 0.39(2) and 0.41(1) respectively.

DFT is an in principle exact approach, widely used in quantum chemistry to describe normal (i.e., non-superfluid) systems, and holding promise for describing nuclear systems [16, 17]. It has recently been extended to describe the unitary gas [6, 18–20]: We build upon one such approach called the Superfluid Local Density Approximation (SLDA). In its original formulation, the SLDA contained three parameters that were constrained by QMC calculations of the continuum state. This form was then validated with QMC calculations in a harmonic trap [21, 22] (see also Fig. 2). The agreement for medium to large systems indicates that corrections to the DFT in the form of density gradients are small, however, the exact nature of the ∼10% disagreements for small systems was not known. Here we focus on translationally invariant systems in a periodic box to isolate the non-gradient finite-size effects. In particular, we find that the inclu-

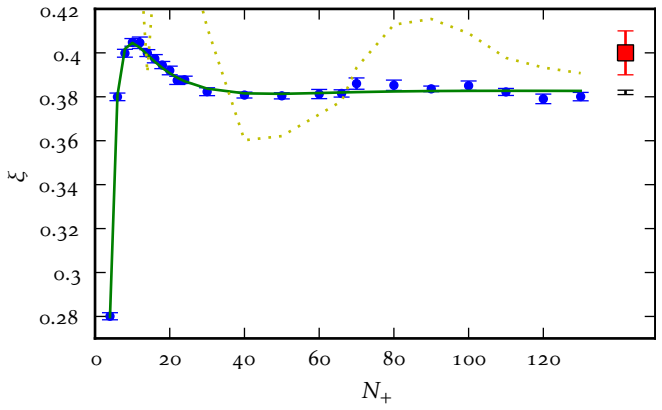

FIG. 1. (color online) Ground-state energy-density $\xi = \mathcal{E}/\mathcal{E}_{FG}$ of N_+ fermions in a periodic cubic box at the unitary limit. The circles with error bars are the result of using a quadratic least-squares extrapolation to zero effective range of our new QMC results. The solid curve is the best fit SLDA DFT. The light dotted curve is the functional considered in [18] with $\alpha = 0.69$. For comparison, we have plotted the previous best estimate $\xi_S = 0.40(1)$ (red square) and the current estimate $\xi_S = 0.383(1)$ below it to the far right of the figure.

sion of an anomalous density is crucial: functionals attempting to model the superfluid by adding only gradient or kinetic corrections [18, 20] are unable to even qualitatively characterize the finite-size effects.

Our QMC results are based on a Diffusion Monte Carlo approach that projects out the excited-state contributions from a variational starting wave function, providing an upper bound for the energy. We take the wave function to have a Jastrow-BCS form, as first discussed in Ref. [7], but implement a more efficient procedure for variationally optimizing its parameters. We thereby obtain a substantially lower bound on the energy than any previously reported QMC calculation.

Our QMC approach simulates the Hamiltonian:

$$\mathcal{H} = \frac{\hbar^2}{2m}\left(-\sum_{k=1}^{N_+}\nabla_k^2 \; - \; 4v_0\mu^2\sum_{i,j'}\mathrm{sech}^2(\mu r_{ij'})\right), \qquad (1)$$

with an inter-species interaction of the modified Pöschl-Teller type (off-resonance intra-species interactions are neglected). We tune the s-wave scattering length to infinity by setting $v_0 = 1$: the effective range becomes $r_e = 2/\mu$. To extrapolate to the zero-range limit, we simulate at $\mu/k_F \in \{12.5, 24, 36, 48, 60\}$. These lead to considerably shorter ranges ($0.03 < k_F r_e < 0.16$) than previously cited in the literature; a careful examination of additional ranges $k_F r_e < 0.35$ for the $N_+ = 40$ and $N_+ = 66$ reveals that a three-parameter quadratic model in r_e is necessary and sufficient to extrapolate our data without a systematic bias: larger ranges require higher order. The extrapolated energies are shown in Fig. 1.

The energies exhibit definite finite-size (shell) effects for $N_+ \lesssim 50$, but are essentially featureless for larger N_+. This lack of structure is confirmed by the best fit DFT (discussed below) and disagrees with the results presented in Ref. [23]. The values of ξ for $N_+ > 50$ are distributed about the best fit value $\xi_S \approx 0.383(1)$, and represent the lowest variational bounds to date. Part of the decrease from previous results is due to the careful extrapolation to zero effective range: the best fit quadratic is concave down, implying that linear extrapolations systematically overestimate ξ_S. The remainder is due to the improved optimization of the variational wave function.

To model the finite-size effects we turn to a local DFT for the unitary Fermi gas that generalizes the SLDA originally presented in Ref. [19]. In addition to the total density n_+, the SLDA includes both a kinetic density τ_+ and an anomalous density ν. (The + index signifies the sum of the contributions coming from the two components a and b.) These are expressed in terms of the Bogoliubov quasiparticle wave functions $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$:

$$\tau_+ = 2\sum_n |\nabla v_n|^2, \quad n_+ = 2\sum_n |v_n|^2, \quad \nu = \sum_n u_n v_n^*.$$

The original 3-parameter SLDA functional has the form

$$\mathcal{E}_{\text{SLDA}} = \frac{\hbar^2}{m}\left(\frac{\alpha}{2}\tau_+ + \beta\frac{3}{10}(3\pi^2)^{2/3}n_+^{5/3}\right) + g\nu^\dagger\nu, \qquad (2)$$

where α is the inverse effective mass; β is the self-energy; and γ, which controls the pairing, enters through the regularized coupling $g = 1/(n_+^{1/3}/\gamma - \Lambda/\alpha)$ where $\Lambda \to \infty$ is a momentum cutoff that we take to infinity (see Ref. [6] for details). Using the equations for homogeneous matter in the thermodynamic limit, one can numerically replace the parameters β and γ with the more physically relevant quantities ξ_S and $\eta = \Delta/E_F$, where Δ is the pairing gap.

In principle, the DFT can be expressed in terms of only the density n_+ and its gradients. Local formulations of this type are referred to as Extended Thomas-Fermi (ETF) functionals and have been considered in Refs. [20]. Since the ground state in a periodic box is homogeneous, the gradient terms vanish, and the functional takes the form $\mathcal{E}_{\text{ETF}}(n_+) = \xi_S\mathcal{E}_{FG}$. The simplest form thus exhibits no shell effects and is in contradiction with the QMC results. This deficiency can be rectified by introducing an explicit dependence on the "dimensionless parameter N_+", but such a functional has no predictive power: each finite-size system must be independently fit.

Reference [18] considered adding the kinetic density τ_+ and effective mass α. This produces shell structure, but without an anomalous density the effects are much too large: the best fit to the QMC results drives $\alpha \to 0$ reproducing the flat ETF results, indicating that the shell structure of this DFT has essentially no correlation with the shell structure exhibited by the QMC. Furthermore,

such a functional can not even qualitatively reproduce the quasiparticle dispersion relationship, an attractive feature of the SLDA.

The best fit to the three-parameter SLDA functional (2) is $\alpha = 1.26(2)$, $\xi_S = 0.3826(5)$, and $\eta = 0.87(2)$. This is shown in Fig. 1 and fits the 23 QMC points from $N_+ = 4$ to $N_+ = 130$ with a reduced chi squared $\chi^2_r = 0.7$, indicating complete consistency. Although quite remarkable, this fit is not completely satisfactory: 1) It does not fit the exact energy for the two-particle box $\xi_2 = -1.5641\cdots$, and 2) the best fit gap parameter η and inverse effective mass α are inconsistent with the values $\eta = 0.50(5)$ and $\alpha = 1.09(2)$ obtained from the $N_+ = 66$ QMC quasiparticle dispersion relation [9, 26], and the values $\eta = 0.45(5)$ [24] and $\eta = 0.44(3)$ [25] extracted from experimental data.

Some of these deficiencies can be remedied by considering a generalization of the SLDA. As noted in Ref. [6], the following combination of divergent kinetic and anomalous densities is finite:

$$K = \frac{\hbar^2\tau_+}{2m} + \frac{g}{\alpha}\nu^\dagger\nu = \frac{\hbar^2\tau_+}{2m} + \frac{\nu^\dagger\nu}{\alpha n_+^{1/3}/\gamma - \Lambda}. \qquad (3)$$

The lack of scales in the unitary Fermi gas thus dictates that the functional have the form:

$$\mathcal{E}(K, n_+) = \xi(Q)\,\mathcal{E}_{FG}(n_+), \qquad Q = K/\mathcal{E}_{FG}(n_+), \qquad (4)$$

where Q is dimensionless. The regularization condition may also depend on Q through a function $\gamma(Q)$. The original SLDA is linear $\xi(Q) = \alpha Q + \beta$: thus, the shell structure of $Q(N_+)$ for the SLDA functional is the same as that of $\xi_S(N_+)$. One can show that if $\xi(N_+)$ is monotonic, then any functional form can be fit with freedom to spare. On one hand, this allows us to modify the functional to additionally fit the exact $N_+ = 2$ point $\xi_2 = -1.5641\ldots$; on the other hand, it also means that the functional is not fully constrained for values of Q corresponding to $N_+ < 6$. The function $\xi(N_+)$ is not monotonic for $N_+ > 6$, however, and, in principle, two branches are sufficient to uniquely determine the functional. For example, requiring that $\xi = \xi_S$ at both $N_+ \approx 6.2(2)$ and $N_+ = \infty$ fixes the ratio of the thermodynamic parameters $\eta/\alpha = 0.69(2)$, in agreement with the best fit SLDA functional discussed above.

In practice, the errors and the discreteness in N_+ still leave room for flexibility in the functional form. This allows us to address the issue of η not matching the quasiparticle dispersion relationship, and we have found several generalized functional forms with $\chi^2_r \approx 1.5$ while constraining $\eta = 0.50$. The constraint $\eta/\alpha = 0.69(2)$ must still be preserved, however, so we cannot simultaneously describe both the gap and the effective mass as currently displayed by the quasiparticle dispersion relationship present in [24]. This is consistent with the traditional interpretation of a DFT where the single-particle states are simply a mathematical tool. Nevertheless, it has been shown perturbatively that an appropriate functional form can reproduce the quasi-particle properties at the Fermi surface [27], which is certainly a desirable property for a DFT. Further generalizations to the functional, such as including non-locality or additional densities, might restore this feature, but we leave this analysis until high-precision odd-even staggering and quasiparticle dispersions are published.

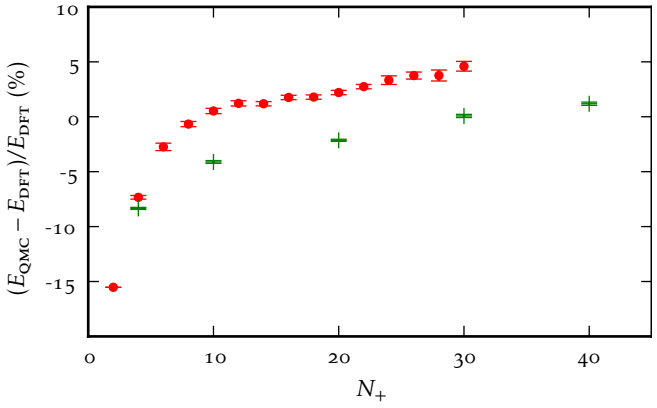

FIG. 2. Relative change (in %) in the ground-state energy of the unitary Fermi gas in a harmonic trap from the QMC results taken from Ref. [22] (upper red dots) for even systems of N_+ from 2 to 30. We have also included preliminary results from Ref. [29] (green pluses) for an interaction with a comparable effective range. These new results significantly lower the energy, suggesting that the wavefunctions in Ref. [22] were not fully optimized. The zero-range extrapolation has not yet been performed, but given the results in the present paper, we expect this to lower the energies by a few percent.

It is quite non-trivial that the simple functional form of Eq. (2) can fully capture all finite-size effects above $N_+ = 4$ to high precision. In particular, we note that no particle-number projection is required. This technique is quite ill-defined in the DFT framework, but nevertheless often considered necessary in the nuclear physics context [28]. Our results suggest that improved functionals should be able to intrinsically capture these effects in a self-consistent manner, possibly requiring additional local densities in the same spirit as ν.

To finish, we compare the best fit SLDA functional with the QMC results of Ref. [22] for harmonically trapped systems in Fig. 2. We see that the DFT still over-estimates the energy for small systems, but that it systematically produces lower energies for large systems. This is consistent with the fact that the wavefunctions used in Ref. [22] have not been as carefully optimized as in the present work, nor have the results been extrapolated to zero effective range. To emphasize this, we have included a few preliminary points from Ref. [29] using optimized wavefunctions of a slightly larger range to show that, indeed, improved wavefunctions yield signif-

icantly lower energies. Even with the improved wavefunction, the DFT predicts slightly lower energies for larger systems: this is fully consistent with a simple estimate of the extrapolation to zero effective range, but we leave this discussion until a careful zero-range extrapolation is published.

We also leave to future work a detailed analysis of the remaining deviations for small systems, but point out that these are likely due to two effects. One is the form of the functional $\xi(Q)$ for the small values of Q seen in the cores of the traps, and for the large values of Q seen in the tails of the traps. These regions of the functional are largely unconstrained by our boxed results which – with the exception of the single $N = 2$ point at negative Q – explore only the region from −26% to +5% of the thermodynamic value. The remaining corrections are likely due to gradient terms in the functional that vanish in homogeneous systems.

To summarize, we present the most precise Quantum Monte Carlo calculations to date of a symmetric unitary Fermi gas in a periodic box comprising 4 to 130 particle. By carefully characterizing and extrapolating these results to zero effective range, we have completely mapped out the finite-size (shell) corrections. These results are used to analyze the structure of a Density Functional Theory for the symmetric unitary gas, and it is shown that the simplest three-parameter form of Eq. (2) fully accounts for all shell effects to within the statistical errors of the QMC results without the need for particle-number projection; a more complicated form, however, is required to capture both the finite-size effects and the quasiparticle dispersions. The DFT predicts that there are no significant shell corrections beyond 50 particles, and the QMC confirms this, allowing us to extract a precise upper bound on the universal equation of state $\xi_S \leq 0.383(1)$: an order of magnitude improvement in precision over previous bounds and the lowest bound of any variational method to date. The functional in its latest form is well constrained, but leads to slight disagreements with QMC predictions for harmonic traps. Removing those (both at the QMC and the DFT level) promises to be a fruitful direction of future research.

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