The Unitary Fermi Gas in a Harmonic Trap and its Static Response

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We use harmonically trapped systems to find the leading gradient corrections of the superfluid local
density approximation (SLDA) – a density functional theory (DFT) describing the unitary Fermi gas
(UFG). We find the leading order correction to be negative, and predict the $q^2$ coefficient of the
long-range static response $c_\chi = 1.5(3)$ – a factor of two smaller than predicted by mean-field theory –
thereby establishing a new and experimentally measurable universal constant.

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Unversally describing two-component Fermi systems with short-range interactions of infinite scattering
length $a_s \to \infty$, the unitary Fermi gas (UFG) [1] not only approximates the dilute neutron matter
found in neutron stars [2], but is directly realized in cold-atom systems [3], allowing experiments to benchmark
many-body techniques used to study astrophysical phenomenology. Despite the simplicity of the system –
the lack of length-scales, for example, implies that the equation of state $E(n) \propto n^{5/3}$ – the system is strongly
interacting and admits no known perturbative expansions: A quantitative description requires experiments or
ab initio computations.

Ab initio techniques, however, can only address a few questions – direct quantum Monte Carlo (QMC) simulations,
for example, can study systems with at most a few hundred particles. It is therefore imperative to benchmark computationally tractable models of macroscopic phenomena so that they can be used to answer outstanding phenomenological questions, such as the
origin of glitching in neutron stars [4].

Density functional theory (DFT) is an in principle exact approach, widely used in nuclear physics (see [5] for a review), and in quantum chemistry to describe normal (i.e., non-superfluid) systems. It provides a framework capable of assimilating ab initio and experimental results into a computationally tractable and predictive framework. In this letter, we extend one such DFT – the superfluid local density approximation (SLDA) – to describe the inhomogeneous behaviour of harmonically trapped systems. We use DFT to analyse recent experimental and theoretical results, noting discrepancies and the asymptotic behaviour toward the thermodynamic limit, and establish the leading order gradient corrections to the SLDA which we find to be negative. The SLDA then uniquely predicts the low-energy static response of the UFG to quadratic order, which is crucial for a proper low-energy description of the UFG: this therefore makes significant progress towards a predictive framework for studying superfluid phenomenology.

At low-energies, the UFG can be characterized by a superfluid effective field theory (EFT) describing phonon
dynamics [6]. The EFT controls a powered-counting scheme: The leading order (LO) contains a single
dimensionless parameter – the Bertsch parameter $\xi$ which characterizes the equation of state $E(n) = E_F G(n)$ where $E_F G = 3/5n E_F$ is the energy density of a free Fermi gas with the same total density $n = k_F^3/(3\pi^2)$, and $E_F = h^2k_F^2/2m$ is the Fermi energy. At next-to-leading order (NLO), two additional dimensionless coefficients $c_\omega$ [8] appear which characterize the static and dynamic low-frequency and low-momentum response. We shall address only the value of the static response $\chi(q)$ as defined by adding small external potential $\delta V_q(x) = \delta \cos(qx)$ to a homogeneous system:

$$\delta n_+(x) = \chi(q) \delta V_q(x) + o(\delta^2) \tag{1}$$

To NLO in the superfluid EFT, the response is

$$\chi(q) = \frac{m k_F}{h^2 \pi^2 \xi} \left[ 1 - \frac{c_\chi q^2}{12 \xi^5 k_F^2} + o(q^4 \ln q) \right] \tag{2}$$

where $c_\chi$ is a universal dimensionless constant [9]. This normalization for $c_\chi$ is numerically close to unity ($c_\chi = 1$ for non-interacting fermions), appears simply in the energy of trapped fermions (see Eq. (6), and is independent of the $\xi$ and pairing parameters in the SLDA. The other universal constant $c_\omega$ describes low-energy dynamical properties, and enters through the phonon dispersion relation $\omega_q/(q c_\omega) = 1 + c_\omega q^2/(24k_F^2) + o(q^4 \ln q)$ where $c_s = h k_F \sqrt{\xi/3}/m$ is the speed of sound.

While many techniques have been employed to calculate the Bertsch parameter $\xi \approx 0.37$ (see [11] for a survey), NLO coefficients have only been considered in a few cases: The $\epsilon$-expansion [12] (expanding in spatial dimension: $\epsilon = 4 - d$) gives $c_\chi \approx 8/5 + o(\epsilon^2)$ and $c_\omega \approx c_\omega + o(\epsilon^2)$ [13], while Bogoliubov-de Gennes (BdG) mean-field theory [14] finds $c_\chi = 7/3$ and $c_\omega \approx 0.7539$.

The EFT breaks down for small systems and near the boundary of clouds, so to connect with finite-size QMC calculations, we use DFT. The Hohenberg-Kohn theorem [14] asserts the existence of a universal functional of the density alone whose minimum describes the ground state of the UFG. The exact form of this functional is
When applied to inhomogeneous systems however, one ETF functional describes well some energetic and dynamical aspects of the UFG. It fails, however, to properly describe finite-size effects in homogeneous systems.

To describe these properties we use the Kohn-Sham formulation which includes an auxiliary kinetic density \( \tau_+ \). While this is formally equivalent to the Hohenberg-Kohn formulation, the addition of a kinetic density allows a local formulation to describe finite-size features of the system. In particular, the finite-size properties of non-interacting systems are exactly reproduced. Interacting versions have been considered, but one finds that the finite-size effects are not properly suppressed. The suppression can be realized by include an additional auxiliary anomalous density, \( \nu \), representing the pairing field, resulting in the SLDA:

\[
\epsilon_{\text{SLDA}} = \frac{\hbar^2}{m} \left( \frac{\alpha}{2} \tau_+ + g \nu \right) + \beta \epsilon_{FG}(n_+) + \frac{\hbar^2 \delta \lambda (\nabla n_+)^2}{8m} n_+,
\]

\[
g^{-1} = \frac{n_+^{1/3}}{\gamma} - \frac{k_c}{2\pi \alpha} \tag{3}
\]

Here \( \alpha \) is the inverse effective mass, \( \beta \) is the self-energy, \( \gamma \) controls the pairing, and \( \delta \lambda \) characterizes the leading order gradient term (known as a Weizsäcker correction). The unitary limit is realized when we take the wave-vector cutoff \( k_c \to \infty \) to infinity (see Ref. \[24\] for details). In homogeneous systems, the gradient corrections vanish, and one can use the equations in the thermodynamic limit to replace the parameters \( \beta \) and \( \gamma \) by the more physically relevant quantities \( \epsilon_S \) and \( \eta = \Delta/E_F \), where \( \Delta \) is the pairing gap (see the appendix of \[20\] for details). When applied to inhomogeneous systems, however, one must hold the parameters \( \beta \) and \( \gamma \) fixed to define the functional.

This form subsumes earlier DFTs. In particular, the well-studied bdc mean-field equations are reproduced with unit effective mass \( \alpha = 1 \), \( \gamma^{-1} = 0 \), no Hartree term \( \beta = 0 \), and no gradient corrections \( \delta \lambda = 0 \). The Kohn-Sham form discussed in \[22\] [23] neglects the \( \nu = 0 \), while the ETF form \[12\] [15] is reproduced if one neglects both the anomalous density \( \nu \) and the kinetic density \( \tau_+ \). As discussed in \[19\], none of these restricted forms can even qualitatively characterize the finite-size effects, but we still consider the ETF functional as it is much easier to solve numerically while retaining the asymptotic properties of trapped systems:

\[
\epsilon_{\text{ETF}} = \xi \epsilon_{FG}(n_+) + \frac{\hbar^2 (1/4 + \delta \lambda) (\nabla n_+)^2}{8m} n_+ \tag{4}
\]

The leading gradient term here derives from a semi-classical expansion of the kinetic energy with an additional Weizsäcker correction \( \delta \lambda \). Superfluid hydrodynamic phenomenology \[17\] and vortex dynamics (appendix \[E\]) suggest that \( \delta \lambda = 0 \). The resulting ETF is completely determined by the value of \( \xi \). A simple calculation shows that the ETF model has \( c_x = c_\omega = 9/4 + 9 \delta \lambda = 9/4 \).

The SLDA was originally constrained by QMC calculations of the continuum state, and validated with QMC calculations in a harmonic trap \[20\] [27]. These validations, however, provided only a weak test of the SLDA form. In particular, the symmetric thermodynamic limit does not provide enough information to constrain the effective mass, and the original variational trap results were not sufficiently accurate to exhibit the appropriate scaling in the thermodynamic limit.

Recently, experimental and \textit{ab initio} QMC results for homogeneous matter in the continuum and in periodic boxes were used to more rigorously test the form of the SLDA: the best fit to current unbiased results is consistent with \( \xi = 0.3742(5) \), \( \alpha = 1.104(8) \), and \( \eta = 0.651(9) \). Here we estimate the leading order gradient correction \( \delta \lambda \) by reconsidering the energies of trapped systems.

The static response in the thermodynamic limit can be calculated using the same techniques as in the bdc \[8\] and one finds

\[
c_x = \frac{7}{3} \alpha + 9 \delta \lambda, \tag{5}
\]

which is independent of \( \xi \) and \( \eta \). This demonstrates how the effective mass and gradient corrections play a similar role, as pointed out in \[29\] [30].

From the NLO superfluid EFT \[6\] [8], one finds the energy of the UFG in an isotropic harmonic trap with trapping frequency \( \omega \) to depend on the coefficients \( \xi \) and \( c_x \):

\[
\frac{E}{\hbar \omega} = \frac{\sqrt{\xi}}{4} (3N_+)^{4/3} \left[ 1 - \frac{c_x}{2\xi (3N_+)^{2/3}} + o \left( \frac{1}{(N^4_+)^{1/9}} \right) \right].
\]

This form naturally suggests the abscissa \( x = (3N_+)^{-2/3} \) so that the asymptotic behavior of \( E \) is linear: we prefer to use the square of the energy \( E^2 \),

\[
y = \frac{16E^2}{\hbar^2 \omega^2 (3N_+)^{8/3}} = \xi + c_x x + o \left( x^{7/6} \right), \tag{6}
\]

as \( \xi \) appears on the intercept, and \( c_x \) appears directly. It is interesting that, in the non-interacting system, shell-effects appear at the same linear order \( x \), leading to a fundamental uncertainty in the coefficient \( \frac{2}{3} \leq c_x \leq 1.7 \). Pairing suppresses these shell effects, yielding a well-defined asymptotic slope \( c_x \), which can also be determined from the semi-classical approximation (see appendix \[F\]).

In Fig. 1 we display QMC results for trapped unitary systems. The dotted lines guide the eye through several variational bounds obtained using fixed-node QMC (FNQMC) calculations. In these methods, one avoids any sign problem by sampling a restricted set of wavefunctions with the same nodal structure as an initial reference
ansatz. By improving the ansatz and varying the parameters, these bounds have come down over time, and the lowest (green) curve [20] represents the best bound to date. Note that this is the only set of results that demonstrates the expected linear scaling [3] predicted by the effective theory. We suspect that numerical issues or the nature of the ansatz in the other cases introduced spurious lengths scales that violate this scaling (see [20] for further discussion.)

The solid (magenta) line guides the eye through calculations based on lattice techniques [11]. In principle, these are unbiased ab initio results, but it is somewhat troubling that most lie significantly above the variational bounds. They also display large shell effects that are virtually absent in the FNQMC results. For comparison, we have included the energies of free particles shown in Fig. 4 as a light (grey) curve, shifted down from 1 to facilitate comparison. As we shall see, although the non-interacting SLDA reproduces these shell-effects, the interacting SLDA exhibits a marked lack of shell effects, consistent with the FNQMC. The lattice results thus seem qualitatively inconsistent with the others.

A third variational technique [12] based on a correlated Gaussian approach provides very tight bounds, but is limited to small systems. These are shown as (black) crosses for \( N_+ \in [2, 4, 6] \). Unfortunately, at these three points, all methods agree, and significant discrepancies between the lattice and FNQMC results only appear at larger \( N_+ \).

Finally, we include the latest experimental results as a (yellow) band [33] and the best fit value of \( \xi = 0.3742(5) \) to all homogeneous ab initio QMC results from [20] at \( x = 0 \). Coordinates have been scaled as in [3] to demonstrate the scaling. The corresponding particle numbers \( N_+ \) are listed along the top axis, and emphasize the closed shells which occur for \( N_+ \in \{2, 8, 20, 40, 70\} \). (Note that all methods agree for the point \( N_+ = 2 \) (not shown) which admits an analytic solution.)
Note that the SLDA predicts higher energies for systems with small particle numbers – especially the \( N_+ \in \{2, 4, 6\} \) systems where all \textit{ab-initio} methods agree. To correct for this, the leading gradient correction needs to be negative \( \lambda < 0 \). We explore these effects in Fig. 3 by perturbatively including the gradient for various values of \( \lambda \). (Note: these corrections are less than 15% for all systems as shown in Fig. 5.) The remaining corrections from a fully self-consistent solution will not significantly alter these results.) One could also increase the effective mass, but to match even the modest correction of \( \lambda \lesssim -0.1 \) requires \( m_{\text{eff}} \gtrsim 1.4m \) which spoils the description of homogeneous systems \cite{19, 20} and quasi-particle dispersions \cite{34}. Higher order gradient corrections might help, however, there are several different gradient corrections – each requiring additional coefficients – and insufficient \textit{ab-initio} results to constrain these. These neglected terms will not affect the coefficient \( c_\chi \). Finally, there is the possibility that the functional could be generalized as discussed in \cite{19}, but the success of the three-parameter SLDA \cite{20} suggests that corrections along this line would be small.

We note that a negative gradient correction is somewhat surprising since a naïve expansion of an attractive non-local interaction \( -V(x-y)n(x)n(y) \) yields a positive gradient correction (see appendix E).

Thus, we conclude from Fig. 3 that the SLDA will require \( \lambda \approx -0.12(3) \) to describe both homogeneous boxes and trapped systems. The SLDA therefore predicts

\[
c_\chi \approx 1.5(3)
\]

indicating that momentum-dependent density fluctuations are suppressed by interaction, though this effect is mostly due to the reduced value of \( \xi \).

As discussed, \( c_\chi \) cannot be directly extracted from the QMC results without a model capable of extrapolating well into the thermodynamic limit. To extract \( c_\chi \) more directly, one should consider systems that minimize the sensitivity to the breakdown of the \textit{eft} at the boundary of the system. To do this, consider how the density \( n \equiv n(x) \) depends on a smoothly varying potential \( V \equiv V(x) \):

\[
n = n_\text{TF}(x) \left\{ 1 - \frac{c_\chi}{64} \frac{(\nabla V)^2 + 4(\mu - V)\nabla^2 V}{(\mu - V)^3} \frac{\hbar^2}{m} + \cdots \right\},
\]

\[
n_{\text{TF}}(x) = \frac{8(\mu - V)^{3/2}}{3 \pi^2 (2\xi)^{3/2}} \left( \frac{m}{\hbar^2} \right)^{3/2}.
\]

This is valid to NLO in a static background with constant phase (i.e. not near a vortex). Thus, one can directly search for deviations from the Thomas-Fermi (TF) profile that are sensitive to gradients in the potential. Applying a modulation \( V \propto \cos(qx) \) directly probes the static response and is feasible in QMC simulations. Optical lattices could be used similarly in experiments, however, measuring the density to sufficient accuracy is likely to be a challenge – to compensate for the numerical suppression \( c_\chi/64 \) while avoiding contamination from higher-order terms will require percent level accuracy. Experiments should thus probably retain traps with axial or spherical symmetry so they can benefit from averaging techniques like the inverse Abel transform to reduce noise in \( n(x) \).

Adding a small dimple to the core of the trap with varying widths will allow experiments to probe the response while retaining the benefits of averaging to reduce noise.

Confirming the value of \( c_\chi \) will provide an important validation of the SLDA functional, and provides another benchmark for models of the \textit{ufg}. To reliably predict low-energy behaviour of the \textit{ufg}, a model should reproduce the LO and NLO coefficients – \( \xi \), \( c_\chi \), and \( c_\omega \) – of the superfluid \textit{eft}.

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Appendix A: Contradictory QMC Results

As noted in Fig. 2, there are unresolved contradictions in the QMC results for larger $N_+$ with the lattice results [31] exceeding the FNQMC variational bounds [20]. It would be useful to have an alternative method calculate the energies for $N_+ = 8$ and $N_+ = 12$ to resolve between these:

$$\frac{E_{\text{lat}}}{h\omega} = 11.64^{+0.16}_{-0.12} \quad \frac{E_{\text{FNQMC}}}{h\omega} \leq 12.01(2) \quad (N_+ = 8)$$

$$\frac{E_{\text{lat}}}{h\omega} = 20.76^{+0.045}_{-0.093} \quad \frac{E_{\text{FNQMC}}}{h\omega} \leq 16.07(2) \quad (N_+ = 12)$$

Appendix B: Semiclassical Expansion

The superfluid EFT is closely related to the well-studied semiclassical expansion (in $\hbar$) [25] for non-interacting systems, and one can derive similar expressions to those arising from the EFT. The utility of the EFT is to organize the universal coefficients for the interacting superfluid system.

The shell effects for non-interacting systems is shown in Fig. 3 (this was shifted down to match $\xi$ for comparison in Fig. 1). The semiclassical expansion systematically organizes contributions from volume effects, surface effects, periodic orbits, etc. It thus provides some insight into the breakdown of the EFT: shell for the harmonic trap, for example, effects appear at the same order as the NLO corrections. These are shown in Fig. 4, demonstrating a fundamental uncertainty in the slope $\frac{2}{3} \leq c_\chi \lesssim 1.7$. Considering the static response allows one to extract the non-interacting value of $c_\chi = 1$, which lies in this band. The fact that these corrections appear at the same order is related to nearby breakdown of the EFT formula, and the subsequent slow approach to the asymptotic scaling in the thermodynamic limit. What is non-trivial is that pairing acts to sufficiently suppress these shell effects so that a well defined slope emerges in harmonically trapped systems. Perhaps this can be explained within the semiclassical theory, but the author is not aware of such a discussion in the literature.

Appendix C: Perturbative Gradient Corrections

![Figure 5](image)

**Figure 4.** (color online) Shell effects in the trapped non-interacting two-component gas. The scaling is the same as in Fig. 3. The asymptotic bounds $\frac{2}{3} \leq c_\chi \lesssim 1.7$ have been drawn as dotted lines.

In Fig. 3 we show the size of the gradient corrections $E_{\text{grad}}$ as a percent of the total energy $E$ for the $\delta \lambda = -0.15$ required to bring the SLDa in rough accordance with the smallest trapped systems. This demonstrates that the gradient corrections may be included perturbatively, simplifying the numerical calculations.

![Figure 6](image)

**Figure 5.** With $E_{\text{grad}}/E$ (in percent) for $\delta \lambda = -0.15$, demonstrating that the correction is indeed perturbative.

In order to perform a fully self-consistent calculation of the gradient corrections, one must modify the single-particle self-energy to include a term

$$U_{\text{grad}} = -\frac{\hbar^2 \delta \lambda}{8m} \left( \frac{\nabla n_+}{n_+} \right) = \frac{\hbar^2}{8m} \left( 4 \frac{\nabla^2 n_+}{\sqrt{n_+}} - \nabla^2 \frac{n_+}{n_+} \right).$$

Accurately computing the derivatives – especially in the tails of the cloud – presents a mild numerical challenge, and will only alter the energies at the percent level, and so is not required for the present analysis. This self-consistency will be important, however, if one wants to compare the density profile of the smallest trapped systems with QMC results.

Appendix D: Asymptotic Behaviour

Figure 6 is a full-sized version of the inset of Fig. 2. This shows on a log-log scale the deviation of the numerically computed $y(x)$ from the EFT model from the expected asymptotic form $y = \xi + c_\chi x - 2.2 x^{7/6} + \cdots$. (We do not claim anything universal about the coefficient 2.2.
Consider a single stationary vortex $\Psi \propto e^{if(r)}$ embedded in a uniform gas with background chemical potential $\mu = \xi E_F(n^+_{\xi}) = br^{4/3}(r = \infty)$. The phase yields a centrifugal term:

$$\left(\frac{h^2}{4m r^2} - \frac{(1 + 4\delta\lambda)h^2\nabla^2}{4m} + br^{4/3}(r - \mu)\right)f(r) = 0. \tag{E1}$$
[1] W. Zwerger, ed., *The BCS–BEC Crossover and the Unitary Fermi Gas*. Lecture Notes in Physics, Vol. 836 (Springer-Verlag, Berlin Heidelberg, 2012).

[2] Dilute neutron matter is also well modelled by the UFG as a consequence of the unnaturally large neutron-neutron scattering length: $a_{nn} \approx -18.9(4)$ fm, while densities are on the order of $k_F^{-1} \sim 1$ fm. The effective $s$ range, however, is not small: $r_{nn} \approx 2.75(11)$ fm implying $k_F r \approx 3$. Thus, range corrections must generally be included to quantitatively describe these systems. Despite this complications, the qualitative properties of dilute neutron matter are well described by the UFG.

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[10] In [5], $c_\omega \equiv -6\pi^2(2\xi)^3/2(c_1 + 3c_2)$ while in [8], $c_\omega \equiv -12\pi^2(2\xi)(c_1 - 3c_2)$.

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