Renormalization factor and effective mass of the two-dimensional electron gas

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We calculate the momentum distribution of the Fermi liquid phase of the homogeneous, two-dimensional electron gas. We show that, close to the Fermi surface, the momentum distribution of a finite system with \( N \) electrons approaches its thermodynamic limit slowly, with leading order corrections scaling as \( N^{-1/4} \). These corrections dominate the extrapolation of the renormalization factor, \( Z \), and the single particle effective mass, \( m^* \), to the infinite system size. We show how convergence can be improved analytically. In the range \( 1 \leq r_s \leq 10 \), we get a lower renormalization factor \( Z \) and a higher effective mass, \( m^* > m \), compared to the perturbative RPA values.

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Landau’s Fermi liquid theory [1] postulates a one-to-one mapping of low energy excitations of an interacting quantum system with that of an ideal Fermi gas via the distribution function of quasiparticles of momentum \( k \). The resulting energy functional has been successfully applied to describe equilibrium and transport properties of quantum Fermi liquids, the most prominent are the Fermi gas [7]. The effective mass is then explicitly given in terms of the energy difference, \( \epsilon_k = E_k^{N+1} - (E_k^N + \mu) \), between single particle excitations of energy \( E_k^{N+1} \) and momentum \( k \), and the \( N \)-particle ground state energy \( E_0^N \) where \( \mu \) is the chemical potential.

Quantum Monte Carlo (QMC) methods provide the most accurate calculations of the ground state energy of the electron gas [10, 11]. However, fermionic QMC calculations suffer from two major drawbacks, the fixed node approximation and finite size errors. For a normal Fermi liquid, the most precise results are obtained using a generalized Slater Jastrow form for the trial wavefunction [12]

\[
\Psi_T \propto D(R) e^{-U(R)}
\]  

where \( R \) indicates a dependance on all particle coordinates. Antisymmetry is assured by a Slater determinant \( D(R) = \det e^{i k_j \cdot \mathbf{a}_i(R)} \) of plane waves inside the Fermi sphere \( |k_j| \leq k_F \) using dressed quasiparticle coordinates \( \mathbf{q}_i(R) \) to account for many-body backflow effects, whereas the many-body Jastrow potential \( U(R) \) is symmetric with respect to particle exchange and accounts for
the singularities in the interparticle potential at the coincidence points. Projector Monte Carlo methods (DMC) can be used to improve the wavefunction stochastically. Many ground-state properties have been successfully calculated using QMC, however, the situation is less clear concerning excited state properties [7].

The Slater determinant of the many-body wavefunction, Eq. (2), directly connects the ground state of the interacting system with the non-interacting one; low-lying excitations are obtained by changing the “occupation numbers” of the plane waves. The energy is therefore a functional of the occupation numbers as postulated within Landau Fermi theory [3]. Whereas this energy functional certainly exists for any finite system, its existence in the thermodynamic limit is non-trivial; a necessary condition is $\lim_{N \to \infty} Z^N_{k_F} > 0$; a central issue of this paper.

We have performed Variational Quantum Monte Carlo calculations (VMC) of the 2DEG; the electrons interact with a $1/r$ potential and with a positive background charge. We have used a Slater-Jastrow backflow wavefunctions (SJ-BF) with an analytical form for the both the Jastrow and backflow potentials [14]; all potentials are split in short and long-range contributions as described in [14]. For $N = 58$ electrons, the DMC ground state energies obtained are $\lesssim 3mRy$ lower than previous calculations using numerically optimized forms [14]. Excited states were formed by adding or subtracting orbitals in the determinant; the backflow and Jastrow forms [14] are independent of the precise occupation of the Slater determinant. Since the trial function had no free parameters, we can study size effects without re-optimizing parameters for different system sizes.

First, we calculated the momentum distribution as explained in Ref. [11]. However, for systems in periodic boundary conditions, the momentum distribution is only given at discrete values $\mathbf{k} = 2\pi(n\hat{x} + m\hat{y})/L$ where $n$ and $m$ are integers and $\hat{x}, \hat{y}$ are the unit vectors in the $x$ and $y$ direction, respectively. Using twisted boundary conditions with twist angles $(\theta_x, \theta_y)2\pi/L$ for the trial wavefunctions, we can obtain a momentum distribution for all values of $\mathbf{k}$ by varying the twist angle. In the limit of an infinite sized system, the Slater determinant of our trial wavefunction approaches a sharp Fermi surface, occupying only wavevectors $|\mathbf{k}| \leq k_F$. For finite systems, the sharp behavior of the occupation numbers inside the Slater determinant is best described by working in the grand-canonical ensemble and for a given twist angle use only orbitals inside the Fermi sphere. This leads to a varying particle number as a function of the twist angle. As described in Ref. [8], the translational invariance of the ground state wavefunction allows us to define pockets inside of which the wavefunction transforms trivially — any change of the twist angle inside a pocket reduces to a change of the total center of mass moment accounted for by a simple phase factor; only a single QMC calculation is needed for each pocket. As shown in Fig. 1 the renormalization factor quantifying the jump in the momentum distribution at $k_F$ can be read-off precisely for any finite system. However, strong size effects around the Fermi surface are still evident.

We can analyze size-effects directly using the analytical form of the SJ-BF trial wavefunction. The momentum distribution is obtained by displacing one particle $\mathbf{r}_j$ a distance $\mathbf{r}$:

\[
\rho_{k_F}^N = \left\langle e^{-i\mathbf{k} \cdot \mathbf{r} - \delta U_N} \frac{D(\mathbf{R} : \mathbf{r}_j + \mathbf{r})}{D(\mathbf{R})} \right\rangle
\]

where $\langle \ldots \rangle$ denotes averaging over $|\Psi_T(\mathbf{R})|^2$ and over a uniform distribution for $\mathbf{r}$. The change of the Jastrow factor in Eq. (1) writes

\[
\delta U_N = \frac{1}{V} \sum_{\mathbf{q} \neq 0} u_q \left[ e^{i\mathbf{q} \cdot \mathbf{r}} \rho_{-\mathbf{q}} - 1 \right] \left[ e^{i\mathbf{q} \cdot \mathbf{r}} - 1 \right]
\]
where $\rho_q = \sum_j e^{i \mathbf{q} \cdot \mathbf{r}_j}$. As described in Ref. 3, the most important finite size-effects can be understood as an integration error by analytical continuation of the finite-size (periodic) wavefunction to an infinite system where the estimator in Eq. (3) would contain the following change in the Jastrow factor

$$\delta U_N \to \int \frac{d^2 \mathbf{q}}{(2\pi)^2} u_q [e^{i \mathbf{q} \cdot \mathbf{r}_q} - 1] [e^{i \mathbf{q} \cdot \mathbf{r}_q} - 1].$$  

(5)

The finite-size correction is then dominated by the non-analyticity of the integrand at $q = 0$

$$\delta U_\infty = \delta U_N \simeq \int_{-\pi/L}^{\pi/L} \frac{d^2 \mathbf{q}}{(2\pi)^2} u_q [e^{i \mathbf{q} \cdot \mathbf{r}_q} - 1] [e^{i \mathbf{q} \cdot \mathbf{r}_q} - 1],$$

and we can calculate the leading order size corrections, $\delta n_k \equiv n_k^\infty - n_k^N$, by expanding $n_k^\infty$, Eq. (3), up to second order in $\delta U_\infty - \delta U_N$. Neglecting mode-coupling terms, we get

$$\delta n_k \simeq \int_{-\pi/L}^{\pi/L} \frac{d^2 \mathbf{q}}{(2\pi)^2} \delta(q) [n_{k+q}^N - n_k^N]$$

$$+ \int_{-\pi/L}^{\pi/L} \frac{d^2 \mathbf{q}}{(2\pi)^2} \int_{-\pi/L}^{\pi/L} \frac{d^2 \mathbf{q}'}{(2\pi)^2} u_q u_q' [1 - S(q) - S(q')]$$

$$\times [n_{k+q+q'}^N - n_{k+q'}^N - n_k^N - n_{k+q'}^N],$$

(6)

where

$$\delta(q) = [u_q (1 - S(q)) - n_q^2 S(q)]$$

(7)

Equation (6) expresses size corrections in terms of the long-wavelength limits of the Jastrow potential and the structure factor, $S(q)$. For the homogenous electron gas, in the limit $q \to 0$, we have:

$$2nu_q \simeq -1 + [1 + (2nu_q/\varepsilon_q)]^{1/2}$$

$$S(q) \simeq \left[2nu_q + 1/S_0(q)\right]^{-1},$$

(8)

where $u_q = 2\pi e^2/\varepsilon_q$, $\varepsilon_q = \hbar^2 q^2/2m$, and $S_0(q)$ is the structure factor of the non-interacting Fermi gas.

As the momentum distribution of a Fermi liquid, Eq. (1), is smooth everywhere away from the Fermi surface, leading order corrections are restricted to a small region around $k_F$, where we can write

$$\delta n_k \simeq Z_{k_F}^N \int_{-\pi/L}^{\pi/L} \frac{d^2 \mathbf{q}}{(2\pi)^2} \delta(q) [\theta(k_F - |k + q|) - \theta(k_F - k)].$$

(9)

In Figure 1 we show the size-corrected momentum distribution for different densities between $r_s = 1$ and $r_s = 10$ using Eq. (9). Close to $k_F$, size effects lead to important qualitative and quantitative changes.

The renormalization factor, $Z$, can be read-off directly from the jump of the momentum distribution at the Fermi surface, $Z_{k_F}^N = n_{k_F+r_s}^N - n_{k_F+r_s}^N$, and its size corrected value may therefore be read of directly from

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure3.png}
\caption{The inverse effective mass $m/m^*$ for $r_s = 10$ as a function of $N^{-1}$, together with the corresponding size corrected values. Dashed lines illustrate the expected size corrections.}
\end{figure}

FIG. 3: The inverse effective mass $m/m^*$ for $r_s = 10$ as a function of $N^{-1}$, together with the corresponding size corrected values. Dashed lines illustrate the expected size corrections.

For a precise evaluation of $Z$ in the thermodynamic limit, we have studied the extrapolation separately. From Eq. (3), one can show that size-corrections of $Z$ can be written as

$$Z_{k_F}^\infty \simeq Z_{k_F}^N e^{-\Delta_N}, \quad \Delta_N = \int_{-\pi/L}^{\pi/L} \frac{d^2 \mathbf{q}}{(2\pi)^2} \delta(q)$$

(10)

which includes the main sub-leading order corrections. Using the analytical forms, Eq. (7) and Eq. (8), the leading order corrections are

$$\Delta_N \simeq \left(\frac{\pi^2}{4N}\right)^{-1/4}$$

for $N \to \infty$. (11)

The asymptotic form, Eq. (10) with Eq. (11), shows that actual QMC calculations with typically $N \sim 10^2$ electrons suffer from very strong size effects. Obscured by the intrinsic noise of QMC calculations, pure numerical analysis of the data might suggest convergence to values far off the exact value in the thermodynamic limit.

In Figure 2 we compare the bare data for $r_s = 1$ and $r_s = 10$ with their size corrected values. Whereas the bare data are in reasonable agreement with previous QMC results [7, 11], a numerical extrapolation of the uncorrected data strongly depends on assumptions on the asymptotic scaling form, as size corrections overwhelmingly dominate the calculation of $Z$. In order to go beyond leading order, we have directly used Eq. (10) together with the asymptotic forms, Eq. (7) and Eq. (8), to correct our bare data analytically. As can be seen from the figure, the size corrected values drastically reduce size effects, as expected. More important, in contrast to the uncorrected data, the extrapolation of the size corrected values is not sensitive to assumptions on the remaining corrections for densities $r_s \geq 3$. Approaching the high density region $r_s \lesssim 1$, the thermodynamic limit extrapolation is getting more difficult, since the asymptotic expansion is singular in the limit $r_s \to 0$. In Table 1 we have summarized our results for the renormalization factor.
Size corrections of the momentum distribution induces size corrections for the total kinetic energy which can be shown to coincide with the two-dimensional analog of Ref. [8]. In two dimensions, leading order size corrections of the kinetic and potential energy per particle scales as $N^{-5/4}$ in the Fermi liquid phase. We have added VMC and DMC energies of the size-extrapolated values of the energy per particle in table I.

Since our class of wavefunction have $Z > 0$, the single particle excitation spectrum should be dominated by quasiparticle excitations with an effective mass $m^\ast$. We have calculated the effective mass by adding an electron with momentum $\mathbf{p}$ with $|\mathbf{p}| > k_F$ to the ground state. The effective mass of an excited state has been determined assuming an expansion of the self energy in powers of $p - k_F$, leading to $2m\varepsilon_p/h^2 = p^2 - k^2_F + 2k_F(m/m^\ast - 1)(p - k_F)$ in the vicinity of $k_F$.

Again, the proper treatment of size effects is essential to extrapolate to the thermodynamic limit. The additional electron at momentum $\mathbf{p}$ will induce size corrections in the momentum distribution which can be estimated as before. The resulting additional finite size error in the total kinetic energy, $\delta T^N_{\mathbf{p}}$, due to the excitation of momentum $\mathbf{p}$, is then given by

$$\delta T^N_{\mathbf{p}} = \frac{\hbar^2}{2m} \mathbf{p}^2 \frac{Z^N}{Z^N_{\mathbf{p}}} \left[ e^{-\Delta^N} - 1 \right]. \quad (12)$$

We see that size-corrections of the effective mass are intrinsically related to those of the renormalization factor, $Z$, leading to a similar asymptotic scaling law, $N^{-1/4}$. Potential energy corrections are independent of $\mathbf{p}$ in leading order, and Eq. (12) dominates finite size corrections for $m/m^\ast$. Note, that the renormalization factor can also be obtained from analyzing the finite-size error of effective mass calculations without explicit calculations of the momentum distribution.

From figure 3, we see that size effects play a similar important role for determining $m^\ast$ as they do for determining $Z$. In particular, for high densities, size effects qualitatively change the conclusion of previous calculations [4]: whereas, in agreement with [4] all bare data indicate an effective mass smaller than the bare mass for $N \lesssim 100$, in the thermodynamic limit the effective mass is increased, as predicted by perturbative RPA calculations [5, 6].

Calculations based on many-body perturbation theory going beyond the perturbative RPA approximation have been suggested. However, based on different approximations, these predictions may lead to an enhancement or depression of $Z$ (or the effective mass) [5] and it is difficult to estimate reliably the validity of the underlying approximations. Our VMC results for $Z$ are always below the corresponding values of the perturbative RPA calculations, whereas we predict a higher effective mass $m^\ast/m$. Our calculations therefore support improved RPA calculations based on many-body local field theory including charge- and spin-density fluctuations as proposed in [6].

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\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
$r_s$ & 1 & 3 & 5 & 10 \\
\hline
$E_{\text{VMC}}$ & -0.4179(2) & -0.4223(1) & -0.2975(1) & -0.16952(1) \\
$E_{\text{DMC}}$ & -0.4206(2) & -0.2991(1) & -0.17070(1) & \\
$Z_{\text{VMC}}$ & 1.26(7) & 1.39(8) & 1.54(7) & 1.729(9) \\
$m^\ast/m_{\text{VMC}}$ & 1.26(7) & 1.39(8) & 1.54(7) & 1.729(9) \\
$Z_{\text{RPA}}$ & 0.66 & 0.44 & 0.34 & 0.24 \\
$m^\ast/m_{\text{RPA}}$ & 1.02 & 1.12 & 1.16 & 1.21 \\
\hline
\end{tabular}
\caption{Energies per particle (in Ry), $E_{\text{VMC}}$, and $E_{\text{DMC}}$, the renormalization factor $Z$ and the effective mass $m^\ast/m$ extrapolated to the thermodynamic limit (both within VMC, and from perturbative RPA calculations [5]). Values in () are standard errors in the last decimal place.}
\end{table}