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Finite-size analysis of the Fermi liquid properties of the homogeneous electron gas

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Abstract. We analyze the extrapolation to the thermodynamic limit of Fermi liquid properties of the homogeneous electron gas in two and three dimensions. Using field theory, we explicitly calculate finite-size effects of the total energy, the renormalization factor, and the effective mass at the Fermi surface within the random phase approximation (RPA) and discuss the validity for general metallic systems.

1. Introduction

We consider the Fermi liquid phase of the (unpolarized) homogeneous electron gas in two and three dimensions ($d = 2, 3$) at zero temperature, $T = 0$. Quantum Monte Carlo (QMC) calculations [1, 2] have not only provided the most precise evaluations of the ground state energy, E, as a function of density, n, but also give access to spectral properties, *e.g.* the momentum distribution, n_k, the effective mass, m^*, of quasiparticle excitations, and the corresponding spectral weight, the renormalization factor Z [2, 3, 4, 5, 6, 7, 8, 9, 10]. Whereas QMC provides a powerful strategy to quantify correlations in Fermi systems, it still suffers from two fundamental limitations: the fixed-node error, and the extrapolation to the thermodynamic limit. As shown recently, calculations of the Fermi liquid parameters are drastically affected by size effects [4, 7], since typical QMC computations are done with $N \lesssim 10^3$ electrons, but extrapolation schemes based on analytical knowledge of underlying properties significantly reduce the finite size error [11, 12, 4, 7]. Here, to provide further insight, we address the issue of extrapolating calculations of finite (small) systems to the infinite volume limit within common language of field theory. Strategies of improving the many-body wave function to reduce the fixed-node error in QMC are discussed elsewhere [13, 14, 15].

At high densities, $r_s \to 0$, the random phase approximations (RPA) is expected to be valid, and we explicitly calculate leading order size corrections within this approximation, and discuss their general validity. Here, $r_s = a/a_B$ with $a = [2(d-1)\pi n/d]^{-1/d}$ is the mean inter particle distance, $a_B = \hbar^2/me^2$ the Bohr radius, and e and m are the charge and mass of the electrons. Our results agree with the leading order corrections in [11, 4, 6, 7] where finite size corrections have been derived from a formulation directly based on the many-body wave function. In the

following, we explicitly concentrate on three fundamental properties, the total energy, E, the renormalization factor, $Z = n_{k_F^-} - n_{k_F^+}$, and the effective mass, m^*, at the Fermi surface, k_F.

2. Formalism

From the dielectric function, $\epsilon(q,\omega)$, the ground state energy per particle, E, inside a box of volume V with periodic boundary conditions, and $n = N/V$, can be obtained via coupling constant integration [16]

$$E = E_0 + \frac{1}{2V}\sum_{\mathbf{q}\neq 0}\left(-v_q - \frac{\hbar}{n}\int_0^1 d\lambda \int_0^\infty \frac{d\omega}{\pi}\left[\frac{1}{\epsilon(q,i\omega;\lambda)} - 1\right]\right) \tag{1}$$

where $v_q = 2(d-1)\pi e^2/q^{d-1}$ is the Coulomb potential and

$$E_0 = \frac{2}{N}\sum_{\mathbf{k}\leq k_F}\varepsilon_k \tag{2}$$

is the ideal gas kinetic energy with $\varepsilon_k = \hbar^2 k^2/2m$. In the following we set $\hbar = 1$. Within the RPA [17, 18], the dielectric function is given in terms of the ideal-gas density-density response function, $\chi_0(k,\omega)$,

$$\epsilon_{RPA}(k,\omega) = 1 - v_k\chi_0(k,\omega) \tag{3}$$

and the coupling constant integration can be done explicitly

$$E_{RPA} = E_0 + \frac{1}{N}\sum_{\mathbf{q}\neq 0}\left[-\frac{v_q}{2n} + \int_0^\infty \frac{d\omega}{2\pi}\log\epsilon_{RPA}(\mathbf{q},i\omega)\right] \tag{4}$$

Spectral properties are obtained from the single particle Green's function, $G(k,\omega)$, which equals

$$G^{-1}(k,\omega) = \omega + \mu - \varepsilon_k - \Sigma(k,\omega) \tag{5}$$

where the self energy, $\Sigma(k,\omega)$ accounts for interaction effects, and μ is the chemical potential which fixes the Fermi energy, $\varepsilon_F = \mu$, via $\varepsilon_F = \varepsilon_{k_F} + \Sigma(k_F, 0; \mu \equiv \varepsilon_F)$. From a frequency integration over the Green's function, the momentum distribution, n_k, can be obtained, and the magnitude of the jump at the Fermi surface, $Z = n_{k_F^-} - n_{k_F^+}$, is directly related to the residual of G at (k_F,ε_F). In general, poles of the Green's function give rise to quasi-particle excitations, whose energies are given in terms of an effective mass m^* at the Fermi surface.

Within the RPA, the self energy equals [19, 20, 21]

$$\begin{aligned}\Sigma_{RPA}(k,\omega) &= -\frac{1}{V}\sum_{\mathbf{q}\neq 0}\left\{\frac{v_q}{2} + \frac{v_q}{\epsilon(q,\varepsilon_{\mathbf{k}+\mathbf{q}}-\omega)}\left[\theta(\varepsilon_F - \varepsilon_{\mathbf{k}+\mathbf{q}}) - \theta(\omega - \varepsilon_{\mathbf{k}+\mathbf{q}})\right]\right. \\ &\left. + \int_{-\infty}^{\infty}\frac{d\nu}{(2\pi)}\frac{v_q}{\epsilon(q,i\nu)}\frac{1}{i\nu + \omega - \varepsilon_{\mathbf{k}+\mathbf{q}}}\right\}\end{aligned} \tag{6}$$

where $\varepsilon_F = k_F^2/2m$ is the unperturbed Fermi energy. From the self-energy, the renormalization factor, Z, at $k = k_F$ is given by

$$Z^{-1} = 1 - \frac{\partial\Sigma(k_F,\omega)}{\partial\omega}\Big|_{\omega=\varepsilon_F} \tag{7}$$

and the effective mass, m^*_σ, which characterizes the quasi-particle dispersion at the Fermi surface, is then obtained via

$$\frac{m}{m^*} = Z\left(1 + \frac{m}{k_F}\frac{\partial\Sigma(k,\varepsilon_F)}{\partial k}\Big|_{k=k_F}\right) = \frac{1 + \frac{m}{k_F}\frac{\partial\Sigma(k,\varepsilon_F)}{\partial k}\Big|_{k=k_F}}{1 - \frac{\partial\Sigma(k_F,\omega)}{\partial\omega}\Big|_{\omega=\varepsilon_F}} \tag{8}$$

Formally, the RPA contains the leading order corrections beyond the independent particle Hartree-Fock approximation, and its validity is restricted to the high density region, $r_s \to 0$. In this limit, it is consistent to expand Eq. (8). This leads to the so-called on-shell approximation (OSA) of the effective mass,

$$\frac{m}{m^*_{OSA}} = 1 + \frac{m}{k_F}\frac{\partial\Sigma(k,\varepsilon_F)}{\partial k}\Big|_{k=k_F} + \frac{\partial\Sigma(k_F,\omega)}{\partial\omega}\Big|_{\omega=\varepsilon_F}. \tag{9}$$

In the literature, there exists a long-standing controversy [19, 22, 23, 24, 25], whether Eq. (8) or Eq. (9) should be used to determine the effective mass. Strictly speaking, the validity of the RPA is confined to the high density region where both formulas essentially agree, $r_s \lesssim 1$, and the validity of RPA or RPA-like results at lower densities essentially relies on cancelation of errors. However, given the exact self-energy beyond RPA, only Eq. (8) provides the effective mass, and our finite-size analysis below is based on Eq. (8) , since, as we will see, our results are not restricted to the RPA.

3. Thermodynamic limit extrapolation of finite system results

All formulas of the previous section are valid for systems of finite size, $L = V^{1/d}$, where wave vectors are discrete. Perturbative expressions for the Green's function and the dielectric functions, as *e.g.* the RPA expressions, are based on the linked-cluster theorem, valid in a grand-canonical ensemble of fixed volume introducing small number fluctuations. Since the non-interacting Green's function does not depend explicitly on the system size, the extrapolation from the finite to the infinite system corresponds to the conversions of all underlying discrete sums to integrals, $(2\pi/L)^d \sum_{\mathbf{q}} \ldots \to \int d\mathbf{q} \ldots$, and finite size corrections are equivalent to discretization errors in quadrature. On this basis, the elimination of the size error in the second term on the rhs of the total energy expression, Eq. (1), is straightforward, leading to the Madelung constant

$$v_M = \sum_{\mathbf{q}} \frac{v_q}{2V} - \int \frac{d\mathbf{q}}{(2\pi)^d}\frac{v_q}{2}. \tag{10}$$

In the following, we show that a similar analysis of the quadrature error can be used to reduce the finite size error in other quantities.

If the integrand is regular, the discretization error is rapidly vanishing (of order $1/N$ or higher). The main contribution of order $N^{-\alpha}$ with $\alpha < 1$ comes from non-analytical points in the integrand. From the general structure of the perturbation expansion there are only certain discrete points where non-analyticities can develop: in the long wavelength limit, $k = 0$, where the Coulomb potential is singular, and for integer multiples of the Fermi wave-vector $k = j\,k_F$ ($j = 1, 2, \ldots$) due to the sharp Fermi surface of the underlying wave function.

Explicitly, the sharp Fermi surface at k_F leads to well-known shell oscillations in the energy, already present in the energy of the ideal Fermi gas, Eq. (2). Twisted boundary conditions strongly reduce these oscillations [26], and grand-canonical twist averaging (GTABC) completely eliminates them [11]. Within GTABC, we have

$$E_0^{GTABC} = \frac{2}{N}\int_{|\vartheta_\alpha|\le\pi/L} \frac{d\vartheta}{(2\pi/L)^d} \sum_{\mathbf{k}_\alpha = 2\pi m/L} \theta(\varepsilon_F - \varepsilon_{\mathbf{k}+\vartheta})\varepsilon_{\mathbf{k}+\vartheta} = \frac{2}{n}\int \frac{d\mathbf{k}}{(2\pi)^d}\theta(\varepsilon_F - \varepsilon_{\mathbf{k}})\varepsilon_{\mathbf{k}} \tag{11}$$

and $E_0^{GTABC} \equiv E_0(N \to \infty)$. Similarly, GTABC also eliminates size effects of other non-interacting properties, *e.g.* in the ideal gas density response, $\chi_0^{GTABC}(q,\omega) \equiv \chi_0(q,\omega;N\to\infty)$, as can be seen from the spectral representation

$$\chi_0^{GTABC}(q,\omega) = \frac{2}{V}\int_{|\theta_\alpha|\le\pi/L}\frac{d\vartheta}{(2\pi/L)^d}\sum_{\mathbf{k}_\alpha=2\pi m/L}\frac{\theta(\varepsilon_F-\varepsilon_{\mathbf{k}+\vartheta})-\theta(\varepsilon_F-\varepsilon_{\mathbf{k}+\vartheta+\mathbf{q}})}{\omega+\varepsilon_{\mathbf{k}+\vartheta}-\varepsilon_{\mathbf{k}+\vartheta+\mathbf{q}}+i\eta} \tag{12}$$

although χ_0 is still only given at discrete wave vectors ($\mathbf{q}_\alpha = 2\pi j/L$ with integer j). Therefore, twisted boundary conditions as well as GTABC do not modify the discrete sum in the exchange-correlation energy on the rhs of Eq. (1). However, GATBC lead to an accelerated convergence of the integrand towards the thermodynamic limit on all allowed wave vectors.

Within GTABC, we assume that size effects in the integrands of all expressions can be neglected, and focus on the presumably largest contributions from the Coulomb singularity at $k = 0$. For the total energy, Eq. (1), we expect that the leading order size corrections of the exchange-correlation energy, δE, is given by

$$\delta E \simeq \int_{|\mathbf{q}_\alpha|\le\pi/L}\frac{d\mathbf{q}}{(2\pi)^d}\int_0^1 d\lambda\int_0^\infty\frac{d\omega}{2\pi n}\left[\frac{1}{\epsilon(q,i\omega;\lambda)}-1\right]. \tag{13}$$

Similarly, the effect of the thermodynamic limit extrapolation on the renormalization factor and the effective mass can be obtained from explicit (approximate) expressions of the self-energy, Eq. (6), together with Eq. (7) and Eq. (8).

4. Results

The Lindhard function, $\chi_0(q,\omega)$, has the following limiting form in the long wave length limit

$$\chi_0(k,\omega) \approx nk^2/m\omega^2, \quad k\to 0 \tag{14}$$

and we have

$$\epsilon(k,\omega) \approx 1-\omega_p^2(k)/\omega^2, \quad k\to 0 \tag{15}$$

where the plasma frequency is given by $\omega_p(k) = (nv_k k^2/m)^{1/2}$.

4.1. Total energy

Inserting the limiting form of the dielectric function in Eq. (4), we obtain

$$\delta E = \frac{1}{n}\int_{|\mathbf{q}_\alpha|\le\pi/L}\frac{d\mathbf{q}}{(2\pi)^d}\int\frac{d\omega}{2\pi}\log(1+\omega_p^2(q)/\omega^2) = \frac{1}{n}\int_{|\mathbf{q}_\alpha|\le\pi/L}\frac{d\mathbf{q}}{(2\pi)^d}\frac{\omega_p(q)}{2} \tag{16}$$

and size corrections in the energy have a simple interpretation in terms of zero point energy of long wavelength plasmon modes. Explicitly, in three dimensions, we have

$$\delta E_{3d} = \frac{\hbar^2}{2ma_B^2}\sqrt{\frac{3}{r_s^3}}\frac{1}{N} \tag{17}$$

in agreement with Ref. [11], and

$$\delta E_{2d} = s_2\frac{\pi}{5}(4\pi)^{1/4}\frac{1}{r_s^{3/2}}\frac{1}{N^{5/4}} \tag{18}$$

in two dimensions [4] where $s_2 = \frac{5}{4\pi}\int_{|q_\alpha|<1}|q|^{1/2} = \frac{4}{\pi}\int_0^1 du\,(1+u^2)^{1/4} \simeq 1.362073657$ accounts for the cubic geometry.

4.2. Renormalization factor and effective mass

For the calculation of the renormalization factor and the effective mass, we need the derivatives of the self energy at the Fermi surface. Within the RPA, we have

$$\frac{\partial\Sigma(k_F,\varepsilon_F)}{\partial\omega} = -\frac{1}{V}\sum_{\mathbf{q}\neq 0}\int_{-\infty}^{\infty}\frac{d\nu}{(2\pi)}\left[\frac{1}{\epsilon(q,i\nu)}-\frac{1}{\epsilon(q,0)}\right]\frac{v_q}{[i\nu+\varepsilon_F-\varepsilon_{k_F+\mathbf{q}}]^2} \quad (19)$$

$$\frac{m}{k_F}\frac{\partial\Sigma(k_F,\varepsilon_F)}{\partial k} = \frac{1}{V}\sum_{\mathbf{q}\neq 0}\int_{-\infty}^{\infty}\frac{d\nu}{(2\pi)}\frac{1}{\epsilon(q,i\nu)}\frac{v_q}{[i\nu+\varepsilon_F-\varepsilon_{k_F+\mathbf{q}}]^2}\left[1+\frac{\mathbf{k}_F\cdot\mathbf{q}}{k_F^2}\right] \quad (20)$$

Since $\chi_0(q,0)=-dn/\varepsilon_F$ for $q\to 0$, the static dielectric function diverges in the long wave length limit,

$$\epsilon_{RPA}(q,0)=1+dnv_q/\varepsilon_F\sim v_q\sim q^{1-d},\quad q\to 0 \quad (21)$$

providing perfect screening, and the dominant size correction, Δ, of $\partial\Sigma/\partial\omega$ exactly equals that of $-\partial\Sigma/\partial k$, and is given by

$$\Delta = -\int_{|\mathbf{q}_\alpha|\leq\pi/L}\frac{d\mathbf{q}}{(2\pi)^d}\int_{-\infty}^{\infty}\frac{d\nu}{(2\pi)}\frac{1}{\epsilon(q,i\nu)}\frac{v_q}{[i\nu+\varepsilon_F-\varepsilon_{k_F+\mathbf{q}}]^2} \quad (22)$$

$$\simeq \int_{|\mathbf{q}_\alpha|\leq\pi/L}\frac{d\mathbf{q}}{(2\pi)^d}\int_{-\infty}^{\infty}\frac{d\nu}{(2\pi)}\frac{v_q}{1+\omega_p^2(q)/\nu^2}\frac{1}{\nu^2} \quad (23)$$

We get

$$\Delta=-\int_{|\mathbf{q}_\alpha|\leq\pi/L}\frac{d\mathbf{q}}{(2\pi)^d}\frac{v_q}{4\omega_p(q)} \quad (24)$$

and we have

$$\Delta_{3d}=-c_3\left(\frac{r_s}{3}\right)^{1/2}\left(\frac{3}{4\pi N}\right)^{1/3} \quad (25)$$

in three dimension [7] with $c_3=\frac{1}{4\pi}\int_{|q_\alpha|<1}|q|^{-2}=\frac{6}{\pi}\int_0^1 du\,\frac{\ln(2+u^2)}{1+u^2}\simeq 1.221374804$, and

$$\Delta_{2d}=-c_2\left(\frac{r_s}{8}\right)^{1/2}\left(\frac{\pi}{N}\right)^{1/4} \quad (26)$$

in two dimensions [4] with $c_2=\frac{5}{4\pi}\int_{|q_\alpha|<1}|q|^{-3/2}=\frac{4}{\pi}\int_0^1 du\,(1+u^2)^{-3/4}\simeq 1.057929920$. The leading order size corrections for the renormalization factor are then given by

$$Z_\infty^{-1}\simeq Z_N^{-1}+\Delta \quad (27)$$

and, using Eq. (8), the effective mass correction writes

$$\frac{m}{m^*}-1\Big|_\infty \simeq \left(\frac{m}{m^*}-1\right)\Big|_N(1+\Delta Z) \quad (28)$$

Note, that, within the validity of the RPA, we may put $Z=1$ on the rhs of Eq. (28). The slow decay of Δ with increasing system size can lead to important qualitative and quantitative changes of spectral quantities when properly extrapolated to the thermodynamic limit with respect to calculations which rely on linear extrapolation schemes.

5. Discussion

We have discussed size effects of the total energy, the renormalization factor, and the effective mass. Particularly, in two dimensions, Z and m^* show an unexpected slowly decaying size effect $\sim N^{-1/4}$. In general, we expect that these size effects are also present in other response quantities, *e.g.* the spin susceptibility, as they are connected to m^* by relations based on Landau's Fermi liquid theory. Our results on the finite size corrections are quite general and do not rely on the validity of the RPA, as they are based on the large wave length behavior of the dielectric function, Eq. (15), which applies to all metallic systems. Further, all results agree with the leading order corrections in [11, 4, 7] where finite size corrections have been derived from a formulation directly based on the many-body wave function.

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