Static Response and Local Field Factor of the Electron Gas

Saverio Moroni,[1] David M. Ceperley,[2] and Gaetano Senatore[3]

[1]*FORUM–INFM, Institute for Condensed Matter Theory, Scuola Normale Superiore, I–56126 Pisa, Italy*

[2]*National Center for Supercomputing Applications, Department of Physics, University of Illinois, Urbana, Illinois 61801*

[3]*Dipartimento di Fisica Teorica, Università di Trieste, Strada Costiera 11, I-34014 Trieste, Italy*

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We have evaluated the density-density static response of the electron gas at zero temperature and in the metallic regime by diffusion Monte Carlo. The computed local field factor $G(q)$ smoothly interpolates between the asymptotic small and large q behavior, with a crossover around $2q_F$. In fact, $G(q)$ appears to be almost completely given by its asymptotes, being accurately reproduced by the local density approximation to density functional theory for $q \lesssim 2q_F$. We give a simple formula to reproduce $G(q)$ at relevant values of the wave vector.

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The electron gas or jellium is an ideal system of electrons in a uniform neutralizing background, characterized at zero temperature by one parameter, the average density $n_0 \equiv 1/(4\pi r_s^3 a_B^3/3)$. In spite of its simplicity, the system is interesting from many points of view. It represents the first approximation to valence electrons in simple metals [1]. It is a nontrivial model for many-body theory [2]. It has a phase diagram that displays, with lowering the density, transitions to states with magnetic ordering and to the Wigner crystal [3]. In addition, it provides the basic ingredient of density functional [4] calculations for real materials, both at the local density level and beyond [5]. All practical density functional schemes, in fact, are concerned with the approximation of the exchange-correlation energy $E_{xc}[n]$ of the inhomogeneous many-electron system in terms of properties of the homogeneous electron gas. One such property is the local field factor $G(q)$, closely related to the exchange-correlation factor $f_{xc}(q)$ [2]:

$$f_{xc}(q) = -v_c(q)G(q), \tag{1}$$

with $v_c(q) = 4\pi e^2/q^2$ the Coulomb coupling. E_{xc} and f_{xc} are directly related in real space,

$$f_{xc}(|\mathbf{r} - \mathbf{r}'|) = \left[\frac{\delta^2 E_{xc}[n]}{\delta n(\mathbf{r})\delta n(\mathbf{r}')}\right]_{n_0}. \tag{2}$$

In this Letter we compute the zero temperature local field factor $G(q)$ of the electron gas from the static density-density (linear) response function $\chi(q)$ [2], obtained from extensive diffusion Monte Carlo (DMC) simulations. The method is very simple [6,7]. One perturbs the otherwise homogeneous many-body system with a static external potential

$$v_{\mathrm{ext}}(\mathbf{r}) = 2v_{\mathbf{q}}\cos(\mathbf{q}\cdot\mathbf{r}), \tag{3}$$

which induces a modulation of the density, with respect to its mean value n_0, and a shift of the ground-state energy (per particle) [6]

$$E_v = E_0 + \frac{\chi(q)}{n_0}v_{\mathbf{q}}^2 + \frac{\chi^{(3)}(\mathbf{q},\mathbf{q},-\mathbf{q})}{4n_0}v_{\mathbf{q}}^4 + \cdots, \tag{4}$$

with $\chi^{(3)}$ the cubic response function. A DMC simulation allows an accurate evaluation of E_v for given $\mathbf{q}$ and $v_{\mathbf{q}}$. By performing simulations at a few coupling strengths $v_{\mathbf{q}}$ one can extract $\chi(q)$ as well as higher order response functions from the calculated E_v, by fitting in powers of $v_{\mathbf{q}}$. Clearly, the procedure must be repeated for each value of the wave vector and of any other relevant parameter characterizing the system. So far applications have been to ^{4}He [6], for which excellent agreement with experiment was obtained, to charged bosons [7] and to 2D electrons [6] within the fixed-node approximation.

In DMC simulations [8] one propagates the wave function in imaginary time, starting from a suitable trial function, to project out higher energy components and filter out the ground state. We have chosen a trial wave function of the form

$$\Psi_T^v = D_\uparrow^v D_\downarrow^v \prod_{i<j}\exp[-u(r_{ij})], \tag{5}$$

with D_s^v a Slater determinant of one-particle orbitals with spin projection s and $u(r)$ the random phase approximation (RPA) pseudopotential [9]. The one-particle orbitals are solutions of the problem of noninteracting particles in an external field $v'(\mathbf{r}) = \alpha\cos(\mathbf{q}\cdot\mathbf{r})$, whose amplitude $\alpha = \alpha(v_{\mathbf{q}})$ is determined by optimizing the variational energy. Clearly, the imposed periodic boundary conditions restrict $\mathbf{q}$ to the reciprocal lattice vectors of the simulation cell. Finite size effects were mitigated by (i) performing the Ewald summation on the infinite periodic replicas of the simulation box, (ii) using a number of particles N corresponding to closed shells of orbitals, and (iii) keeping $v_{\mathbf{q}}$ weak enough not to alter the orbital filling appropriate to $v_{\mathbf{q}} = 0$. We performed simulations with 38, 54, and 66 particles.

We have studied the unpolarized electron gas in the metallic regime at few values of the density parameter, $r_s = 2, 5, 10$. By fitting the calculated ground-state energies to the polynomial of Eq. (4) we immediately obtain the static response $\chi(q)$. In Fig. 1 we show our fixed-node results at $r_s = 5$. Comparison with the mean-field RPA [2], which is also shown, reveals that the effects of

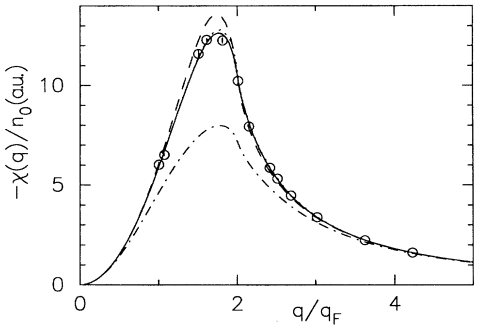

FIG. 1. Linear static response function $\chi(q)$ of the electron gas at $r_s = 5$. The circles give the present MC results, with the full curve being an interpolation of the calculated points [see Eq. (7)]. Error bars are reported on each MC point. The dash-dotted curve is the RPA [2]; dots and dashes give, respectively, the approximations of Geldart and Taylor [14] and of Farid *et al.* [15].

correlation (and exchange) are large at this density. A direct measure of such effects is provided by the exchange-correlation factor [2], giving the deviation of the full response from its RPA counterpart:

$$-f_{xc}(q) = \frac{1}{\chi(q)} - \frac{1}{\chi_{\mathrm{RPA}}(q)} = \frac{1}{\chi(q)} - \frac{1}{\chi_0(q)} + v_c(q). \quad (6)$$

Note that the RPA corresponds to $f_{xc}(q) = 0$ [$G(q) = 0$], while Lindhard noninteracting response $\chi_0(q)$ is obtained for $f_{xc}(q) = -v_c(q)$ [$G(q) = 1$]. Clearly, working with $f_{xc}(q)$ or $G(q)$ is equivalent in view of Eq. (1).

The limiting behavior of $G(q)$ at small and large q is exactly known. From Eqs. (1) and (2) it follows that, as $q \to 0$, $G(q) = A(q/q_F)^2$ to dominant order, with $A(r_s) = 1/4 + (-d\mu_c/dn_0)/(4\pi e^2/q_F^2)$, $q_F = (3\pi^2 n_0)^{1/3}$ the Fermi wave vector, and μ_c the correlation contribution to the chemical potential of the uniform electron gas. The large q behavior is given by [10] $G(q) = C(q/q_F)^2 + B$, where C is related to the fractional change of kinetic energy, δ_2, in going from noninteracting to interacting electrons: $C(r_s) = (\pi/2e^2 q_F)[-d(r_s\varepsilon_c)/dr_s]$, with ε_c the correlation energy per particle; $B(r_s)$ has a simple expression in terms of δ_2, the fractional change of the squared kinetic energy δ_4, and the pair correlation function at contact $g(0)$. $A(r_s)$ and $C(r_s)$ (or δ_2) can be readily calculated from an accurate parametrization [11] of the equation of state of the uniform electron gas [12]. To evaluate B in the metallic regime we have used recent DMC results [13] on the electron gas momentum distribution $n(q)$ and contact correlation, in conjunction with δ_2 obtained from the equation of state. We find that for $0 \le r_s \le 10$ our calculated B (for $r_s = 0.8, 1, 2, 3, 5, 8, 10$), together with the known result $B(0) = 1/3$ [10], can be reproduced with a precision of about 1% by $B(r_s) = (1 + a_1 x + a_2 x^3)/(3 + b_1 x + b_2 x^3)$, where $x = \sqrt{r_s}$ and $a_1 = 2.15$, $a_2 = 0.435$, $b_1 = 1.57$, $b_2 = 0.409$.

In Fig. 2 we give our fixed-node results for the exchange-correlation factor of the electron gas at $r_s = 5$. The asymptotic behaviors are also shown. It is evident that $f_{xc}(q)$ does not have much structure, and it can be essentially reproduced by taking its small-q constant value, for $q \lesssim 2q_F$, and the large-q behavior, for $q \gtrsim 2q_F$. An interpolation scheme embodying the behavior $f_{xc}(q) \simeq f_{xc}(0)$, $q \lesssim 2q_F$, though yielding $f_{xc}(\infty) = 0$, is due to Geldart and Taylor [14]. As seen from the figure, it appears to provide a reasonable account of our data for $q \lesssim 4q_F$, as well. We also report the prediction of an approximation due to Farid *et al.* [15], which has the correct functional form at large q [10]. There are quantitative deviations from our DMC points, from below for $q < 2q_F$ and from above for $q > 2q_F$. The latter discrepancy is easily traced to an underestimate of the constant B, since the approximation of [15] embodies the correct value of C. In Figs. 3 and 4 we give our results for the local field factor at $r_s = 2$ and 10. It is clear that considerations similar to those valid for $r_s = 5$ apply also to $r_s = 2$ and 10, with the obvious changes implied by Eq. (1). Having the response function $\chi(q)$ one can also evaluate the static dielectric function of the electron gas [2], via $1/\epsilon(q) = 1 + v_c(q)\chi(q)$. We find that between $r_s = 5$ and $r_s = 10$ antiscreening [16] [i.e., $1/\epsilon(q) < 0$] sets in. In fact, the dielectric function is positive at $r_s = 5$, while displaying at $r_s = 10$ a negative region for $0 < q \lesssim 2q_F$.

Numerical simulations yield estimates for a finite number of particles, which need to be extrapolated to $N = \infty$. We find that size effects, which are known to be fairly large for the total energy of electrons [9,13] especially at small r_s, are also pronounced for the static response.

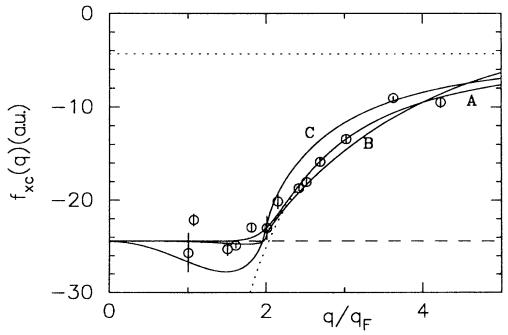

FIG. 2. Exchange-correlation factor $f_{xc}(q)$ of the electron gas at $r_s = 5$. The circles give the present MC results, with the curve A being an interpolation of the calculated points [see Eq. (7)] and curves B and C showing two approximations [14,15]. The horizontal dashed and dotted lines give, respectively, $f_{xc}(0)$ and $f_{xc}(\infty)$, while the dotted curve gives the large q behavior of $f_{xc}(q)$.

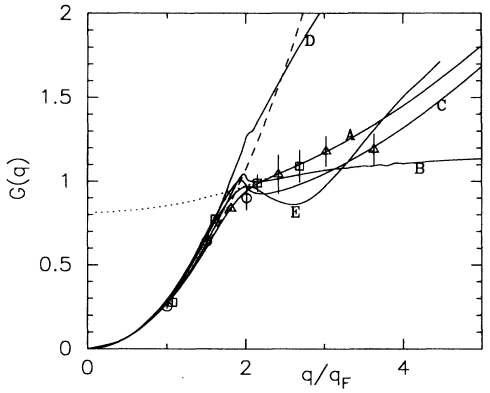

FIG. 3. Local field factor $G(q)$ of the electron gas at $r_s = 2$. The triangles, squares, and circles give the present MC results with 38, 54, and 66 particles, respectively, with the curve A being an interpolation of the calculated points [see Eq. (7)]. Curves B, C, and D, E, respectively, show the predictions of [14,15] and [17]. The dashed and dotted parabolas give, respectively, the small and large q behaviors of $G(q)$.

In fact, the restriction of $\mathbf{q}$ to reciprocal lattice vectors of the simulation box yields different sets of allowed wave vectors for different N, and this makes a systematic extrapolation in N of $\chi(\mathbf{q}, N)$ somewhat difficult. However, a little reflection suggests that one may define a local field factor for finite systems through $\chi^{-1}(\mathbf{q}, N) = \chi_0^{-1}(\mathbf{q}, N) - v_c(q) + v_c(q)G(\mathbf{q}, N)$ and, on the physical ground that $G(q)$ should describe short range correlations among the electrons (beyond RPA), one may assume $G(q) \equiv G(q, \infty) \simeq G(\mathbf{q}, N)$. This amounts to attribute all the N dependence of $\chi^{-1}(\mathbf{q}, N)$, whose additive structure [2] directly follows from density functional theory, to its noninteracting part $\chi_0^{-1}(\mathbf{q}, N)$. All the data presented here are obtained with this extrapolation procedure. Even at the smallest r_s, shown in Fig. 3, no residual size dependence can be appreciated within statistical error.

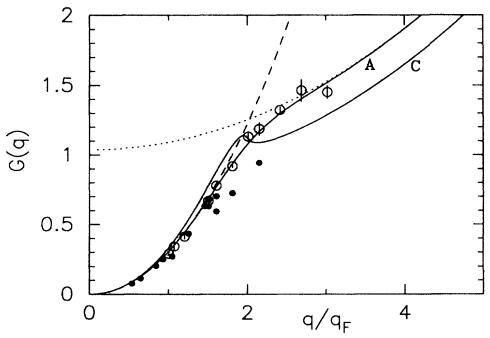

FIG. 4. Local field factor $G(q)$ of the electron gas at $r_s = 10$. The open circles give the present MC results, with the curve A being an interpolation of the calculated points [see Eq. (7)] and curve C showing the approximation of [15]. The solid circles are the MC results of [18]. The dashed and dotted parabolas give, respectively, the small and large q behaviors of $G(q)$.

In some approximations the local field factor exhibits a hump around $2q_F$, in the metallic regime. As is clear from Figs. 2–4, within statistical error and to the accuracy of our extrapolation procedure we find no evidence of such a structure, though we cannot conclusively rule it out. In Fig. 3 we also report (curve D) the predictions of a recent screened Hartree-Fock approximation [17] . This treatment yields a very small, hardly distinguishable hump in $G(q)$ at $2q_F$, and a sizable overestimate of our MC results for $q \gtrsim 2q_F$. We also report in the same figure a simple parametrization due to [17] (curve E), which embodies the leading asymptotic behavior of the local field factor at small and large q.

All our results for the local field factor of the unpolarized electron gas in the metallic regime are recorded in Table I. We have found that a simple interpolation formula (ignoring the possibility of humps at $2q_F$) is able to capture the main quantitative features of our fixed-node local field,

$$G(q) = \left(\left[(A - C)^{-n} + \left(\frac{q^2}{Bq_F^2} \right)^n \right]^{-1/n} + C \right) \left(\frac{q}{q_F} \right)^2, \tag{7}$$

with $n \simeq 8$ for $r_s = 2$ and $r_s = 5$ and $n \simeq 4$ for $r_s = 10$. This can be explicitly checked from Figs. 1–4, where Eq. (7) is given by the full line. We conjecture that Eq. (7), with $n = 8$ and A, B, C calculated as explained above, should also give a good account of the local field for $2 \lesssim r_s \lesssim 5$ and $0 < q \lesssim 3q_F$. We note that extracting the local field from the response function for $q \gtrsim 3q_F$ is very difficult as can be appreciated from Fig. 1, since full and RPA responses become very close. In fact, it is easy to show that both decay as $1/q^2$, with

TABLE I. Electron gas local field factor $G(q)$, for selected values of the wave vector q and of the density parameter r_s, from fixed-node diffusion Monte Carlo simulations.

r_s	2	5	10
q/q_F			
1.01	0.25(1)	0.30(2)	0.29(1)
1.08	0.28(2)	0.30(1)	0.24(3)
1.21			0.41(2)
1.51	0.64(2)	0.67(2)	0.67(1)
1.61	0.77(1)	0.76(1)	0.78(1)
1.81	0.84(1)	0.88(2)	0.92(1)
2.01	0.90(7)	1.09(6)	1.13(4)
2.15	0.99(5)	1.09(4)	1.19(5)
2.42	1.04(12)	1.28(2)	1.32(2)
2.51		1.33(3)	
2.69	1.09(10)	1.34(4)	1.46(8)
3.02	1.18(9)	1.44(4)	1.45(4)
3.63	1.19(9)	1.39(3)	
4.23		1.99(12)	

their difference being of order $1/q^4$. It is unclear at present whether the fine details of $G(q)$ beyond $3q_F$ are of any practical importance.

The fact that the local field factor appears to follow the small wave vector behavior up to q as large as $2q_F$ has some bearing on the accuracy of the local density approximation (LDA) [4] to density functional theory. In fact in LDA, as in any scheme giving a prescription to construct $E_{xc}[n]$ from the one-body density $n(\mathbf{q})$, one can generate a corresponding exchange-correlation factor by using Eq. (2), and from it a local field by virtue of Eq. (1). It is a simple matter to show [2] that the LDA local field is $G_{\mathrm{LDA}}(q) = A(q/q_F)^2$, with $A(r_s)$ as specified above. Thus, as far as we can judge at present, LDA correctly reproduces the static response for all $q \lesssim 2q_F$, if the exact equation of state of the electron gas is used to calculate A.

In summary, we have presented extensive accurate results for the local field factor of the unpolarized electron gas, obtained with the fixed-node diffusion Monte Carlo simulation. We have shown that our results correctly satisfy the asymptotic behaviors, which can be independently determined, and, in fact, appear to be dominated by them. In this connection the ability of LDA to correctly reproduce the static response to wave vectors as large as $2q_F$ is intriguing. We plan to investigate this point more closely in the near future. We have also given a simple formula that reproduces the main quantitative features of the MC local field in the metallic regime, to facilitate its use in the areas of many-body and density functional theories.

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Note added.—After this work was submitted for publication, a MC study by Bowen, Sugiyama, and Alder [18] appeared, with calculations similar to ours for $r_s = 1, 4, 6, 10$. A direct comparison is possible at $r_s = 10$, and we make it in Fig. 4. We find that the points of [18] are systematically lower than ours for $q \gtrsim 1.5q_F$. With reference to this discrepancy, we note the following. (i) The scatter of the data of [18] is reduced if our size extrapolation scheme is used on their own data, as is the discrepancy with our data. (ii) We have verified that the remaining sizable discrepancy is mostly due to their use of a trial function with nodes different from ours (in the presence of the modulating potential), yielding higher energies. (iii) Being fixed-node DMC variational, our response is more accurate around $2q_F$.

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