THE LOCAL FIELD OF THE ELECTRON GAS

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We review recent diffusion Monte Carlo (DMC) results for the static response of the electron gas in 3 dimensions. A detailed discussion focussing on the extraction of the local field factor G(q) from the calculated response is given, with emphasis on size effects and on alternative definitions of G(q) present in the literature.

1 Introduction

The local field factor $G(q)$ is a convenient measure of exchange and correlation effects beyond RPA in the problem of the linear screening of an external charge by the electron gas [1,2], which involves the dielectric function

$$\epsilon(q) = 1 - v_c(q)\chi_0(q)/[1 + v(q)G(q)\chi_0(q)]. \quad (1)$$

Above, $v_c(q) = 4\pi e^2/q^2$ is the Coulomb coupling and

$$\chi_0(q) = -\frac{m}{\pi^2}\frac{1}{q}\int_o^\infty dppn^0(p)\ln\left|\frac{q+2p}{q-2p}\right| \quad (2)$$

is the Lindhard function, with the non-interacting momentum distribution, $n^0(q) = 1, q \leq q_F$ and $n^0(q) = 0, q > q_F$. Evidently, $G(q) = 0$ yields the RPA, $\epsilon_{RPA}(q) = 1 - v(q)\chi_0(q)$. Over the years many approximations have been developed for $G(q)$, their accuracy being indirectly tested [1,2] through the predictions of quantities like correlation energy and pair correlation functions. It has been only recently that computer simulations of the dielectric screening in the electron gas have been performed, in two [3] and in three dimensions [4,5], yielding very accurate information on the local field factor $G(q)$.

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The local field factor of a many-electron system is of importance in various problems. Thus it provides information on the exchange-correlation functional $E_{xc}[n]$ of density functional theory [6], which is widely applied to the study of real materials [7]. Moreover, it is a basic ingredient of the pseudopotential perturbation treatment of simple metals, in that it directly determines the effective inter-ionic pair potential $\phi(r)$ [8]. Application of our accurate DMC local field to calculate $\phi(r)$ in test cases like Na and Al has appeared elsewhere [9]. Here we shall focus on the extraction of the local field $G(q)$, in the bulk limit, from the calculated DMC static response $\chi(q,N)$ at finite particle number N. Moreover we shall investigate the consequences of an alternative definition [10] of the local field, which replaces $\chi_0(q)$ in Eq. 1 with a modified reference function $\chi_I(q)$, obtained using, in Eq. 2, the interacting momentum distribution $n(q)$ instead of $n^0(q)$. We shall denote this modified or Niklasson local field with $G_I(q)$.

2 Local field from DMC

Calculating the static response of a quantum fluid with numerical simulations is in fact straightforward [3,5]. One perturbs the otherwise homogeneous many-body system with a static external potential

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

which induces a modulation of the density, with respect to its mean value $n_0 = N/V$, and a shift of the ground state energy (per particle) [3]

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

with χ and $\chi^{(3)}$ the linear and cubic response functions. DMC allows an accurate evaluation of E_v for given $\mathbf{q}$ and $v_{\mathbf{q}}$. By performing simulations at 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 wavevector and of any other relevant parameter characterizing the system, which makes it somewhat demanding computationally.

The local field factor $G(q)$ of the electron gas is immediately extracted from the computed χ by combing Eq. (1) with the exact relation $1/\epsilon(q) = 1 + v_c(q)\chi(q)$, which yields

$$v_c(q)G(\mathbf{q};N) = \chi^{-1}(\mathbf{q};N) - \chi_0^{-1}(\mathbf{q};N) + v_c(q). \tag{5}$$

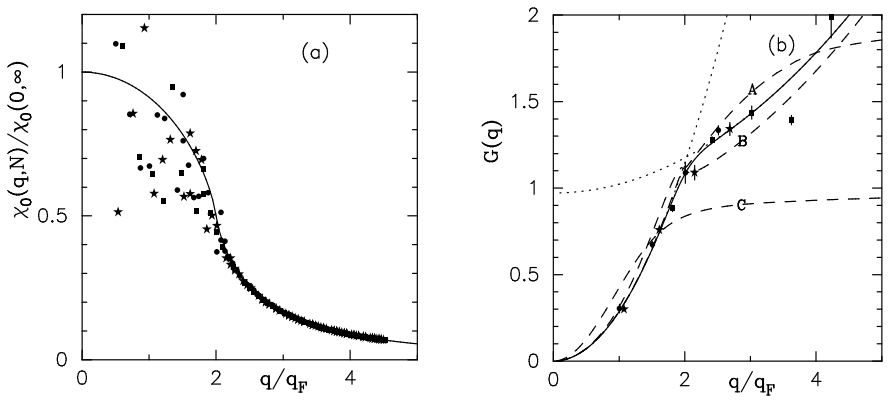

Figure 1: (a) Lindhard function at different values of N. Squares, stars and circles refer to $N = 38, 54, 68$, respectively. The curve gives the bulk limit $N = \infty$. (b) Local field $G(q)$ at $r_s = 5$. Squares, stars and circles are our DMC results for $N = 38, 54, 68$, respectively. The two dotted parabolas give the small and large q behaviour[5] and the dashed curves A,B,C give three approximations[16,13,17]. The full curve is a fit to the calculated points[5].

Evidently, simulations yield estimates at finite N, which one wants to extrapolate to the bulk limit, $N = \infty$. The size effects, which are known to be fairly large for the total energy of electrons[11,12] especially at small r_s, are also pronounced for the static response. In fact in the present case the extrapolation is not straightforward, as we argue below.

3 Number extrapolation

Simulations are performed with a finite number of particles N, in a box that we chose cubic and is periodically repeated in space (Ewald summation) to mitigate size effects. Thus the wavevector $\mathbf{q}$ is restricted to reciprocal lattice vectors of the simulation box. We find that the sets of allowed wavevectors are generally different for different N, as may be appreciated from Fig. 1a, where we show the dependence of $\chi_0(\mathbf{q}; N)$ on N and on the orientation of $\mathbf{q}$. This rules out the possibility of a systematic extrapolation in N for fixed $\mathbf{q}$.

The size dependence of $\chi_0(\mathbf{q}; N)$ is quite substantial for the typical N that can be used in practice and in fact it does not display any sign of saturation even at $N = 1000$, which is already prohibitively large. However, one may argue that a similar number dependence should be present in the full response $\chi(\mathbf{q}; N)$, so that when this is combined with $\chi_0(\mathbf{q}; N)$ as in Eq. 5, most of the dependence cancels out. In fact, $G(\mathbf{q}; N)$ describes short range correlations (beyond RPA) and one would expect it to be a smooth function of N.

This is indeed the case as it can be seen from Fig. 1b, where the local field for a density corresponding to $r_s = 5$ is given. Here, as it is customary, $n_0 =$

Table 1: Parameters of the fit of Eq. 7 to the DMC [12] momentum distribution, with the wavevector in units of q_F. For each r_s, three of the five fit parameters where eliminated by imposing: (i) the normalization of $n(q)$; (ii)the kinetic energy, as obtained from an accurate fit [18] to the known equation of state of the electron gas [19]; (iii) the exact large q behaviour [20] $n(q) \approx a_4/q^8$, with $a_4 = \hbar^4\omega_p^4 g(0)/32\epsilon_F$, and $g(0)$ from DMC simulations [12].

r_s	a_1	a_2	a_3	a_4	a_5
0.8	1.0001	-0.0194	0.0049	0.0104	0.9651
1.0	1.0017	-0.0283	0.0067	0.0165	1.0494
2.0	0.9933	-0.0677	0.0154	0.1119	1.3988
3.0	0.9838	-0.0959	0.0203	0.1372	1.2539
5.0	0.9658	-0.1591	0.0142	0.2437	1.2019
8.0	0.9018	-0.1698	0.0079	0.3270	1.1122
10.0	0.9007	-0.2198	0.0059	0.2970	0.9967

$1/(4\pi r_s^3 a_B^3/3)$ and a_B is the Bohr radius. It is evident that, within error bars, $G(\mathbf{q}; N)$ has little number dependence left, if any, in contrast to what happens with the response function. Thus we assume $G(q) \equiv G(q; N = \infty) \simeq G(\mathbf{q}; N)$.

4 Niklasson local field

As we have mentioned above, one may define a modified reference function $\chi_I(q)$, using in Eq. 2 the interacting momentum distribution $n(q)$ instead of $n^0(q)$, and a modified local field $G_I(q)$, by replacing $\chi_0(q)$ with $\chi_I(q)$ in Eq. 1. It follows that

$$v_c(q)G_I(q) = v_c(q)G(q) - [\chi_I^{-1}(q) - \chi_0^{-1}(q)]. \tag{6}$$

We have utilized recent DMC results for the momentum distribution [12], which we have fitted with a simple formula previously suggested by Farid *et al* [13],

$$n(q) = [a_0 + a_1 q^2]\theta(q_F - q) + [a_3/q^8 + a_4 e^{-a_5 q^2}]\theta(q - q_F), \tag{7}$$

to obtain the Niklasson function $\chi_I(q)$ at relevant values of r_s, from Eq. 2.

Using the results for $\chi_I(q)$ given in Fig. 2a it is a simple matter to obtain $G_I(q)$, which we show in Fig. 2b. It is evident that Niklasson definition yields indeed a local field with a pronounced peak at about $2q_F$, as it was predicted

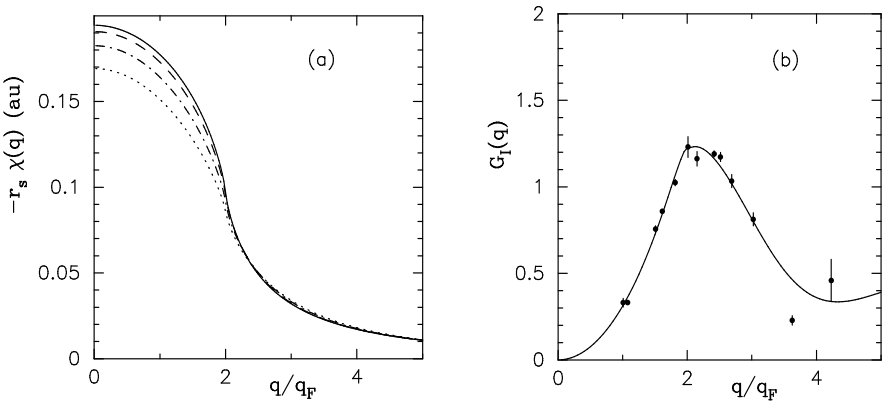

Figure 2: (a) Lindhard and Niklasson response functions: the full curve gives $\chi_0(q)$ while the dashed, dash-dotted, and dotted curve give $\chi_I(q)$ for $r_s = 2, 5, 10$, respectively. (b) Niklasson local field at $r_s = 5$. Circles and curve give the predictions obtained using Eq. 6 and respectively the DMC points and the fit shown Fig. 1.

in Hartree-Fock theory [14], though much lower and broader. The difference between $G_I(q)$ and $G(q)$ is fairly large. In particular it increases with q, in spite of the fact that the deviations of $\chi_I(q)$ from $\chi_0(q)$ become smaller with increasing q, as it is clear from Fig. 2a. We also note that the asymptotic large q value [10] of Niklasson local field, $G_I(\infty) = (2/3)[1 - g(0)]$, with $g(r)$ the pair correlation function, appears to have not been attained yet at $q \simeq 5q_F$, as at the $r_s = 5$ $g(0) \approx 0$ and $G_I(\infty) \simeq 0.66$. This is at variance with the behaviour of $G(q)$, which appears to reach its large q behaviour much sooner [5].

5 Conclusions

Above we have discussed in some detail the extraction of the local field factor $G(q)$ in the bulk limit from the DMC static response at finite N. We have argued that, in spite of the impossibility of a systematic extrapolation in which one fixes $\mathbf{q}$ and varies N, a meaningful extrapolation is still feasible.

We have also analyzed our DMC results in terms of the modified local field defined by Niklasson. Apart from the big differences at large q, first pointed out by Holas [15], we note that $G_I(q)$ and $G(q)$ have an overall different shape, with $G_I(q)$ indeed possessing a pronounced peak at $q \simeq 2q_F$. We should emphasize however that this is a property of $G_I(q)$ which is not shared by the

more commonly used local field $G(q)$.

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