Analytical expressions for the charge-charge local-field factor and the exchange-correlation kernel of a two-dimensional electron gas

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We present an analytical expression for the static many-body local field factor $G_+(q)$ of a homogeneous two-dimensional electron gas, which reproduces diffusion Monte Carlo data and embodies the exact asymptotic behaviors at both small and large wave number q. This allows us to also provide a closed-form expression for the exchange and correlation kernel $K_{xc}(r)$, which represents a key input for density functional studies of inhomogeneous systems.

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The static charge-charge response function $\chi_C(q)$ of a paramagnetic electron gas (EG) can be written in terms of the Lindhard function $\chi_0(q)$ by means of the spin-symmetric many-body local field $G_+(q)$ through the relationship

$$\chi_C(q)=\frac{\chi_0(q)}{1-v_q[1-G_+(q)]\chi_0(q)}. \tag{1}$$

Thus $G_+(q)$ is a fundamental quantity for the determination of many properties of a general electron system. By definition $G_+(q)$ is meant to represent the effects of the exchange and correlation hole surrounding each electron in the fluid and is therefore a key input in the density functional theory (DFT) of the inhomogeneous electron gas[1] and in studies of quasiparticle properties (such as the effective mass and the effective Landè g factor) in the electronic Fermi liquid.[2]

For what concerns DFT calculations, a common approximation to the unknown exchange-correlation energy functional $E_{xc}[n]$ appeals to its second functional derivative

$$K_{xc}(\bar{n},|\mathbf{r}-\mathbf{r}'|)\equiv\left.\frac{\delta^2 E_{xc}[n]}{\delta n(\mathbf{r})\,\delta n(\mathbf{r}')}\right|_{\bar{n}}, \tag{2}$$

where $\bar{n}$ is the average local density of the EG. The local field factor and the exchange-correlation kernel are simply related in Fourier transform by

$$\tilde{K}_{xc}(q)\equiv\int d^d r e^{-i\mathbf{q}\cdot\mathbf{r}}K_{xc}(r)=-v_q G_+(q), \tag{3}$$

where d is the dimensionality of the system and v_q is the Fourier transform of the Coulomb potential e^2/r. In what follows we shall only consider the case of two spatial dimensions, with $d=2$ and $v_q=2\pi e^2/q$. The corresponding three-dimensional case was discussed in Ref. 3.

A number of exact asymptotic properties of the static local field factor in two dimensions are readily proven. In particular,

$$\lim_{q\to 0}G_+(q)=A_+\frac{q}{k_F} \tag{4}$$

with

$$A_+=\frac{1}{r_s\sqrt{2}}\left(1-\frac{\kappa_0}{\kappa}\right), \tag{5}$$

where $k_F=\sqrt{2\pi n}=\sqrt{2}/r_s a_B$ is the Fermi wave number, $r_s=\sqrt{\pi n a_B^2}$ is the usual EG density parameter with a_B the Bohr radius, $\kappa_0=\pi r_s^4/2$ is the compressibility of the ideal gas in units of a_B^2/Ryd, while κ is the compressibility of the interacting system. By making use of the thermodynamic definition of κ we can write

$$\frac{\kappa_0}{\kappa}=1-\frac{\sqrt{2}}{\pi}r_s+\frac{r_s^4}{8}\left[\frac{d^2\epsilon_c(r_s)}{dr_s^2}-\frac{1}{r_s}\frac{d\epsilon_c(r_s)}{dr_s}\right], \tag{6}$$

where $\epsilon_c(r_s)$ is the correlation energy per particle. Once this function is known, it is possible to calculate A_+. For the present purpose $\epsilon_c(r_s)$ can be taken from the Monte Carlo data of Ref. 4.

The asymptotic behavior of $G_+(q)$ at large q is also known exactly:[5,6]

$$\lim_{q\to\infty}G_+(q)=C_+\frac{q}{k_F}+B_+, \tag{7}$$

where C_+ is proportional to the difference in kinetic energy between the interacting and the ideal gas,

$$C_+=\frac{t-t_0}{2\pi n e^2}k_F=-\frac{r_s}{2\sqrt{2}}\frac{d}{dr_s}[r_s\epsilon_c(r_s)]. \tag{8}$$

Moreover $B_+=1-g(0)$, $g(0)$ being the value of the pair-correlation function at the origin. For $g(0)$ we use the simple expression

$$g(0)=\frac{1/2}{1+1.372r_s+0.0830r_s^2}, \tag{9}$$

which has been derived[7] by an interpolation between the result of a low-r_s expansion, including the second order direct and exchange contributions to the energy in the paramagnetic state, and the result of a partial-wave phase-shift analysis near Wigner crystallization. This interpolation for-

mula is in excellent agreement with many-body calculations based on the ladder approximation.[8,9]

In this work we fit the values of $G_+(q)$ originally obtained by the diffusion Monte Carlo (DMC) method in Ref. 10 in such a way as to obtain analytical expressions for both $\tilde{K}_{\rm xc}(q)$ and $K_{\rm xc}(r)$. Our formula for $G_+(q)$ reads

$$G_+(\bar{q}) = A_+\bar{q}\left[\frac{e^{r_s/10}}{\sqrt{1+(A_+e^{r_s/10}\bar{q}/B_+)^2}} + (1-e^{r_s/10})e^{-\bar{q}^2/4}\right] + C_+\bar{q}(1-e^{-\bar{q}^2}) + \mathrm{P}_+(\bar{q})e^{-\alpha_+\bar{q}^2}, \tag{10}$$

where $\bar{q}=q/k_F$ and $\mathrm{P}_+(\bar{q})$ is the polynomial $\mathrm{P}_+(\bar{q})=g_2\bar{q}^2+g_4\bar{q}^4+g_6\bar{q}^6+g_8\bar{q}^8$.

Some comments are needed in order to appreciate the correct physics which has been incorporated in Eq. (10). (i) Our functional form embodies the exact asymptotic behaviors already introduced in Eqs. (4) and (7). (ii) The exponential factor $e^{r_s/10}$ ensures that $G_+(q)$ rapidly reaches the asymptotic behavior given by Eq. (7), a fact that is borne out by the DMC data at $r_s=10$. (iii) In the high-density limit ($r_s\to 0$) the term in square brackets tends to a two-dimensional Hubbard-like term,[11] while the second and third terms tend to zero. (iv) The introduction of the high-degree polynomial $\mathrm{P}_+(q)$ serves to reproduce the rich structure at intermediate wave number which is exhibited by $G_+(q)$ as compared to the three-dimensional case.[12]

The only free parameters are contained in the last term in Eq. (10) and are fitted so as to minimize the differences from the DMC numerical results. For practical reasons it proves useful to have a continuous parametrization of the coefficients of the polynomial $P_+(q)$, which is at least valid in the range $0\leqslant r_s\leqslant 10$. We therefore propose the following:

$$\alpha_+(r_s)=\frac{0.1598+0.8931(r_s/10)^{0.9218}}{1+0.8793(r_s/10)^{0.9218}},$$

$$g_2(r_s)=0.5824(r_s/10)^2-0.4272(r_s/10),$$

$$g_4(r_s)=0.2960(r_s/10)-1.003(r_s/10)^{5/2}+0.9466(r_s/10)^3,$$

$$g_6(r_s)=-0.0585(r_s/10)^2,$$

$$g_8(r_s)=0.0131(r_s/10)^2. \tag{11}$$

In Fig. 1 we compare the fit given by Eqs. (10) and (11) with the DMC data for $r_s=1,2,5$, and 10. In Fig. 2 we show the local field factor $G_+(q)$ as from Eq. (10) for various values of r_s: the evolution from the low-r_s regime to the high-r_s one is clear. The fact that the highest peak in $G_+(q)$ occurs at $r_s=5$ is due to the behavior of $C_+(r_s)$: this is a function that increases up to $r_s\simeq 3.5$, reaches a maximum and then decreases. Thus, the value of C_+ at $r_s=5$ is larger than that at $r_s=10$.

We turn next to the evaluation of $K_{\rm xc}(r)$. From Eqs. (3) and (10) the expression of the exchange-correlation kernel in real space (in Ryd) is readily obtained as

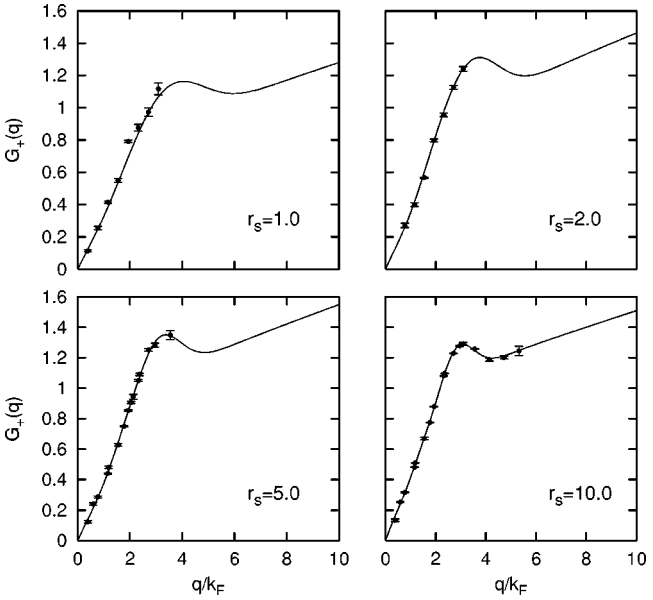

FIG. 1. The local field factor $G_+(\bar{q})$ for various values of r_s as computed according to Eq. (10), in comparison with the DMC data of Ref. 10.

$$K_{\rm xc}(r)=M_1\frac{\delta^{(2)}(\mathbf{r})}{k_F^2}+M_2\frac{\exp[-B_+k_Fr/(A_+e^{r_s/10})]}{k_Fr} + M_3e^{-(k_Fr)^2}+M_4e^{-(k_Fr)^2/4} + \sum_{n=1}^{4}M_{5,2n}F_{2n}(\alpha_+,k_Fr), \tag{12}$$

where $M_1=-4\pi\sqrt{2}C_+/r_s$, $M_2=-2\sqrt{2}B_+/r_s$, $M_3=-4\sqrt{2}A_+(1-e^{r_s/10})/r_s$, $M_4=\sqrt{2}C_+/r_s$ and $M_{5,n}=-2^{\frac{3}{2}}g_n/r_s$. The function $F_n(\alpha,x)$ is given by

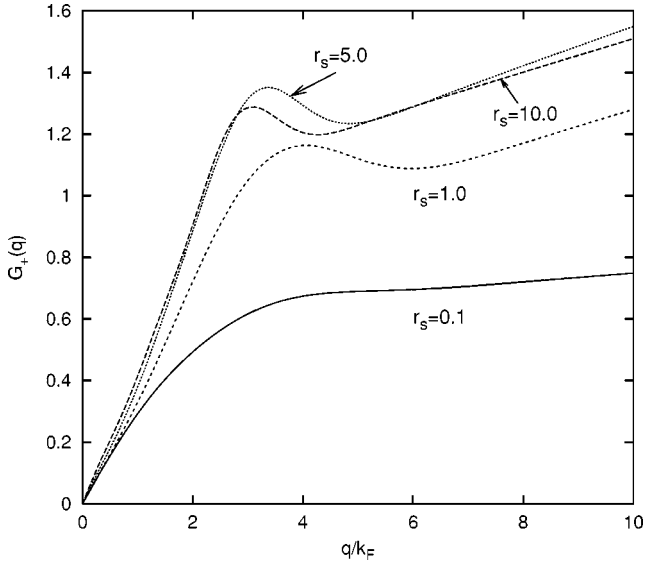

FIG. 2. The local field factor $G_+(q)$ as from Eq. (10) for various values of r_s.

$$F_n(\alpha,x)=\int_0^\infty dy y^n J_0(xy)e^{-\alpha y^2}$$
$$=\frac{1}{2}\alpha^{-(1+n)/2}\Gamma\left(\frac{1+n}{2}\right){}_1\mathrm{F}_1\left(\frac{1+n}{2};1;-\frac{x^2}{4\alpha}\right), \tag{13}$$

where $\Gamma(z)$ is Euler's Gamma function and ${}_1\mathrm{F}_1(a;b;z)$ is Kummer's function. In practice the function $F_n(\alpha,x)$ can be obtained via the recursive relation

$$F_{n+2}(\alpha,x)=-\frac{dF_n(\alpha,x)}{d\alpha},$$
$$F_2(\alpha,x)=\frac{\sqrt{\pi}}{16\alpha^{5/2}}\left[(4\alpha-x^2)I_0\left(\frac{x^2}{8\alpha}\right)\right.$$
$$\left.+x^2 I_1\left(\frac{x^2}{8\alpha}\right)\right]e^{-x^2/8\alpha}, \tag{14}$$

where $I_n(z)$ is the modified Bessel function of order n. It is also useful to recall that $dI_0(z)/dz=I_1(z)$ and that $dI_1(z)/dz=I_0(z)-I_1(z)/z$.

In Fig. 3 we show the exchange-correlation kernel $K_{\mathrm{xc}}(r)$ for various values of r_s as from Eq. (12) (without the first term, which contains a two-dimensional δ function). It is pleasing to note that no long-range oscillations are present in $K_{\mathrm{xc}}(r)$. Notice that the M_2 term in Eq. (12) diverges for $k_F r\to 0$.

In conclusion, we have presented an analytic parametrization of the local field factor entering the dielectric response of the two-dimensional electron gas in the paramagnetic state, incorporating the known asymptotic behaviors and giving an accurate description of the available quantum Monte Carlo data. We have obtained from it an analytic expression of the exchange-correlation kernel for density-functional calculations on inhomogeneous two-dimensional electronic systems.

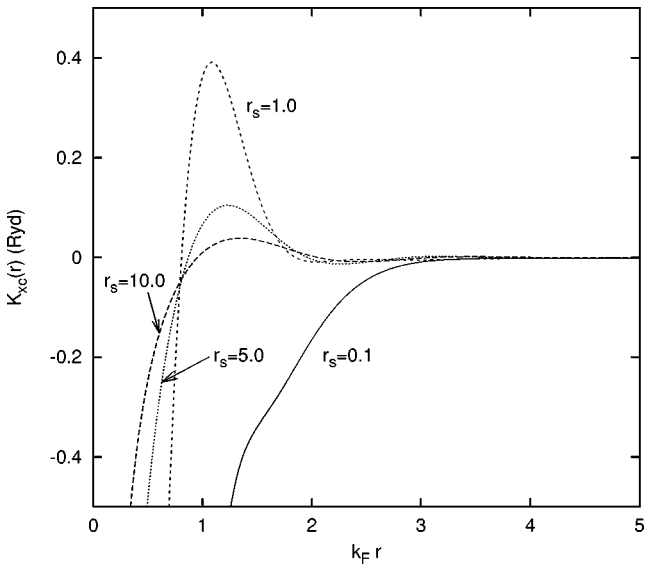

FIG. 3. The exchange-correlation kernel $K_{\mathrm{xc}}(r)$ as from Eq. (12) for various values of r_s.

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