Analytical expressions for the spin-spin local-field factor and the spin-antisymmetric 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 spin-antisymmetric exchange and correlation kernel $K^-_{xc}(r)$ which represents a key input for spin-density functional studies of inhomogeneous electronic systems.

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

$$\chi_S(q)=-\mu_B^2\frac{\chi_0(q)}{1+v_qG_-(q)\chi_0(q)}, \tag{1}$$

where μ_B is the Bohr magneton. Thus $G_-(q)$ is a fundamental quantity for the determination of many properties of a general electron system. It is a key input, together with the charge-charge local-field factor $G_+(q)$, in the spin-density functional theory (SDFT) of the inhomogeneous electron gas[1,2] and in studies of quasiparticle properties (such as the effective mass and the effective Landé g factor) in the electronic Fermi liquid.[3,4]

For what concerns SDFT calculations, a common approximation to the unknown exchange-correlation energy functional $E_{xc}[n,\zeta]$ of electron density n and spin polarization ζ appeals to its second functional derivatives,

$$K^{\sigma\sigma'}_{xc}(\overline{n},\overline{\zeta};|\mathbf{r}-\mathbf{r}'|)\equiv\left.\frac{\delta^2E_{xc}[n,\zeta]}{\delta n_\sigma(\mathbf{r})\,\delta n_{\sigma'}(\mathbf{r}')}\right|_{n=\overline{n},\zeta=\overline{\zeta}}, \tag{2}$$

where $\overline{n}=\overline{n}_\uparrow+\overline{n}_\downarrow$ is the average local density of the EG and $\overline{\zeta}=(\overline{n}_\uparrow-\overline{n}_\downarrow)/\overline{n}$ is the average local spin polarization. The local-field factors $G_{\sigma\sigma'}(q)$ and the matrix of the exchange-correlation kernels are simply related in Fourier transform by

$$\tilde{K}^{\sigma\sigma'}_{xc}(q)\equiv\int d^dr\,e^{-i\mathbf{q}\cdot\mathbf{r}}K^{\sigma\sigma'}_{xc}(r)=-v_qG_{\sigma\sigma'}(q), \tag{3}$$

where d is the dimensionality of the system and v_q is the Fourier transform of the Coulomb potential e^2/r. In the paramagnetic state the following relation holds between the charge-charge and spin-spin local-field factors $G_\pm(q)$ and $G_{\sigma\sigma'}(q)$:

$$G_\pm(q)=\frac{G_{\uparrow\uparrow}(q)\pm G_{\uparrow\downarrow}(q)}{2}. \tag{4}$$

Thus, from Eqs. (3) and (4), one obtains that the spin-symmetric and the spin-antisymmetric exchange and correlation kernels $K^\pm_{xc}(r)$ are related to $G_\pm(q)$ by

$$\tilde{K}^\pm_{xc}(q)\equiv\frac{\tilde{K}^{\uparrow\uparrow}_{xc}(q)\pm\tilde{K}^{\uparrow\downarrow}_{xc}(q)}{2}\equiv\int d^dr\,e^{-i\mathbf{q}\cdot\mathbf{r}}K^\pm_{xc}(r)$$
$$=-v_qG_\pm(q). \tag{5}$$

In what follows we shall only consider $K^-_{xc}(r)$ in the case of two spatial dimensions, with $d=2$ and $v_q=2\pi e^2/q$. An analytical expression for $K^+_{xc}(r)$ has already been given in Ref. 5.

A number of exact asymptotic properties of $G_-(q)$ in two dimensions are readily proved. In particular,[6]

$$\lim_{q\to0}G_-(q)=A_-\frac{q}{k_F}, \tag{6}$$

with

$$A_-=\frac{1}{r_s\sqrt{2}}\left(1-\frac{\chi_0}{\chi}\right), \tag{7}$$

where $k_F=\sqrt{2\pi n}=\sqrt{2}/r_sa_B$ is the Fermi wave number, $r_s=\sqrt{\pi na_B^2}$ is the usual EG density parameter with a_B the Bohr radius, and $\chi_0=\mu_B^2m/\pi\hbar^2$ is the (Pauli) spin susceptibility of the ideal Fermi gas, while χ is the spin susceptibility of the interacting system. By making use of the thermodynamic definition of χ we can write

$$\frac{\chi_0}{\chi}=1-\frac{\sqrt{2}}{\pi}r_s+\frac{r_s^2}{2}\left.\frac{\partial^2\epsilon_c}{\partial\zeta^2}\right|_{\zeta=0}, \tag{8}$$

where ϵ_c is the correlation energy per particle in the spin-polarized fluid. Unfortunately the correlation energy at finite spin polarization is poorly known. By extrapolating the diffusion Monte Carlo (DMC) data[7] for $G_-(q)$ to $q=0$ and by observing from Eq. (8) that $A_-\to1/\pi$ for $r_s\to0$, we obtain the following parametrization of A_- in the range $0\leqslant r_s\leqslant10$ where simulation data are available:

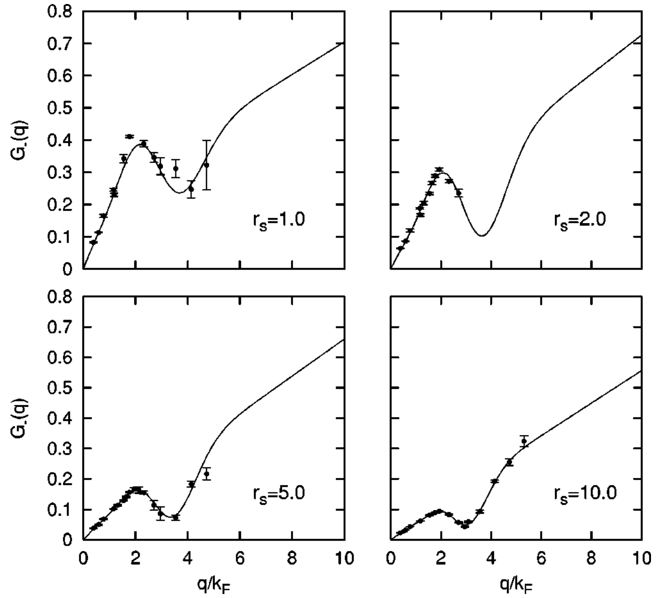

FIG. 1. The local-field factor $G_-(\overline{q})$ for various values of r_s as computed according to Eq. (12), in comparison with the DMC data of Ref. 7.

$$A_-=\frac{1}{\pi+1.4954r_s+0.3193\sqrt{r_s}}. \tag{9}$$

The asymptotic behavior of $G_-(q)$ at large q is also known exactly,[6,8]

$$G_-(q)\sim C_-\frac{q}{k_F}+B_-, \tag{10}$$

for $q\to\infty$, where C_- is proportional to the difference in kinetic energy between the interacting and the ideal gas,

$$C_-=\frac{t-t_0}{2\pi ne^2}k_F=-\frac{r_s}{2\sqrt{2}}\frac{d}{dr_s}[r_s\epsilon_c(r_s)]. \tag{11}$$

The correlation energy per particle $\epsilon_c(r_s)$ in the paramagnetic fluid is available from Monte Carlo data.[9] Finally $B_-=g(0)$, $g(0)$ being the value of the pair-correlation function at the origin.[10]

In this work we fit the values of $G_-(q)$ originally obtained by DMC in Ref. 7 in such a way as to obtain analytical expressions for both $\tilde{K}^-_{\rm xc}(q)$ and $K^-_{\rm xc}(r)$. The functional form previously employed[5] for the charge-charge local-field factor $G_+(q)$ is also suitable for $G_-(q)$:

$$G_-(\overline{q})=A_-\overline{q}\left[\frac{\kappa_-(r_s)}{\sqrt{1+(A_-\kappa_-(r_s)\overline{q}/B_-)^2}}+[1-\kappa_-(r_s)]e^{-\overline{q}^2/4}\right]+C_-\overline{q}(1-e^{-\beta_-\overline{q}^2})+P_-(\overline{q})e^{-\alpha_-\overline{q}^2}, \tag{12}$$

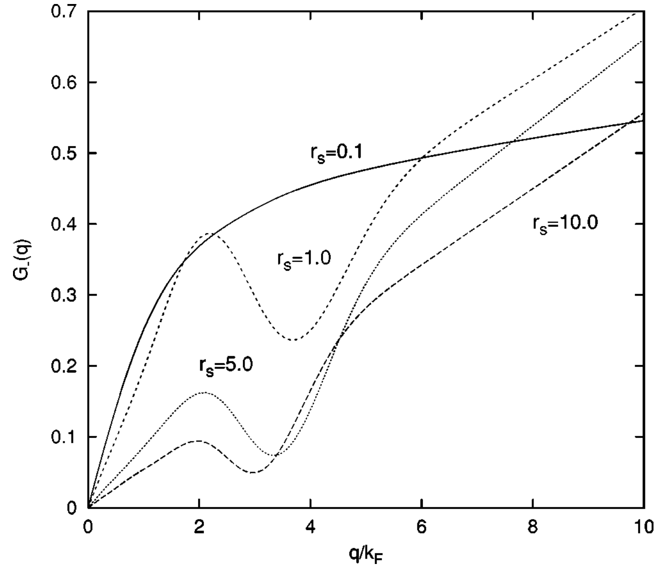

FIG. 2. The local-field factor $G_-(q)$ as from Eq. (12) for various values of r_s.

where $\overline{q}=q/k_F$, $\kappa_-(r_s)=\sqrt{1+0.0082r_s^2}$, and $P_-(\overline{q})$ is the polynomial $P_-(\overline{q})=h_2\overline{q}^2+h_4\overline{q}^4+h_6\overline{q}^6+h_8\overline{q}^8$. The free parameters α_-, β_-, and $h_2,\ldots,h_8$ are fitted so as to minimize the differences from the DMC numerical results. As for $G_+(q)$, it proves useful to have a continuous parametrization of these parameters at least in the range $0\leqslant r_s\leqslant 10$ where simulation data are available. We propose the following:

$$\alpha_-(r_s)=\exp\left(-\frac{0.2231+81.2115(r_s/10)}{1+54.6665(r_s/10)+50.7534(r_s/10)^2}\right),$$

$$\beta_-(r_s)=0.8089-0.4025(r_s/10)^3-0.0941(r_s/10)^{1/2},$$

$$h_2(r_s)=\exp\left(-\frac{12.6262+20.9673(r_s/10)}{1+12.4002(r_s/10)}\right),$$

$$h_4(r_s)=0.0531(1-e^{-2.154r_s^2})-0.4984(r_s/10)^{3/2}+0.4021(r_s/10)^2,$$

$$h_6(r_s)=-0.0076(1-e^{-r_s})+0.0977(r_s/10)^{3/2}-0.0726(r_s/10)^2,$$

$$h_8(r_s)=-0.0027\,(r_s/10). \tag{13}$$

In Fig. 1 we compare the fit given by Eq. (12) 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. (12) for various values of r_s.

We turn next to the evaluation of $K^-_{\rm xc}(r)$. From Eqs. (5) and (12), the expression of the spin-antisymmetric exchange-correlation kernel in real space (in Ry) is readily obtained as

$$K_{\rm xc}^{-}(r)=N_1\frac{\delta^{(2)}(\mathbf{r})}{k_F^2}+N_2\frac{\exp\{-B_-k_Fr/[A_-\kappa_-(r_s)]\}}{k_Fr}$$
$$+N_3e^{-(k_Fr)^2}+N_4e^{-(k_Fr)^2/4\beta_-}$$
$$+\sum_{n=1}^{4}N_{5,2n}F_{2n}(\alpha_-,k_Fr), \tag{14}$$

where $N_1=-4\pi\sqrt{2}C_-/r_s$, $N_2=-2\sqrt{2}B_-/r_s$, $N_3=-4\sqrt{2}A_-[1-\kappa_-(r_s)]/r_s$, $N_4=\sqrt{2}C_-/r_s\beta_-$, and $N_{5,n}=-2^{2/3}h_n/r_s$. The function $F_n(\alpha,x)$ is given by

$$F_n(\alpha,x)=\int_0^\infty dy\, y^n J_0(xy)e^{-\alpha y^2}$$
$$=\frac{1}{2}\alpha^{-(1+n)/2}\,\Gamma\left(\frac{1+n}{2}\right){}_1\mathrm{F}_1\left(\frac{1+n}{2};1;-\frac{x^2}{4\alpha}\right), \tag{15}$$

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

$$F_{n+2}(\alpha,x)=-\frac{dF_n(\alpha,x)}{d\alpha},$$

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

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 matrix elements $K_{\rm xc}^{\sigma\sigma'}(r)$ of the exchange-correlation kernel for various values of r_s. These kernels describe the local structure (Pauli-Coulomb hole) of the paramagnetic electron fluid around an electron of a given spin. $K_{\rm xc}^{\uparrow\uparrow}(r)$, being the sum of $K_{\rm xc}^{+}(r)$ and $K_{\rm xc}^{-}(r)$, has the same behavior of these two components: namely, no structure at both small and high r_s. The situation is different for $K_{\rm xc}^{\uparrow\downarrow}(r)$, which is instead given by the difference of $K_{\rm xc}^{+}(r)$ and $K_{\rm xc}^{-}(r)$. Although these two components are structureless at small r_s, the difference between them around $k_Fr\simeq 1$ is large and this is reflected in the large structure shown in Fig. 3.

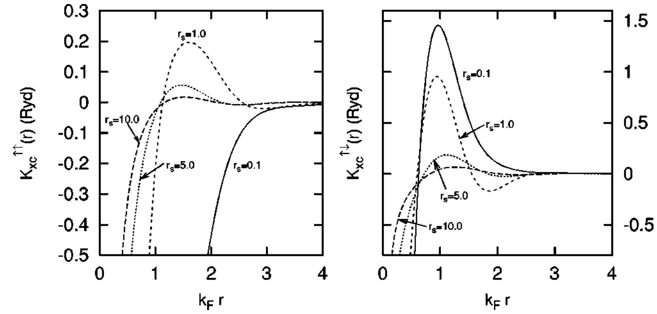

FIG. 3. The matrix elements $K_{\rm xc}^{\uparrow\uparrow}(r)$ and $K_{\rm xc}^{\uparrow\downarrow}(r)$ of the exchange-correlation kernel for various values of r_s.

In conclusion, we have presented an analytic parametrization of the local-field factor entering the spin response of the two-dimensional electron gas in the paramagnetic state, incorporating the known asymptotic behaviors and giving an accurate representation of the available quantum Monte Carlo data. We have obtained from it and from our earlier results on the dielectric response[5] analytic expressions of the exchange-correlation kernels for spin-density functional calculations on inhomogeneous two-dimensional electronic systems.

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