PHYSICAL REVIEW B **74**, 193108 (2006)

Analytic expression for the diamagnetic susceptibility of a uniform electron gas

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(Received 31 July 2006; revised manuscript received 29 September 2006; published 30 November 2006)

The diamagnetic (Landau) susceptibility is a key ingredient in current-density functional theory. We calculate this quantity of a uniform electron gas beyond the random-phase approximation and present an analytic expression for it which recovers the exact high-density limit.

DOI: 10.1103/PhysRevB.74.193108 PACS number(s): 71.15.Mb, 31.15.Ew, 71.45.Gm

Current-density functional theory (CDFT)[1,2] is a very useful extension of Kohn-Sham density functional theory[3] to describe a system in the presence of a magnetic field **B** which induces an orbital current of electrons. In this theory, the exchange-correlation (XC) energy must be approximated as a functional of the electron density $n(\mathbf{r})$ and the (paramagnetic) current density $\mathbf{j}_p(\mathbf{r})$ (Refs. 4–6)

$$\mathbf{j}_p(\mathbf{r}) = \frac{\hbar}{2mi}\sum_{k=1}^{\text{occup}}[\psi_k^*\nabla\psi_k - \psi_k\nabla\psi_k^*], \tag{1}$$

where ψ_k are the occupied Kohn-Sham orbitals. As shown by Tao and Perdew,[7,8] current-density functionals may be constructed from ordinary density functionals[9,10]: $E_{\rm xc}[n,\mathbf{j}_p] = E_{\rm xc}[n,\mathbf{j}_p=0] + \Delta E_{\rm xc}^{\rm VR}[n,\mathbf{j}_p]$, where

$$\Delta E_{\rm xc}^{\rm VR}[n,\mathbf{j}_p] = \int d^3r\, n\epsilon_{\rm x}^{\rm unif}(n)\frac{m}{18\pi n e^2}\left[1 - \frac{\chi_{\rm L}(n)}{\chi_{\rm L}^0(n)}\right] \times |\nabla\times(\mathbf{j}_p/n)|^2 \tag{2}$$

is the Vignale-Rasolt second-order energy shift[1,11] and $E_{\rm xc}[n,\mathbf{j}_p=0]$ is the gauge-invariant XC functional obtained by zeroing out the possible second-order energy shift contribution from an ordinary functional. Here $\epsilon_{\rm x}^{\rm unif}(n) = -e^2(3/4\pi)(3\pi^2 n)^{1/3}$ is the exchange energy per electron of the uniform gas, and $\chi_{\rm L}$ and $\chi_{\rm L}^0 = -e^2 v_{\rm F}/(12\pi^2 c^2)$, where $v_{\rm F}$ is the Fermi velocity and c is the speed of light, are the diamagnetic (Landau) susceptibilities of the interacting and noninteracting electron gas of uniform density n.

Practical application of current-density functional theory relies on the knowledge of the diamagnetic susceptibility of the interacting electron gas. Because of its significance in current-density functional theory, this quantity has received much attention in recent years. The problem is to calculate the effect of electron-electron interactions on the diamagnetic susceptibility $\chi_{\rm L}$. Several calculations[12–16] have been performed in this respect. In particular, making use of the double-time Green's-function method, Singh and Pathak[15] calculated the static part of the diamagnetic susceptibility by assuming the Coulomb interaction potential to be screened by the static Thomas-Fermi screening function. More than ten years later Vignale, Rasolt, and Geldart (VRG)[16] recalculated the diamagnetic susceptibility including the dynamical screening of the electron-electron interaction within the random phase approximation (RPA). Their result has been analytically parametrized by several authors[8,17,18] and has served as the standard input for current-density functional calculations in the weak magnetic field regime.

In their calculation VRG separated the dynamically screened electron-electron interaction into a statically screened component and a remainder, and calculated the contributions of these two parts separately before combining them in the final result. This suggests that the static and dynamical contributions to the diamagnetic susceptibility could be approximated independently.

In this paper we develop this idea by making use of the Singh and Pathak method [with the static structure factor obtained by Gori-Giorgi, Sacchetti, and Bachelet[19] (GSB)] to calculate the static component of the diamagnetic susceptibility of the interacting uniform electron gas. Then we follow VRG in the calculation of the dynamical part of $\chi_{\rm L}$ within the RPA; but in doing this we employ the Perdew-Wang[20] RPA chemical potential, which is more accurate than the von Barth-Hedin[21] RPA chemical potential used by VRG. Finally we present an analytic expression which reproduces the calculated $\chi_{\rm L}$ in the range for $r_s = 0-20$.

Consider an interacting electron gas of uniform density n. In the static ($\omega\to 0$) and the long-wavelength ($q\to 0$) limit, the Fourier transform of the tranverse current-current response function $\chi_{\rm T}$ is related to the Landau (L) diamagnetic susceptibility of the system through the relation (Refs. 12 and 22)

$$\chi_{\rm L} = -\lim_{q\to 0}\frac{e^2}{c^2 q^2}\left[\chi_{\rm T}(q,0) + \frac{n}{m}\right]. \tag{3}$$

Singh and Pathak[15] calculated the static and long-wavelength limit of the tranverse current-current response $\chi_{\rm T}(q,0)$ by making use of the (Hartree-Fock-like) mode-decoupling approximation for the four-point functions (i.e., the average of the product of four operators). Assuming the Coulomb interaction to be screened by the static Thomas-Fermi screening function

$$V_{\rm TF}(\mathbf{q}) = \frac{4\pi e^2}{q^2 + 4k_{\rm F}^2\lambda}, \tag{4}$$

where $\lambda = \alpha r_s/\pi$ and $\alpha = (4/9\pi)^{1/3}$, they obtained

TABLE I. Values of γ.

r_s	0.1	0.2	0.5	1	2	3	4	5	6	7	8	9	10
γ	0.392	0.402	0.425	0.451	0.484	0.506	0.523	0.536	0.547	0.556	0.564	0.571	0.578

$$\chi_{\mathrm{T}}(q,0) = \frac{\chi_{\mathrm{T}}^0(q,0)}{1 - F(q,0)}, \tag{5}$$

where $\chi_{\mathrm{T}}^0(q,0)=v_F q^2/(12\pi^2)-n/m$ is the noninteracting version of the tranverse current-current response and

$$F(q,0) = -\frac{(4+6\lambda)/(1+\lambda)-(1+6\lambda)\ln(1+1/\lambda)}{1+4\lambda\gamma/3}\frac{q^2\lambda}{24k_{\mathrm{F}}^2}, \tag{6}$$

$$\gamma = -\frac{1}{2k_{\mathrm{F}}}\int_0^\infty dq[S(q)-1]. \tag{7}$$

In Eq. (7), $S(q)$ is the static structure factor.[2,19,23] Substituting Eqs. (5) and (6) into Eq. (3) and taking the $q\to 0$ limit, the contribution of the static part of the interaction to the diamagnetic susceptibility is then obtained as

$$(\chi_{\mathrm{L}}^{\mathrm{int}})_{\mathrm{static}} = \chi_{\mathrm{L}}^0 \frac{(4+6\lambda)/(1+\lambda)-(1+6\lambda)\ln(1+1/\lambda)}{1+4\lambda\gamma/3}\frac{\lambda}{6}. \tag{8}$$

Notice that γ takes into account the XC effects beyond RPA. [γ would vanish if we were to ignore the Pauli exclusion principle and Coulomb XC effects, because in that case $S(q)=1$.]

We now turn to the dynamical part. Within the RPA, VRG (Ref. 16) derived

$$\chi_{\mathrm{L}}^{\mathrm{int}} = -\frac{e^2}{m^2c^2}\int\frac{d^3q}{(2\pi)^3}\int\frac{d\omega}{2\pi i}\, v(\mathbf{q},\omega)I(\mathbf{q},\omega) + \frac{\Sigma(k_{\mathrm{F}},\mu)}{12\pi^2 k_{\mathrm{F}}}, \tag{9}$$

where $\Sigma(k_{\mathrm{F}},\mu)=\partial(n\epsilon_{\mathrm{xc}}^{\mathrm{RPA}})/\partial n$ is the RPA XC contribution to the chemical potential[24] at the Fermi surface. $I(\mathbf{q},\omega)$ can be calculated analytically[25,26] from the noninteracting Green's function. VRG divided the RPA dynamically screened interaction into a statically screened Thomas-Fermi part and a dynamical part,

$$V(\mathbf{q},\omega) = \frac{4\pi e^2}{q^2+4k_{\mathrm{F}}^2\lambda} + \left[\frac{4\pi e^2}{q^2\epsilon(\mathbf{q},\omega)} - \frac{4\pi e^2}{q^2+4k_{\mathrm{F}}^2\lambda}\right], \tag{10}$$

and calculated separately the contribution of each part to the diamagnetic susceptibility. While the contribution of static part has the simple analytic expression

$$(\chi_{\mathrm{L}}^{\mathrm{int}})_{\mathrm{TF}} = \chi_{\mathrm{L}}^0\left[\frac{4+6\lambda}{1+\lambda} - (1+6\lambda)\ln\left(1+\frac{1}{\lambda}\right)\right]\frac{\lambda}{6}, \tag{11}$$

[i.e., Eq. (8) with $\gamma=0$], the dynamical part is the sum of three terms,

$$(\chi_{\mathrm{L}}^{\mathrm{int}})_{\mathrm{dyn}} = -\chi_{\mathrm{L}}^0\frac{12\pi^2}{v_{\mathrm{F}}}\left[(P_2^{\mathrm{int}})_{\mathrm{dyn}} + \frac{\Sigma(k_{\mathrm{F}},\mu)-\Sigma_{\mathrm{TF}}(k_{\mathrm{F}})}{12\pi^2 k_{\mathrm{F}}} + (P_2^\infty)_{\mathrm{dyn}}\right], \tag{12}$$

where

$$(P_2^{\mathrm{int}})_{\mathrm{dyn}} = \frac{2e^2}{\pi^4}\int_0^\infty dx\, x^3\int_0^\infty dy\,\tilde{I}(x,y) \times\left[\frac{1}{x^2+\lambda R(x,y)} - \frac{1}{x^2+\lambda}\right], \tag{13}$$

with $x=q/2k_{\mathrm{F}}$, $y=\omega/iqv_{\mathrm{F}}$, and $\tilde{I}(x,y)=4\pi^2v_{\mathrm{F}}^3I(x,y)$ being a dimensionless function defined below, $\Sigma_{\mathrm{TF}}(k_{\mathrm{F}})=-(e^2k_{\mathrm{F}}/\pi)\times[1+\lambda\ln(1+1/\lambda)-2\lambda^{1/2}\tan^{-1}(1/\lambda^{1/2})]$ the Thomas-Fermi self-energy, and $(P_2^\infty)_{\mathrm{dyn}}=e^2\lambda^{1/2}/12\pi^2$. Here $R(x,y)$ is a dimensionless function[25,26] defined by

$$R(x,y) = -\frac{\mathrm{Re}\,\chi^0(x,y)}{2N(0)}, \tag{14}$$

where $N(0)=m^2v_{\mathrm{F}}/2\pi^2$ and $\mathrm{Re}\,\chi^0(x,y)$ is the real part of the Lindhard function[2] given by

TABLE II. Diamagnetic Landau susceptibility de-enhancement $\chi_{\mathrm{L}}/\chi_{\mathrm{L}}^0$.

	$\chi_{\mathrm{L}}/\chi_{\mathrm{L}}^0$	
r_s	Present	RPA
0.01	0.999	0.999
0.1	0.994	0.994
0.5	0.987	0.987
1.0	0.981	0.982
2.0	0.968	0.971
3.0	0.951	0.957
4.0	0.935	0.943
5.0	0.918	0.927
6.0	0.901	0.911
7.0	0.884	0.895
8.0	0.867	0.879
9.0	0.851	0.863
10.0	0.835	0.847
12.0	0.804	0.817
14.0	0.774	0.787
16.0	0.747	0.759
18.0	0.720	0.732
20.0	0.697	0.709

TABLE III. Parameters of Eq. (20).

	a_2	a_3	a_4	a_5	a_6	a_7	a_8	a_9	a_{10}
RPA	2.8	1.1029	−0.4995	0.4425	−0.0664	0.00086	0.041	0.027	0.041
Present	2.5	1.1	−0.49	0.438	−0.07	0.00182	0.054	0.02	0.05

$$\mathrm{Re}\,\chi^0(x,y) = -2N(0)\left\{\frac{1}{2} - \frac{1}{4x}\,\mathrm{Re}\left[(\alpha_-^2-1)\ln\left(\frac{\alpha_- -1}{\alpha_- +1}\right)\right]\right\}, \tag{15}$$

with $\alpha_- = iy - x$. The crucial function $\widetilde{I}(x,y)$ can be calculated analytically following the procedures described by Ma and Brueckner (MB) in their pioneering work on gradient corrections.[25] The result is

$$\widetilde{I} = \frac{1}{48x^3}\ln\frac{(x+1)^2+y^2}{(x-1)^2+y^2} + \mathrm{Re}\left[\frac{1+2x^2}{12x^3}\left(\frac{\alpha_-}{\alpha_-^2-1}\right) - \frac{1+4x^2}{18x^3}\frac{\alpha_-}{(\alpha_-^2-1)^2} - \frac{2}{9x^2}\frac{1}{(\alpha_-^2-1)^2}\right]. \tag{16}$$

The diamagnetic susceptibility of the interacting electron gas is the sum of three terms,

$$\chi_{\mathrm{L}} = \chi_{\mathrm{L}}^0 + (\chi_{\mathrm{L}}^{\mathrm{int}})_{\mathrm{static}} + (\chi_{\mathrm{L}}^{\mathrm{int}})_{\mathrm{dyn}}, \tag{17}$$

where the last two terms are from the Coulomb interaction. The corresponding RPA version is just to replace the second term $(\chi_{\mathrm{L}}^{\mathrm{int}})_{\mathrm{static}}$ on the right-hand side of Eq. (17) with $(\chi_{\mathrm{L}}^{\mathrm{int}})_{\mathrm{TF}}$ of Eq. (11).

From Eq. (8) we can see that the static part of the diamagnetic susceptibility depends upon the γ value of Eq. (7). It is clear from Eqs. (8) and (11) that within the RPA, $(\chi_{\mathrm{L}}^{\mathrm{int}})_{\mathrm{static}}$ reduces exactly to $(\chi_{\mathrm{L}}^{\mathrm{int}})_{\mathrm{TF}}$, as we have seen, because γ vanishes identically within the RPA, suggesting that the dynamical part was completely ignored in the Sing-Pathak calculation. At the exchange-only level, i.e., $S(q)=S_0(q)$, where

$$S_0(q) = \begin{cases} \dfrac{3}{4}\dfrac{q}{k_{\mathrm{F}}} - \dfrac{1}{16}\dfrac{q^3}{k_{\mathrm{F}}^3}, & 0 \le q \le 2k_{\mathrm{F}}, \\ 1, & q \ge 2k_{\mathrm{F}}. \end{cases} \tag{18}$$

is the static structure factor of the noninteracting electron gas, $\gamma = 3/8$. In the present work, γ is evaluated using the more accurate GSB parametrization[19] of the static structure factor. The results are displayed in Table I. We observe that with these values of γ the static contribution to χ_{L} is slightly smaller than in the exchange-only approximation. This tendency becomes stronger at lower densities, reflecting the fact that in the low-density region the correlation is more important, and more correction to the exchange-only result is needed. However, the value of γ does not affect the leading contribution to the high-density expansion [Eq. (19)] where the RPA is exact. $\Sigma(k_{\mathrm{F}},\mu)$ needed in the calculation of the second term of $(\chi_{\mathrm{L}}^{\mathrm{int}})_{\mathrm{dyn}}$ may be calculated using the Perdew-Wang parametrization[20] of $\epsilon_{\mathrm{xc}}^{\mathrm{RPA}}$. The results are shown in Table II. The corresponding RPA values are also listed for comparision.

From Table II we can see that the diamagnetic susceptibility of an interacting electron gas is slightly smaller than the the corresponding RPA value, as expected, suggesting a stronger effect of the Coulomb interaction on the diamagnetic susceptibility of the noninteracting electron gas than the RPA screened interaction. In the high-density limit, Eq. (8) gives the exact behavior

$$\chi_{\mathrm{L}} = \chi_{\mathrm{L}}^0\left[1 + \frac{\alpha r_s}{6\pi}\ln r_s\right]. \tag{19}$$

Since the diamagnetic susceptibility in the high-density limit may be important for a finite system, our analytic parametrization should reproduce this limit exactly. The fit proposed by Tao and Perdew satisfied this requirement. On the other hand, while in the original RPA calculation of VRG the RPA XC potential was evaluated from the Hedin-von Barth[21] parametrization of the RPA XC energy per electron, in the present calculation the Perdew-Wang RPA parametrization is used instead. To account for this small difference, we reparametrize our RPA calculation by slightly adjusting the parameters of Eq. (21) of Ref. 8. For simplicity, we use the same form for our diamagnetic susceptibility de-enhancement

$$\chi_{\mathrm{L}}/\chi_{\mathrm{L}}^0 = [(1 + a_1 r_s \ln r_s)e^{-a_2 r_s} + (1 - e^{-a_2 r_s}) \times (a_3 + a_4 r_s^{1/3} + a_5 r_s^{1/2} + a_6 r_s + a_7 r_s^2)]e^{-a_8 r_s} + (1 - e^{-a_8 r_s})(1 + a_9 r_s)e^{-a_{10} r_s}, \tag{20}$$

where $a_1 = \alpha/6\pi$ determined by the high-density limit of Eq. (19). All other parameters fixed by a fit to the numerical data

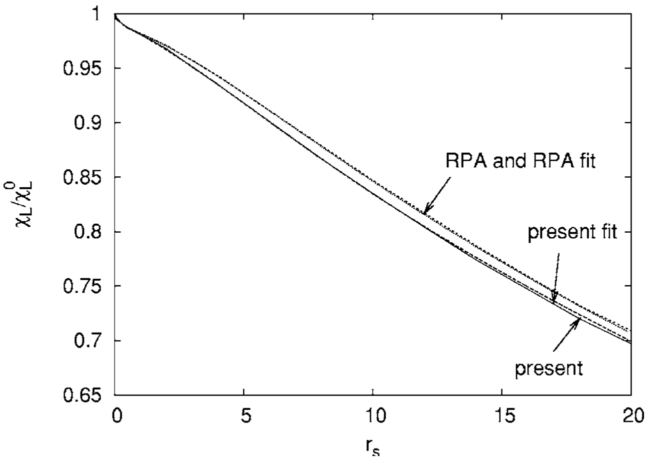

FIG. 1. Diamagnetic Landau susceptibility de-enhancement $\chi_{\mathrm{L}}/\chi_{\mathrm{L}}^0$ as a function of r_s: the numerical values (present) and the parametrization of Eq. (17) (present fit), and the numerical RPA values (RPA) and the parametrization (RPA fit).

in Table II are given in Table III. In Fig. 1, we compare the analytic expression of the diamagnetic susceptibility deenhancement with the numerical values in Table II. The corresponding numerical RPA and the parametrization are also displayed in Fig. 1 for comparison. Since the diamagnetic susceptibility proposed in this work is smaller than the corresponding RPA value, this may improve the description of the current-density meta-generalized gradient approximation functional for atomic and molecular degeneracy problems.[27]

In conclusion, we have presented a parametrization of the diamagnetic susceptibility of the interacting uniform electron gas. Our analytic form fits the numerical data with remarkable accuracy and thus may improve the performance of current-density functionals when the density is away from the high-density regime.

This work was supported by DOE under Grant No. DE-FG02-05ER46203. We acknowledge very helpful discussions with John P. Perdew. Part of the computational work was done at Tulane University.

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