Spin-resolved second-order correlation energy of the two-dimensional uniform electron gas

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Abstract. For the two-dimensional electron gas, the exact high-density limit of the correlation energy is evaluated here numerically for all values of the spin polarization. The result is spin-resolved into $\uparrow\uparrow$, $\uparrow\downarrow$, and $\downarrow\downarrow$ contributions and parametrized analytically. Interaction-strength interpolation yields a simple model (LSD) for the correlation energy at finite densities.

In recent years, two-dimensional (2D) electron systems have become the subject of extensive research [1]. The 2D version of density functional theory (DFT) has proven particularly successful in studying quantum dots [2, 3, 4]. The local spin-density approximation (LSD) of DFT requires the correlation energy of the spin-polarized uniform electron gas. This quantity in 2D is known accurately for a wide range of densities and spin polarizations from fixed-node diffusion Monte Carlo simulations [5]. Its high-density limit is known exactly in terms of six-dimensional momentum-space integrals [6]. Resolved into contributions due to $\uparrow\uparrow$, $\uparrow\downarrow$, and $\downarrow\downarrow$ excitation electron pairs, these integrals are evaluated here numerically. The analytical parametrization of the results, Eqs. (16) and (17) below, is a crucial ingredient for the construction of the spin-resolved correlation energy at finite densities, performed recently for the 3D electron gas [7]. It is also required for studying the magnetic response of the spin-polarized 2D electron gas [8, 9]. Generally, it provides a fundamental test for numerical parametrizations of the correlation energy [5].

In the 2D uniform electron gas, the electrons are moving on a plane at uniform density $\rho=\frac{\pi (r_s a_B)^2}{2}$, where $a_B=0.529$ Å is the Bohr radius and $r_s$ is the dimensionless density parameter (Seitz radius). We consider lowest-energy states with a given spin polarization

$$\zeta \equiv \frac{\rho_\uparrow - \rho_\downarrow}{\rho},$$

where $\rho_\uparrow$ and $\rho_\downarrow \equiv \rho - \rho_\uparrow$, respectively, are the (uniform) densities of spin-up and spin-down electrons. Including a neutralizing positive background, the total energy per electron is a unique function of the dimensionless parameters $r_s$ and $\zeta$,

$$e_{\text{tot}}(r_s, \zeta) = t_s(r_s, \zeta) + e_x(r_s, \zeta) + e_c(r_s, \zeta).$$

The non-interacting kinetic and exchange energies,

$$t_s(r_s, \zeta) = \frac{1 + \zeta^2}{2} \frac{1}{r_s^2}, \quad e_x(r_s, \zeta) = -\frac{4\sqrt{2}}{3\pi} \left( \frac{1+\zeta}{2} \right)^{3/2} \left( \frac{1-\zeta}{2} \right)^{3/2} \frac{1}{r_s}$$

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(all energies are given in units of 1 Ha $\equiv e^2/a_B = 27.21$ eV in the following), may be understood as the 0th- and the 1st-order terms of a perturbation expansion for the electron-electron interaction (where $r_s$ turns out to be the expansion parameter).

The remaining correlation energy in Eq. (2) appears to have the perturbation (high-density) expansion \[10, 11\]

\[
e_c(r_s, \zeta) = \sum_{n=0}^{\infty} \left[ a_n(\zeta) \ln(r_s) + b_n(\zeta) \right] r_s^n \quad (r_s \ll 1).
\] (4)

For the 2D electron gas (but not for the 3D one), the first coefficient vanishes, $a_0(\zeta) \equiv 0$. Consequently, the second-order ($n = 0$) term is $e_c^{(2)}(\zeta) \equiv b_0(\zeta)$, representing the high-density ($r_s \to 0$) limit of $e_c(r_s, \zeta)$. It can be split into an exchange ("2b") and a ring-diagram ("2r") term \[6\],

\[
e_c^{(2)}(\zeta) = e_c^{(2b)} + e_c^{(2r)}(\zeta).
\] (5)

The exchange term has only equal-spins contributions, $e_c^{(2b)} = e_c^{(2b)}(\uparrow\uparrow) + e_c^{(2b)}(\downarrow\downarrow)$, given by the $\delta_{\sigma_1\sigma_2}$ term of Eq. (14) in Ref. \[6\] (we choose the $k_x$ axis in the direction of $q$),

\[
e_c^{(2b)}(\zeta) = \frac{1}{8\pi^2} \int_0^\infty dq \int A[\kappa, q] d^2k_1 \int A[\kappa, q] d^2k_2 \frac{1}{q + k_{1x} + k_{2x}}.
\] (6)

Here, $q$, $k_1$, and $k_2$ are dimensionless, $\sigma \in \{\uparrow, \downarrow\}$, and the domain of the 2D integrals is

\[
A[\kappa, q] \equiv \left\{ k \in \mathbb{R}^2 \mid |k| < \kappa, \quad |q + q e_x| > \kappa \right\}, \quad \kappa(\zeta) \equiv \left[ 1 + \text{sgn}(\zeta) \right]^{1/2}.
\] (7)

[$\kappa(\zeta)$ is the Fermi wave vector for spin-$\sigma$ electrons in units of its value at $\zeta = 0$.] Scaling the integration variables by some constant $\kappa$, $q = \kappa Q$ and $k = \kappa K$, we have generally

\[
\int_0^\infty dq A[\kappa, q] = \kappa^2 \int_0^\infty Q A[1, Q] = \kappa^2 \int_0^\infty K A[1, K].
\] (8)

Applying this rule to the integrals in Eq. (6), we find \[6\]

\[
e_c^{(2b)}(\zeta) = \left[ 1 + \text{sgn}(\zeta) \right] J^{(2b)}.
\] (9)

Consequently \[6\], the full second-order exchange term $e_c^{(2b)} = e_c^{(2b)}(\uparrow\uparrow) + e_c^{(2b)}(\downarrow\downarrow) \equiv 2J^{(2b)}$ is $\zeta$-independent. A Monte Carlo integration yields

\[
J^{(2b)} \equiv e_c^{(2b)}(0) = (57.15 \pm 0.05) \text{ mHa} \quad (1\text{ mHa} = 10^{-3}\text{ Ha}).
\] (10)
The ring-diagram term \( e_c^{(2r)}(\zeta) \) is the remaining part of expression (14) in Ref. [6], with the contributions

\[
e_c^{(2r)}(\zeta) = -\frac{1}{8\pi^2} \int_0^\infty dq \frac{d^2k_1}{q^2} (A[\kappa_{\sigma_1}(\zeta),q] \int d^2k_2 \frac{1}{q + k_{1x} + k_{2x}}).
\]

The equal-spins terms \((\sigma_1 = \sigma_2)\) can be treated in the same way as the integral (6),

\[
e_c^{(2r)}_{\sigma_1\sigma_2}(\zeta) = -\left[1 + \text{sgn}(\sigma_1)\zeta\right] J^{(2r)}, \\
J^{(2r)} = (76.69 \pm 0.03) \text{mHa}.
\]

The only non-trivial \(\zeta\)-dependence is in the opposite-spins term \(e_c^{(2r)}(\zeta) \equiv e_{c_{\uparrow \downarrow}^{(2r)}}(\zeta)\),

\[
e_{c_{\uparrow \downarrow}^{(2r)}}(\zeta) = e_{c_{\uparrow \downarrow}^{(2r)}}(0) \left[1 - f(\zeta)\right].
\]

By definition, \(f(0) = 0\), and, since \(A[\kappa_{\downarrow}(1),q] = \emptyset, f(1) = 1\). Moreover, \(e_{c_{\uparrow \downarrow}^{(2r)}}(0) = -J^{(2r)}\).

When the results of a Monte Carlo evaluation of \(f(\zeta)\) at different values of \(\zeta\) are compared with the functions \(f_\alpha(\zeta) \equiv [(1+\zeta)^\alpha + (1-\zeta)^\alpha - 2]/(2^\alpha - 2)\), particularly good agreement (specially for \(\zeta \rightarrow 0\) and \(\zeta \rightarrow 1\)) is found in the limit \(\alpha \rightarrow 1\) (Fig. 1a),

\[
f(\zeta) = f_1(\zeta) + \delta f(\zeta), \\
f_1(\zeta) \equiv \frac{(1+\zeta) \ln(1+\zeta) + (1-\zeta) \ln(1-\zeta)}{2 \ln 2}.
\]

[Note that \(f_\alpha(\zeta)\) also represents the \(\zeta\)-dependence of \(t_s\) \((\alpha = 2)\) and \(e_x(\alpha = \frac{3}{2})\) in Eq. [3].] The small deviation \(\delta f(\zeta)\) is accurately fitted by a polynomial (Fig. 1b)

\[
\delta f(\zeta) \approx 0.0636 \zeta^2 - 0.1024 \zeta^4 + 0.0389 \zeta^6.
\]

The small minimum of \(\delta f(\zeta)\) indicated by the numerical data (dots in Fig. 1b) at \(\zeta \approx 0.98\) is probably real, since a similar peculiarity is observed for the 3D electron gas (see the inset in Fig. 1 of Ref. [12]).

In summary, the second-order correlation energy \(e_c^{(2)}(\zeta) \equiv e_c^{(2b)} + e_c^{(2r)}(\zeta)\) is

\[
e_c^{(2)}(\zeta) \equiv e_{c_{\uparrow \downarrow}^{(2)}}(\zeta) + 2e_{c_{\uparrow \downarrow}^{(2)}}(\zeta) + e_{c_{\uparrow \downarrow}^{(2)}}(\zeta) = [153.38 f(\zeta) - 192.46] \text{mHa},
\]

where \(f(\zeta)\) is given by Eqs. [14] and [15]. The spin resolution is fixed by

\[
e_{c_{\uparrow \downarrow}^{(2)}}(\zeta) \equiv e_{c_{\downarrow \downarrow}^{(2)}}(-\zeta) = -(1 + \zeta) \times 19.54 \text{mHa}.
\]

\(e_c^{(2)}(\zeta) \equiv e_c(0,\zeta)\) is the high-density limit of the general correlation energy \(e_c(r_s,\zeta)\). To illustrate the relevance of this limit for finite densities \((r_s > 0)\), the present result can be used in the interaction-strength interpolation (ISI) of Ref. [13]. This approach does not require the higher-order \((n \geq 1)\) terms of the expansion [14] (which is expected
to have only a finite radius of convergence). Instead, information beyond the second order is taken from the low-density (strong-interaction or Wigner-crystal) limit of the exchange-correlation energy \( e_{xc} \equiv e_x + e_c \) (per electron),

\[
e_{xc}(r_s, \zeta) \to \frac{a_{\infty}}{r_s} + \frac{b_{\infty}}{r_s^{3/2}} \quad (r_s \to \infty).
\]

The coefficients \( a_{\infty} \approx -1.1061 \) and \( b_{\infty} \approx \frac{1}{2} \) are independent of \( \zeta \), since any spatial overlap between two electrons is strongly suppressed in this limit, no matter whether their spins are parallel or not \[15\]. The resulting ISI expression for the exchange-correlation energy at finite densities reads \[13\]

\[
e_{xc}^{ISI}(r_s, \zeta) = \frac{a_{\infty}}{r_s} + \frac{2 X}{Y} \left[ (1 + Y)^{1/2} - 1 - Z \ln \left( \frac{(1 + Y)^{1/2} + Z}{1 + Z} \right) \right].
\]

Using \( b_{\infty} = \frac{1}{2} \) and writing \( e_x(r_s, \zeta) = c_x(\zeta)/r_s \), we have explicitly \[13\]

\[
X(r_s, \zeta) = \frac{-b_0(\zeta)}{[c_x(\zeta) - a_{\infty}]^2} \frac{1}{r_s}, \\
Y(r_s, \zeta) = \frac{4 b_0(\zeta)^2}{[c_x(\zeta) - a_{\infty}]^4} r_s, \\
Z(\zeta) = \frac{-b_0(\zeta)}{[c_x(\zeta) - a_{\infty}]^3} - 1.
\]

Eq. (19) provides a simple explicit LSD,

\[
E_{xc}^{LSD}[\rho_\uparrow, \rho_\downarrow] = \int d^2 r \rho(\mathbf{r}) e_{xc}^{ISI}(r_s(\mathbf{r}), \zeta(\mathbf{r})),
\]

for treating arbitrary 2D electron systems (also finite ones such as quantum dots) by the Kohn-Sham Equations of DFT. In Eq. (21), \( r_s(\mathbf{r}) = a_B^{-1}[\pi \rho(\mathbf{r})]^{-1/2} \) and \( \zeta(\mathbf{r}) = [\rho_\uparrow(\mathbf{r}) - \rho_\downarrow(\mathbf{r})]/\rho(\mathbf{r}) \).

In Fig. 2a, the ISI prediction \( e_{xc}^{ISI}(r_s, \zeta) = e_{xc}^{ISI} - e_x \) for the correlation energy of the unpolarized uniform electron gas (\( \zeta = 0 \)) is compared with the accurate parametrization of the fixed-node diffusion Monte Carlo results in Ref. \[5\]. \( e_{xc}^{ISI} \) differs slightly from the latter by up to 4%. This mild deviation might be cured by including in the ISI a simple model for the next-order coefficient of expansion \[14\] \[16\]. In the high-density limit \( (r_s \to 0) \), however, where the present result is exact, the parametrization in Ref. \[5\] has for \( 0.7 < \zeta < 0.95 \) a small positive deviation \[5\], shown in Fig. 2b.
Figure captions:

Fig. 1. (a) Numerical results (dots) for the function $f(\zeta)$ of Eq. (13) obtained by Monte Carlo integrations of expression (11) (with $\sigma_1 \sigma_2 = \uparrow \downarrow$) at selected values of $\zeta$. The analytical function $f_1(\zeta)$ of Eq. (14) is plotted as a dashed curve. The solid curve represents the accurate fit $f_1(\zeta) + \delta f(\zeta)$, using Eq. (15) for $\delta f(\zeta)$. (b) The fit (solid curve) compared to the true deviation (dots) of the Monte-Carlo-integration results from $f_1(\zeta)$.

Fig. 2. The correlation energy of Ref. [5] (dotted curves) versus the present ISI results (solid curves).

References

[1] E. Abrahams, S. V. Kravchenko, and M. P. Sarachik, Rev. Mod. Phys. 73, 251 (2001).
[2] S.M. Reimann and M. Manninen, Rev. Mod. Phys. 74, 1283 (2002).
[3] H. Jiang, H.U. Baranger, and W. Yang, Phys. Rev. B 68, 165337 (2003).
[4] H. Saarikoski, E. Räsänen, S. Siljamäki, A. Harju, M.J. Puska, R.M. Nieminen, Phys. Rev. B 67, 205327 (2003).
[5] C. Attaccalite, S. Moroni, P. Gori-Giorgi, and G. B. Bachelet, Phys. Rev. Lett. 88, 256601 (2002).
[6] A.K. Rajagopal and J.C. Kimball, Phys. Rev. B 15, 2819 (1977).
[7] P. Gori-Giorgi and J.P. Perdew, Phys. Rev. B (to appear; cf. cond-mat/0305250).
[8] J. Moreno and D.C. Marinescu, Phys. Rev. B 68, 195210 (2003).
[9] M. Polini and M.P. Tosi, Phys. Rev. B 63, 045118 (2001).
[10] W. Macke, Z. Naturforsch. A 5A, 192 (1950).
[11] W.J. Carr and A.A. Maradudin, Phys. Rev. 133, A371 (1964).
[12] G.G. Hoffman, Phys. Rev. B 45, 8730 (1992).
[13] M. Seidl, J.P. Perdew, and S. Kurth, Phys. Rev. Lett. 84, 5070 (2000).
[14] L. Bonsall and A.A. Maradudin, Phys. Rev. B 15, 1959 (1977).
[15] M. Seidl, J.P. Perdew, and S. Kurth, Phys. Rev. A 62, 012502 (2000).
[16] M. Seidl and J.P. Perdew (unpublished).
Figure 1: (a) Numerical results (dots) for the function $f(\zeta)$ of Eq. (13) obtained by Monte Carlo integrations of expression (11) (with $\sigma_1 \sigma_2 = \uparrow \downarrow$) at selected values of $\zeta$. The analytical function $f_1(\zeta)$ of Eq. (14) is plotted as a dashed curve. The solid curve represents the accurate fit $f_1(\zeta) + \delta f(\zeta)$, using Eq. (15) for $\delta f(\zeta)$. (b) The fit (solid curve) compared to the deviation (dots) of the Monte-Carlo-integration results from $f_1(\zeta)$. 
Figure 2: The correlation energy of Ref. [5] (dotted curves) versus the present ISI results (solid curves).