Exact energy of the spin-polarized two-dimensional electron gas at high density

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(Dated: January 14, 2013)

Abstract

We derive the exact expansion, to $O(r_s)$, of the energy of the high-density spin-polarized two-dimensional uniform electron gas, where $r_s$ is the Seitz radius.

PACS numbers: 71.10.Ca, 73.20.-r, 31.15.E-

Keywords: jellium; uniform electron gas; correlation energy; high-density limit
The three-dimensional uniform electron gas is a ubiquitous paradigm in solid-state physics and quantum chemistry, and has been extensively used as a starting point in the development of exchange-correlation density functionals in the framework of density-functional theory. The two-dimensional version of the electron gas has also been the object of extensive research because of its intimate connection to two-dimensional or quasi-two-dimensional materials, such as quantum dots.

The two-dimensional gas (or 2-jellium) is characterized by a density $\rho = \rho_\uparrow + \rho_\downarrow$, where $\rho_\uparrow$ and $\rho_\downarrow$ are the (uniform) densities of the spin-up and spin-down electrons, respectively. In order to guarantee its stability, the electrons are assumed to be embedded in a uniform background of positive charge. We will use atomic units throughout.

It is known from contributions by numerous workers that the high-density (i.e. small-$r_s$) expansion of the energy per electron (or reduced energy) in 2-jellium is

$$E(r_s, \zeta) = \frac{\varepsilon_{-2}(\zeta)}{r_s^2} + \frac{\varepsilon_{-1}(\zeta)}{r_s} + \varepsilon_0(\zeta) + \varepsilon_\ell(\zeta) r_s \ln r_s + O(r_s),$$

where $r_s = (\pi \rho)^{-1/2}$ is the Seitz radius, and

$$\zeta = \frac{\rho_\uparrow - \rho_\downarrow}{\rho}$$

is the relative spin polarization. Without loss of generality, we assume $\rho_\downarrow \leq \rho_\uparrow$, i.e. $\zeta \in [0, 1]$.

The first two terms of the expansion are the kinetic and exchange energies, and their sum gives the Hartree-Fock (HF) energy. The paramagnetic ($\zeta = 0$) coefficients are

$$\varepsilon_{-2}(0) = +\frac{1}{2},$$

$$\varepsilon_{-1}(0) = -\frac{4\sqrt{2}}{3\pi},$$

and their spin-scaling functions are

$$\Upsilon_{-2}(\zeta) = \frac{\varepsilon_{-2}(\zeta)}{\varepsilon_{-2}(0)} = \frac{(1-\zeta)^2 + (1+\zeta)^2}{2},$$

$$\Upsilon_{-1}(\zeta) = \frac{\varepsilon_{-1}(\zeta)}{\varepsilon_{-1}(0)} = \frac{(1-\zeta)^{3/2} + (1+\zeta)^{3/2}}{2}.$$
The logarithmic coefficient \( \varepsilon_\ell(\zeta) \) can be obtained by a Gell-Mann–Brueckner resummation\(^{21}\) of the most divergent terms in the infinite series in (1), and this yields\(^{13}\)

\[
\varepsilon_\ell(\zeta) = -\frac{1}{12\sqrt{2}\pi} \int_{-\infty}^{\infty} \left[ R \left( \frac{u}{k_\uparrow} \right) + R \left( \frac{u}{k_\downarrow} \right) \right]^3 du,
\]

where

\[
R(u) = 1 - \frac{1}{\sqrt{1 + 1/u^2}},
\]

and

\[
k_{\uparrow, \downarrow} = \sqrt{1 \pm \zeta}
\]

is the Fermi wave vector associated with the spin-up and spin-down electrons, respectively. After an unsuccessful attempt by Zia\(^{11}\) the paramagnetic (\( \zeta = 0 \)) and ferromagnetic (\( \zeta = 1 \)) values,

\[
\varepsilon_\ell(0) = -\sqrt{2} \left( \frac{10}{3\pi} - 1 \right) = -0.0863136 \ldots,
\]

\[
\varepsilon_\ell(1) = \frac{1}{4\sqrt{2}} \varepsilon_\ell(0) = -\frac{1}{4} \left( \frac{10}{3\pi} - 1 \right) = -0.0152582 \ldots,
\]

were found by Rajagopal and Kimball\(^{13}\) and the spin-scaling function,

\[
\Upsilon_\ell(\zeta) = \frac{\varepsilon_\ell(\zeta)}{\varepsilon_\ell(0)} = \frac{1}{8} \left[ k_\uparrow + k_\downarrow + \frac{3F(k_\uparrow, k_\downarrow) + F(k_\downarrow, k_\uparrow)}{10 - 3\pi} \right],
\]

was obtained 30 years later by Chesi and Giuliani\(^{18}\) The explicit expression for \( F(x, y) \) is

\[
F(x, y) = 4(x + y) - \pi x - 4xE \left( \frac{1 - y^2}{x^2} \right) + 2x^2 \kappa(x, y),
\]

where

\[
\kappa(x, y) = \begin{cases} 
(x^2 - y^2)^{-1/2} \arccos(y/x), & x \leq y, \\
(y^2 - x^2)^{-1/2} \arccosh(x/y), & x > y,
\end{cases}
\]

and \( E(x) \) is the complete elliptic integral of the second kind\(^{22}\)

The constant coefficient \( \varepsilon_0(\zeta) \) can be written as the sum

\[
\varepsilon_0(\zeta) = \varepsilon_0^a(\zeta) + \varepsilon_0^b
\]

of a direct (“ring-diagram”) term \( \varepsilon_0^a(\zeta) \) and an exchange term \( \varepsilon_0^b \). Following Onsager’s work\(^{23}\) on the three-dimensional gas, the exchange term was found by Isihara and Ioriatti\(^{13}\) to be

\[
\varepsilon_0^b = \beta(2) - \frac{8}{\pi^2} \beta(4) = +0.114357 \ldots,
\]
where $\beta$ is the Dirichlet beta function and $G = \beta(2)$ is Catalan’s constant. We note that $\varepsilon^b_0$ is independent of $\zeta$ and the spin-scaling function therefore takes the trivial form

$$\Upsilon^b_0(\zeta) = \frac{\varepsilon^b_0(\zeta)}{\varepsilon^b_0(0)} = 1. \quad (17)$$

The direct term has not been found in closed form, but we now show how this can be achieved. Following Rajagopal and Kimball, we write the direct term as the double integral

$$\varepsilon^b_0(\zeta) = -\frac{1}{8\pi^3} \int_{-\infty}^{\infty} \int_0^\infty \left[ Q_{q/k_{\uparrow}}\left(\frac{u}{k_{\uparrow}}\right) + Q_{q/k_{\downarrow}}\left(\frac{u}{k_{\downarrow}}\right) \right]^2 dq\,du, \quad (18)$$

where

$$Q_q(u) = \frac{\pi}{q} \left[ q - \sqrt{\left(\frac{q}{2} - iu - 1\right) \left(\frac{q}{2} - iu + 1\right)} - \sqrt{\left(\frac{q}{2} + iu - 1\right) \left(\frac{q}{2} + iu + 1\right)} \right]. \quad (19)$$

In the paramagnetic ($\zeta = 0$) case, the transformation $s = q^2/4 - u^2$ and $t = qu$ yields

$$\varepsilon^b_0(0) = -\frac{1}{2\pi} \int_{-\infty}^{\infty} \int_0^\infty \frac{1}{\sqrt{s^2 + t^2}} \left[ 1 - \left(\frac{\sqrt{(s-1)^2 + t^2} + s - 1}{\sqrt{s^2 + t^2} + s}\right)^{1/2} \right]^2 dt\,ds. \quad (20)$$
and, if we adopt polar coordinates, this becomes

\[
\varepsilon_0^a(0) = -\frac{1}{2\pi} \int_0^\infty \int_0^\pi \left[ 1 - \sqrt{\frac{1 - 2r \cos \theta + r^2 - 1 + r \cos \theta}{r(1 + \cos \theta)}} \right]^2 d\theta dr
\]

\[
= -\frac{1}{2\pi} \int_0^\pi \left[ 2 \ln 2 - (\pi - \theta) \tan \frac{\theta}{2} - 2 \tan^2 \frac{\theta}{2} \ln \left( \sin \frac{\theta}{2} \right) \right] d\theta
\]

\[
= \ln 2 - 1
\]

\[
= -0.306853 \ldots,
\]

which confirms Seidl’s numerical estimate

\[
\varepsilon_0^a(0) = -0.30682 \pm 0.00012.
\] (22)

In the ferromagnetic (\(\zeta = 1\)) case, Eq. (18) yields

\[
\varepsilon_0^a(1) = \frac{1}{2} \varepsilon_0^a(0) = \frac{\ln 2 - 1}{2} = -0.153426 \ldots.
\] (23)

In intermediate cases, where \(0 < \zeta < 1\), we define the spin-scaling function

\[
\Upsilon_0^a(\zeta) = \frac{\varepsilon_0^a(\zeta)}{\varepsilon_0^a(0)},
\] (24)

and, from (18), we have

\[
\Upsilon_0^a(\zeta) = \frac{1}{2} - \frac{1}{4\pi(\ln 2 - 1)} \int_0^\infty \int_{-1}^1 P_{k_\uparrow}(r, z) P_{k_\downarrow}(r, z) \frac{idz}{z} dr,
\] (25)

where

\[
P_k(r, z) = 1 - \frac{\sqrt{rz - k^2} + \sqrt{r/z - k^2}}{\sqrt{r}(\sqrt{z} + 1/\sqrt{z})}.
\] (26)

Integrating over \(r\) gives

\[
\Upsilon_0^a(\zeta) = \frac{1}{2} - \frac{1}{4\pi(\ln 2 - 1)} \int_{-1}^1 L_{k_\uparrow, k_\downarrow}(z) \frac{idz}{z},
\] (27)

where

\[
L_{k_\uparrow, k_\downarrow}(z) = -k_\uparrow \ln k_\uparrow - k_\downarrow \ln k_\downarrow
\]

\[
+ \frac{1}{(z + 1)^2} \left[ (zk_\uparrow - k_\downarrow)^2 \ln(zk_\uparrow - k_\downarrow) + (zk_\downarrow - k_\uparrow)^2 \ln(zk_\downarrow - k_\uparrow)
\]

\[
- i\pi(k_\uparrow^2 - 2zk_\uparrow k_\downarrow + k_\downarrow^2) + 2z(k_\uparrow + k_\downarrow)^2 \ln(k_\uparrow + k_\downarrow) - z(zk_\uparrow^2 - 2k_\uparrow k_\downarrow + zk_\downarrow^2) \ln z \right],
\] (28)
TABLE I. Energy coefficients and spin-scaling functions for 2-jellium in the high-density limit.

| Term          | Coefficient | \(\varepsilon(0)\) | \(\varepsilon(1)\) | \(\Upsilon(\zeta)\) |
|---------------|-------------|---------------------|---------------------|----------------------|
| \(r_s^{-2}\)  | \(\varepsilon_{-2}(\zeta)\) | \(\frac{1}{2}\)     | 1                   | Eq. (5)              |
| \(r_s^{-1}\)  | \(\varepsilon_{-1}(\zeta)\) | \(-\frac{4\sqrt{2}}{3\pi}\) | \(-\frac{8}{3\pi}\) | Eq. (6)              |
| \(r_s^{0}\)   | \(\varepsilon_{0}^a(\zeta)\) | \(\ln 2 - 1\)      | \(\frac{\ln 2 - 1}{2}\) | Eq. (29)             |
| \(r_s\ln r_s\)| \(\varepsilon_{\ell}(\zeta)\) | \(-\sqrt{2}\left(\frac{10}{3\pi} - 1\right)\) | \(-\frac{1}{4}\left(\frac{10}{3\pi} - 1\right)\) | Eq. (12)             |

and contour integration over \(z\) eventually yields

\[
\Upsilon_{0}^{a}(\zeta) = \frac{1}{2} + \frac{1 - \zeta}{4(\ln 2 - 1)} \left[ 2\ln 2 - 1 - \sqrt{\frac{1 + \zeta}{1 - \zeta}} \right.
\left. + \frac{1 + \zeta}{1 - \zeta}\ln \left( 1 + \sqrt{\frac{1 - \zeta}{1 + \zeta}} \right) - \ln \left( 1 + \sqrt{\frac{1 + \zeta}{1 - \zeta}} \right) \right]. \tag{29}
\]

This is plotted in Fig. 1 and agrees well with Seidl’s approximation\(^{\text{[17]}}\) deviating by a maximum of 0.0005 near \(\zeta = 0.9815\).

In conclusion, we have shown that the energy of the high-density spin-polarized two-dimensional uniform electron gas can be found in closed form up to \(O(r_s)\). We believe that these new results, which are summarized in Table I, will be useful in the future development of exchange-correlation functionals within density-functional theory.

We thank Prof. Stephen Taylor for helpful discussions. P.M.W.G. thanks the NCI National Facility for a generous grant of supercomputer time and the Australian Research Council (Grants DP0984806 and DP1094170) for funding.

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