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

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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.

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The three-dimensional uniform electron gas is a ubiquitous paradigm in solid-state physics[1] and quantum chemistry,[2] and has been extensively used as a starting point in the development of exchange-correlation density functionals in the framework of density-functional theory.[3] The two-dimensional version of the electron gas has also been the object of extensive research[4,5] because of its intimate connection to two-dimensional or quasi-two-dimensional materials, such as quantum dots.[6,7]

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.[8] We will use atomic units throughout.

It is known from contributions by numerous workers[9–19] that the high-density (i.e., small r_s) expansion of the energy per electron (or reduced energy) in 2-jellium is

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

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

$$\zeta = \frac{\rho_\uparrow - \rho_\downarrow}{\rho} \tag{2}$$

is the relative spin polarization.[8] Without loss of generality, we assume $\rho_\downarrow \leqslant \rho_\uparrow$, i.e., $\zeta \in [0,1]$.

The first two terms of the expansion (1) are the kinetic and exchange energies, and their sum gives the Hartree-Fock (HF) energy. The paramagnetic ($\zeta = 0$) coefficients are

$$\varepsilon_{-2}(0) = +\frac{1}{2}, \tag{3}$$

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

and their spin-scaling functions are

$$\Upsilon_{-2}(\zeta) = \frac{\varepsilon_{-2}(\zeta)}{\varepsilon_{-2}(0)} = \frac{(1-\zeta)^2 + (1+\zeta)^2}{2}, \tag{5}$$

$$\Upsilon_{-1}(\zeta) = \frac{\varepsilon_{-1}(\zeta)}{\varepsilon_{-1}(0)} = \frac{(1-\zeta)^{3/2} + (1+\zeta)^{3/2}}{2}. \tag{6}$$

In this Brief Report, we show that the next two terms, which dominate the expansion of the reduced correlation energy,[20] can also be obtained in closed form for any value of the relative spin polarization ζ.

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 Eq. (1), and this yields[13]

$$\varepsilon_\ell(\zeta) = -\frac{1}{12\sqrt{2}\pi} \int_{-\infty}^{\infty} \left[R\left(\frac{u}{k_\uparrow}\right) + R\left(\frac{u}{k_\downarrow}\right) \right]^3 du, \tag{7}$$

where

$$R(u) = 1 - \frac{1}{\sqrt{1 + 1/u^2}}, \tag{8}$$

and

$$k_{\uparrow,\downarrow} = \sqrt{1 \pm \zeta} \tag{9}$$

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,

$$\varepsilon_\ell(0) = -\sqrt{2}\left(\frac{10}{3\pi} - 1\right) = -0.086\,3136\ldots, \tag{10}$$

$$\varepsilon_\ell(1) = \frac{1}{4\sqrt{2}}\varepsilon_\ell(0) = -\frac{1}{4}\left(\frac{10}{3\pi} - 1\right) = -0.015\,2582\ldots, \tag{11}$$

were found by Rajagopal and Kimball[13] and the spin-scaling function,

$$\Upsilon_\ell(\zeta) = \frac{\varepsilon_\ell(\zeta)}{\varepsilon_\ell(0)} = \frac{1}{8}\left[k_\uparrow + k_\downarrow + 3\frac{F(k_\uparrow,k_\downarrow) + F(k_\downarrow,k_\uparrow)}{10 - 3\pi} \right], \tag{12}$$

was obtained 30 years later by Chesi and Giuliani.[18] The explicit expression for $F(x,y)$ is

$$F(x,y) = 4(x+y) - \pi x - 4x E\left(1 - \frac{y^2}{x^2}\right) + 2x^2 \kappa(x,y), \tag{13}$$

where

$$\kappa(x,y) = \begin{cases} (x^2 - y^2)^{-1/2} \arccos(y/x), & x \leqslant y, \\ (y^2 - x^2)^{-1/2} \operatorname{arccosh}(x/y), & x > y, \end{cases} \tag{14}$$

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

$$\varepsilon_0(\zeta) = \varepsilon_0^{\mathrm{a}}(\zeta) + \varepsilon_0^{\mathrm{b}} \tag{15}$$

of a direct ("ring-diagram") term $\varepsilon_0^{\mathrm{a}}(\zeta)$ and an exchange term $\varepsilon_0^{\mathrm{b}}$. Following Onsager's work[23] on the three-dimensional gas, the exchange term was found by Isihara and Ioriatti[14] to be

$$\varepsilon_0^{\mathrm{b}} = \beta(2) - \frac{8}{\pi^2}\beta(4) = +0.114\,357\ldots, \tag{16}$$

where β is the Dirichlet beta function[22] and $G = \beta(2)$ is Catalan's constant. We note that $\varepsilon_0^{\mathrm{b}}$ is independent of ζ and the spin-scaling function therefore takes the trivial form

$$\Upsilon_0^{\mathrm{b}}(\zeta) = \frac{\varepsilon_0^{\mathrm{b}}(\zeta)}{\varepsilon_0^{\mathrm{b}}(0)} = 1. \tag{17}$$

The direct term has not been found in closed form, but we now show how this can be achieved. Following Rajagopal and Kimball,[13] we write the direct term as the double integral

$$\varepsilon_0^{\mathrm{a}}(\zeta) = -\frac{1}{8\pi^3}\int_{-\infty}^{\infty}\int_0^{\infty}\left[Q_{q/k_\uparrow}\left(\frac{u}{k_\uparrow}\right) + Q_{q/k_\downarrow}\left(\frac{u}{k_\downarrow}\right)\right]^2 dq\,du, \tag{18}$$

where

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

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

$$\varepsilon_0^{\mathrm{a}}(0) = -\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_0^{\infty}\frac{1}{\sqrt{s^2+t^2}} \times \left[1 - \left(\frac{\sqrt{(s-1)^2+t^2}+s-1}{\sqrt{s^2+t^2}+s}\right)^{1/2}\right]^2 dt\,ds, \tag{20}$$

and, if we adopt polar coordinates, this becomes

$$\begin{aligned}\varepsilon_0^{\mathrm{a}}(0) &= -\frac{1}{2\pi}\int_0^{\infty}\int_0^{\pi}\left[1 - \sqrt{\frac{\sqrt{1-2r\cos\theta+r^2}-1+r\cos\theta}{r(1+\cos\theta)}}\right]^2 d\theta\,dr \\ &= -\frac{1}{2\pi}\int_0^{\pi}\left[2\ln 2 - (\pi-\theta)\tan\frac{\theta}{2} - 2\tan^2\frac{\theta}{2}\ln\left(\sin\frac{\theta}{2}\right)\right]d\theta = \ln 2 - 1 = -0.306\,853\ldots,\end{aligned} \tag{21}$$

which confirms Seidl's numerical estimate[17]

$$\varepsilon_0^{\mathrm{a}}(0) = -0.306\,82 \pm 0.000\,12. \tag{22}$$

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

$$\varepsilon_0^{\mathrm{a}}(1) = \frac{1}{2}\varepsilon_0^{\mathrm{a}}(0) = \frac{\ln 2 - 1}{2} = -0.153\,426\ldots. \tag{23}$$

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

$$\Upsilon_0^{\mathrm{a}}(\zeta) = \frac{\varepsilon_0^{\mathrm{a}}(\zeta)}{\varepsilon_0^{\mathrm{a}}(0)}, \tag{24}$$

and, from (18), we have

$$\Upsilon_0^{\mathrm{a}}(\zeta) = \frac{1}{2} - \frac{1}{4\pi(\ln 2 - 1)}\int_0^{\infty}\int_{-1}^{1} P_{k_\uparrow}(r,z)P_{k_\downarrow}(r,z)\frac{i\,dz}{z}\,dr, \tag{25}$$

where

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

Integrating over r gives

$$\Upsilon_0^{\mathrm{a}}(\zeta) = \frac{1}{2} - \frac{1}{4\pi(\ln 2 - 1)}\int_{-1}^{1} L_{k_\uparrow,k_\downarrow}(z)\frac{i\,dz}{z}, \tag{27}$$

where

$$\begin{aligned}L_{k_\uparrow,k_\downarrow}(z) = {} & -k_\uparrow\ln k_\uparrow - k_\downarrow\ln k_\downarrow + \frac{1}{(z+1)^2}[(zk_\uparrow - k_\downarrow)^2 \\ & \times \ln(zk_\uparrow - k_\downarrow) + (zk_\downarrow - k_\uparrow)^2\ln(zk_\downarrow - k_\uparrow) \\ & - i\pi(k_\downarrow^2 - 2zk_\uparrow k_\downarrow + k_\downarrow^2) + 2z(k_\uparrow + k_\downarrow)^2\ln(k_\uparrow \\ & + k_\downarrow) - z(zk_\uparrow^2 - 2k_\uparrow k_\downarrow + zk_\downarrow^2)\ln z],\end{aligned} \tag{28}$$

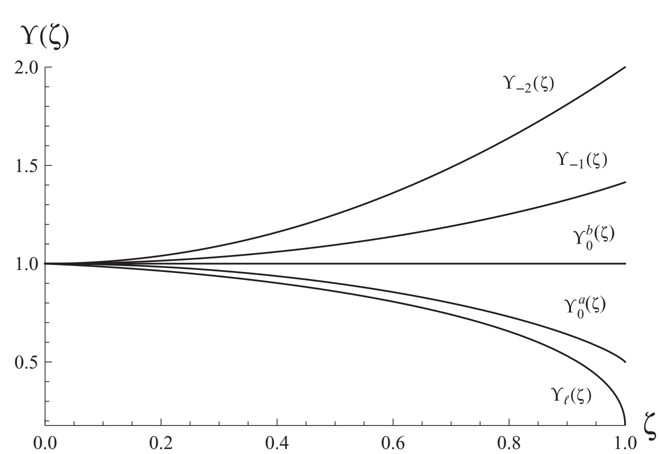

FIG. 1. $\Upsilon_{-2}(\zeta)$, $\Upsilon_{-1}(\zeta)$, $\Upsilon_0^{\mathrm{a}}(\zeta)$, $\Upsilon_0^{\mathrm{b}}(\zeta)$, and $\Upsilon_\ell(\zeta)$ as functions of ζ.

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}	$\varepsilon_0^{\mathrm{a}}(\zeta)$	$\ln 2 - 1$	$\frac{\ln 2 - 1}{2}$	Eq. (29)
	$\varepsilon_0^{\mathrm{b}}(\zeta)$	$\beta(2) - \frac{8}{\pi^2}\beta(4)$	$\beta(2) - \frac{8}{\pi^2}\beta(4)$	1
$r_s \ln r_s$	$\varepsilon_\ell(\zeta)$	$-\sqrt{2}\left(\frac{10}{3\pi} - 1\right)$	$-\frac{1}{4}\left(\frac{10}{3\pi} - 1\right)$	Eq. (12)

and contour integration over z eventually yields

$$\Upsilon_0^{\mathrm{a}}(\zeta) = \frac{1}{2} + \frac{1-\zeta}{4(\ln 2 - 1)}\left[2\ln 2 - 1 - \sqrt{\frac{1+\zeta}{1-\zeta}} + \frac{1+\zeta}{1-\zeta} \times \ln\left(1 + \sqrt{\frac{1-\zeta}{1+\zeta}}\right) - \ln\left(1 + \sqrt{\frac{1+\zeta}{1-\zeta}}\right)\right]. \quad (29)$$

This is plotted in Fig. 1 and agrees well with Seidl's approximation,[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 results, which are summarized in Table I, will be useful in the future development of exchange-correlation functionals within density-functional theory.

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