Brief Reports

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Correlation energy of a spin-polarized electron gas at high density

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This paper extends the result of Gell-Mann and Brueckner to include spin polarization. The contributions to the correlation energy of a spin-polarized electron gas that do not vanish in the high-density limit are evaluated exactly. In the process a closed-form expression is given for the generalization of an integral that has previously been evaluated numerically.

The spin-polarized electron gas is characterized by two quantities: the Wigner-Seitz radius r_s,[1] defined in terms of the number density ρ by

$$\rho^{-1}=\frac{4\pi}{3}a_0^3r_s^3\ , \tag{1}$$

where $a_0=\hbar^2/me^2$ is the Bohr radius, and the spin polarization ζ, defined in terms of the spin number densities ρ_+ and ρ_-, by

$$\zeta=\frac{\rho_+-\rho_-}{\rho}\ . \tag{2}$$

The ground-state energy of this system is conveniently expressed as a function of these two parameters.

At high electron densities, where the Wigner-Seitz radius becomes small, the correlation energy per electron in the ground state of a spin-polarized electron gas can be expanded in r_s as

$$\varepsilon_c=\frac{me^4}{2\hbar^2}(A_\zeta\ln r_s+C_\zeta+\cdots)\ . \tag{3}$$

The function A_ζ has been evaluated recently[2] to be

$$A_\zeta=\frac{1}{2\pi^2}\left[2(1-\ln2)+x_1x_2(x_1+x_2)-x_1^3\ln\left[\frac{x_1+x_2}{x_1}\right]-x_2^3\ln\left[\frac{x_1+x_2}{x_2}\right]\right]\ , \tag{4}$$

where $x_1=(1-\zeta)^{1/3}$ and $x_2=(1+\zeta)^{1/3}$. The function C_ζ is the coefficient of r_s^0. It has been evaluated numerically[3] for $\zeta=0$ to be $C_0=-0.096\pm0.002$. A scaling argument[4] then yields a value for $\zeta=1$ of $C_1=-0.053\pm0.001$. The higher-order terms represented by the ellipsis in Eq. (3) vanish in the limit of high densities. This paper presents an exact evaluation of the function C_ζ for all spin polarizations. In the process, an integral is evaluated analytically that has, until now, been evaluated only numerically.

The correlation energy can be separated into three terms:

$$\varepsilon_c=\frac{me^4}{2\hbar^2}(\varepsilon_b^{(2)}+\varepsilon_r+\varepsilon_\delta)\ . \tag{5}$$

The first term, $\varepsilon_b^{(2)}$, is the second-order exchange term, evaluated[5] to be

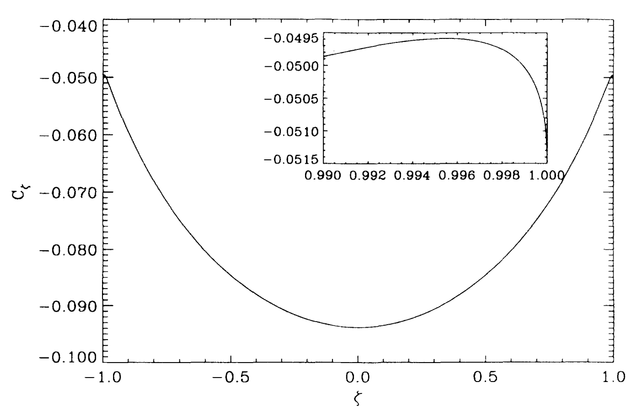

FIG. 1. C_ζ as a function of ζ. The inset shows greater detail of the maximum near $\zeta=0.996$.

$$\varepsilon_b^{(2)} \equiv \frac{3}{16\pi^5} \int \frac{d^3q}{q^2} \int_{\substack{p_1<1 \\ |\mathbf{p}_1+\mathbf{q}|>1}} d^3p_1 \int_{\substack{p_2<1 \\ |\mathbf{p}_2+\mathbf{q}|>1}} d^3p_2 \frac{1}{|\mathbf{q}+\mathbf{p}_1+\mathbf{p}_2|^2} \frac{1}{q^2+\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2)}$$

$$= \tfrac{1}{3}\ln 2 - \frac{3}{2\pi^2}\zeta(3) \; . \tag{6}$$

The second term is given by[3,6]

$$\varepsilon_r = \frac{3\alpha^2}{4\pi r_s^2} \int_{-\infty}^{\infty} du \int_0^{\infty} dq\, q^3 \left[\ln\left[1+\frac{r_s Q_\zeta(q,u)}{\alpha\pi^2 q^2}\right] - \frac{r_s Q_\zeta(q,u)}{\alpha\pi^2 q^2} \right] , \tag{7}$$

where $\alpha=(9\pi/4)^{1/3}$ and $Q_\zeta(q,u)$ is defined by

$$Q_\zeta(q,u) = \tfrac{1}{2}\int_{-\infty}^{\infty} dt\, e^{ituq} \sum_{s=1}^{2} \int_{\substack{p<x_s \\ |\mathbf{p}+\mathbf{q}|>x_s}} d^3p\, e^{-|t|(q^2/2+\mathbf{q}\cdot\mathbf{p})}$$

$$= \pi \sum_{s=1}^{2} \left\{ \frac{x_s^2-q^2/4+u^2}{2q} \ln\left[\frac{(x_s+q/2)^2+u^2}{(x_s-q/2)^2+u^2}\right] - u\left[\arctan\left[\frac{x_s+q/2}{u}\right] + \arctan\left[\frac{x_s-q/2}{u}\right]\right] + x_s \right\} . \tag{8}$$

The final quantity in Eq. (5), ε_δ, vanishes in the limit of $r_s \to 0$ and so is not considered any more.

Of interest is the $r_s \to 0$ limit of ε_c, and hence, of ε_r. Simply letting r_s vanish in the integrand of ε_r, however, leads to a divergent integral due to the behavior of the integrand in the $q \to 0$ limit. The proper approach is to separate the integral over q into two parts at some arbitrary, but small, value of q, denoted by β. For q greater than β, it is proper to let r_s vanish in the integrand, after which the remaining integrations can be solved in closed form. For q less than β, the integrand is replaced by its small-q limit, after which the integration over q can be performed explicitly. After this is done, r_s is allowed to vanish and the remaining integrals performed. The two parts of the integral are then recombined and the limit $\beta \to 0$ is taken.

For small q,

$$Q_\zeta(q,u) \sim 4\pi R_\zeta(u) \quad \text{as } q \to 0 \; , \tag{9}$$

where

$$R_\zeta(u) = \frac{1}{2}\left\{ \left[(1-\zeta)^{1/3} - u \arctan\left[\frac{(1-\zeta)^{1/3}}{u}\right]\right] + \left[(1+\zeta)^{1/3} - u\arctan\left[\frac{(1+\zeta)^{1/3}}{u}\right]\right]\right\} . \tag{10}$$

This function is independent of q, simplifying subsequent integrations significantly. Therefore, assuming β to be small,

$$\varepsilon_r \sim \frac{3\alpha^2}{4\pi r_s^2} \lim_{\beta\to 0} \int_{-\infty}^{\infty} du \left\{ \int_0^{\beta} q^3 dq \left[\ln\left[1+\frac{4 r_s R_\zeta(u)}{\alpha\pi q^2}\right] - \frac{4 r_s R_\zeta(u)}{\alpha\pi q^2}\right] + \int_\beta^\infty q^3 dq \left[\ln\left[1+\frac{r_s Q_\zeta(q,u)}{\alpha\pi^2 q^2}\right] - \frac{r_s Q_\zeta(q,u)}{\alpha\pi^2 q^2}\right]\right\} \quad \text{as } r_s \to 0$$

$$\sim \frac{3}{2\pi^3} \lim_{\beta\to 0} \int_{-\infty}^{\infty} du \left[-R_\zeta^2(u) + 2R_\zeta^2(u) \ln\left[\frac{4 r_s R_\zeta(u)}{\alpha\pi\beta^2}\right] - \frac{1}{4\pi^2}\int_\beta^\infty \frac{dq}{q} Q_\zeta^2(q,u)\right] \quad \text{as } r_s \to 0$$

$$= \lim_{\beta\to 0} \left\{ A_\zeta \ln r_s + A_\zeta\left[\ln\left[\frac{4}{\alpha\pi}\right] + \langle \ln R_\zeta\rangle_{\text{av}} - \frac{1}{2}\right] - \frac{3}{8\pi^5}\int_{-\infty}^{\infty} du \int_\beta^\infty \frac{dq}{q} Q_\zeta^2(q,u)\right\} , \tag{11}$$

where A_ζ is given by Eq. (4) and

$$\langle \ln R_\zeta \rangle_{\text{av}} = \frac{\int_{-\infty}^{\infty} du\, R_\zeta^2(u) \ln[R_\zeta(u)]}{\int_{-\infty}^{\infty} du\, R_\zeta^2(u)} \; . \tag{12}$$

The final integral can be evaluated in closed form. Using the definition of $Q_\zeta(q,u)$ in the first line of Eq. (8),

$$\int_{-\infty}^{\infty} du\, Q_\zeta^2(q,u) = \frac{\pi}{q} \sum_{s,s'} I(q; x_s, s_{s'}) \; , \tag{13}$$

where

$$I(q;x_s,x_s')=\int_{\substack{p<x_s,\\ |\mathbf{p}+\mathbf{q}|>x_s}} d^3p \int_{\substack{p'<x_{s'},\\ |\mathbf{p}'+\mathbf{q}|>x_{s'}}} d^3p' \frac{1}{\mathbf{q}\cdot(\mathbf{q}+\mathbf{p}+\mathbf{p}')} \ . \tag{14}$$

Due to the restrictions on the integrations, it is necessary to specify the quantities $x_< = \min(x_s,x_{s'})$ and $x_> = \max(x_s,x_{s'})$. The function $I(q;x_s,x_{s'})$ is symmetric in the two arguments x_s and $x_{s'}$, so this does not cause any difficulties in what follows. Using the coordinate transformation defined by Macke,[7] the integrals over $\mathbf{p}$ and $\mathbf{p}'$ are readily performed to yield

$$\begin{aligned} I(q;x_<,x_>)=\frac{\pi^2}{q}\Bigg\{ & \frac{11x_>^3+18x_>^2x_<+18x_>x_<^2+11x_<^3}{30}q^2-\frac{x_>+x_<}{40}q^4 \\ & -\frac{2(x_>^5-5x_>^3x_<^2-5x_>^2x_<^3+x_<^5)}{15}\ln[1-q^2/(x_>+x_<)^2] \\ & -\tfrac{2}{3}q^2\left[x_>^3\ln\left[\frac{(x_>+x_<)^2-q^2}{x_>^2-q^2/4}\right]+x_<^3\ln\left[\frac{(x_>+x_<)^2-q^2}{x_<^2-q^2/4}\right]\right] \\ & +\left[\frac{x_>^4q}{2}+\frac{x_>^2q^3}{4}-\frac{q^5}{96}\right]\ln\left[\frac{x_>+q/2}{x_>-q/2}\right]+\left[\frac{x_<^4q}{2}+\frac{x_<^2q^3}{4}-\frac{q^5}{96}\right]\ln\left[\frac{x_<+q/2}{x_<-q/2}\right] \\ & +\left[-\frac{(x_>^2-x_<^2)^2q}{2}-\frac{(x_>^2+x_<^2)q^3}{3}+\frac{q^5}{30}\right]\ln\left[\frac{x_>+x_<+q}{x_>+x_<-q}\right]\Bigg\},\quad q<2x_< \ ; \end{aligned} \tag{15a}$$

$$\begin{aligned} I(q;x_<,x_>)=\frac{\pi^2}{q}\Bigg[& \frac{11x_>x_<(x_>^2+x_<^2)q}{15}+\frac{x_<(18x_>^2+11x_<^2)q^2}{30}+\frac{x_>x_<q^3}{15} \\ & -\frac{x_<q^4}{40}-\frac{2(x_>^5-5x_>^3x_<^2-5x_>^2x_<^3+x_<^5)}{15}\ln[1+q/(x_>+x_<)] \\ & +\frac{2(x_>^5-5x_>^3x_<^2+5x_>^2x_<^3-x_<^5)}{15}\ln[1+q/(x_>-x_<)] \\ & -\frac{2x_<^3q^2}{3}\ln\left[\frac{(x_>+q)^2-x_<^2}{q^2/4-x_<^2}\right]+\left[\frac{x_<^4q}{2}+\frac{x_<^2q^3}{4}-\frac{q^5}{96}\right]\ln\left[\frac{q/2+x_<}{q/2-x_<}\right] \\ & +\left[-\frac{(x_>^2-x_<^2)^2q}{2}-\frac{2x_>^3q^2}{3}-\frac{(x_>^2+x_<^2)q^3}{3}+\frac{q^5}{30}\right]\ln\left[\frac{x_>+x_<+q}{x_>-x_<+q}\right]\Bigg],\quad 2x_<<q<2x_> \ ; \end{aligned} \tag{15b}$$

$$\begin{aligned} I(q;x_<,x_>)=\frac{\pi^2}{q}\Bigg[& \frac{22x_>x_<(x_>^2+x_<^2)q}{15}+\frac{2x_>x_<q^3}{15} \\ & +\left[-\frac{(x_>^2-x_<^2)^2q}{2}-\frac{(x_>^2+x_<^2)q^3}{3}+\frac{q^5}{30}\right]\ln\left[\frac{q^2-(x_>+x_<)^2}{q^2-(x_>-x_<)^2}\right] \\ & +\left[-\frac{2(x_>^5-5x_>^3x_<^2-5x_>^2x_<^3+x_<^5)}{15}-\frac{2(x_>^3+x_<^3)q^2}{3}\right]\ln\left[\frac{q+x_>+x_<}{q-(x_>+x_<)}\right] \\ & +\left[\frac{2(x_>^5-5x_>^3x_<^2+5x_>^2x_<^3-x_<^5)}{15}+\frac{2(x_>^3-x_<^3)q^2}{3}\right]\ln\left[\frac{q+x_>-x_<}{q-(x_>-x_<)}\right]\Bigg],\quad 2x_><q \ . \end{aligned} \tag{15c}$$

The integral over q is readily performed assuming β to be small. To order β^2,

$$\begin{aligned} -\frac{3}{8\pi^5}\int_{-\infty}^{\infty}du\int_{\beta}^{\infty}\frac{dq}{q}Q_\zeta^2(q,u) &= -\frac{3}{8\pi^2}[\gamma(x_1,x_1)+\gamma(x_2,x_2)+2\gamma(x_1,x_2)] \\ &\quad +2A_\zeta\ln\beta-\frac{(x_1+x_2)^2+2x_1^2+2x_2^2}{32\pi^2(x_1+x_2)}\beta^2+\cdots \ , \end{aligned} \tag{16}$$

where

$$\gamma(x_<,x_>)=\tfrac{11}{9}x_>x_<(x_>+x_<)+\tfrac{4}{3}x_>x_<(x_>+x_<)\ln 2$$
$$+\frac{2x_>^3}{3}\left\{-\frac{\pi^2}{6}-\left[\mathrm{Li}_2(x_</x_>)+\mathrm{Li}_2(-x_</x_>)+2\,\mathrm{Li}_2\left[-\frac{x_>-x_<}{x_>+x_<}\right]\right]\right.$$
$$\left.+\ln\left[\frac{(x_>+x_<)^2}{2x_>}\right]\ln\left[\frac{x_>-x_<}{x_>+x_<}\right]+2\ln(2x_<)\ln(x_>)-\ln(x_>^2-x_<^2)\ln(2x_<)\right\}$$
$$+\frac{2x_<^3}{3}\left\{-\frac{2\pi^2}{3}+\left[\mathrm{Li}_2(x_</x_>)+\mathrm{Li}_2(-x_</x_>)+2\,\mathrm{Li}_2\left[\frac{2x_<}{x_>+x_<}\right]\right]\right.$$
$$\left.-2\ln\left[\frac{x_>+x_<}{x_<}\right]\ln(2x_<)-\ln\left[\frac{x_>^2-x_<^2}{x_<x_>}\right]\ln\left[\frac{x_>}{x_<}\right]\right\}$$
$$+\tfrac{4}{9}[x_<^2(3x_>-x_<)\ln(x_<)-x_>^2(x_>-3x_<)\ln(x_>)]$$
$$-(\tfrac{7}{18}x_>^2-\tfrac{11}{9}x_>x_<+\tfrac{7}{18}x_<^2)(x_>+x_<)\ln(x_>+x_<)+\tfrac{5}{6}(x_>^2-x_<^2)(x_>-x_<)\ln(x_>-x_<) \quad (17)$$

and $\mathrm{Li}_2(z)$ is the dilogarithm function,[8] given by

$$\mathrm{Li}_2(z)=-\int_0^z\frac{\ln(1-t)}{t}dt\ . \quad (18)$$

In the special case where $x_>=x_<=1$, Eq. (16) takes the much simpler form

$$-\frac{3}{8\pi^5}\int_{-\infty}^{\infty}du\int_\beta^\infty\frac{dq}{q}Q_\zeta^2(q,u)=-\frac{3}{2\pi^2}\left[\tfrac{22}{9}-\frac{\pi^2}{3}+\tfrac{32}{9}\ln(2)-\tfrac{8}{3}\ln^2(2)-\tfrac{8}{3}[1-\ln(2)]\ln(\beta)+\frac{\beta^2}{12}\right]$$
$$=-2[0.025\,68-0.062\,18\ln\beta+0.006\,333\beta^2]\ . \quad (19)$$

This may be compared with the numerical result of Pines.[9]

Putting everything together, the correlation energy is indeed found to have the form presented in Eq. (3). The coefficient of $\ln r_s$ is found to be A_ζ, as required, and

$$C_\zeta=\tfrac{1}{3}\ln(2)-\frac{3}{2\pi^2}\zeta(3)+A_\zeta\left[\ln\left[\frac{4}{\alpha\pi}\right]+\langle\ln R_\zeta\rangle_{\mathrm{av}}-\frac{1}{2}\right]-\frac{3}{8\pi^2}[\gamma(x_1,x_1)+\gamma(x_2,x_2)+2\gamma(x_1,x_2)]\ . \quad (20)$$

Although $\langle\ln R_\zeta\rangle_{\mathrm{av}}$ must still be evaluated numerically, this can be done to high precision. The denominator of Eq. (12) can be evaluated in closed form, and the numerator can be converted to an integral over a finite range. Equation (20) can be evaluated exactly, for all intents and purposes.

For $\zeta=0$, Eq. (20) becomes

$$C_0=\tfrac{1}{3}\ln(2)-\frac{3}{2\pi^2}\zeta(3)+\frac{2}{\pi^2}[1-\ln(2)]\left[\ln\left[\frac{4}{\alpha\pi}\right]+\langle\ln R_0\rangle_{\mathrm{av}}-\frac{1}{2}\right]-\frac{3}{2\pi^2}\left[\tfrac{22}{9}-\frac{\pi^2}{3}+\tfrac{32}{9}\ln(2)-\tfrac{8}{3}\ln^2(2)\right]$$
$$=-0.093\,841\ . \quad (21)$$

For $\zeta=1$, Eq. (20) becomes

$$C_1=\tfrac{1}{3}\ln(2)-\frac{3}{2\pi^2}\zeta(3)+\frac{1}{\pi^2}[1-\ln(2)]\left[\ln\left[\frac{4}{\alpha\pi}\right]+\langle\ln R_1\rangle_{\mathrm{av}}-\frac{1}{2}\right]-\frac{3}{4\pi^2}\left[\tfrac{22}{9}-\frac{\pi^2}{3}+\tfrac{32}{9}\ln(2)-\tfrac{8}{3}\ln^2(2)\right]$$
$$-\frac{2}{3\pi^2}[1-\ln(2)]\ln(2)=-0.051\,475\ . \quad (22)$$

These two values are in accord with the scaling relation of Misawa.[4] The function C_ζ is plotted in Fig. 1. It is interesting to note the maxima near $\zeta=\pm 0.996$.

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