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# Analysis of the second-order exchange self-energy of a dense electron gas

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**Abstract**
We evaluate the six-fold integral representation for the second-order exchange contribution to the self-energy of a dense three-dimensional electron gas on the Fermi surface.

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## Introduction

The second-order exchange energy contributes importantly to the correlation energy of a dense electron gas [1]. It is given by the nine-fold integral

$$E_{2x} = \frac{3}{32\pi^4}\int \mathrm{d}^3 p_1 \int \mathrm{d}^3 p_2 \int \frac{\mathrm{d}q^3}{q^2}\frac{f_{p_1} f_{p_2} f'_{p_1+q} f'_{p_2+q}}{(\vec{q}+\vec{p}_1+\vec{p}_2)^2(q^2+\vec{p}_1\cdot\vec{q}+\vec{p}_2\cdot\vec{q})} \qquad (1)$$

in three dimensions, where $f_p$ denotes the Fermi distribution function for electrons of wave vector $\vec{p}$ and $f'_p$ denotes that for holes. In a remarkable display of mathematical virtuosity (1) was evaluated in closed form by Onsager [2] and Onsager, Mittag and Stephen [3] who found

$$E_{2x} = \frac{1}{6}\ln(2) - \frac{3}{4\pi^2}\zeta(3). \qquad (2)$$

Subsequently, Ishihara and Ioratti [4] worked out the corresponding value for a two-dimensional system, and the $d$-dimensional case was evaluated by Glasser [5].

Recently the second-order exchange term in the electron self-energy has been studied by Ziesche [6]. It is given, in three dimensions, by the six-fold integral

$$\Sigma_{2x}(k) = \frac{1}{4\pi^4}\int \frac{\mathrm{d}^3 q}{q^2}\int \mathrm{d}^3 p \frac{f_p f_{k+q} f_{p+q} f'_p f'_{p+q}}{(\vec{k}+\vec{p}+\vec{q})^2(q^2+\vec{k}\cdot\vec{q}+\vec{p}\cdot\vec{q})}. \qquad (3)$$

For $k = k_F (=1)$ Ziesche succeeded in decomposing (3) into the sum $\Sigma_{2x} = -(X_1+X_2)/4\pi^2$ of the two simpler integrals

$$X_1 = \int \frac{d^3q_1}{q_1^2} \int \frac{d^3q_2}{q_2^2} \frac{f_{k+q_1+q_2} f'_{k+q_1} f'_{k+q_2}}{\vec{q}_1 \cdot \vec{q}_2}$$
$$X_2 = -\int \frac{d^3q_1}{q_1^2} \int \frac{d^3q_2}{q_2^2} \frac{f'_{k+q_1+q_2} f_{k+q_1} f_{k+q_2}}{\vec{q}_1 \cdot \vec{q}_2} \tag{4}$$

and by following the procedure in [3], he managed to perform three of the integrations, thereby obtaining

$$X_1 = -16\pi \int_0^1 dp \int_0^1 dq \int_{-1}^1 \frac{dx}{(1-p^2q^2)} \frac{F[p,q,x]}{1+q^2}$$
$$X_2 = 16\pi \int_0^1 dp \int_0^1 dq \int_{-1}^1 \frac{dx}{(1-p^2q^2)} \frac{q^2 F[p,q,x]}{1+q^2} \tag{5}$$

where

$$\alpha = \frac{1-q^2}{2q}, \qquad \beta = \frac{1-p^2}{2p}, \qquad a = \frac{1+p^2q^2}{2pq}$$
$$F[p,q,x] = \frac{2}{a^2-x^2} \tan^{-1}\left[\frac{\alpha x + \beta}{\sqrt{(1+\alpha^2)(1-x^2)}}\right]. \tag{6}$$

The integrals in (6) are amenable to numerical evaluation and Ziesche found $X_1 = -30.705\,98\ldots$, $X_2 = 21.284\,90\ldots$.

According to the Hugenholtz–van Hove–Luttinger–Ward theorem [7] $\Sigma_{2x} = E_{2x}$, giving

$$X_1 + X_2 = 3\zeta(3) - \frac{2\pi^2}{3}\ln(2). \tag{7}$$

The aim of this paper is to evaluate $X = X_2 - X_1$, so as to obtain closed form expressions for the integrals in (4).

## Calculation

From (5) we have

$$X = 16\pi \int_0^1 dq \int_0^1 dp \int_{-1}^1 dx \frac{F[p,q,x]}{1-p^2q^2}. \tag{8}$$

Since the limits on the $x$-integral are symmetric, we retain only the even part of the integrand of (8) by averaging $X$ and the integral obtained by $x \to -x$; after combining the two arctangents, one obtains

$$X = 16\pi \int_0^1 dp \int_0^1 dq \int_0^1 dx \frac{\tan^{-1}\left[\frac{2\beta\sqrt{(1+\alpha^2)(1-x^2)}}{\alpha^2-\beta^2+1-x^2}\right]}{(1-p^2q^2)(a^2-x^2)}. \tag{9}$$

Next, we set $q = e^{-u}$, $p = e^{-v}$, $x = \sin\phi$, so $\alpha = \sinh u$, $\beta = \sinh v$, $a = \cosh(u+v)$, and find that

$$X = 8\pi \int_0^\infty du \int_0^\infty dv \int_0^{\pi/2} d\phi \cos\phi \frac{\tan^{-1}\left[\frac{(\sinh(u+v)+\sinh(v-u))\cos\phi}{\sinh(u+v)\sinh(u-v)+\cos^2\phi}\right]}{\sinh(u+v)[\sinh^2(u+v)+\cos^2\phi]}. \tag{10}$$

We next make the coordinate transformation $r = v+u$, $s = v-u$, having Jacobian $1/2$, to obtain

$$X = 4\pi \int_0^\infty dr \int_{-r}^r ds \int_0^{\pi/2} d\phi \cos\phi \frac{\tan^{-1}\left[\frac{(\sinh r+\sinh s)\cos\phi}{\cos^2\phi-\sinh r\sinh s}\right]}{\sinh r(\sinh^2 r+\cos^2\phi)}. \tag{11}$$

Since

$$\tan^{-1}\left[\frac{\cos\phi(\sinh r + \sinh s)}{\cos^2\phi - \sinh r\sinh s}\right] = \mathrm{Im}\ln[(\cos\phi + \mathrm{i}\sinh r)(\cos\phi + \mathrm{i}\sinh s)]$$
$$= \tan^{-1}\left(\frac{\sinh r}{\cos\phi}\right) + \tan^{-1}\left(\frac{\sinh s}{\cos\phi}\right), \quad (12)$$

(11) becomes

$$X = 4\pi\int_0^\infty \mathrm{d}r \int_{-r}^{r}\mathrm{d}s\int_0^{\pi/2}\mathrm{d}\phi\cos\phi\frac{\tan^{-1}(\sec\phi\sinh r) + \tan^{-1}(\sec\phi\sinh s)}{\sinh r(\cos^2\phi + \sinh^2 r)}. \quad (13)$$

Once again, the term in the integrand of (13) odd in $s$ may be dropped and following the elementary $s$-integration, one has

$$X = 8\pi\int_0^\infty \frac{r\,\mathrm{d}r}{\sinh r}\int_0^{\pi/2}\mathrm{d}\phi\tan^{-1}\left(\frac{\sinh r}{\cos\phi}\right)\frac{\cos\phi}{\cos^2\phi + \sinh^2 r}. \quad (14)$$

To evaluate the $\phi$-integral, we set $\tan\psi = \sec\phi\sinh r$, $\mu = \tan^{-1}(\sinh r) = \cos^{-1}(\mathrm{sech}\, r)$, to transform (14) into

$$X = 8\pi\int_0^\infty \frac{r\,\mathrm{d}r}{\sinh r}\cos\mu\int_\mu^{\pi/2}\frac{\psi\cos\psi\,\mathrm{d}\psi}{\sqrt{\sin^2\psi - \sin^2\mu}}. \quad (15)$$

The $\psi$-integral is tabulated [8] and $X$ is reduced to

$$X = 4\pi^2\int_0^\infty \frac{r\,\mathrm{sech}\, r\ln(1 + \mathrm{sech}\, r)}{\sinh r}\,\mathrm{d}r. \quad (16)$$

To evaluate the remaining integral, let

$$f(a) = \int_0^\infty \frac{r\ln(1 - a\,\mathrm{sech}\, r)}{\sinh r\cosh r}\,\mathrm{d}r \quad (17)$$

for which $f(1) = X/4\pi^2$ and $f(0) = 0$. By differentiation with respect to $a$ and partial fraction decomposition, we obtain

$$(1-a^2)\frac{\mathrm{d}f}{\mathrm{d}a} = \int_0^\infty \frac{r\,\mathrm{d}r}{\sinh r} - 2a\int_0^\infty\frac{r\,\mathrm{d}r}{\sinh 2r} - \frac{1}{a}\int_0^\infty r\sinh r\left[\frac{1}{\cosh r} - \frac{1}{\cosh r + a}\right]. \quad (18)$$

The first two integrals on the right-hand side of (18) are tabulated [9] and, after an integration by parts, we find

$$(1-a^2)\frac{\mathrm{d}f}{\mathrm{d}a} = \frac{\pi^2}{8}(2-a) - \frac{1}{a}\int_0^\infty \ln(1 + a\,\mathrm{sech}\, r)\,\mathrm{d}r. \quad (19)$$

The substitution $u = \mathrm{sech}\, r$ leads to another tabulated integral [10], giving

$$\frac{\mathrm{d}f}{\mathrm{d}a} = -\frac{\pi^2}{8a}\left(\frac{1-a}{1+a}\right) + \frac{1}{2a}\frac{(\cos^{-1}a)^2}{1-a^2}, \quad (20)$$

which, with the substitution $a = \cos\theta$, yields

$$X = 4\pi^2\int_0^1\frac{\mathrm{d}f}{\mathrm{d}a}\mathrm{d}a = \pi^4\ln(2) + 4\pi^2\int_0^{\pi/2}\frac{\mathrm{d}\theta}{\sin 2\theta}\left[\theta^2 - \frac{\pi^2}{8}(1 - \cos(2\theta))\right]. \quad (21)$$

Finally, we find by setting $\phi = 2\theta$, and folding the new range of integration $[\pi/2, \pi]$ back to $[0, \pi/2]$

$$X = \pi^4\ln(2) + 4\pi^2\int_0^{\pi/2}\frac{4\phi(\phi-\pi)}{\sin\phi}d\phi$$
$$= \pi^4\ln(2) - \frac{7}{2}\pi^2\zeta(3), \quad (22)$$

where we have used [11]

$$\int_0^{\pi/2} \frac{\phi\, \mathrm{d}\phi}{\sin\phi} = 2\mathbf{G}, \qquad \int_0^{\pi/2} \frac{\phi^2 \mathrm{d}\phi}{\sin\phi} = 2\pi\mathbf{G} - \frac{7}{2}\zeta(3) \tag{23}$$

in which **G** denotes Catalan's constant.

## Discussion

In conclusion, we have obtained closed form expressions for the two six-fold integrals in (4)

$$X_1 = -\pi^4\left[\frac{4}{3}\ln(2) - \frac{5}{\pi^2}\zeta(3)\right]$$
$$= -30.705\,985\,239\,248\,899\,257\,622\,684\,446\,084\,815\,368\,758\,552\,081\,659\,459\,189\,816\,458\,46\ldots. \tag{24}$$

$$X_2 = \pi^4\left[\frac{2}{3}\ln(2) - \frac{2}{\pi^2}\zeta(3)\right]$$
$$= 21.284\,905\,670\,516\,337\,983\,402\,598\,547\,497\,784\,400\,625\,730\,440\,810\,132\,220\,995\,696\,061\ldots. \tag{25}$$

This gives the value

$$\Sigma_{2x} = 0.024\,179\,158\,918\,144\,405\,895\,450\,762\,162\,898\,431\,404\,915\,238\,425\,120\,733\,594\,530\,9986\ldots, \tag{26}$$

in agreement with Ziesche's [6] seven place calculation. We hope to extend the calculation to an electron gas of arbitrary dimension, as was done for $E_{2x}$.

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## References

[1] Gell-Mann M and Brueckner K 1957 *Phys. Rev.* **106** 364
[2] Onsager L Unpublished
[3] Onsager L, Mittag L and Stephen M J 1966 *Ann. Phys., Lpz* **18** 71
[4] Isihara A and Ioriatti L 1980 *Phys. Rev.* B **22** 214
[5] Glasser M L 1984 *J. Comput. Appl. Math.* **10** 293
[6] Ziesche P 2007 *Ann. Phys., Lpz* **16** 45
[7] Luttinger J M and Ward J C 1960 *Phys. Rev.* **118** 1417
[8] Gradshteyn I S and Ryzhik I M 2000 *Table of Integrals, Series and Products* 6th edn (New York: Academic) p 466 no. 3.842(2)
[9] Gradshteyn I S and Ryzhik I M 2000 *Table of Integrals, Series and Products* 6th edn (New York: Academic) p 369, no. 3.521(1)
[10] Gradshteyn I S and Ryzhik I M 2000 *Table of Integrals, Series and Products* 6th edn (New York: Academic) p 554, no. 4.292(5)
[11] Gradshteyn I S and Ryzhik I M 2000 *Table of Integrals, Series and Products* 6th edn (New York: Academic) p 427, nos. 3.747(1,2)