Second order exchange energy of a d-dimensional electron fluid.

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Abstract. A method is presented for reducing a 3d-fold integral occurring in higher order many-body integrals for a d-dimensional electron gas to a double integral. The result is applied to the second order exchange energy for a d-dimensional uniform electron fluid. The cases $d = 2, 3$ are examined in detail.

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1. Introduction

In their classic work on the ground-state energy of an interacting electron gas[1] Gell-Mann and Brueckner encountered the second order exchange term

$$E_{2b} = \frac{3p_F^3 e^4}{16\pi^5} \int d\vec{p}d\vec{k}d\vec{q} \frac{f_{\vec{p}} f_{\vec{k}}(1 - f_{\vec{p}+\vec{q}})(1 - f_{\vec{k}+\vec{q}})}{q^2(\vec{p} + \vec{k} + \vec{q})^2 \vec{q} \cdot (\vec{p} + \vec{k} + \vec{q})}, \quad (1)$$

where f_p is the Fermi distribution function and p_F denotes the Fermi momentum. Gell-Mann's assistant, H. Kahn, estimated by Monte-Carlo integration the value as -0.044 and in a 1965 lecture in Istambul[2] L. Onsager claimed that the exact value is $(\ln 2)/3 - 3\zeta(3)/2\pi^2$, which remained unproven till eight years later when Onsager, Mittag and Stephen published a lengthy derivation[2]. In 1980, Ishihara and Ioriatti[3] evaluated the two-dimensional analogue of (1) and In 1984 the author published a note[4] indicating how such integrals might be handled in d-dimensions. But, due to a number of misprints [4] is difficult to follow and it seems appropriate to present a simplified and corrected version, particularly since the method has been found useful in other contexts[5] and, due to an oversight, it erroneously stated that the value given in [3] was confirmed. The dimension d will be treated as continuous by means of the expedient integration rule for an azimuthally symmetric integrand

$$\int dk^d = \frac{2\pi^{(d-1)/2}}{\Gamma\left[\frac{1}{2}(d-1)\right]} \int_0^\infty dk k^{d-1} \int_0^\pi d\theta \sin^{d-2}\theta$$

The following section covers the reduction of a basic 9d-dimensional integral to more manageable 3d+2-dimensional form which, in section 3, is applied to the second order exchange energy. The last section gives the results for $d = 2$ and $d = 3$.

2. Basic Integral Identity

The units $\hbar = 2m = 1$, will be used along with the notation

$$f_p = [1 + \exp[\beta(p^2 - p_F^2)]^{-1}, \quad Q(p) = f_p(1 - f_{\vec{p}+\vec{q}}), \quad Q'(p) = f_{\vec{p}+\vec{q}}(1 - f_p) \qquad (2)$$

$$\Delta(p) = f_{\vec{p}+\vec{q}} - f_{\vec{p}}, \quad \delta(p) = (\vec{p}+\vec{q})^2 - p^2, \qquad (3)$$

All vectors are d-dimensional and vector integrals are over all space.

Lemma. In the zero temperature limit

$$\frac{Q(p)Q(k) - Q'(p)Q'(k)}{\vec{q}\cdot(\vec{p}+\vec{k}+\vec{q})} = -\frac{1}{\pi}\int_{-\infty}^{\infty} dz \frac{\Delta(p)}{z - i\delta(p)} \frac{\Delta(k)}{z + i\delta(k)}. \qquad (4)$$

The proof follows closely the derivation of a similar result in Appendix A of [3].

Theorem 1. For real $\vec{r}$ and $t \geq 0$

$$\int d\vec{p}\, e^{i[\vec{r}\cdot\vec{p}+\delta(p)t]}\Delta(p) = -2i\left(\frac{2\pi p_F}{\xi}\right)^{d/2} e^{-\frac{1}{2}i\vec{r}\cdot\vec{q}} \sin\left(\frac{1}{2}\vec{q}\cdot\vec{\xi}\right) J_{d/2}\left(p_F\xi\right), \qquad (5)$$

where $\vec{\xi} = \vec{r} + 2t\vec{q}$.

Proof. First of all note that $\Delta(p)$ is simply a rectangular pulse with height 1 and width q, so has the inverse Laplace transform representation

$$\Delta(p) = \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i s} e^{sp_F^2}[e^{-s(\vec{p}+\vec{q})^2} - e^{-sp^2}], \quad c > 0. \qquad (6)$$

By substituting (6) into (5) one obtains the difference of two integrals. In the first make the change of variable $\vec{p} \to -\vec{p} - \vec{q}$. This gives

$$\int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i s} e^{sp_F^2}\{e^{-i\vec{r}\cdot\vec{q}}e^{-itq^2}C(-\vec{r} - 2t\vec{q}) - e^{itq^2}C(\vec{r} + 2t\vec{q})\} \qquad (9)$$

$$C(\vec{\xi}) = \int d\vec{p}\, e^{i\vec{p}\cdot\vec{\xi}} e^{-sp^2} = \left(\frac{\pi}{s}\right)^{d/2} e^{-\xi^2/4s}.$$

Next, one has

$$\int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{p_F^2 s} s^{-1-d/2} e^{-\xi^2/4s} = \left(\frac{2p_F}{\xi}\right)^{d/2} J_{d/2}(p_F\xi), \qquad (10)$$

which gives for (9)

$$\left(\frac{2p_F\pi}{\xi}\right) J_{d/2}(p_F\xi)e^{itq^2}[e^{-i\vec{q}\cdot\vec{\xi}}-1] = -2i\left(\frac{2p_F\pi}{\xi}\right) J_{d/2}\left(p_F\xi\right) e^{-\frac{1}{2}i\vec{r}\cdot\vec{q}}\sin(\frac{1}{2}\vec{q}\cdot\vec{\xi}) \quad (11)$$

QED

Now, we choose, from among other possibilities,

$$\alpha(\vec{q}) = \int \frac{e^{i\vec{r}\cdot\vec{q}}}{r}d\vec{r} \quad (12)$$

and define

$$A(\vec{q}) = \int d\vec{p}d\vec{k}\,\alpha(\vec{p}+\vec{k}+\vec{q})\,\frac{Q(p)Q(k)}{\vec{q}\cdot(\vec{p}+\vec{k}+\vec{q})}. \quad (13)$$

By making the substitution $\vec{p}\to-\vec{p}-\vec{q}$, $\vec{k}\to-\vec{k}-\vec{q}$, and adding the result back to (13), we find, using the identity in the Lemma,

$$\begin{aligned} A(q) &= -\frac{1}{2\pi}\int_{-\infty}^{\infty}dz\int d\vec{p}d\vec{k}\,\alpha(\vec{p}+\vec{k}+\vec{q})\frac{\Delta(p)\Delta(k)}{(z+i\delta(p))(z-i\delta(k))} \quad (14)\\ &= -\frac{1}{2\pi}\int\frac{d\vec{r}}{r}\int_{-\infty}^{\infty}dzB(\vec{r},z)B(-\vec{r},z) \end{aligned}$$

with

$$B(\vec{r},z) = \int d\vec{p}e^{i\vec{r}\cdot\vec{p}}\frac{\Delta(p)}{z+i\delta(p)} = \int_0^{\infty}dt\,e^{-zt}\int d\vec{p}\,e^{i[\vec{r}\cdot\vec{p}+t\delta(p)]}\Delta(p). \quad (15)$$

By applying Theorem 1 and performing the elementary $z-$ integration, we have, after scaling q out of t_j,

Theorem 2.

$$A(q) =$$

$$\frac{2}{\pi q}\left(2\pi p_F\right)^d\int\frac{d\vec{r}}{r}\int_0^{\infty}\int_0^{\infty}\frac{dt_1dt_2}{t_1+t_2}\frac{\sin\left(\frac{1}{2}q\xi_1\right)\sin\left(\frac{1}{2}q\xi_2\right)}{(\xi_1\xi_2)^{d/2}}J_{d/2}(p_F\xi_1)J_{d/2}(p_F\xi_2), \quad (16)$$

$$\vec{\xi_1} = \vec{r}+2t_1\hat{q}, \quad \vec{\xi_2} = \vec{r}-2t_2\hat{q}.$$

3. Application to Second Order Exchange

For our choice of Coulomb interaction

$$\alpha(q) = e^2\frac{(4\pi)^{(d-1)/2}}{q^{d-1}}\Gamma\left(\frac{d-1}{2}\right) \quad (17)$$

which requires $d>1$.

The second order exchange contribution to the ground-state energy per unit volume, of a d-dimensional electron fluid is

$$E_{2x} = \frac{1}{(2\pi)^{2d}}\int\alpha(q)A(q)d\vec{q}. \quad (18)$$

For $d > 2$ we take the polar axis as the $\hat{q}$-direction and apply Theorem 2. The q-integration is elementary and we have

$$E_{2x} = K_d \int d\Omega_q \int \frac{d\vec{r}}{r} \int_0^\infty \int_0^\infty \frac{dt_1 dt_2}{t_1 + t_2} \ln\left|\frac{\xi_1 + \xi_2}{\xi 1 - \xi_2}\right| \frac{J_{d/2}(p_F\xi_1)J_{d/2}(p_F\xi_2)}{(\xi_1\xi_2)^{d/2}}, \tag{19}$$

where K_d collects all the numerical prefactors and powers of p_F (for $d = 2$ $\int d\Omega_q = 2\pi$) and will be made explicit in the final result. Now set $t_2 = ut_1$ and $\vec{r} \to t_1\vec{r}$, so

$$E_{2x} = K_d \int d\Omega_q \int_0^\infty \frac{du}{u+1} \int \frac{d\vec{r}}{r(\eta_1\eta_2)^{d/2}} \ln\left|\frac{\eta_1 + \eta_2}{\eta_1 - \eta_2}\right| \int_0^\infty \frac{dt}{t} J_{d/2}(p_F t\eta_1)J_{d/2}(p_F t\eta_2), \tag{20}$$

where $\eta_1 = |\vec{r} + 2\hat{q}|$, $\eta_2 = |\vec{r} - 2u\hat{q}|$. The $\theta, t-$ integrals can be done next, yielding

$$E_{2x} = K_d \int_0^\infty \frac{du}{u+1} \int \frac{d\vec{r}}{r\eta_>^d} \ln\left|\frac{\eta_1 + \eta_2}{\eta_1 - \eta_2}\right|, \quad (d > 2) \tag{21}$$

For $d > 2$ we can switch to $d-$dimensional cylindrical coordinates with axis along $\hat{q}$. Since the integrand is independent of the azimuthal angle

$$\int d\vec{r} = \frac{2\pi^{(d-1)/2}}{\Gamma(\frac{1}{2}(d+1))} \int_{-\infty}^\infty dz \int_0^\infty \rho^{d-2} d\rho. \tag{22}$$

Next, after the successive transformations $t = (z-1)/(z+1)$ and $\rho = 2s/(1-t)$ we have

$$E_{2x} = K_d \int_{-1}^1 \frac{dt}{1-t} \ln\left(\frac{1+t}{1-t}\right) F(t)$$

$$F(t) = \int_0^\infty \frac{s^{d-2} ds}{(s^2+1)^{d/2}} \int_t^1 \frac{dy}{\sqrt{y^2+s^2}}. \tag{23}$$

Carrying out the $s-$integration, we come to

$$F(t) = \frac{1}{d-1} \int_t^1 \frac{dy}{|y|}\ {}_2F_1\left(\frac{1}{2}, \frac{1}{2}(d-1); \frac{1}{2}(d+1); 1 - y^{-2}\right). \tag{24}$$

By integrating by parts and noting that ${}_2F_1(\frac{1}{2}, a; a+1; 1-y^{-2}) = \frac{2|y|}{1+|y|}\ {}_2F_1\left(1, 1-a; a+1; \frac{1-|y|}{1+|y|}\right)$, we arrive at the principal result

Theorem 3

The second order exchange contribution to the ground-state energy of a $d > 2-$dimensional electron fluid is

$$E_{2x} = K_d G(d)$$

$$G(d) = \int_0^1 \frac{dy}{y+1} \left[\frac{\pi^2}{3} - \ln^2 y\right]\ {}_2F_1\left[1, \frac{1}{2}(3-d); \frac{1}{2}(1+d); y\right]. \tag{25}$$

4. Discussion

Equation (25) is as far as one can proceed without specifying the dimensionality. For $d = 3$, we find, since the hypergeometric function reduces to unity,

$$E_{2x} = K_3 G(3) = \frac{e^4 p_F^3}{4\pi^2} \int_0^1 \frac{dy}{1+y} \left(\frac{\pi^2}{3} - \ln^2 y \right) = \frac{1}{6}(\pi^2 \ln 4 - 9\zeta(3)). \qquad (26)$$

which is exactly the Onsager-Stephen-Mittag value, since they have $e^2 = 2$ and $p_F = 1$.

For the case $d = 2$ we itake the limit of (25) which gives

$$G(2) = 2 \int_0^1 \left(\frac{\pi^2}{3} - 4 \ln^2 y \right) \frac{\tan^{-1} y}{y^2 + 1} dy \qquad (27)$$

which, unlike the corresponding integral in [3] does not seem to be analytically evaluable. This gives

$$E_{2x} = K_2 G(2) = \frac{p_F^2 e^4}{32\pi^4}(18.0586) \qquad (28)$$

about 30% less than the value $(p_F^2 e^4/32\pi^4)(28.3664)$ in [3]. A possible reason is that in [3,(14)] the argument of the second Bessel function is $|\vec{r} - 2\hat{u}t|$ and after making the substitution $\vec{r} \to (t + x)\vec{r} + \hat{u}(x - t)$, in [3,(16)] the authors present it as $(x + t)|\vec{r} - \hat{u}|$, which is incorrect. It is this error which renders the remainder of the evaluation analytically tractable. An attempt to continue the calculation after correcting this was stymied by a further difficulty in [3,(14)]; the factor of 2 in the numerator of the argument of the logarithm means that, as $x \to \infty$ this argument tends to 2, rather than unity as required for convergence at the upper limit of the $x-$ integration.

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