The self-energy of the uniform electron gas in the second order of exchange

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The on-shell self-energy of the homogeneous electron gas in second order of exchange, $\Sigma_{2x} = \text{Re} \Sigma_{2x}(k_F, k^2_F/2)$, is given by a certain integral. This integral is treated here in a similar way as Onsager, Mittag, and Stephen [Ann. Physik (Leipzig) 18, 71 (1966)] have obtained their famous analytical expression $e_{2x} = \frac{1}{6} \ln 2 - \frac{3}{4} \frac{\zeta(3)}{\pi^2}$ (in atomic units) for the correlation energy in second order of exchange. Here it is shown that the result for the corresponding on-shell self-energy is $\Sigma_{2x} = e_{2x}$. The off-shell self-energy $\Sigma_{2x}(k, \omega)$ correctly yields $2e_{2x}$ (the potential component of $e_{2x}$) through the Galitskii-Migdal formula. The quantities $e_{2x}$ and $\Sigma_{2x}$ appear in the high-density limit of the Hugenholtz-van Hove (Luttinger-Ward) theorem.
I. INTRODUCTION

Although not present in the Periodic Table the homogeneous electron gas (HEG) is still an important model system for electronic structure theory, cf. e.g. [1]. In its spin-unpolarized version the HEG ground state is characterized by only one parameter $r_s$, such that a sphere with the radius $r_s$ contains on average one electron [2]. It determines the Fermi wave number as $k_F = 1/(\alpha r_s)$ with $\alpha = (4/(9\pi))^{1/3}$ and it measures simultaneously the interaction strength and the density such that high density corresponds to weak interaction and hence weak correlation. For recent papers on this limit cf. [3, 4, 5]. Naively one should expect that in this weak-correlation limit the Coulomb repulsion $\alpha r_s/r$ (where lengths and energies are measured in units of $k_F^{-1}$ and $k_F^2$, respectively) can be treated as perturbation. But in the early theory of the HEG, Heisenberg [6] has shown, that ordinary perturbation theory does not apply. With $e_0$ being the energy per particle of the ideal Fermi gas and $e_x$ being the exchange energy in lowest (1st) order, the total energy $e = e_0 + e_x + e_c$ defines the correlation energy $e_c = e_2 + e_3 + \cdots$. In 2nd order, there is a direct (d) term $e_{2d}$ and an exchange (x) term $e_{2x}$, so that $e_2 = e_{2d} + e_{2x}$. Whereas $e_{2x}/(\alpha r_s)^2$ is a pure finite number $b_x$, the direct term $e_{2d}$ logarithmically diverges along the Fermi surface (i.e. for vanishing transition momenta $q$): $e_{2d} \to \ln q$ for $q \to 0$. This failure of perturbation theory has been repaired by Macke [7] with an appropriate partial summation of higher-order terms up to infinite order. The result of this (ring-diagram) summation for the correlation energy in its weak-correlation limit is $e_c/(\alpha r_s)^2 = a \ln r_s + \cdots$ with $a = (1 - \ln 2)/\pi^2 \approx 0.031091$. This has been confirmed later by Gell-Mann and Brueckner [8], who in addition to the logarithmic term numerically calculated contributions to the next (constant, i.e. not depending on $r_s$) term $b$, namely $b_t$ and $b_d$ arising from the ring-diagram summation and from $e_{2d}$, respectively: $b_t \approx a \ln 2 - 0.001656 \approx -0.057514$ and $b_d \approx -0.013586$. The total constant term is $b = b_t + b_d + b_x \approx -0.046921$, where the exchange term $b_x = \frac{1}{6} \ln 2 - \frac{3}{4} \zeta(3) \approx +0.0241792$ has been analytically calculated by Onsager, Mittag, and Stephen in a very tricky way [9]. Although the integrand is rather simple, the Pauli principle causes complicated boundary conditions, which need a sophisticated treatment through several substitutions of the integral variables.

Here their method is used to calculate the analog term of the self-energy on the energy shell,
namely $\Sigma_{2x} = \text{Re} \Sigma_{2x}(1, 1/2)$ [with $k$ measured in units of $k_F$ and $\omega$ measured in units of $k_F^2$]. The more general quantity $\Sigma_{2x}(k, \omega)$ appears (i) in a recent study of the spectral moments of the HEG \[11\], (ii) in the context of self-consistent GW calculations \[12\], and within a project 'spectral functions for a hydrogen plasma' \[13\]. For $k = 1$, $\omega = \mu$ it appears in the Hugenholtz-van Hove (Luttinger-Ward) identity \[14\], which relates the chemical potential $\mu$ to the self-energy $\Sigma(k, \omega)$ according to $\mu - \mu_0 = \Sigma(1, \mu)$. The chemical potential follows from the total energy according to $\mu = (\frac{5}{3} - \frac{1}{3} r_s \frac{d}{dr_s}) e$. In the weak-correlation limit $r_s \to 0$ the total energy $e = e_0 + e_x + e_c$ and the chemical potential $\mu = \mu_0 + \mu_x + \mu_c$ are given by

$$e_0 = \frac{3}{10}, \quad e_x = -\frac{3}{4} \frac{\alpha r_s}{\pi}, \quad e_c = (\alpha r_s)^2 \left[ a \ln r_s + b + O(r_s) \right],$$

$$\mu_0 = \frac{1}{2}, \quad \mu_x = -\frac{\alpha r_s}{\pi}, \quad \mu_c = (\alpha r_s)^2 \left[ a \ln r_s + \left( -\frac{1}{3} a + b \right) + O(r_s) \right]. \quad (1.1)$$

Because of the above mentioned identity the self-energy $\Sigma(1, \mu)$ must have a corresponding behavior. The exchange in lowest order yields $\Sigma_x(1) = -\frac{\alpha r_s}{\pi}$ or $\mu_x = \Sigma_x(1)$, exactly in agreement with the mentioned identity. To obtain also the logarithmic term of $\Sigma(1, 1/2)$ the ring-diagram summation has to be done for the self-energy \[15\]. To the next term beyond the logarithmic term contributes the 2nd-order exchange self-energy $\Sigma_{2x} = \text{Re} \Sigma_{2x}(1, 1/2)$. Just this term is calculated here using the tricky method of Onsager, Mittag, and Stephen \[9\]. The Feynman diagrams of $e_{2x}$ and $\Sigma_{2x}$ are given in Figs. 1 and 2. As shown in the Appendix, from the Feynman diagram rules it follows $\Sigma_{2x} = -\frac{(\alpha r_s)^2}{4 \pi^4} (X_1 + X_2)$, where $X_{1,2}$ mean the integrals defined in Eqs. \[A.10\] and \[A.11\]. They are calculated in the following sections. The final results are $X_1 = -\pi^4 \left[ \frac{1}{3} \ln 2 - \frac{5}{\pi^2} \frac{\zeta(3)}{\pi^2} \right]$, $X_2 = \pi^4 \left[ \frac{2}{3} \ln 2 - \frac{2}{\pi^2} \frac{\zeta(3)}{\pi^2} \right]$, thus $\Sigma_{2x} = (\alpha r_s)^2 \left[ \frac{1}{6} \ln 2 - \frac{3}{4} \frac{\zeta(3)}{\pi^2} \right] = e_{2x}$, thus $\mu_{2x} = \Sigma_{2x}$. This relation appears in the weak-correlation limit of the above mentioned Hugenholtz-van Hove theorem \[14\]. This paper is a contribution to the mathematics of the weakly-correlated (high-density) HEG.

**II. THE INTEGRAL $X_1$**

In Eq. \[A.10\], new variables $q' = (q_1 + q_2)/2$, $p' = (q_1 - q_2)/2$, and $s' = e + (q_1 + q_2)/2$ lead to

$$q_1 = q' + p', \quad (e + q_1)^2 = (s' + p')^2, \quad (e + q_2)^2 = (s' - p')^2, \quad q_2 = q' - p', \quad (e + q_1 + q_2)^2 = (s' + q')^2, \quad e^2 = (s' - q')^2. \quad (2.1)$$
Therefore (with $\Theta(x) =$ Heaviside step function)

$$X_1 = \int d^3q' d^3p' \frac{2^3}{q'^2 - p'^2} \frac{1}{(p' + q')^2(p' - q')^2} \times$$

$$\times \int \frac{d^2s'}{\pi} \delta((s' - q')^2 - 1)\Theta[1 - (s' + q')^2] \Theta[(s' + p')^2 - 1] \Theta[(s' - p')^2 - 1].$$

(2.2)

The next step scales $q'$, $p'$, $s'$ with $\lambda = 1/\sqrt{1 - s'^2}$ according to $q = \lambda q'$, $p = \lambda p'$, $s = \lambda s'$ with the consequences

$$1 - s'^2 = \frac{1}{1 + s'^2}, \quad d^2s' = \frac{d^2s}{(1 + s'^2)^2},$$

$$\delta((s' - q')^2 - 1) = (1 + s'^2) \delta(q'^2 - 2sq - 1),$$

$$\pm 2sp + p^2 > 1, \quad 2sq + q^2 < 1, \quad -2sq + q^2 = 1,$$  

(2.3)

from which follow $p \geq 1$ and $q \leq 1$ (what makes the energy denominator $q^2 - p^2$ negative) and $sq < 0, s \geq \alpha$. Thus

$$X_1 = -\int_{0}^{1} dq \int_{1}^{\infty} dp \int_{-1}^{+1} dx \frac{16 \pi}{p^2 - q^2} \int_{-1}^{+1} dx \frac{8 q^2 p^2}{(p^2 + q^2)^2 - (2qp)^2} \times$$

$$\times \int_{s \geq \alpha, \cos \varphi_q < 0} d^2s \frac{d^2s'}{1 + s'^2} \delta(q'^2 - 1 - 2sq) \Theta(p^2 - 1 + 2sp) \Theta(p^2 - 1 - 2sp).$$

(2.4)

Here and in the following of Sec. II the abbreviations

$$\alpha = \frac{1 - q^2}{2q} \geq 0, \quad \beta = \frac{p^2 - 1}{2p} \geq 0, \quad a = \frac{q^2 + p^2}{2qp} \geq 1,$$

$$\frac{t}{s} = \cos \varphi_p = \cos \varphi(s, p), \quad x = \cos \varphi = \cos \varphi(q, p), \quad y = \cos \varphi_q = \cos \varphi(q, s)$$

(2.5)

are used:

$$X_1 = -\int_{0}^{1} dq \int_{1}^{\infty} dp \frac{16 \pi}{p^2 - q^2} \int_{-1}^{+1} dx \frac{1}{a^2 - x^2} \int_{s \geq \alpha, \cos \varphi_q < 0} sds \frac{d\varphi_q}{1 + s^2} \frac{1}{2sq} \delta \left(\frac{\alpha}{s} + y\right) \Theta(\beta - |t|)$$

(2.6)

$t$ is introduced to replace $s$ after having done the $\varphi_q$ integration. To this purpose the relation between $t$ and $s$ is needed. It follows from $\varphi_q + \varphi_p = \varphi$ or $\varphi_p = \varphi - \varphi_q$, therefore $\cos \varphi_p = \cos(\varphi - \varphi_q) = \cos \varphi \cos \varphi_q + \sin \varphi \sin \varphi_q$; what is in terms of $t/s, x,$ and $y$ (the latter quantity equals $-\alpha/s$ because of the delta function):

$$\frac{t}{s} = x \left(-\frac{\alpha}{s}\right) \pm \sqrt{1 - x^2} \sqrt{1 - \left(\frac{\alpha}{s}\right)^2} \quad \text{or} \quad (t + \alpha x)^2 = (1 - x^2)(s^2 - \alpha^2).$$

(2.7)
This has the consequences

\[ s^2 - \alpha^2 = \frac{(t + \alpha x)^2}{1 - x^2}, \quad (2.8) \]

\[ \frac{sds}{1 + s^2} = \frac{(t + \alpha x)dt}{(t + \alpha x)^2 + (1 + \alpha^2)(1 - x^2)}. \quad (2.9) \]

With the help of Eq. (2.8) the \( \varphi_q \) integration yields a function depending on \( s \) (respectively on \( t \)). Note that \( \cos \varphi_q = -\frac{\alpha}{s} \) has two solutions \( \varphi_{q1} \) and \( \varphi_{q2} \) with \( |\sin \varphi_{q1}| = |\sin \varphi_{q2}| = \sqrt{1 - \left(\frac{\alpha}{s}\right)^2} : \)

\[ \int_0^{2\pi} \frac{d\varphi_q}{s} \left[ \delta(-\sin \varphi_{q1} \cdot (\varphi_q - \varphi_{q1})) + \delta(-\sin \varphi_{q2} \cdot (\varphi_q - \varphi_{q2})) \right] \]

\[ = \int_0^{2\pi} \frac{d\varphi_q}{s} \left[ \frac{\varphi_q - \varphi_{q1}}{\sqrt{1 - \left(\frac{\alpha}{s}\right)^2}} + \frac{\varphi_q - \varphi_{q2}}{\sqrt{1 - \left(\frac{\alpha}{s}\right)^2}} \right] = \frac{2}{\sqrt{s^2 - \alpha^2}} = 2 \frac{\sqrt{1 - x^2}}{|t + \alpha x|}. \quad (2.10) \]

Thus

\[ \int_{s \geq \alpha, \cos \varphi_q} sds \frac{d\varphi_q}{2sq} \delta \left( \frac{\alpha}{s} + y \right) \Theta(\beta - |t|) = \frac{\sqrt{1 - x^2}}{q} \int_{t_0}^{t_1} \frac{\text{sign}(t + \alpha x) \ dt}{(t + \alpha x)^2 + (1 + \alpha^2)(1 - x^2)} \]

\[ = \frac{2}{1 + q^2} \arctan \frac{t + \alpha x}{\sqrt{(1 + \alpha^2)(1 - x^2)}} \bigg|_{t_0}^{t_1} \quad (2.11) \]

\(|t| \leq \beta \) contains the upper limit of the \( t \)-integration as \( t \leq \beta =: t_1 \). What concerns its lower limit \( t_0 \), the relation \( t \geq -\beta \) competes with \( t \geq -\alpha x \), as it follows from Eq. (2.7) for the lower limit \( \alpha \) of the \( s \)-integration. This means for the ranges of the \( t \)- and \( x \)-integrations, one has in the (vertical) stripe \( q = 0 \cdots 1, p = 1 \cdots \infty \) of the \( q,p \)-plane to distinguish between the two regions, cf. Fig. 3:

(a) region A with \( qp \geq 1 \) or \( \alpha \leq \beta \) or \( -\alpha x \geq -\alpha \geq -\beta \), hence \( t_0 = -\alpha x \), and

(b) region B with \( qp \leq 1 \) or \( \alpha \geq \beta \) or \( -\alpha \leq \beta \).

In the case (b) one has again to distinguish between

(i) \( x = -\beta/\alpha \cdots + \beta/\alpha \), with the consequence \( t_0 = -\alpha x \) and

(ii) \( x = \beta/\alpha \cdots 1 \), with the consequence \( t_0 = -\beta \).

Thus it is

\[ \int_{-1}^{+1} dx \int_{t_0}^{+\beta} dt = \begin{cases} 
\int_{-1}^{+\beta} dx \int_{-1}^{+\beta} dt & \text{for } qp \geq 1 \text{ or } \alpha \leq \beta, \\
\int_{-\beta}^{+\beta} dx \int_{-\beta}^{+\beta} dt + \int_{-\beta}^{+\beta} dx \int_{-\beta}^{+\beta} dt & \text{for } qp \leq 1 \text{ or } \alpha \geq \beta.
\end{cases} \quad (2.12) \]
With the abbreviations (2.5) and
\[ f(t, x) = \frac{2}{a^2 - x^2} \arctan \frac{t + \alpha x}{\sqrt{(1 + \alpha^2)(1 - x^2)}}, \] (2.13)

Eq. (2.6) can be written as (note that \( f(-\alpha x, x) = 0 \))
\[
X_1 = -\int_0^1 dq \int_1^{\infty} dp \frac{16 \pi}{(p^2 - q^2)} \frac{1}{1 + q^2} \left\{ \Theta(qp - 1) \int_{-1}^{+1} dx f(\beta, x) \right. \\
+ \Theta(1 - qp) \left[ \int_{-\beta/\alpha}^{+1} dx f(\beta, x) + \int_{-\beta/\alpha}^{+1} dx [f(\beta, x) - f(-\beta, x)] \right] \right\}. \tag{2.14}
\]

With
\[
\int_{+\beta/\alpha}^{+1} dx (-1)f(-\beta, x) = \int_{+\beta/\alpha}^{+1} dx f(\beta, -x) = \int_{-1}^{+1} dx f(\beta, x) \tag{2.15}
\]
the terms for \( qp \leq 1 \) can be comprised as \( \int_{-1}^{+1} dx f(\beta, x) \). Therefore
\[
X_1 = -\int_0^1 dq \int_1^{\infty} dp \int_{-1}^{+1} dx \frac{16 \pi}{p^2 - q^2} \frac{1}{1 + q^2} f(\beta, x). \tag{2.16}
\]

The final substitution \( p = 1/k \) transforms the region of the last two integrations from the (vertical) stripe \( q = 0 \cdots 1, p = 1 \cdots \infty \) to the more simple unit square \( q = 0 \cdots 1, k = 0 \cdots 1 \).

With the abbreviations
\[
\alpha = \frac{1 - q^2}{2q} \geq 0, \quad \beta = \frac{1 - k^2}{2k} \geq 0, \quad a = \frac{1 + q^2k^2}{2qk} \geq 1 \tag{2.17}
\]

it is:
\[
X_1 = -\int_0^1 dq \int_0^1 dk \int_{-1}^{+1} dx \frac{16 \pi}{1 - q^2k^2} \frac{1}{1 + q^2} f(\beta, x) \approx -30.70598 \cdots . \tag{2.18}
\]

The coefficients \( \alpha, \beta, \) and \( a \) of Eq. (2.17) make the integrand of (2.18) functions of \( q \) and \( k \).

Mathematica5.2 \[17\] yields the given figure. It seems to hold
\[
X_1 = -\pi^4 \left[ \frac{4}{3} \ln 2 - 5 \zeta(3) \right] \approx -30.705985239248893 \cdots \tag{2.19}
\]

How to derive this analytically? Is this possible with the method of ref. \[18\]?
The whole procedure of Sec. II is repeated here step by step. In Eq. (A.11), new variables

\[ q' = (q_1 + q_2)/2, \quad p' = (q_1 - q_2)/2, \quad \text{and} \quad s' = e + (q_1 + q_2)/2 \]

lead to

\[ q_1 = q' + p', \quad (e + q_1)^2 = (s' + p')^2, \quad (e + q_2)^2 = (s' - p')^2, \]
\[ q_2 = q' - p', \quad (e + q_1 + q_2)^2 = (s' + q')^2, \quad e^2 = (s' - q')^2. \quad (3.1) \]

Therefore

\[
X_2 = \int d^3q' d^3p' \frac{2^3}{q'^2 - p'^2} \frac{1}{(q' + p')(q' - p')} \times \]
\[
\times \int \frac{d^2s'}{\pi} \delta((s' - q')^2 - 1)\Theta((s' + q')^2 - 1)\Theta[1 - (s' + p')^2]\Theta[1 - (s' - p')^2]. \quad (3.2)
\]

The next step scales \( q', p', s' \) with \( \lambda = 1/\sqrt{1 - s'^2} \) according to \( q = \lambda q', p = \lambda p', s = \lambda s' \) with the consequences

\[
1 - s'^2 = \frac{1}{1 + s'^2}, \quad d^2s' = \frac{d^2s}{(1 + s'^2)^2}, \quad \delta((s' - q')^2 - 1) = (1 + s'^2) \delta(q'^2 - 2sq - 1), \]
\[
\pm 2sp + p^2 < 1, \quad 2sq + q^2 > 1, \quad -2sq + q^2 = 1, \quad (3.3)
\]

from which follow \( q \geq 1 \) and \( p \leq 1 \) (what makes the energy denominator \( q^2 - p^2 \) positive) and \( sq > 0, s \geq \bar{\alpha} \). Thus

\[
X_2 = \int dq \int^1_0 dp \frac{16 \pi}{q^2 - p^2} \int^{+1}_1 dx \frac{8 q^2 p^2}{(p^2 + q^2)^2 - (2qp)^2} \times \]
\[
\times \int_{s \geq \bar{\alpha}, \cos \varphi_q > 0} \frac{d^2s}{1 + s^2} \delta(q^2 - 1 - 2sq)\Theta(1 - p^2 - 2sp)\Theta(1 - p^2 + 2sp). \quad (3.4)
\]

Here and in the following of Sec. III the abbreviations

\[
\bar{\alpha} = \frac{q^2 - 1}{2q} \geq 0, \quad \bar{\beta} = \frac{1 - p^2}{2p} \geq 0, \quad \bar{a} = \frac{q^2 + p^2}{2qp} \geq 1,
\]
\[
t = \cos \varphi_p = \cos \chi(s,p), \quad x = \cos \varphi = \cos \chi(q,p), \quad y = \cos \varphi_q = \cos \chi(q,s) \quad (3.5)
\]

are used:

\[
X_2 = \int dq \int^1_0 dp \frac{16 \pi}{q^2 - p^2} \int^{+1}_1 dx \frac{sdq}{a^2 - \tilde{x}^2} \int_{s \geq \bar{\alpha}, \cos \varphi_q > 0} ds dq \frac{1}{2sq} \delta \left( \frac{\bar{\alpha}}{s} - y \right) \Theta(\bar{\beta} - |t|). \quad (3.6)
\]
$t$ is introduced to replace $s$ after having done the $\varphi_q$ integration. To this purpose the relation between $t$ and $s$ is needed. It follows from $\varphi_q + \varphi_p = \varphi$ or $\varphi_p = \varphi - \varphi_q$, therefore $\cos \varphi_p = \cos(\varphi - \varphi_q) = \cos \varphi \cos \varphi_q + \sin \varphi \sin \varphi_q$, what is in terms of $t/s$, $x$, and $y$ (which equals $+\tilde{\alpha}/s$ because of the delta function):

$$
\frac{t}{s} = x\frac{\tilde{\alpha}}{s} \pm \sqrt{1 - x^2} \sqrt{1 - \left(\frac{\tilde{\alpha}}{s}\right)^2} \quad \text{or} \quad (t - \tilde{\alpha} x)^2 = (1 - x^2)(s^2 - \tilde{\alpha}^2).
$$

(3.7)

This has the consequences

$$
s^2 - \tilde{\alpha}^2 = \frac{(t - \tilde{\alpha} x)^2}{1 - x^2},
$$

(3.8)

$$
\frac{sds}{1 + s^2} = \frac{(t - \tilde{\alpha} x)dt}{(t - \tilde{\alpha} x)^2 + (1 + \tilde{\alpha}^2)(1 - x^2)}.
$$

(3.9)

With the help of Eq. (3.8) the $\varphi_q$ integration yields a function depending on $s$ (respectively on $t$). Note that $\cos \varphi_q = +\frac{\tilde{\alpha}}{s}$ has two solutions $\varphi_{q,1}$ and $\varphi_{q,2}$ with $|\sin \varphi_{q,1}| = |\sin \varphi_{q,2}| = \sqrt{1 - \left(\frac{\tilde{\alpha}}{s}\right)^2}$:

$$
\int_0^{2\pi} \frac{d\varphi_q}{s} \left[ \delta(+ \sin \varphi_{q,1} \cdot (\varphi_q - \varphi_{q,1})) + \delta(+ \sin \varphi_{q,2} \cdot (\varphi_q - \varphi_{q,2})) \right]
\int_0^{2\pi} \frac{d\varphi_q}{s} \frac{\delta(\varphi_q - \varphi_{q,1}) + \delta(\varphi_q - \varphi_{q,2})}{\sqrt{1 - \left(\frac{\tilde{\alpha}}{s}\right)^2}} = \frac{2}{\sqrt{s^2 - \tilde{\alpha}^2}} = 2 \frac{1 - x^2}{|t - \tilde{\alpha} x|}.
$$

(3.10)

Thus

$$
\int_{s \geq \tilde{\alpha}, \cos \varphi_q > 0} \frac{sds}{1 + s^2} \frac{1}{2sq} \delta \left(\frac{\tilde{\alpha}}{s} - y\right) \Theta(\beta - |t|) = \frac{\sqrt{1 - x^2}}{q} \int_{t_0}^{t_1} \frac{\text{sign}(t - \tilde{\alpha} x) dt}{(t - \tilde{\alpha} x)^2 + (1 + \tilde{\alpha}^2)(1 - x^2)}
$$

$$
= \frac{2}{1 + q^2} \arctan \frac{t - \tilde{\alpha} x}{\sqrt{(1 + \tilde{\alpha}^2)(1 - x^2)}} \bigg|_{t_0}^{t_1}.
$$

(3.11)

$|t| \leq \tilde{\beta}$ contains the upper limit of the $t$-integration as $t \leq \tilde{\beta} =: t_1$. What concerns its lower limit $t_0$, the relation $t \geq -\tilde{\beta}$ competes with $t \geq \tilde{\alpha} x$, as it follows from Eq. (3.7) for the lower limit $\tilde{\alpha}$ of the $s$-integration. This means for the ranges of the $t$- and $x$-integrations, one has in the (horizontal) stripe $q = 1 \cdots \infty, p = 0 \cdots 1$ of the $q$-$p$-plane to distinguish between the two regions, cf. Fig. 4:

(a) region A with $qp \geq 1$ or $\tilde{\alpha} \geq \tilde{\beta}$ or $-\tilde{\alpha} \leq -\tilde{\beta}$, and

(b) region B with $qp \leq 1$ or $\tilde{\alpha} \leq \tilde{\beta}$ or $\tilde{\alpha} x \leq \tilde{\alpha} \leq \tilde{\beta}$, hence $t_0 = \tilde{\alpha} x$. 
In the case (a) one has again to distinguish between

(i) \( x = -1 \cdots -\bar{\beta}/\bar{\alpha} \), with the consequence \( t_0 = -\bar{\beta} \) and

(ii) \( x = -\bar{\beta}/\bar{\alpha} \cdots + \bar{\beta}/\bar{\alpha} \), with the consequence \( t_0 = \bar{\alpha} x \).

Thus it is

\[
\int_{-1}^{1} \int_{t_0}^{+\beta} dx \int_{-1}^{+\beta} dt = \begin{cases} 
\int_{-1}^{+\beta} dx \int_{-1}^{+\beta} dt + \int_{-1}^{+\beta} dx \int_{-1}^{+\beta} dt \quad \text{for } qp \geq 1 \text{ or } \bar{\alpha} \geq \bar{\beta}, \\
\int_{-1}^{+\beta} dx \int_{-1}^{+\beta} dt \quad \text{for } qp \leq 1 \text{ or } \bar{\alpha} \leq \bar{\beta}. 
\end{cases}
\]  

(3.12)

With the abbreviations (3.5) and with

\[
\bar{f}(t, x) = \frac{2}{\bar{\alpha}^2 - x^2} \arctan \frac{t - \bar{\alpha}x}{\sqrt{(1 + \bar{\alpha}^2)(1 - x^2)}},
\]  

(3.13)

Eq. (3.6) can be written as (note that \( \bar{f}(\bar{\alpha}x, x) = 0 \))

\[
X_2 = \int_{1}^{\infty} dq \int_{0}^{1} dp \frac{16 \pi}{q^2 - p^2} \frac{1}{1 + q^2} \left\{ \Theta(1 - qp) \int_{-1}^{+1} dx \ \bar{f}(\bar{\beta}, x) \\
+ \Theta(qp - 1) \left[ \int_{-1}^{-\beta/\bar{\alpha}} dx \ [\bar{f}(\bar{\beta}, x) - \bar{f}(\bar{\beta}, -x)] + \int_{-\beta/\bar{\alpha}}^{+\beta/\bar{\alpha}} dx \ \bar{f}(\bar{\beta}, x) \right] \right\}. 
\]  

(3.14)

With the identity

\[
\int_{-1}^{-\beta/\bar{\alpha}} dx \ (-1)\bar{f}(\bar{\beta}, x) = \int_{-1}^{+1} dx \ \bar{f}(\bar{\beta}, -x) = \int_{-1}^{+1} dx \ \bar{f}(\bar{\beta}, x)
\]  

(3.15)

the terms for \( qp \geq 1 \) can be comprised as \( \int_{-1}^{+1} dx \ \bar{f}(\bar{\beta}, x) \). Therefore

\[
X_2 = \int_{1}^{\infty} dq \int_{0}^{1} dp \int_{-1}^{+1} dx \frac{16 \pi}{q^2 - p^2} \frac{1}{1 + q^2} \ \bar{f}(\bar{\beta}, x). 
\]  

(3.16)

This is similar to Eq. (2.10), but there are also differences. The substitution \( q = 1/k \) transforms the region of the last two integrations from the (horizontal) stripe \( q = 1 \cdots \infty \), \( p = 0 \cdots 1 \) to the more simple unit square \( k = 0 \cdots 1 \), \( p = 0 \cdots 1 \). With the abbreviations

\[
\bar{\alpha} = \frac{1 - k^2}{2k}, \quad \bar{\beta} = \frac{1 - p^2}{2p}, \quad \tilde{\alpha} = \frac{1 + k^2 p^2}{2kp},
\]  

(3.17)
it is
\[X_2 = \int_0^1 dq \int_0^1 dk \int_{-1}^{+1} dx \frac{16 \pi}{1 - q^2 k^2} \frac{1}{1 + k^2} \frac{1}{1 + k^2} \tilde{f}(\beta, x).\]

Changing finally the notation with \(k \to q\) and \(p \to k\) makes \(\alpha = \alpha, \beta = \beta,\) and \(\bar{a} = a,\) cf. Eq. (2.17). With these identities and with \(\tilde{f}(t, -x) = f(t, x)\) a further rewriting yields
\[X_2 = \int_0^1 dq \int_0^1 dk \int_{-1}^{+1} dx \frac{16 \pi}{1 - q^2 k^2} \frac{q^2}{1 + q^2} f(\beta, x) \approx 21.284906 \cdots. \tag{3.18}\]

This integral differs from Eq. (2.18) 'only' in an additional factor of \(-q^2\) in the nominator of the integrand. Mathematica5.2 yields the given figure. It seems to hold
\[X_2 = \pi^4 \left[ \frac{2}{3} \ln 2 - 2 \frac{\zeta(3)}{\pi^2} \right] \approx 21.284905670516334 \cdots. \tag{3.19}\]

How to derive this analytically? Is this possible with the method of ref. [18]?

IV. THE CALCULATION OF \(X\)

With Eqs. (2.13), (2.18), (3.18), and with \(a, \alpha, \beta\) being defined in Eq. (2.17) the result for \(X = X_1 + X_2\) is
\[X = -\int_0^1 dq \int_0^1 dk \int_{-1}^{+1} dx \frac{16 \pi}{1 - q^2 k^2} \frac{1 - q^2}{1 + q^2} \frac{2}{a^2 - x^2} \arctan \frac{\beta + \alpha x}{\sqrt{(1 + \alpha^2)(1 - x^2)}} \approx -9.42108 \cdots. \tag{4.1}\]

It seems to hold \([18, 19]\)
\[X = -\pi^4 \left[ \frac{2}{3} \ln 2 - 3 \frac{\zeta(3)}{\pi^2} \right] \approx -9.421079568732553 \cdots. \tag{4.2}\]

The final result \([20]\)
\[\Sigma_{2x} = -\frac{(\alpha r_s)^2}{4\pi^4} X = e_{2x} \quad \text{with} \quad \frac{e_{2x}}{(\alpha r_s)^2} = \frac{1}{6} \ln 2 - \frac{3}{4} \frac{\zeta(3)}{\pi^2} \approx 0.0241792 \tag{4.3}\]
appears in the weak-correlation limit of the Hugenholtz-van Hove (Luttinger-Ward) theorem \([14, 15]\). Because of \(\mu_{2x} = e_{2x}\) it holds the sum rule \(\mu_{2x} = \Sigma_{2x}\) analogous to \(\mu_x = \Sigma_x\). Whether perhaps also the more general expression \(\Sigma_{2x}(k, \omega)\) can be calculated in a similar way, has to be studied.
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[20] This result should be comparable to calculations by E. Shirley [12] if one considers in his Fig. 1 the contribution of the second (exchange) Feynman diagram to the on-shell self-energy $\Sigma(1,1/2)$ in the limit $r_s \to 0$, where the effectively screened Coulomb repulsion $W(12)$ is replaced by the bare Coulomb repulsion $\nu(12)$.

APPENDIX A: DERIVATION OF $\Sigma_{2x}$

The one-body Green’s function of the non-interacting system (ideal Fermi gas)

$$G_0(k, \omega) = \theta(k - 1) \frac{\omega - \frac{1}{2}k^2 + i\delta}{\omega - \frac{1}{2}k^2 - i\delta} + \theta(1 - k) \frac{\omega - \frac{1}{2}k^2 - i\delta}{\omega - \frac{1}{2}k^2 + i\delta}$$  \hspace{1cm} (A.1)

(with $\theta(x)$ = Heaviside step function) and $G(k, \omega)$, the one-body Green’s function of the fully interacting system, define the self-energy $\Sigma(k, \omega)$ through

$$G(k, \omega) = G_0(k, \omega) + G_0(k, \omega) \Sigma(k, \omega) G(k, \omega) \ .$$  \hspace{1cm} (A.2)

$\Sigma(k, \omega)$ appears in the Hugenholtz-van Hove theorem (in the Luttinger-Ward form $\mu - \mu_0 = \Sigma(1, \mu)$ with $\mu$ = chemical potential) [14] and in the Galitskii-Migdal formula [16]

$$v = \frac{1}{2} \int d(k)^3 \int \frac{d\omega}{2\pi i} e^{i\omega\delta} G(k, \omega) \Sigma(k, \omega) \ , \ \delta > 0 \ .$$  \hspace{1cm} (A.3)

$v$ is the potential component of $e$, the total energy per particle. The contour of the $\omega$-integration is to be closed in the upper complex $\omega$-plane. In lowest order it is $\Sigma_x(k) = -(1 + \frac{1-k^2}{2k} \ln |1+k|_{1-k})$. This makes $v_x = -\frac{3\alpha_r^2}{4\pi}$, in agreement with $v_x = e_x$, what
follows from the virial theorem \( v = r_s \frac{d}{dr_s} \epsilon \).

From the Feynman diagram for the exchange term of the 2nd-order self-energy it follows

\[
\Sigma_{2x}(k, \omega) = \frac{(\alpha r_s)^2}{4\pi^4} \int \frac{d^3q_1 d^3q_2}{q_1^2 q_2^2} \int \frac{d\eta_1 d\eta_2}{(2\pi i)^2} \times \\
\times G_0(|k + q_2|, \omega + \eta_2)G_0(|k + q_1 + q_2|, \omega + \eta_1 + \eta_2)G_0(|k + q_1|, \omega + \eta_1) \\
(A.4)
\]

One may check this expression by using it in the Galitskii-Migdal formula \(A.3\). Its lhs is known from the virial theorem as \( v_{2x} = 2e_{2x} \) with \( e_{2x} = \text{energy in second order of exchange} \), calculated by Onsager et al. \[9\]. Its rhs gives with Eqs. \(A.1\) and \(A.5\)

\[
\text{rhs} = -\frac{3(\alpha r_s)^2}{(2\pi)^5} \left[ \int \frac{d^3k d^3q_1 d^3q_2}{q_1^2 q_2^2} \Theta(1-k)\Theta(1-|k + q_1 + q_2|)\Theta(|k + q_1| - 1)\Theta(|k + q_2| - 1) \\
\times \frac{q_1 \cdot q_2 + i\delta}{q_1 \cdot (-q_2) + i\delta} \right] \Theta(k-1)\Theta(|k + q_1 + q_2| - 1)\Theta(1-|k + q_1| - 1)\Theta(1-|k + q_2|) \\
(A.6)
\]

It is easy to show with the help of the substitutions \( q_1 \rightarrow q'_1, q_2 \rightarrow -q'_2, k \rightarrow -(k' + q'_1) \) that the second term equals the first one. Thus

\[
\text{Re rhs} = -2\frac{3(\alpha r_s)^2}{(2\pi)^5} \int \frac{d^3k d^3q_1 d^3q_2}{q_1^2 q_2^2} \frac{P}{q_1 \cdot q_2} \times \\
\times \Theta(1-k)\Theta(1-|k + q_1 + q_2|)\Theta(|k + q_1| - 1)\Theta(|k + q_2| - 1) = 2e_{2x}. \\
(A.7)
\]

\( P \) means the Cauchy principle value. This is in agreement with the above mentioned relation. That \( e_{2x} \) of Eq. \(A.7\) really agrees with the integral calculated by Onsager et al. \[9\] follows from the substitutions \( k \rightarrow k_1, q_1 \rightarrow q, q_2 \rightarrow -(k_1 + k_2 + q) \). From Eq. \(A.5\) also follows \( n_{2x}(k) \), the second-order-in-exchange contribution to the momentum distribution. It is again easy to derive the well-known asymptotics \( n_{2x}(k \rightarrow \infty) = -\frac{4}{9\pi^2} \frac{(\alpha r_s)^2}{k^3} \).
After this control of $\Sigma_{2x}(k, \omega)$, the formula for $\Sigma_{2x} = \text{Re} \, \Sigma_{2x}(1, 1/2)$ follows from Eq. (A.5) as $\Sigma_{2x} = -\frac{(\alpha r)^2}{4\pi^2} (X_1 + X_2)$, where $X_{1,2}$ mean the integrals

$$X_1 = \int d^3q_1 \, d^3q_2 \, \frac{P}{q_1 \cdot q_2} \frac{1}{q_1^2 q_2^2} \Theta[1 - (e + q_1 + q_2)^2] \Theta[(e + q_1)^2 - 1] \Theta[(e + q_2)^2 - 1] ,$$  

(A.8)

$$X_2 = \int d^3q_1 \, d^3q_2 \, \frac{P}{q_1 \cdot q_2} \frac{1}{q_1^2 q_2^2} \Theta[(e + q_1 + q_2)^2 - 1] \Theta[1 - (e + q_1)^2] \Theta[1 - (e + q_2)^2] .$$  

(A.9)

They contain $q_1 \cdot q_2$ as the energy denominator. $1/q_{1,2}^2$ arises from the Coulomb repulsion and the remainder is due to the Pauli principle. $e$ is a unit vector. Note that $q_1 \cdot q_2 < 0$ for $X_1$, because of $(2e + q_1) \cdot q_1 > 0$ and $(2e + q_2) \cdot q_2 > 0$ in combination with $(2e + q_1) \cdot q_1 + (2e + q_2) \cdot q_2 + 2q_1 \cdot q_2 < 0$. This latter inequality enforces $q_1 \cdot q_2 < 0$. Thus $X_1 < 0$. It follows similarly $X_2 > 0$. The integrals $X_{1,2}$ do not depend on $e$. Therefore application of $\hat{O} = \int d^3e/(4\pi^2) \, 2 \, \delta(e^2 - 1)$ does not change them (notice $2 \, \delta(e^2 - 1) = \delta(e - 1)$). Following Onsager et al. (9), $e$ is resolved into its components perpendicular to the $q_1 - q_2$-plane $e_\perp$, and in the plane $e_\parallel$: $\hat{O} = \int de_\perp/2 \, \int d^2e_\parallel/(2\pi) \, 2 \, \delta(e_{\parallel}^2 + e_{\perp}^2 - 1)$. The integration over $e_\perp$ may be done immediately by means of a change in scale: $q_1 = \tilde{q}_1 \sqrt{1-e_{\perp}^2}$, $q_2 = \tilde{q}_2 \sqrt{1-e_{\perp}^2}$, $e_\parallel = \tilde{e}_\parallel \sqrt{1-e_{\perp}^2}$. The results are (denoting $\tilde{e}_\parallel$ as $\tilde{e}$ and deleting also all the other tildes for simplicity)

$$X_1 = \int d^3q_1 \, d^3q_2 \, \frac{P}{q_1 \cdot q_2} \frac{1}{q_1^2 q_2^2} \int \frac{d^2e}{2\pi} \, 2 \, \delta(e^2 - 1) \times \Theta[1 - (e + q_1 + q_2)^2] \Theta[(e + q_1)^2 - 1] \Theta[(e + q_2)^2 - 1] ,$$  

(A.10)

$$X_2 = \int d^3q_1 \, d^3q_2 \, \frac{P}{q_1 \cdot q_2} \frac{1}{q_1^2 q_2^2} \int \frac{d^2e}{2\pi} \, 2 \, \delta(e^2 - 1) \times \Theta[(e + q_1 + q_2)^2 - 1] \Theta[1 - (e + q_1)^2] \Theta[1 - (e + q_2)^2] .$$  

(A.11)

Whereas the two terms of $\Sigma_{2x}(k, \omega)$, cf. (A.6) each contributes $e_{2x}$ to $v_{2x}$ (thus $v_{2x} = 2e_{2x}$) as shown above, cf. (A.7), $X_1$ and $X_2$ contribute different values to $\Sigma_{2x}(1, 1/2)$ as shown in Secs. II and III.
FIG. 1: The Feynman diagram of $e_{2x}$, analytically calculated by Onsager et al. 

FIG. 2: The Feynman diagram of $\Sigma_{2x}(k, \omega)$, (semi)analytically calculated in this paper.
FIG. 3: The dashed area is the region of integration described by Eq. (2.12).

FIG. 4: The dashed area is the region of integration described by Eq. (3.12).