

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, $\Sigma_{2x} = \text{Re } \Sigma_{2x}(k_F, k_F^2/2)$, 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 Σ_{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. [3–5]. 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 $e_c = e_2 + e_3 + \dots$. 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): $e_{2d} \rightarrow \ln q$ for $q \rightarrow 0$. 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 $e_c/(\alpha r_s)^2 = a \ln r_s + \dots$ 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_r and b_d arising from the ring-diagram summation and from e_{2d} , respectively: $b_r \approx a \ln \frac{\alpha}{\pi} - 0.001656 \approx -0.057514$ and $b_d \approx -0.013586$. The total constant term is $b = b_r + b_d + b_x \approx -0.046921$, where the exchange term $b_x = \frac{1}{6} \ln 2 - \frac{3}{4} \frac{\zeta(3)}{\pi^2} \approx +0.0241792$ 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 ω 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 μ 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 $r_s \rightarrow 0$ the total energy $e = e_0 + e_x + e_c$ and the chemical potential $\mu = \mu_0 + \mu_x + \mu_c$ are given by

$$\begin{aligned} e_0 &= \frac{3}{10}, & e_x &= -\frac{3}{4} \frac{\alpha r_s}{\pi}, & e_c &= (\alpha r_s)^2 [a \ln r_s + b + O(r_s)], \\ \mu_0 &= \frac{1}{2}, & \mu_x &= -\frac{\alpha r_s}{\pi}, & \mu_c &= (\alpha r_s)^2 \left[a \ln r_s + \left(-\frac{1}{3}a + b \right) + O(r_s) \right]. \end{aligned} \quad (1.1)$$

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] *mutatis mutandi*. The Feynman diagrams of e_{2x} and Σ_{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 $X_1 = -\pi^4 \left[\frac{4}{3} \ln 2 - 5 \frac{\zeta(3)}{\pi^2} \right]$, $X_2 = \pi^4 \left[\frac{2}{3} \ln 2 - 2 \frac{\zeta(3)}{\pi^2} \right]$, 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, 15]. 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 $\mathbf{q}' = (\mathbf{q}_1 + \mathbf{q}_2)/2$, $\mathbf{p}' = (\mathbf{q}_1 - \mathbf{q}_2)/2$, and $\mathbf{s}' = \mathbf{e} + (\mathbf{q}_1 + \mathbf{q}_2)/2$ lead to

$$\begin{aligned} \mathbf{q}_1 &= \mathbf{q}' + \mathbf{p}', & (\mathbf{e} + \mathbf{q}_1)^2 &= (\mathbf{s}' + \mathbf{p}')^2, & (\mathbf{e} + \mathbf{q}_2)^2 &= (\mathbf{s}' - \mathbf{p}')^2, \\ \mathbf{q}_2 &= \mathbf{q}' - \mathbf{p}', & (\mathbf{e} + \mathbf{q}_1 + \mathbf{q}_2)^2 &= (\mathbf{s}' + \mathbf{q}')^2, & e^2 &= (\mathbf{s}' - \mathbf{q}')^2. \end{aligned} \quad (2.1)$$

Therefore (with $\Theta(x) = \text{Heaviside step function}$)

$$X_1 = \int d^3 q' d^3 p' \frac{2^3}{q'^2 - p'^2} \frac{1}{(\mathbf{p}' + \mathbf{q}')^2 (\mathbf{p}' - \mathbf{q}')^2} \times \\ \times \int \frac{d^2 s'}{\pi} \delta((\mathbf{s}' - \mathbf{q}')^2 - 1) \Theta[1 - (\mathbf{s}' + \mathbf{q}')^2] \Theta[(\mathbf{s}' + \mathbf{p}')^2 - 1] \Theta[(\mathbf{s}' - \mathbf{p}')^2 - 1]. \quad (2.2)$$

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

$$1 - s'^2 = \frac{1}{1 + s^2}, \quad d^2 s' = \frac{d^2 s}{(1 + s^2)^2}, \\ \delta((\mathbf{s}' - \mathbf{q}')^2 - 1) = (1 + s^2) \delta(q^2 - 2\mathbf{s}\mathbf{q} - 1), \\ \pm 2\mathbf{s}\mathbf{p} + p^2 > 1, \quad 2\mathbf{s}\mathbf{q} + q^2 < 1, \quad -2\mathbf{s}\mathbf{q} + q^2 = 1, \quad (2.3)$$

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

$$X_1 = - \int_0^1 dq \int_1^\infty dp \frac{16 \pi}{p^2 - q^2} \int_{-1}^{+1} \frac{dx}{2} \frac{8 q^2 p^2}{(p^2 + q^2)^2 - (2\mathbf{q}\mathbf{p})^2} \times \\ \times \int_{s \geq \alpha, \cos \varphi_q < 0} \frac{d^2 s}{1 + s^2} \delta(q^2 - 1 - 2\mathbf{s}\mathbf{q}) \Theta(p^2 - 1 + 2\mathbf{s}\mathbf{p}) \Theta(p^2 - 1 - 2\mathbf{s}\mathbf{p}). \quad (2.4)$$

Here and in the following of Sec. II the abbreviations

$$\alpha = \frac{1 - q^2}{2q} \geq 0, \quad \beta = \frac{p^2 - 1}{2p} \geq 0, \quad a = \frac{q^2 + p^2}{2qp} \geq 1, \\ \frac{t}{s} = \cos \varphi_p = \cos \sphericalangle(\mathbf{s}, \mathbf{p}), \quad x = \cos \varphi = \cos \sphericalangle(\mathbf{q}, \mathbf{p}), \quad y = \cos \varphi_q = \cos \sphericalangle(\mathbf{q}, \mathbf{s}) \quad (2.5)$$

are used:

$$X_1 = - \int_0^1 dq \int_1^\infty dp \frac{16 \pi}{p^2 - q^2} \int_{-1}^{+1} \frac{dx}{a^2 - x^2} \int_{s \geq \alpha, \cos \varphi_q < 0} \frac{s ds d\varphi_q}{1 + s^2} \frac{1}{2sq} \delta\left(\frac{\alpha}{s} + y\right) \Theta(\beta - |t|) \quad (2.6)$$

t is introduced to replace s after having done the φ_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):

$$\frac{t}{s} = x \left(-\frac{\alpha}{s}\right) \pm \sqrt{1 - x^2} \sqrt{1 - \left(\frac{\alpha}{s}\right)^2} \quad \text{or} \quad (t + \alpha x)^2 = (1 - x^2)(s^2 - \alpha^2). \quad (2.7)$$

This has the consequences

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

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

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

$$\begin{aligned} & \int_0^{2\pi} \frac{d\varphi_q}{s} [\delta(-\sin \varphi_{q,1} \cdot (\varphi_q - \varphi_{q,1})) + \delta(-\sin \varphi_{q,2} \cdot (\varphi_q - \varphi_{q,2}))] \\ &= \int_0^{2\pi} \frac{d\varphi_q}{s} \frac{\delta(\varphi_q - \varphi_{q,1}) + \delta(\varphi_q - \varphi_{q,2})}{\sqrt{1 - (\frac{\alpha}{s})^2}} = \frac{2}{\sqrt{s^2 - \alpha^2}} = 2 \frac{\sqrt{1 - x^2}}{|t + \alpha x|}. \end{aligned} \quad (2.10)$$

Thus

$$\begin{aligned} \int_{s \geq \alpha, \cos \varphi_q} \frac{s ds}{1 + s^2} \frac{d\varphi_q}{2sq} \frac{1}{2sq} \delta\left(\frac{\alpha}{s} + y\right) \Theta(\beta - |t|) &= \frac{\sqrt{1 - x^2}}{q} \int_{t_0}^{t_1} \frac{\text{sign}(t + \alpha x) dt}{(t + \alpha x)^2 + (1 + \alpha^2)(1 - x^2)} \\ &= \frac{2}{1 + q^2} \arctan \frac{t + \alpha x}{\sqrt{(1 + \alpha^2)(1 - x^2)}} \Bigg|_{t_0}^{t_1}. \end{aligned} \quad (2.11)$$

$|t| \leq \beta$ 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 α 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

$$\int_{-1}^{+1} dx \int_{t_0}^{+\beta} dt = \begin{cases} \int_{-1}^{+1} dx \int_{-\alpha x}^{+\beta} dt & \text{for } qp \geq 1 \text{ or } \alpha \leq \beta, \\ \int_{-\beta/\alpha}^{+\beta/\alpha} dx \int_{-\alpha x}^{+\beta} dt + \int_{+\beta/\alpha}^{+1} dx \int_{-\beta}^{+\beta} dt & \text{for } qp \leq 1 \text{ or } \alpha \geq \beta. \end{cases} \quad (2.12)$$

With the abbreviations (2.5) and

$$f(t, x) = \frac{2}{a^2 - x^2} \arctan \frac{t + \alpha x}{\sqrt{(1 + \alpha^2)(1 - x^2)}}, \quad (2.13)$$

Eq. (2.6) can be written as (note that $f(-\alpha x, x) = 0$)

$$X_1 = - \int_0^1 dq \int_1^\infty dp \frac{16 \pi}{(p^2 - q^2)} \frac{1}{(1 + q^2)} \left\{ \Theta(qp - 1) \int_{-1}^{+1} dx f(\beta, x) + \Theta(1 - qp) \left[\int_{-\beta/\alpha}^{+\beta/\alpha} dx f(\beta, x) + \int_{+\beta/\alpha}^{+1} dx [f(\beta, x) - f(-\beta, x)] \right] \right\}. \quad (2.14)$$

With

$$\int_{+\beta/\alpha}^{+1} dx (-1) f(-\beta, x) = \int_{+\beta/\alpha}^{+1} dx f(\beta, -x) = \int_{-1}^{-\beta/\alpha} dx f(\beta, x) \quad (2.15)$$

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

$$X_1 = - \int_0^1 dq \int_1^\infty dp \int_{-1}^{+1} dx \frac{16 \pi}{p^2 - q^2} \frac{1}{1 + q^2} f(\beta, x). \quad (2.16)$$

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

$$\alpha = \frac{1 - q^2}{2q} \geq 0, \quad \beta = \frac{1 - k^2}{2k} \geq 0, \quad a = \frac{1 + q^2 k^2}{2qk} \geq 1 \quad (2.17)$$

it is:

$$X_1 = - \int_0^1 dq \int_0^1 dk \int_{-1}^{+1} dx \frac{16 \pi}{1 - q^2 k^2} \frac{1}{1 + q^2} f(\beta, x) \approx -30.70598 \cdots \quad (2.18)$$

The coefficients α , β , 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

$$X_1 = -\pi^4 \left[\frac{4}{3} \ln 2 - 5 \frac{\zeta(3)}{\pi^2} \right] \approx -30.705985239248893 \cdots \quad (2.19)$$

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

III. THE INTEGRAL X_2

The whole procedure of Sec. II is repeated here step by step. In Eq. (A.11), new variables $\mathbf{q}' = (\mathbf{q}_1 + \mathbf{q}_2)/2$, $\mathbf{p}' = (\mathbf{q}_1 - \mathbf{q}_2)/2$, and $\mathbf{s}' = \mathbf{e} + (\mathbf{q}_1 + \mathbf{q}_2)/2$ lead to

$$\begin{aligned} \mathbf{q}_1 &= \mathbf{q}' + \mathbf{p}', & (\mathbf{e} + \mathbf{q}_1)^2 &= (\mathbf{s}' + \mathbf{p}')^2, & (\mathbf{e} + \mathbf{q}_2)^2 &= (\mathbf{s}' - \mathbf{p}')^2, \\ \mathbf{q}_2 &= \mathbf{q}' - \mathbf{p}', & (\mathbf{e} + \mathbf{q}_1 + \mathbf{q}_2)^2 &= (\mathbf{s}' + \mathbf{q}')^2, & \mathbf{e}^2 &= (\mathbf{s}' - \mathbf{q}')^2. \end{aligned} \quad (3.1)$$

Therefore

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

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

$$\begin{aligned} 1 - s'^2 &= \frac{1}{1 + s^2}, & d^2s' &= \frac{d^2s}{(1 + s^2)^2}, \\ \delta((\mathbf{s}' - \mathbf{q}')^2 - 1) &= (1 + s^2) \delta(q^2 - 2\mathbf{s}\mathbf{q} - 1), \\ \pm 2\mathbf{s}\mathbf{p} + p^2 < 1, & 2\mathbf{s}\mathbf{q} + q^2 > 1, & -2\mathbf{s}\mathbf{q} + q^2 = 1, \end{aligned} \quad (3.3)$$

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

$$\begin{aligned} X_2 &= \int_1^\infty dq \int_0^1 dp \frac{16\pi}{q^2 - p^2} \int_{-1}^{+1} \frac{dx}{2} \frac{8q^2p^2}{(p^2 + q^2)^2 - (2\mathbf{q}\mathbf{p})^2} \times \\ &\times \int_{s \geq \bar{\alpha}, \cos \varphi_q > 0} \frac{d^2s}{1 + s^2} \delta(q^2 - 1 - 2\mathbf{s}\mathbf{q}) \Theta(1 - p^2 - 2\mathbf{s}\mathbf{p}) \Theta(1 - p^2 + 2\mathbf{s}\mathbf{p}). \end{aligned} \quad (3.4)$$

Here and in the following of Sec. III the abbreviations

$$\begin{aligned} \bar{\alpha} &= \frac{q^2 - 1}{2q} \geq 0, & \bar{\beta} &= \frac{1 - p^2}{2p} \geq 0, & \bar{a} &= \frac{q^2 + p^2}{2qp} \geq 1, \\ \frac{t}{s} &= \cos \varphi_p = \cos \sphericalangle(\mathbf{s}, \mathbf{p}), & x &= \cos \varphi = \cos \sphericalangle(\mathbf{q}, \mathbf{p}), & y &= \cos \varphi_q = \cos \sphericalangle(\mathbf{q}, \mathbf{s}) \end{aligned} \quad (3.5)$$

are used:

$$X_2 = \int_1^\infty dq \int_0^1 dp \frac{16\pi}{q^2 - p^2} \int_{-1}^{+1} \frac{dx}{\bar{a}^2 - x^2} \int_{s \geq \bar{\alpha}, \cos \varphi_q > 0} \frac{s ds d\varphi_q}{1 + s^2} \frac{1}{2sq} \delta\left(\frac{\bar{\alpha}}{s} - y\right) \Theta(\bar{\beta} - |t|). \quad (3.6)$$

t is introduced to replace s after having done the φ_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 $+\bar{\alpha}/s$ because of the delta function):

$$\frac{t}{s} = x \frac{\bar{\alpha}}{s} \pm \sqrt{1-x^2} \sqrt{1 - \left(\frac{\bar{\alpha}}{s}\right)^2} \quad \text{or} \quad (t - \bar{\alpha}x)^2 = (1-x^2)(s^2 - \bar{\alpha}^2). \quad (3.7)$$

This has the consequences

$$s^2 - \bar{\alpha}^2 = \frac{(t - \bar{\alpha}x)^2}{1-x^2}, \quad (3.8)$$

$$\frac{sds}{1+s^2} = \frac{(t - \bar{\alpha}x)dt}{(t - \bar{\alpha}x)^2 + (1 + \bar{\alpha}^2)(1-x^2)}. \quad (3.9)$$

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

$$\begin{aligned} & \int_0^{2\pi} \frac{d\varphi_q}{s} [\delta(+\sin \varphi_{q,1} \cdot (\varphi_q - \varphi_{q,1})) + \delta(+\sin \varphi_{q,2} \cdot (\varphi_q - \varphi_{q,2}))] \\ &= \int_0^{2\pi} \frac{d\varphi_q}{s} \frac{\delta(\varphi_q - \varphi_{q,1}) + \delta(\varphi_q - \varphi_{q,2})}{\sqrt{1 - \left(\frac{\bar{\alpha}}{s}\right)^2}} = \frac{2}{\sqrt{s^2 - \bar{\alpha}^2}} = 2 \frac{\sqrt{1-x^2}}{|t - \bar{\alpha}x|}. \end{aligned} \quad (3.10)$$

Thus

$$\begin{aligned} \int_{s \geq \bar{\alpha}, \cos \varphi_q > 0} \frac{sds}{1+s^2} \frac{d\varphi_q}{2sq} \delta\left(\frac{\bar{\alpha}}{s} - y\right) \Theta(\beta - |t|) &= \frac{\sqrt{1-x^2}}{q} \int_{t_0}^{t_1} \frac{\text{sign}(t - \bar{\alpha}x) dt}{(t - \bar{\alpha}x)^2 + (1 + \bar{\alpha}^2)(1-x^2)} \\ &= \frac{2}{1+q^2} \arctan \frac{t - \bar{\alpha}x}{\sqrt{(1 + \bar{\alpha}^2)(1-x^2)}} \Bigg|_{t_0}^{t_1} \end{aligned} \quad (3.11)$$

$|t| \leq \bar{\beta}$ contains the upper limit of the t -integration as $t \leq \bar{\beta} =: t_1$. What concerns its lower limit t_0 , the relation $t \geq -\bar{\beta}$ competes with $t \geq \bar{\alpha}x$, as it follows from Eq. (3.7) for the lower limit $\bar{\alpha}$ 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 $\bar{\alpha} \geq \bar{\beta}$ or $-\bar{\alpha} \leq -\bar{\beta}$, and
- (b) region B with $qp \leq 1$ or $\bar{\alpha} \leq \bar{\beta}$ or $\bar{\alpha}x \leq \bar{\alpha} \leq \bar{\beta}$, hence $t_0 = \bar{\alpha}x$.

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

$$\int_{-1}^{+1} dx \int_{t_0}^{+\bar{\beta}} dt = \begin{cases} \int_{-1}^{-\bar{\beta}/\bar{\alpha}} dx \int_{-\bar{\beta}}^{+\bar{\beta}} dt + \int_{-\bar{\beta}/\bar{\alpha}}^{+\bar{\beta}/\bar{\alpha}} dx \int_{\bar{\alpha}x}^{+\bar{\beta}} dt & \text{for } qp \geq 1 \text{ or } \bar{\alpha} \geq \bar{\beta}, \\ \int_{-1}^{+1} dx \int_{\bar{\alpha}x}^{+\bar{\beta}} dt & \text{for } qp \leq 1 \text{ or } \bar{\alpha} \leq \bar{\beta}. \end{cases} \quad (3.12)$$

With the abbreviations (3.5) and with

$$\bar{f}(t, x) = \frac{2}{\bar{a}^2 - x^2} \arctan \frac{t - \bar{\alpha}x}{\sqrt{(1 + \bar{\alpha}^2)(1 - x^2)}}, \quad (3.13)$$

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

$$X_2 = \int_1^\infty dq \int_0^1 dp \frac{16\pi}{q^2 - p^2} \frac{1}{1 + q^2} \left\{ \Theta(1 - qp) \int_{-1}^{+1} dx \bar{f}(\bar{\beta}, x) \right. \\ \left. + \Theta(qp - 1) \left[\int_{-1}^{-\bar{\beta}/\bar{\alpha}} dx [\bar{f}(\bar{\beta}, x) - \bar{f}(-\bar{\beta}, x)] + \int_{-\bar{\beta}/\bar{\alpha}}^{+\bar{\beta}/\bar{\alpha}} dx \bar{f}(\bar{\beta}, x) \right] \right\}. \quad (3.14)$$

With the identity

$$\int_{-1}^{-\bar{\beta}/\bar{\alpha}} dx (-1) \bar{f}(-\bar{\beta}, x) = \int_{-1}^{-\bar{\beta}/\bar{\alpha}} dx \bar{f}(\bar{\beta}, -x) = \int_{+\bar{\beta}/\bar{\alpha}}^{+1} dx \bar{f}(\bar{\beta}, x) \quad (3.15)$$

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

$$X_2 = \int_1^\infty dq \int_0^1 dp \int_{-1}^{+1} dx \frac{16\pi}{q^2 - p^2} \frac{1}{1 + q^2} \bar{f}(\bar{\beta}, x). \quad (3.16)$$

This is similar to Eq. (2.16), 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

$$\bar{\alpha} = \frac{1 - k^2}{2k}, \quad \bar{\beta} = \frac{1 - p^2}{2p}, \quad \bar{a} = \frac{1 + k^2 p^2}{2kp} \quad (3.17)$$

it is

$$X_2 = \int_0^1 dk \int_0^1 dp \int_{-1}^{+1} dx \frac{16 \pi}{1 - k^2 p^2} \frac{k^2}{1 + k^2} \bar{f}(\bar{\beta}, x) .$$

Changing finally the notation with $k \rightarrow q$ and $p \rightarrow k$ makes $\bar{\alpha} = \alpha$, $\bar{\beta} = \beta$, and $\bar{a} = a$, cf. Eq. (2.17). With these identities and with $\bar{f}(t, -x) = f(t, x)$ a further rewriting yields

$$X_2 = \int_0^1 dq \int_0^1 dk \int_{-1}^{+1} dx \frac{16 \pi}{1 - q^2 k^2} \frac{q^2}{1 + q^2} f(\beta, x) \approx 21.284906 \dots . \quad (3.18)$$

This integral differs from Eq. (2.18) 'only' in an additional factor of $-q^2$ in the nominator of the integrand. Mathematica5.2 [17] yields the given figure. It seems to hold

$$X_2 = \pi^4 \left[\frac{2}{3} \ln 2 - 2 \frac{\zeta(3)}{\pi^2} \right] \approx 21.284905670516334 \dots . \quad (3.19)$$

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, α, β being defined in Eq. (2.17) the result for $X = X_1 + X_2$ is

$$X = - \int_0^1 dq \int_0^1 dk \int_{-1}^{+1} dx \frac{16 \pi}{1 - q^2 k^2} \frac{1 - q^2}{1 + q^2} \frac{2}{a^2 - x^2} \arctan \frac{\beta + \alpha x}{\sqrt{(1 + \alpha^2)(1 - x^2)}} \approx -9.42108 \dots . \quad (4.1)$$

It seems to hold [18, 19]

$$X = -\pi^4 \left[\frac{2}{3} \ln 2 - 3 \frac{\zeta(3)}{\pi^2} \right] \approx -9.421079568732553 \dots . \quad (4.2)$$

The final result [20]

$$\Sigma_{2x} = -\frac{(\alpha r_s)^2}{4\pi^4} X = e_{2x} \quad \text{with} \quad \frac{e_{2x}}{(\alpha r_s)^2} = \frac{1}{6} \ln 2 - \frac{3}{4} \frac{\zeta(3)}{\pi^2} \approx 0.0241792 \quad (4.3)$$

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 $r_s \rightarrow 0$, where the effectively screened Coulomb repulsion $W(12)$ is replaced by the bare Coulomb repulsion $\nu(12)$.

APPENDIX A: DERIVATION OF Σ_{2x}

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

$$G_0(k, \omega) = \frac{\Theta(k-1)}{\omega - \frac{1}{2}k^2 + i\delta} + \frac{\Theta(1-k)}{\omega - \frac{1}{2}k^2 - i\delta} \quad (\text{A.1})$$

(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

$$G(k, \omega) = G_0(k, \omega) + G_0(k, \omega)\Sigma(k, \omega)G(k, \omega) . \quad (\text{A.2})$$

$\Sigma(k, \omega)$ 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]

$$v = \frac{1}{2} \int d(k)^3 \int \frac{d\omega}{2\pi i} e^{i\omega\delta} G(k, \omega)\Sigma(k, \omega) , \quad \delta \rightarrow 0^+ . \quad (\text{A.3})$$

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

follows from the virial theorem $v = r_s \frac{d}{dr_s} e$.

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

$$\begin{aligned} \Sigma_{2x}(k, \omega) &= \frac{(\alpha r_s)^2}{4\pi^4} \int \frac{d^3 q_1 d^3 q_2}{q_1^2 q_2^2} \int \frac{d\eta_1 d\eta_2}{(2\pi i)^2} \times \\ &\times G_0(|\mathbf{k} + \mathbf{q}_2|, \omega + \eta_2) G_0(|\mathbf{k} + \mathbf{q}_1 + \mathbf{q}_2|, \omega + \eta_1 + \eta_2) G_0(|\mathbf{k} + \mathbf{q}_1|, \omega + \eta_1) \end{aligned} \quad (\text{A.4})$$

Use of (A.1) yields

$$\begin{aligned} \Sigma_{2x}(k, \omega) &= -\frac{(\alpha r_s)^2}{4\pi^4} \int \frac{d^3 q_1 d^3 q_2}{q_1^2 q_2^2} \left[\frac{\Theta(|\mathbf{k} + \mathbf{q}_1 + \mathbf{q}_2| - 1) \Theta(1 - |\mathbf{k} + \mathbf{q}_1|) \Theta(1 - |\mathbf{k} + \mathbf{q}_2|)}{\omega - \frac{1}{2}k^2 + \mathbf{q}_1 \cdot \mathbf{q}_2 - i\delta} \right. \\ &\quad \left. + \frac{\Theta(1 - |\mathbf{k} + \mathbf{q}_1 + \mathbf{q}_2|) \Theta(|\mathbf{k} + \mathbf{q}_1| - 1) \Theta(|\mathbf{k} + \mathbf{q}_2| - 1)}{\omega - \frac{1}{2}k^2 + \mathbf{q}_1 \cdot \mathbf{q}_2 + i\delta} \right]. \end{aligned} \quad (\text{A.5})$$

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} = energy in second order of exchange, calculated by Onsager et al. [9]. Its rhs gives with Eqs. (A.1) and (A.5)

$$\begin{aligned} \text{rhs} &= -\frac{3(\alpha r_s)^2}{(2\pi)^5} \left[\int \frac{d^3 k d^3 q_1 d^3 q_2}{q_1^2 q_2^2} \frac{\Theta(1 - k) \Theta(1 - |\mathbf{k} + \mathbf{q}_1 + \mathbf{q}_2|) \Theta(|\mathbf{k} + \mathbf{q}_1| - 1) \Theta(|\mathbf{k} + \mathbf{q}_2| - 1)}{\mathbf{q}_1 \cdot \mathbf{q}_2 + i\delta} \right. \\ &\quad \left. + \int \frac{d^3 k d^3 q_1 d^3 q_2}{q_1^2 q_2^2} \frac{\Theta(k - 1) \Theta(|\mathbf{k} + \mathbf{q}_1 + \mathbf{q}_2| - 1) \Theta(1 - |\mathbf{k} + \mathbf{q}_1| - 1) \Theta(1 - |\mathbf{k} + \mathbf{q}_2|)}{\mathbf{q}_1 \cdot (-\mathbf{q}_2) + i\delta} \right]. \end{aligned} \quad (\text{A.6})$$

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

$$\begin{aligned} \text{Re rhs} &= -2 \frac{3(\alpha r_s)^2}{(2\pi)^5} \int \frac{d^3 k d^3 q_1 d^3 q_2}{q_1^2 q_2^2} \frac{P}{\mathbf{q}_1 \cdot \mathbf{q}_2} \times \\ &\times \Theta(1 - k) \Theta(1 - |\mathbf{k} + \mathbf{q}_1 + \mathbf{q}_2|) \Theta(|\mathbf{k} + \mathbf{q}_1| - 1) \Theta(|\mathbf{k} + \mathbf{q}_2| - 1) = 2e_{2x}. \end{aligned} \quad (\text{A.7})$$

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 $\mathbf{k} \rightarrow \mathbf{k}_1$, $\mathbf{q}_1 \rightarrow \mathbf{q}$, $\mathbf{q}_2 \rightarrow -(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{q})$. 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 $n_{2x}(k \rightarrow \infty) = -\frac{4}{9\pi^2} \frac{(\alpha r_s)^2}{k^8}$.

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 $\Sigma_{2x} = -\frac{(\alpha r_s)^2}{4\pi^4}(X_1 + X_2)$, where $X_{1,2}$ mean the integrals

$$X_1 = \int d^3 q_1 d^3 q_2 \frac{P}{\mathbf{q}_1 \cdot \mathbf{q}_2} \frac{1}{q_1^2 q_2^2} \Theta[1 - (\mathbf{e} + \mathbf{q}_1 + \mathbf{q}_2)^2] \Theta[(\mathbf{e} + \mathbf{q}_1)^2 - 1] \Theta[(\mathbf{e} + \mathbf{q}_2)^2 - 1], \quad (\text{A.8})$$

$$X_2 = \int d^3 q_1 d^3 q_2 \frac{P}{\mathbf{q}_1 \cdot \mathbf{q}_2} \frac{1}{q_1^2 q_2^2} \Theta[(\mathbf{e} + \mathbf{q}_1 + \mathbf{q}_2)^2 - 1] \Theta[1 - (\mathbf{e} + \mathbf{q}_1)^2] \Theta[1 - (\mathbf{e} + \mathbf{q}_2)^2]. \quad (\text{A.9})$$

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

$$X_1 = \int d^3 q_1 d^3 q_2 \frac{P}{\mathbf{q}_1 \cdot \mathbf{q}_2} \frac{1}{q_1^2 q_2^2} \int \frac{d^2 e}{2\pi} 2 \delta(\mathbf{e}^2 - 1) \times \\ \times \Theta[1 - (\mathbf{e} + \mathbf{q}_1 + \mathbf{q}_2)^2] \Theta[(\mathbf{e} + \mathbf{q}_1)^2 - 1] \Theta[(\mathbf{e} + \mathbf{q}_2)^2 - 1], \quad (\text{A.10})$$

$$X_2 = \int d^3 q_1 d^3 q_2 \frac{P}{\mathbf{q}_1 \cdot \mathbf{q}_2} \frac{1}{q_1^2 q_2^2} \int \frac{d^2 e}{2\pi} 2 \delta(\mathbf{e}^2 - 1) \times \\ \times \Theta[(\mathbf{e} + \mathbf{q}_1 + \mathbf{q}_2)^2 - 1] \Theta[1 - (\mathbf{e} + \mathbf{q}_1)^2] \Theta[1 - (\mathbf{e} + \mathbf{q}_2)^2]. \quad (\text{A.11})$$

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.

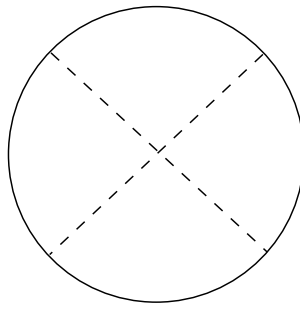


FIG. 1: The Feynman diagram of e_{2x} , analytically calculated by Onsager et al. [9].

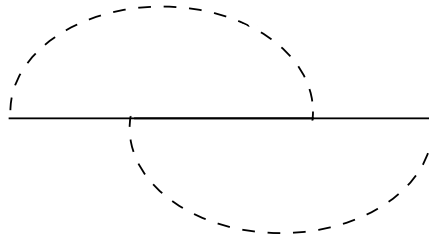


FIG. 2: The Feynman diagram of $\Sigma_{2x}(k, \omega)$, (semi)analytically calculated in this paper.

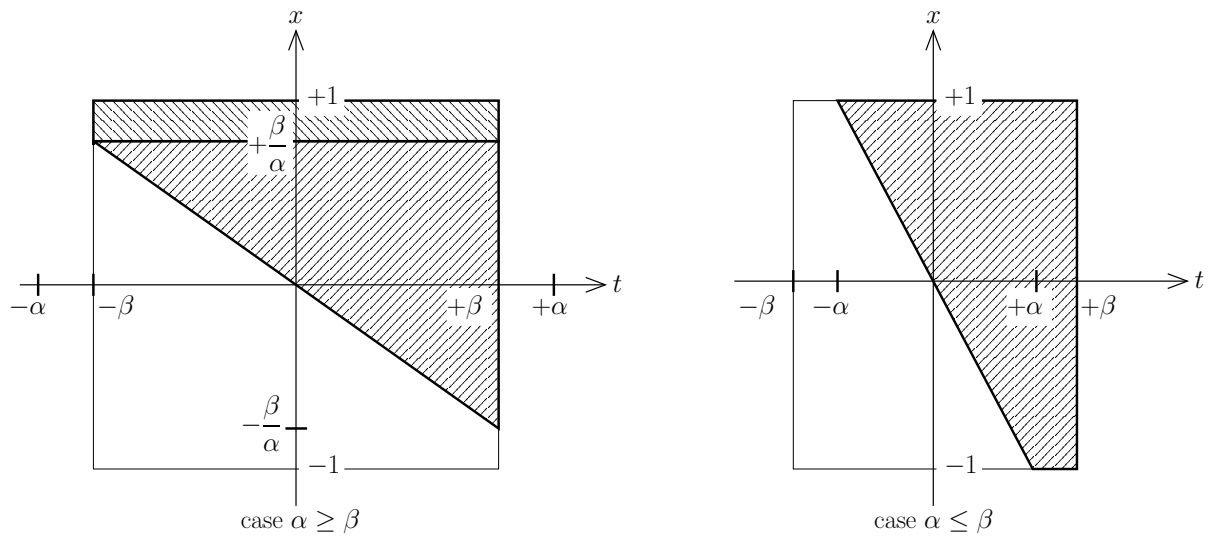


FIG. 3: The dashed area is the region of integration described by Eq. (2.12).

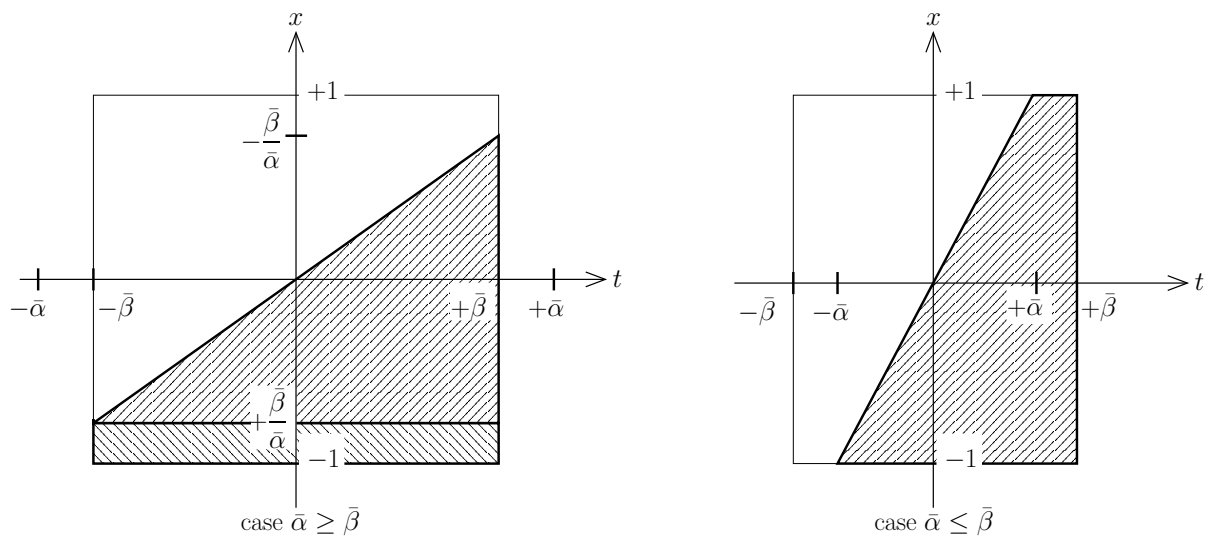


FIG. 4: The dashed area is the region of integration described by Eq. (3.12).