Structural Expansion for the Ground-State Energy of Simple Metals. II

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A self-consistent treatment is given for the Green's function which determines the structure-dependent part of the ground-state energy for simple metals. An expansion in the resulting screened interactions is given exactly up to fourth order. In addition to the previously examined one-electron terms (I), which are the most important ones, the present paper treats the next important terms which may be related to the first-order effect of the exchange energy due to inhomogeneous charge distribution. In fourth order of the expansion, the mentioned term shows the same singularity as the third-order one-electron term, Brovman and Kagan's singularity. It is proved that the Hartree-Fock result exaggerates the first-order exchange effect, most strikingly in the close vicinity of the singular point. Effect of the dynamical shielding on the considered term is also studied, particularly in the third-order term of the expansion.

§ 1. Introduction

In a previous paper, hereafter referred to as I, we have discussed the expansion of the structure-dependent ground-state energy of simple metals, in the Hartree-Fock approximation (HFA). A further expansion in terms of Lindhard's dielectric function manifests an important role of the vertex function, in fourth order. The resulting term has dropped out of the existing theories, which are based on a simple electron-ion coupling reduced by the static dielectric function, $\varepsilon(q, 0)$.

In the present paper, we shall study the same problem by taking account of the electron correlation. Needless to say, a great deal of studies have accumulated for the many-electron effect on the properties of metals, such as on the effective pseudo-potential in simple metals. With them our study has a close contact. In particular, we mention the studies for $\varepsilon(q, 0)$ and for the correlation energy. Most of them have focussed their relevance on the region of the electron density for common metals ($r_s = 3 \sim 5$), which is much lower than our density region ($r_s \leq 2$). This is the region relevant to the high-density hydrogen. Here we mention Geldart et al. whose study on $\varepsilon(q, 0)$ stands on the same footing as ours. It is pointed out that some possibly important terms have dropped out of their treatments.

The present formalism follows I. We expand the structure-dependent thermodynamic potential $\Omega' = \Omega - \Omega_{\text{ex}}$, where $\Omega$ denotes the thermodynamic potential of
the real system and $Q_{\text{ag}}$ that of the electron gas system. In the expansion, a new method is presented for dealing with the self-energy parts ($\S$ 2). The expansion of $Q_{\text{ag}}$ is given exactly up to fourth order ($\S\S$ 3 and 4). We note that at zero temperature $Q_{\text{ag}}$ is identical to the ground-state energy of the system, provided that the deformation energy of the Fermi surface is disregarded.

In each order of the expansion, the one-electron terms, which contain no momentum-transfer between electrons through the screened interactions, are the most important ones and identical to those dealt with in I. Thus we shall here evaluate the next important terms, which contain one momentum-transfer between electrons. Effect of the dynamical screening is studied carefully in third order ($\S$ 5). And, in fourth order, the singular behavior of the considered term is figured out ($\S$ 6). This manifests a striking exaggeration of HFA in the close vicinity of the singular point. The results will be applied to hydrogen and helium at high density in separate papers.

$\S$ 2. Self-energy part

Following I, we consider the thermal Green’s function $G(p, p + \mathbf{g} ; \zeta)$ for the system of the Hamiltonian $H = H_0 + H_1 + H_2$. Here $H_0$ denotes the kinetic term, $H_1$ the electron-ion interaction and $H_2$ the electron-electron one. And $p$ denotes the electron momentum, $\mathbf{g}$ the reciprocal lattice vector and $\zeta_\ell = \mu + \pi i (2\ell + 1)/\beta$, where $\mu$ is the chemical potential, $\beta = 1/k_B T$ and $\ell = 0, \pm 1, \pm 2, \ldots$. For the sake of brevity, let us introduce the four-dimensional ‘vectors’ $p$ and $\mathbf{g}$ respectively by $p = (p, \zeta_\ell)$ and $\mathbf{g} = (\mathbf{g}, 0)$.

Let $G_0(p)$ be the Green’s function of a free particle. Then we write down the Dyson equation in the form

$$G(p, p') = G_0(p) \delta_{pp'} + \sum_{\mathbf{g}} G_0(p) \Sigma(p, p + \mathbf{g}) G(p + \mathbf{g}, p').$$  (2.1)

The known self-energy $\Sigma(p, p + \mathbf{g})$ may be written as

$$\Sigma(p, p + \mathbf{g}) = -\lambda v_1(\mathbf{g}) + \int_{p' \neq p} 2 v_2(\mathbf{g}) G(p', p' + \mathbf{g}) e^{i\mathbf{g} \cdot \mathbf{r}}$$
$$- \int_{p' \neq p} v_2(p - p') G(p', p' + \mathbf{g}) e^{i\mathbf{g} \cdot \mathbf{r}}$$
$$- \sum_{\mathbf{g}'} \int_{p'} v_2(p + \mathbf{g} - p')$$
$$\times [2v_2(p - p') - v_2(p - p')] G(p', p' + \mathbf{g}')$$
$$\times G(p'', p'' + \mathbf{g}'') G(p'' + p'' - p + g'' - p', p'' + p'' - p) + \cdots. $$  (2.2)

In the above expression, $v_1(\mathbf{g})$ denotes the electron-ion coupling and $v_2(\mathbf{q})$ the
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electron-electron one, being in accord with I. Here we use the abbreviation $f_p = N^{-1} \sum_p \beta^{-1} \sum_{q}$. On the right-hand side of Eq. (2.2), a factor 2 comes in due to spin multiplicity.

We first note that the HF result comes out by truncating $\Sigma(p, p+g)$ up to first order in $v_2(g)$. Instead, if we want to get higher-order effects, such bare form of the self-energy parts as Eq. (2·2) is awkward to handle. It is because the series (2·2) has proved divergent in the small momentum region. This divergence has told us the bare interaction to be screened such that

$$v_2(q) = \frac{v_2(q)}{1 - v_2(q) \Pi(q)}, \quad (2·3)$$

where $\Pi(q)$ is a polarization. The above expression in turn gives us

$$v_1(q) = \frac{v_1(q)}{1 + v_2(q) \Pi(q)}. \quad (2·4)$$

Now, by a simple substitution of $v_2$ for $v_1$ in Eq. (2·1), one might commit over-counting of some graphs, because in the expression of the self-energy, Eq. (2·2), the Green’s function is already dressed. The difficulty can be avoided by substituting Eq. (2·4) for $v_2(q)$ in Eq. (2·2).

By expanding the resulting self-energy in $v_2$, we get

$$\Sigma(p, p+g) = - U_g - \int_{p'} [v_2(p-p') G(p', p' + g) \epsilon^{\gamma p'} - \frac{v_2 (p-p') }{1 - v_2(q) \Pi(q)} G(p', p' + g) \epsilon^{\gamma p'} - \frac{v_2 (p-p') }{1 + v_2(q) \Pi(q)} G(p', p' + g) \epsilon^{\gamma p'} - \sum_{g'} \int_{p'} [v_2(p-p') G(p', p' + g-g') \epsilon^{\gamma p'}] \times [2v_2(p-p') - v_2(p-p'')] G(p', p' + g') \times [G(p'', p'' + g'') G(p'' + g'' - p + g' + g'' - g, p' + p'' - p) + \ldots \quad (2·5)$$

up to second order of $v_2$, where we put

$$U_g = \lambda v_1(g) - \int_p 2v_2(g) G(p, p+g) \epsilon^{\gamma p}. \quad (2·6)$$

Notice the third term on the right, which is a correction to the result of the simple substitution. This correction is necessitated in order to get the fourth-order terms correctly.

Let $G(p)$ be the true Green’s function in the electron-gas system with Hamiltonian $H_{eg} = H_0 + H_4$. Then, the polarization, $\Pi(q)$, may be of the form

$$\Pi(q) = 2 \int_p G(p) G(p+q) A(q, p). \quad (2·7)$$

With neglect of an unknown function $A(q, p)$, which may be determined self-
consistently, we shall later assume \( \Pi(q) \) in the form

\[
\Pi^{(0)}(q) = 2 \int G(p) G(p+q). \tag{2.8}
\]

The ambiguity in choice of \( \Pi(q) \) does not matter, because the only thing we have done is a rearrangement of the series. However the rearranged series for \( \Sigma(p, p+g) \) is well convergent, allowing us to study the structural energy straightforwardly.

§ 3. Structural expansion

Following I, we expand \( G, \Sigma, U_g \) in \( \lambda \):

\[
G(p, p+g) = \sum_{n=0}^{\infty} \lambda^n G^{(n)}(p, p+g), \quad \Sigma(p, p+g) = \sum_{n=0}^{\infty} \lambda^n \Sigma^{(n)}(p, p+g),
\]

\[
U_g = \sum_{n=0}^{\infty} \lambda^n U_g^{(n)}, \tag{3.1}
\]

where the zeroth-order terms are relevant to the electron-gas system of the Hamiltonian \( H_{eg} \):

\[
G^{(0)}(p, p+g) = G(p) \delta_{p, g}, \quad \Sigma^{(0)}(p, p+g) = \Sigma(p) \delta_{p, g}. \tag{3.2}
\]

Now, let us rewrite the Dyson equation (2.1) as

\[
G(p, p+g) = G(p) \delta_{p, g} + \sum_{p'} G(p) \Sigma(p, p+g') G(p'+g', p+g) + G(p) \left[ \Sigma(p, p) - \Sigma^{(0)}(p) \right] G(p, p+g). \tag{3.3}
\]

In the self-energy part, Eq. (2.5), we replace \( \bar{v}_2 \) by

\[
\bar{v}_2^{(0)}(q) = v_2(q) / [1 - v_2(q) II^{(0)}(q)] \tag{3.4}
\]

with \( II^{(0)}(q) \) defined by Eq. (2.8).

Thus, the zeroth-order solutions are given by

\[
[G(p)]^{-1} = [G^{(0)}(p)]^{-1} - \Sigma^{(0)}(p), \tag{3.5}
\]

\[
\Sigma^{(0)}(p) = - \int_{p'} \bar{v}_2^{(0)}(p-p') G(p') e^{i v} + \int_{p'} \int_{p''} \bar{v}_2^{(0)}(p-p') \bar{v}_2^{(0)}(p-p'') G(p') G(p''(p'') G(p' + p'' - p) + \cdots. \tag{3.6}
\]

Next, the first-order solution must be of the form:

\[
G^{(1)}(p, p+g) = G(p) \Sigma^{(0)}(p, p+g) G(p+g), \quad (g \neq 0) \tag{3.7}
\]

as seen from Eq. (3.3). Substituting Eq. (3.7) into the right-hand side of Eq.
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We have an integral equation in $\Sigma^{(0)}(p,p+g)$, including $U_g^{(0)}$ as an inhomogeneous term. The solution is assumed to be

$$\Sigma^{(0)}(p,p+g) = -U_g^{(0)}A_g(p). \quad (3\cdot8)$$

With the substitution of Eq. (3·8), the integral equation becomes

$$A_g(p) = 1 - \int_{p'} \bar{\varphi}_{1}^{(0)}(p-p')G(p')G(p'+g)A_g(p')$$

$$+ \int_{p'} \int_{p''} \bar{\varphi}_{1}^{(0)}(p-p')\bar{\varphi}_{1}^{(0)}(p-p'')$$

$$\times \left[ G(p')G(p'+g)A_g(p')G(p''+p''-p) + G(p'+g)G(p'+p''-p)G(p'+p''-p+g) \right]$$

$$= 1 - \int_{p'} \bar{\varphi}_{1}^{(0)}(p-p')G(p)G(p+g)G(p')G(p'+g)A_g(p')$$

$$+ \int_{p'} \int_{p''} \bar{\varphi}_{1}^{(0)}(p-p')\bar{\varphi}_{1}^{(0)}(p-p'')$$

$$\times \left[ G(p')G(p'+g)A_g(p')G(p''+p''-p) + G(p'+g)G(p'+p''-p)G(p'+p''-p+g) \right]$$

$$\times A_g(p'+p''-p-g)] - 2 \int_{p'} \int_{p''} \bar{\varphi}_{1}^{(0)}(p-p')\bar{\varphi}_{1}^{(0)}(p-p'+g)$$

$$\times \left[ G(p')G(p'+g)A_g(p')G(p''+p''-p) + G(p'+g)G(p'+p''-p)G(p'+p''-p+g) \right]$$

$$\times A_g(p'+p''-p-g)]. \quad (3\cdot9)$$

Now, from Eq. (2·6) we obtain the first-order term of $U_g$ with the help of Eqs. (3·7) and (3·8):

$$U_g^{(0)} = v_1(g) \varepsilon(g), \quad (3\cdot10)$$

where $\varepsilon(g)$ is the exact static-dielectric function

$$\varepsilon(g) = 1 - v_1(g)\Pi(g), \quad \Pi(g) = 2 \int_{p'} G(p')G(p'+g)A_g(p'). \quad (3\cdot11)$$

The vertex function $A_g(p)$ may be obtained from Eq. (3·9) by the iteration method. The solution up to second order of $\varphi_{1}^{(0)}$ is inserted into $\Pi(g)$ with the following result:

$$\Pi(g) = \Pi_{1,0}(g) + \Pi_{1,1}(g) + \Pi_{1,2}(g) + \Pi_{1,3}(g) + \Pi_{1,4}(g) + \cdots \quad (3\cdot12)$$

using suffices in conformity with the expansion of $\Omega_{\alpha}$. Here $\Pi_{1,0}(g)$ is identical to $\Pi^{(0)}(g)$ defined by Eq. (2·8) and

$$\Pi_{1,1}(g) = -2 \int_{p} \int_{p'} \bar{\varphi}_{1}^{(0)}(p-p')G(p)G(p+g)G(p'+g), \quad (3\cdot13)$$

$$\Pi_{1,2}(g) = 2 \int_{p} \int_{p'} \bar{\varphi}_{1}^{(0)}(p-p')\bar{\varphi}_{1}^{(0)}(p'-p'')$$

$$\times G(p)G(p+g)G(p'+g)G(p''+g), \quad (3\cdot14)$$
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\[ \bar{H}_{\text{eff}}(g) = 2 \int p \int p' \int p'' \bar{v}_{1}(p - p') \bar{v}_{1}(p - p'') G(p) G(p + g) \]

\[ \times [G(p') G(p' + g) G(p'') G(p' + p'' - p) + G(p' + g) G(p'') G(p' + p'' - p) G(p' + p'' - p + g)] \]

\[ \bar{H}_{\text{eff}}(g) = -4 \int p \int p' \int p'' \bar{v}_{1}(p - p') \bar{v}_{1}(p - p' - g) G(p) G(p + g) \]

\[ \times [G(p') G(p' + g) G(p' + p'' - p) + G(p' + g) G(p') G(p' + p'' - p - g) G(p' + p'' - p + g)]. \] (3.15)

For the higher-order terms we have the following equations:

\[ G^{(n)}(p, p + g) = G(p) [v_{g}^{(n)}(p) + \Sigma^{(n)}(p, p + g)] G(p + g) \] (3.17)

\[ \Sigma^{(n)}(p, p + g) = 2v_{2}(g) \int p' G^{(n)}(p', p' + g) \]

\[ - \int p' \bar{v}_{2}(p - p') G^{(n)}(p', p' + g) + \cdots. \] (3.18)

Here an effective field in n-th order, \( v_{g}^{(n)}(p) \), is defined by

\[ v_{g}^{(n)}(p) = [G(p + g)]^{-1} \sum_{\gamma=1}^{n-1} \sum_{\gamma=1}^{n-\gamma} \gamma^{(\gamma)}(p, p + g') G^{(n-\gamma)}(p + g, p + g). \] (3.19)

A set of Eqs. (3.17) and (3.18) is successively solved to be

\[ G^{(n)}(p, p + g) = G(p) G(p + g) \left\{ v_{g}^{(n)}(p) \right\} \]

\[ - \int p' \bar{v}_{2}(p - p') G(p') G(p' + g) v_{g}^{(n)}(p') \]

\[ + 2 \left[ v_{2}(g) G^{(n)}(p', p' + g) v_{g}^{(n)}(p') \right] \left\{ \int p' G(p') G(p' + g) v_{g}^{(n)}(p') \right\} \]

\[ - \int p' \int p'' G(p') G(p' + g) \bar{v}_{2}(p' - p'' G(p'' + g) v_{g}^{(n)}(p'') + \cdots \} \right\}, \] (3.20)

by the same way as described in I. In the above expression we put

\[ \varepsilon^{(n)}(g) = 1 - v_{2}(g) H^{(n)}(g). \] (3.21)

Now, the structure-dependent thermodynamic potential is obtained by the same procedure as in I:

\[ Q_{n} = \int \frac{d\lambda}{\lambda} \langle \lambda H \rangle = Q_{1} + Q_{2} + Q_{3} + \cdots, \] (3.22)
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$$\Omega_{n+1} = -\frac{2N}{n+1} \sum_{\boldsymbol{g}} \nu_1(-\boldsymbol{g}) \int_{\boldsymbol{p}} G^{(n)}(\boldsymbol{p} + \boldsymbol{g}).$$ \quad (n \geq 1) \tag{3.23}

With the help of Eqs. (3.7), (3.8) and (3.11), we obtain

$$\Omega_2 = N/2 \sum_{\boldsymbol{g}} \left[ \nu_1(\boldsymbol{g}) \right] ^{1/2} \left[ \nu_2(\boldsymbol{g}) \right] ^{-1} \left[ \nu_3(\boldsymbol{g}) \right]$$

$$= \bar{\Omega}_{2,1} + \bar{\Omega}_{2,2} + \bar{\Omega}_{2,3} + \cdots.$$ \quad (3.24)

In the above, the last line comes out by an expansion of \(1/\nu_2(\boldsymbol{g})\), where \(\bar{\Omega}_{2,1}\) is given by the first line of Eq. (3.24) with replacement of \(\nu_2(\boldsymbol{g})\) by \(\nu_2^{(0)}(\boldsymbol{g})\), and

$$\bar{\Omega}_{2,1} = N/2 \sum_{\boldsymbol{g}} \left[ \nu_2^{(0)}(\boldsymbol{g}) \right] \bar{\nu}_1(\boldsymbol{g}),$$

$$\bar{\Omega}_{2,i} = N/2 \sum_{\boldsymbol{g}} \left[ \nu_2^{(0)}(\boldsymbol{g}) \right] \bar{\nu}_i(\boldsymbol{g}). \quad (i = a, b, c) \tag{3.25}

Here \(\nu_1^{(0)}(\boldsymbol{g}) = \nu_1(\boldsymbol{g})/\nu_2^{(0)}(\boldsymbol{g})\) is a screened interaction with the use of Eq. (3.21).

Similarly we obtain \(\Omega_3\) from Eq. (3.20):

$$\Omega_3 = \Omega_{3,0} + \Omega_{3,1} + \cdots,$$ \quad (3.26)

where

$$\bar{\Omega}_{3,0} = -N/3 \sum_{\boldsymbol{g}, \boldsymbol{g}', \boldsymbol{g}''} \nu_3^{(0)}(-\boldsymbol{g}) \nu_2^{(0)}(\boldsymbol{g} - \boldsymbol{g}') \nu_1^{(0)}(\boldsymbol{g}') \bar{\nu}_3(\boldsymbol{g}, \boldsymbol{g}''),$$ \quad (3.27)

$$\bar{\nu}_3(\boldsymbol{g}, \boldsymbol{g}'') = 2 \int_{\boldsymbol{p}} G(\boldsymbol{p}) G(\boldsymbol{p} + \boldsymbol{g}) G(\boldsymbol{p} + \boldsymbol{g}'').$$ \quad (3.28)

And \(\bar{\Omega}_{3,1}\) is given by Eq. (3.27) if one replaces \(\bar{\nu}_3(\boldsymbol{g}, \boldsymbol{g}'')\) by \(\bar{\nu}_3(\boldsymbol{g})\) defined as

$$\bar{\nu}_3(\boldsymbol{g}) = 2 \int_{\boldsymbol{p}} G(\boldsymbol{p}) G(\boldsymbol{p} + \boldsymbol{g}) G(\boldsymbol{p} + \boldsymbol{g}'),$$

$$\times \int_{\boldsymbol{p}'} \nu_2^{(0)}(-\boldsymbol{p} - \boldsymbol{p}') \left[ G(\boldsymbol{p}') G(\boldsymbol{p}' + \boldsymbol{g}) + G(\boldsymbol{p}' + \boldsymbol{g}') G(\boldsymbol{p}') \right].$$ \quad (3.29)

In deriving these expressions we use Eq. (3.20), in which the effective field \(\nu^{(n)}_\theta\) is written particularly for \(n = 2\) as

$$\nu^{(n)}_\theta(\boldsymbol{p}) = \sum_{\boldsymbol{g}} G(\boldsymbol{p} + \boldsymbol{g}) U^{(n)}_\theta A(\boldsymbol{p}) U^{(0)}_{\theta - \theta'} A(\boldsymbol{p} + \boldsymbol{g}')$$

$$= \sum_{\boldsymbol{g}} G(\boldsymbol{p} + \boldsymbol{g}') \nu_1^{(0)}(\boldsymbol{g}') \nu_2^{(0)}(\boldsymbol{g} - \boldsymbol{g}')$$

$$\times \left[ 1 - \int_{\boldsymbol{p}'} \nu_2^{(0)}(-\boldsymbol{p} - \boldsymbol{p}') \left[ G(\boldsymbol{p}') + G(\boldsymbol{p}' + \boldsymbol{g}) \right] \right] \times G(\boldsymbol{p}' + \boldsymbol{g}') e^{i \omega n} + \cdots.$$ \quad (3.30)
Finally $\Omega_i$ is obtained similarly and may be omitted here. The contributions to $\Omega$ are given graphically in Fig. 1.

§ 4. Expansion in the free propagator

In the preceding section, we have obtained the expressions for the thermodynamic potential by expansion in $\varphi_1^{(0)}$, $\varphi_2^{(0)}$ and $G$, where $\varphi_1^{(0)}$ and $\varphi_2^{(0)}$ are the dressed interactions as determined by Eq. (3·4). To evaluate the relevant quantities, we shall further expand $G(p)$ in $G^0(p)$, the free propagator.

In the considered expansion, the primary term of $\varphi_2^{(0)}(q)$ is

$$\varphi_2^S(q) = \varphi_2(q)/\varepsilon(q),$$

where $\varepsilon(q)$ is Lindhard's dielectric function as given by

$$\varepsilon(q) = 1 - v_b(q)\Pi^b(q), \quad \Pi^b(q) = 2 \int_0^t G^d(p)G^a(p+q).$$

However, it is proved that the difference between $\varphi_1^{(0)}(q)$ and $\varphi_2^S(q)$ comes out in higher-order terms than the third-order one of $\varphi_2^S(q)$. Therefore, all expressions given before remain valid by a simple replacement of $\varphi_2^{(0)}(q)$ by $\varphi_2^S(q)$.

Now we expand $G(p)$ in $G^0(p)$, by making use of Eqs. (3·5) and (3·6). The expanded result is substituted for $G(p)$ in $\Pi_{i,m}(q)$, which are given in Eqs. (3·12) ~ (3·16), (3·28) ~ (3·29), and in which $\varphi_2^{(0)}(q)$ is simply replaced by $\varphi_2^S(q)$.

First, $\Pi_{2,1}$ and $\Pi_{4,3}$, both with substitutions of $G^0$ for $G$, will be denoted by $\Pi_{2,1}^{(0)}$ and $\Pi_{4,3}^{(0)}$, respectively, where $i = a, b, c$.

Second, $\Pi_{4,0}^{(0)}(q)$ is expanded as

$$\Pi_{4,0}^{(0)}(q) = \Pi_{4,0}^{(0)}(q) + \Pi_{4,1}^{(0)}(q) + \Pi_{4,1}^{(0)}(q) + \Pi_{4,1}^{(0)}(q) + \cdots,$$
where $\Pi_{2,1}(q)$ is identical to $\Pi^0(q)$ defined by Eq. (4.2), and

$$
\Pi_{2,1}^{(0)}(q) = -2 \int \int \bar{v}^2_\Sigma(p-p')G^\rho(p)G^\rho(p+q)
\times \left[ G^\rho(p)G^\rho(p') + G^\rho(p+q)G^\rho(p'+q) \right],
$$

(4.4)

$$
\Pi_{2,1}^{(2)}(q) = 2 \int \int \int \bar{v}^2_\Sigma(p-p') \bar{v}^2_\Sigma(p'-p'')e^{iv_0G^\rho(p)}G^\rho(p+q)
\times \left\{ G^\rho(p)\left[ G^\rho(p')G^\rho(p'') + G^\rho(p'+q)G^\rho(p' + q) \right] \right\},
$$

(4.5)

Similarly, we have

$$
\Pi_{2,1}(q) = \Pi_{2,1}^{(0)}(q) + \Pi_{2,1}^{(2)}(q) + \cdots
$$

(4.8)

Our results are summarized to be

$$
\Pi(q) = \Pi_{2,1}(q) + \sum_{i=\infty}^b \Pi_{2,1}^{(i)}(q) + \sum_{i=\infty}^\delta \Pi_{2,1}^{(i)}(q) + \cdots
$$

(4.10)

The contributions obtained above are exact up to second order in $v^2_\Sigma$. For them the graphical representations are shown in Fig. 2. Hereafter, we put

$$
\Pi_{2,1}^{(0)} = \Pi_{2,1}^{(0)} + 2\Pi_{2,1}^{(2)} + \Pi_{2,1}^{(4)},
$$

$$
\Pi_{2,1}^{(2)} = \Pi_{2,1}^{(2)} + \Pi_{2,1}^{(4)},
$$

(4.11)

The term $\Pi_{2,1}^{(4)}$ is composed of graphs topologically equivalent to those appearing
Fig. 2. Diagrams for contributions to the thermodynamic potential. (B) The solid lines represent the free electron lines. The broken lines represent the electron-electron interactions and the crosses the electron-ion ones, both interactions shielded by Lindhard's dielectric function.

in HFA (see I). The term $\Pi_{a b}^{(g)}$ is composed of graphs with two crossing interaction-lines. On the other hand, $\Pi_{a b}^{(f)}$ is the term studied by Geldart et al.\(^{10}\) We mention $\Pi_{A}^{(g)}$, $\Pi_{B}^{(g)}$ and $\Pi_{C}^{(g)}$, which are in accord with $\Pi_{A}$, $\Pi_{B}$ and $\Pi_{C}$ in their papers, respectively.

In accordance with Eq. (4·10), the thermodynamic potential is also expanded. In the first line of Eq. (3·24), we expand $1/\varepsilon(g)$ in $1/\varepsilon^{0}(g)$. Then, $\Omega_{a b}$, the primary contributions to $\Omega_{a}$ is identical to the first line of Eq. (3·24) with $\varepsilon(g)$ replaced by $\varepsilon^{0}(g)$. The other contributions are

$$\Omega_{a b}^{(i)} = \frac{N}{2} \sum_{g} \bar{v}_{i}^{g}(g) | \Pi_{a b}^{(i)}(g) |, \quad (i = a, b) \tag{4·12}$$

$$\Omega_{A, B, C}^{(i)} = \frac{N}{2} \sum_{g} \bar{v}_{i}^{g}(g) | \Pi_{A, B, C}^{(i)}(g) |, \quad (i = A, B, C) \tag{4·13}$$

where $\bar{v}_{i}^{g}(g) = v_{i}(g) / \varepsilon^{0}(g)$ is the screened interaction with the use of Lindhard's function (4·2).

In the same way, the third-order terms are written down as

$$\Pi_{a b}^{(g)}(g, g') = \Pi_{a b}^{(g)}(g, g') + \Pi_{a b}^{(g)}(g, g') + \cdots \tag{4·14}$$

$$\Pi_{A, B, C}^{(g)}(g, g') = \Pi_{A, B, C}^{(g)}(g, g') + \cdots \tag{4·15}$$

Here, $\Pi_{a b}$ and $\Pi_{A, B, C}^{(g)}$ are obtained from Eqs. (3·28) and (3·29) by substitutions of $G^{e}$ for $G$ and of $\bar{v}_{i}^{g}$ for $\bar{v}_{i}^{0}$, respectively. And a new term $\Pi_{A, B, C}^{(g)}$ proves to be
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\[ \Pi_{m}^{\omega}(g, g') = 2 \int \int \frac{\bar{\varphi}_{\omega}^{\diamond}(p - p') G_{\omega}^{\gamma}(p) G_{\gamma}^{\gamma}(p + g) G_{\omega}^{\gamma}(p + g')}{[G_{\omega}^{\gamma}(p) G_{\gamma}^{\gamma}(p') + G_{\omega}^{\gamma}(p + g) G_{\gamma}^{\gamma}(p') + G_{\omega}^{\gamma}(p + g') G_{\gamma}^{\gamma}(p' + g')] e^{\gamma \omega}}. \]  

(4.16)

The one-electron terms \( \Pi_{m}^{\omega} \) are identical to those given in I, where the detailed treatments have been given for them. The terms \( \Pi_{m}^{\omega} \) are of forms similar to those in HFA, apart from \( \bar{\varphi}_{\omega}^{\diamond} \) which is a dynamically screened interaction, and which replaces \( \psi_{\nu} \), the bare interaction, in HFA.

§ 5. Third-order terms, \( \Pi_{m}^{(3)} \) and \( \Pi_{m}^{(3)} \)

Let us rewrite Eq. (3.13) more explicitly as

\[ \Pi_{m}^{(3)}(g, g') = -\frac{1}{N^2} \sum_{p, p'} \frac{1}{\delta_{p'}} \bar{\varphi}_{\omega}^{\diamond}(p - p', \zeta_{i} - \zeta_{i'}) \times G_{\omega}^{\gamma}(p, \zeta_{i}) G_{\omega}^{\gamma}(p + g, \zeta_{i}) G_{\gamma}^{\gamma}(p', \zeta_{i}) G_{\omega}^{\gamma}(p' + g, \zeta_{i}). \]  

(5.1)

We then write down the screened interaction \( \bar{\varphi}_{\omega}^{\diamond}(p - p', \zeta_{i} - \zeta_{i'}) \) as \( \psi_{\nu}(p - p') \) divided by \( \varepsilon'_{i}(p - p', \zeta_{i} - \zeta_{i'}) \). Here we use

\[ \varepsilon'_{i}(q, \nu) = 1 + \frac{2}{\beta} v_{i}(q) \sum_{p} \left\{ \frac{f(\varepsilon_{p})}{\varepsilon_{p} + q - \varepsilon_{p} + \nu} + \frac{f(\varepsilon_{p})}{\varepsilon_{p} - \varepsilon_{p} - \nu} \right\}, \]  

(5.2)

where \( f(\varepsilon_{p}) \) is the Fermi factor for a free electron of the energy \( \varepsilon_{p} \).

As can be seen by rewriting \( G_{\omega}^{\gamma}(p) G_{\gamma}^{\gamma}(p + g) \) as \( \{G_{\omega}^{\gamma}(p + g) - G_{\omega}^{\gamma}(p)\}/(\varepsilon_{p + g} - \varepsilon_{p}) \), the frequency sum in Eq. (5.1) proves to be of the form

\[ F_{q}(p, p') = \frac{1}{\beta} \sum_{\nu} \varepsilon_{\nu}(q, \zeta_{i} - \zeta_{i'}) \varepsilon_{\nu}^{\gamma}(p, \zeta_{i}) G_{\omega}^{\gamma}(p, \zeta_{i}) G_{\omega}^{\gamma}(p', \zeta_{i}). \]  

(5.3)

Replacing the sum over \( \nu \) by the corresponding integral, one has

\[ \frac{1}{\beta} \sum_{\nu} \varepsilon_{\nu}^{\gamma}(q, \zeta_{i} - \zeta_{i'}) = -\frac{1}{2\pi i} \int_{\gamma} d\zeta' e^{\beta(\zeta'_{i} - \zeta_{i})} \frac{1}{\varepsilon^{\gamma}(q, \zeta_{i} - \zeta_{i'}) (\zeta'_{i} - \varepsilon_{p})}, \]  

(5.4)

where the contour encircles counterclockwise the vertical line at \( \zeta'_{i} = \mu \) in the complex \( \zeta'_{i} \)-plane. We evaluate the above integral at poles lying outside the prescribed contour, being located at \( \zeta'_{i} = \varepsilon_{p} \) and at zeros of \( \varepsilon^{\gamma}(q, \zeta_{i} - \zeta_{i'}) \). The resulting expression is multiplied by \( \beta^{-2} G_{\gamma}(p, \zeta_{i}) \) and then the second frequency-summation is performed similarly. Thus we obtain

\[ F_{q}(p, p') = \frac{1}{\varepsilon^{\gamma}(q, \zeta_{i} - \zeta_{i'})} \frac{1}{\varepsilon_{p} - (\zeta_{i} - \zeta_{i'}) \nu_{i}}. \]  

(5.5)
Here \( \varepsilon''(q, \nu) \) is the derivative of \( \varepsilon'(q, \nu) \) at \( \nu = \nu_i \), in which \( \nu_i \) denotes a root of \( \varepsilon'(q, \nu) = 0 \), lying on the real axis. In the limit of the continuous momentum, Eq. (5.5) turns out to be

\[
F_q(p, p') = f(\varepsilon_p) f(\varepsilon_{p'}) \Re \left\{ \frac{1}{\varepsilon'(q, \varepsilon_p - \varepsilon_{p'} - i\Omega^+)} \right\} \\
+ \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{d\omega}{\omega - (\varepsilon_p - \varepsilon_{p'})} \cdot \frac{f(\varepsilon_p) - e^{-\beta\omega} f(\varepsilon_{p'})}{1 - e^{-\beta\omega}} \Im \left\{ \frac{1}{\varepsilon'(q, \omega - i\Omega^+)} \right\}.
\]

(5.6)

Next, the evaluation of \( \Pi_{\text{HF}}^{(0)} \), Eq. (4.4), reduces to that of \( \partial F_q(p, p') / \partial \varepsilon_p \). In differentiating \( 1/\varepsilon'(q, \varepsilon_p - \varepsilon_{p'} - i\Omega^+) \) we use the Kramers-Kronig relation

\[
\Re \left\{ \frac{1}{\varepsilon'(q, \nu - i\Omega^+)} \right\} = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{d\omega}{\omega - \nu} \Im \left\{ \frac{1}{\varepsilon'(q, \omega - i\Omega^+)} \right\}.
\]

(5.7)

In the above integral, a contribution from poles due to plasmon may come in. In this way we write down

\[
\frac{\partial}{\partial \varepsilon_p} F_q(p, p') = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{d\omega}{\omega - (\varepsilon_p - \varepsilon_{p'})} \Im \left\{ \frac{1}{\varepsilon'(q, \omega - i\Omega^+)} \right\} \\
+ \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{d\omega}{\omega - (\varepsilon_p - \varepsilon_{p'})} \cdot \frac{f(\varepsilon_p) - e^{-\beta\omega} f(\varepsilon_{p'})}{1 - e^{-\beta\omega}} \Im \left\{ \frac{1}{\varepsilon'(q, \omega - i\Omega^+)} \right\} \\
+ R.
\]

(5.8)

In the above, a remainder, \( R \), includes the derivative of the Fermi factor. We shall discuss such terms at the end of this section.

Using these results we obtain \( \Pi_{\text{HF}}^{(0)} \) and \( \Pi_{\text{HF}}^{(0)} \), which are combined to be

\[
\Pi_{\text{HF}}^{(0)}(g) + \Pi_{\text{HF}}^{(0)}(g) = \Pi_{\text{HF}}^{(0)}(g) + \Pi_{\text{HF}}^{(0)}(g).
\]

(5.9)

Here \( \Pi_{\text{HF}}^{(0)} \) is a modification of the HF term as given by

\[
\Pi_{\text{HF}}^{(0)}(g) = \frac{2}{N^2} \sum_{p, p'} \Re \left\{ \left( \frac{1}{\varepsilon_p - \varepsilon_{p' + g}} - \frac{1}{\varepsilon_{p'} - \varepsilon_{p' + g}} \right) \varepsilon'(p - p') \right\} \\
\times \left\{ \frac{1}{\varepsilon_p - \varepsilon_{p' + g}} + \frac{1}{\varepsilon_{p'} - \varepsilon_{p' + g}} \right\} \\
\times \varepsilon''(p + p' + g, \varepsilon_p - \varepsilon_{p'} - i\Omega^+).
\]

(5.10)

And, at zero temperature \( \Pi_{\text{HF}}^{(0)} \) is written as

\[
\Pi_{\text{HF}}^{(0)}(g) = \frac{2}{N^2} \sum_{p, p'} \Im \left\{ \frac{2}{\pi} \int_{0}^{\infty} \frac{d\omega}{\omega - (\varepsilon_p - \varepsilon_{p'})} \left( \frac{1}{\varepsilon_p - \varepsilon_{p' + g}} - \frac{1}{\varepsilon_{p'} - \varepsilon_{p' + g}} \right) \right\} \\
\times \varepsilon''(p - p', \omega - i\Omega^+) \\
\times \left\{ \frac{1}{\varepsilon_p - \varepsilon_{p' + g}} + \frac{1}{\varepsilon_{p'} - \varepsilon_{p' + g}} \right\}.
\]
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\[ \times \frac{\nu_2(p + p' + g)}{\varepsilon^8(p + p' + g; \omega - i0^+)} + \frac{2}{\pi} \int_0^\infty d\omega \left( \frac{1}{\varepsilon_{p} - \varepsilon_{p' + g}} - \frac{1}{\varepsilon_{p'} - \varepsilon_{p' + g}} \right) \]

\[ \times \frac{\nu_2(p - p')}{\varepsilon^8(p - p'; \omega - i0^+)} \left[ \frac{f^+(\varepsilon_p) f(\varepsilon_{p'})}{\omega + (\varepsilon_p - \varepsilon_{p'})} \right]^2 \]

(5.11)

with \( f^+(\varepsilon_p) = 1 - f(\varepsilon_p) \).

We compute \( \Pi^{(0)}_{21}(\omega) \) by using the known expression:

\[ \text{Re} \varepsilon(q, \omega - i0^+) = 1 + \frac{(4/\pi) \alpha r_s / q^2}{\left[ 1 - \left( \frac{q^2 + \omega^2}{2q} \right)^2 \right] \ln \left[ \frac{2q + q^2 + \omega^2}{2q - q^2 - \omega^2} \right]} \]

\[ + \frac{1}{2} \left[ 1 - \left( \frac{q^2 - \omega^2}{2q} \right)^2 \right] \ln \left[ \frac{2q + q^2 - \omega^2}{2q - q^2 + \omega^2} \right] \]

\[ \text{Im} \varepsilon(q, \omega^* - i0^+) = \left\{ \begin{array}{ll}
\frac{-\alpha r_s}{q^2} \left[ 1 - \left( \frac{\omega^* - q^2}{2q} \right)^2 \right], & |q^2 - 2q| \leq \omega^* \leq 2q + \omega^2; \\
-\frac{\alpha r_s}{q^2}, & q^2 \leq 2, \omega^* \leq 2q - q^2; 0, \text{ otherwise}
\end{array} \right. \]

(5.12)

for \( \omega^* = (\alpha r_s)^2 q^2 > 0 \). Some results are shown in Fig. 3 for several values of \( r_s \).

In the same figure, the computed results are shown also in two kinds of approximations; we replace the dynamical dielectric-function, \( \varepsilon^0(q, \omega - i0^+) \), first by the static one, \( \varepsilon(q, 0) \), and second by the Thomas-Fermi (TF) dielectric function:

\[ \varepsilon_{TF}(q, 0) = 1 + \left( \frac{\kappa^2}{q^2} \right) \]

\[ \kappa^2 = \frac{4}{\pi} \alpha r_s. \quad (5.13) \]

In the limit \( r_s = 0 \), \( \Pi^{(0)}_{21}(\omega) \) reduces to an unscreened result. This HF result is also shown in Fig. 3. We note here that the TF screening underestimates \( \Pi^{(0)}_{21}(\omega) \) considerably.

Fig. 3. The curves for \( \Pi^{(0)}_{21}(\omega) \) as a function of \( g \).

The curves for \( \Pi^{(0)}_{21}(\omega) \) are shown for \( r_s = 1 \) and \( r_s = 2 \). The corresponding results are shown also in the approximations with static screening, with the Thomas-Fermi screening and with no screening.\(^{12,13}\)
The term $II_{x1}^{(a)}(g)$ may be regarded as a fourth-order one. The estimate of it has proved to be about 10% of $II_{x1}^{(a)}(g)$ at $r_s=1$ and in the limit $g=0$. The above dielectric term will be treated elsewhere together with $II_{x1}^{(a)}$ in Eq. (4·13).

Incidentally, we mention an anomalous term, $II_{x1}^{(a)}(g)^4$, including the derivative of the Fermi factor. The mentioned term proves to be

$$II_{x1}^{(a)}(g)^4 = \mu_{b,1} \partial II^1(g) / \partial \mu$$

from Eq. (4·4). Here $\mu_{b,1}$ is defined by

$$\mu_{b,1} = - \int \int \partial \psi^*(p-p') [G^a(p)]^2 G^a(p') e^{i\phi} / \int \int [G^a(p)]^2,$$ (5·15)

and stands for the first-order shift of the chemical potential from its free-electron value, in the electron-gas system. This is proved, if we put the first-order contribution to $\Omega_{eq}$ in the known form

$$\Omega_{b,1} = N \int \ln [1 - v_1(q) II^1(q)].$$ (5·16)

Note that Eq. (5·15) is equivalent to $\mu_{b,1} = - \Omega_{b,1}'(\mu) / \Omega_{b,1}''(\mu)$, being in conformity with 1. Here $\Omega_{b,1}$ is the primary term of $\Omega_{eq}$, and the prime indicates the derivative.

The above observation due to Luttinger and Ward\textsuperscript{13} proves important for evaluation of the higher-order terms (§ 6).

§ 6. The terms $II_{x1}^{(a)}(g, g')$

As seen in the preceding section, contributions from the zeros of the dynamical dielectric function to $[II_{x1}^{(a)} + II_{x1}^{(b)}]$ are of next higher order in the perturbation series. Moreover, the use of the static dielectric function may not cause any serious error. Thus we shall evaluate $II_{x1}^{(a)}(g, g')$ in the TF approximation, where $\psi^*(q)$ is replaced by $v_1^{TF}(q) = v_1(q) / e^{TF}(q)$. However one must remember a certain underestimation to occur in this approximation, as manifested in Fig. 3.

Now, $II_{x1}^{(a)}(g, g')$ is given by Eq. (3·29) with replacement of $v_1^{(0)}(p-p')$ by $v_1^{(a)}(p-p')$ and $II_{x1}^{(a)}(g, g')$ by Eq. (4·16). Let us put

$$J^{(a)}(g, g') = 2 \int \int v_1^{TF}(p-p') G^a(p) G^a(p+g) G^a(p+g') \times G^a(p') G^a(p'+g),$$ (6·1)

$$J^{(b)}(g, g') = 2 \int \int v_1^{TF}(p-p') [G^a(p)]^2 G^a(p+g) G^a(p+g') \times G^a(p') e^{i\phi}.$$ (6·2)

Then, $II_{x1}^{(a)}$ is written down as
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\[ H_{\text{int}}(g, g') = J^{(i)}(g, g') + J^{(i)}(g', g) + J^{(i)}(-g', g - g') \quad (i = a, b) \]  

\[ (6.3) \]

We evaluate \( J^{(i)}(g, g') \) with the help of Feynman's parametrization procedure (I). First, Eq. (6.1) is written as

\[
J^{(i)}(g, g') = 2 \int \int \psi_T^* (p - p') \int d\alpha_1 \int d\alpha_2 \int d\alpha_3 \\
\times \delta \left( 1 - \sum \frac{\alpha_i}{\alpha} \right) \int d\tau_1 \int d\tau_2 \delta \left( 1 - \sum \frac{\tau_i}{\tau} \right) \\
\times \left( \xi - \alpha_i \xi + \alpha_i \xi + \gamma \right)^{1} \left( \xi' - \gamma' \xi + \gamma' \xi + \gamma \right)^{1}, \quad (6.4)
\]

where \((\alpha, \alpha, \alpha)\) and \((\gamma, \gamma)\) are Feynman's parameters. By the same procedure as in I, we first perform the frequency summation and then integrate in \( dp_p \) and \( dp'_p \):

\[
J^{(i)}(g, g') = \frac{3}{16\pi} \left( \alpha \tau \right)^4 \int_0^1 \int_0^1 \int_0^1 \int_0^1 d\alpha_1 d\alpha_2 d\alpha_3 d\tau' \quad (6.5)
\]

Here we put

\[
P^1 = \mu^1 + (\alpha_i g + \alpha_i g')^2 - (\alpha_i g + \alpha_i g')^2,
\]

\[
P^2 = \mu^2 + \gamma (\gamma - 1) g^2, \quad Q = |(\alpha_i - \gamma) g + \alpha_i g'|
\]

with \( \mu^1 = (\alpha \tau) \mu \). In Eq. (6.5), the integrations over \( \alpha_i \), \( \alpha_i \) and \( \gamma \) are confined to the region satisfying \( P^2 \) and \( P^2 \geq 0 \).

Second, for Eq. (6.2) one could obtain an expression similar to Eq. (6.5). However the resulting expression is divergent under a certain condition to be described later. Then the quantity of reality must be

\[
J^{(i)}(g, g') = \frac{3}{16\pi} \left( \alpha \tau \right)^4 \left[ \frac{\partial}{\partial \mu^1} \int_0^1 \int_0^1 \int_0^1 \int_0^1 d\alpha_1 d\alpha_2 d\alpha_3 d\tau' \right] F(P, P'; Q) \quad (6.7)
\]

a similar procedure as taken in Eq. (I.5.4). Here \( F(P, P'; Q) \) is given by

\[
F(P, P'; Q) = \frac{1}{QP} \left[ P^2 + \kappa^2 - (Q + P)^2 \right] \ln \left( \frac{Q + P + P'}{Q + P - P'} \right)^2 + \kappa^2 \\
+ \left[ P^2 + \kappa^2 - (Q - P)^2 \right] \ln \left( \frac{Q - P + P'}{Q - P - P'} \right)^2 + \kappa^2 \\
- 4\kappa (Q + P) \left[ \ln \left( \frac{Q + P + P'}{\kappa} \right) - \ln \left( \frac{Q + P - P'}{\kappa} \right) \right]
\]
for which \( Q, P \) and \( P' \) are given by

\[
P^2 = Q^2 - \alpha_1 g^2 + a_2 g'^2, \quad P'^2 = \mu^* - Q = |\alpha g + \alpha g'|.
\]

As is easily seen, \( \partial(P^2) F(P, P'; Q) \) includes a factor \( P^{-1} \), which brings us a divergent integral if \( P^2 \) becomes negative in the region of \( \alpha_1 \) and \( \alpha_2 \) satisfying \( \alpha_1 + \alpha_2 \leq 1 \). However the derivative of the integral, being prescribed in Eq. (6·7), remains finite; the same procedure as for the evaluation of \( \Pi_4 \) in I. A technique is needed for computing such singular integrals as Eq. (6·7) (Appendix).

Now, in Eq. (6·7) we have taken an anomalous term into account. This term comes from the double pole in Eq. (6·2) and must be eliminated. The anomalous term proves to be of a form similar to Eq. (5·14):

\[
\Pi_{3,3}^{\alpha, \alpha'}(g, g') = \mu_4^{\alpha, \alpha'} \varphi \Pi_{3,3}(g, g') / \partial \mu.
\]

In the above expression, \( \Pi_{3,3}^{\alpha, \alpha'} \) is given by Eq. (3·28) with replacement of \( G \) by \( G^* \), and is identical to \( \Pi_3 \) in I. And \( \mu_4^{\alpha, \alpha'} \) is given by Eq. (5·15) with \( v_4^{\alpha, \alpha'}(q) \) substituted for \( \delta_4^{\alpha, \alpha'}(q) \). This approximate shift of the chemical potential is evaluated to be

\[
\mu_4^{\alpha, \alpha'} = -2 \frac{\sqrt{\mu^*}}{\alpha_4} \left( 1 - \frac{\kappa}{\sqrt{\mu^*}} \right) \left[ \frac{2\sqrt{\mu^*} \kappa \text{arctan} \left( \frac{2\sqrt{\mu^*}}{\kappa} \right) + \kappa^2}{4 \mu^*} \ln \left( \frac{4\mu^* + \kappa^2}{\kappa^2} \right) \right].
\]

Thus we calculate

\[
\Pi_{3,3}^{\alpha, \alpha'}(g, g') = \Pi_{3,3}^{\alpha, \alpha'}(g, g') + \Pi_{3,3}^{\alpha, \alpha'}(g, g') / \partial \mu.
\]

where \( \Pi_{3,3}^{\alpha, \alpha'}(g, g') = \Pi_{3,3}^{\alpha, \alpha'}(g, g') - \mu_4^{\alpha, \alpha'} \varphi \Pi_{3,3}^{\alpha, \alpha'}(g, g') / \partial \mu \). The above subtraction proves equivalent to replacing \( F(P, P'; Q) \) in Eq. (6·8) by

\[
F(P, P'; Q) = F(P, P'; Q) + 4\pi \arctan \mu_4^{\alpha, \alpha'} / P.
\]

In Fig. 4 we show some computed results. We note that \( \Pi_{3,3}^{\alpha, \alpha'}(g, g') \) has the same singularity as \( \Pi_{3,3}^{\alpha, \alpha'}(g, g') \), namely Brovman and Kagan’s singularity (see I). Consider a triangle whose two sides are \( g \) and \( g' \). Then, \( \Pi_{3,3}^{\alpha, \alpha'} \) has a singularity of the cusp type if the triangle is of the acute form while it is not the case for obtuse triangles. For acute triangles, the singularity occurs if the circumscribing circle has the same radius as that of the Fermi sphere. This is just what happens in \( \Pi_{3,3}^{\alpha, \alpha'}(g, g') \). See Fig. 4 for different behaviors of \( \Pi_{3,3}^{\alpha, \alpha'}(g, g') \) for the two different kinds of configurations pointed out above. In the same figure, the broken curves with \( r_s = 0 \) stand for the HF results. These curves are much higher than the solid ones. This HF exaggeration is the most striking in the close vicinity of the singular point.
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In Fig. 4 we also show the case where $\mathbf{g}$ and $\mathbf{g}'$ are parallel to each other. For the colinear case with $\mathbf{g}' = \gamma \mathbf{g}$, we expand a product of the Green's functions, $G^0(\mathbf{p})G^0(\mathbf{p} + \mathbf{g})G^0(\mathbf{p} + \mathbf{g}')$, in a partial series (I). By this way one has

$$J^{(c)}(\mathbf{g}, \mathbf{g}') = \frac{(\alpha \gamma)^2}{\gamma (1 - \gamma) g^2} [S_1(\mathbf{g}, \mathbf{g}) - \gamma S_1(\mathbf{g}', \mathbf{g}) - (1 - \gamma) S_1(\mathbf{g}' - \mathbf{g}, - \mathbf{g})],$$

where

$$S_1(\mathbf{g}, \mathbf{g}') = 2 \int_0^1 \int_0^1 \frac{1}{\pi} \frac{d\alpha_1}{\alpha_1} \frac{d\alpha_2}{\alpha_2} \left[ \ln \left( (\mathbf{Q} + \mathbf{P} + \mathbf{P}')^2 + \kappa^2 \right) 
+ (\mathbf{Q} - \mathbf{P} - \mathbf{P}') \ln \left( (\mathbf{Q} - \mathbf{P} - \mathbf{P}')^2 + \kappa^2 \right) 
- (\mathbf{Q} + \mathbf{P} - \mathbf{P}') \ln \left( (\mathbf{Q} + \mathbf{P} - \mathbf{P}')^2 + \kappa^2 \right) 
+ (\mathbf{Q} - \mathbf{P} + \mathbf{P}') \ln \left( (\mathbf{Q} - \mathbf{P} + \mathbf{P}')^2 + \kappa^2 \right) 
+ 2\kappa \left\{ \arctan \left( \frac{\mathbf{Q} + \mathbf{P} + \mathbf{P}'}{\kappa} \right) + \arctan \left( \frac{\mathbf{Q} - \mathbf{P} - \mathbf{P}'}{\kappa} \right) 
- \arctan \left( \frac{\mathbf{Q} + \mathbf{P} - \mathbf{P}'}{\kappa} \right) - \arctan \left( \frac{\mathbf{Q} - \mathbf{P} + \mathbf{P}'}{\kappa} \right) \right\} \right].$$

(6.14)
with \( Q = |\alpha, g - \alpha, g'|, \ P^2 = \mu^2 + \alpha_i (\alpha_i - 1) g^2 \) and \( P'^2 = \mu^2 + \alpha_i (\alpha_i - 1) g'^2 \). The other integral \( J^{(b)}(g, g') \) is similarly dealt with.

**Appendix**

---Method for Evaluating a Singular Integral---

A method is described for computing the singular integral with particular reference to Eq. (6·7) of the text.

In the integrand of Eq. (6·7), \( F(P, P'; Q) \) is singular at \( P = 0 \), and hence we subtract its principal part at the singular point, which is denoted by \( F_s(P, P'; Q) \), from \( F(P, P'; Q) \). The subtracted expression turns out to be

\[
\left( \frac{\partial}{\partial \mu^*} \right) \int_0^1 d\alpha_i \int_0^{1-\alpha_i} d\alpha_2 (1-\alpha_i-\alpha_2) \left[ F(P, P'; Q) - F_s(P, P'; Q) \right], \tag{A1}
\]

by considering Eq. (6·13). Here the differentiation can be interchanged with the integrations. This allows us to compute Eq. (A1).

Let us then consider

\[
J_s = \int_0^1 d\alpha_i \int_0^{1-\alpha_i} d\alpha_2 (1-\alpha_i-\alpha_2) F_s(P, P'; Q). \tag{A2}
\]

Referring to § 5(a) in I, we now transform the integration variables \((\alpha_i, \alpha_2)\) into \((x_1, x_2)\). In the new integration variables, the momentum \( P \), which corresponds to \( J (x_1, x_2) \) in I, is obtained from \( P^2 = r^2 - R^2 + \mu^2 \). Here \((r, \theta)\) denote the polar coordinates and \( R \) the radius of the circumscribing circle of a triangle formed by \( g \) and \( g' \). Let \((\lambda_1, \lambda_2)\) be the eigenvalues of a \( 2 \times 2 \) matrix \( (g_i | g_j) \) with \( g_i = g \) and \( g_j = g' \). The eigenvectors belonging to \( \lambda_1 \) and \( \lambda_2 \) are denoted by \((c_{11}, c_{12})\) and \((c_{21}, c_{22})\) respectively. Then one has

\[
Q^2 = r^2 + \frac{\sigma_1}{\sqrt{\lambda_1}} + \frac{\sigma_2}{\sqrt{\lambda_2}} + R^2, \tag{A3}
\]

where \( \sigma_i = \sum c_i g_j^2 \). We note here \( R^2 = (1/4) \sum \sigma_i / \lambda_i \).

In the coordinate system described above, we obtain

\[
F_s(P, P'; Q) = \frac{2}{PQ_i} \left\{ (P'^2 + \kappa^2 - Q_i^2) \ln \frac{(Q_i + P')^2 + \kappa^2}{(Q_i - P')^2 + \kappa^2} - 4\kappa Q_i \left[ \arctan \frac{Q_i + P'}{\kappa} - \arctan \frac{Q_i - P'}{\kappa} \right] \right. \\
\left. + 4P' Q_i + 4\kappa \mu_i^2 \frac{\alpha r_x}{P} \right\}. \tag{A4}
\]

In the above, \( Q_i \) denotes \( Q \) at \( P = 0 \), which is given by Eq. (A3) if one replaces \( r \) by \( r_x = \sqrt{\mu^2 - R^2} \).
Now, in Eq. (A2) with Eq. (A4), we perform the integration over $r$ analytically, with integration region lying inside the triangle. The integrated result, which is still an integral over $\theta$, is now regular, and hence the differentiation with respect to $\mu^*$ can be performed under the integral sign. The angular integration is carried out numerically. The numerical value thus obtained is added to that of Eq. (A1).

References

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