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Green Function Method for Electron Gas. III

——*Diamagnetism*——

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The Green function method is applied to the calculation of the diamagnetic susceptibility of a dense electron gas. The exact high density value for the correction to the Landau diamagnetism is calculated.

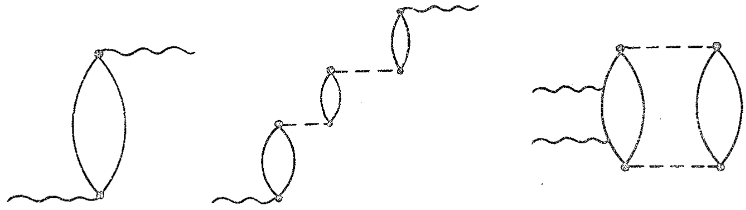
§ 1. Introduction

The influence of Coulomb interaction between electrons on the diamagnetism was treated by March and Donovan,[1] and Kanazawa.[2] March and Donovan, and Fletcher and Larson[3] inserted one-electron energy spectrum, which was obtained by Bohm-Pines theory, into the formula for the diamagnetic susceptibility for the quasi-bound electrons :[4]

$$\chi=-\frac{e^2k_0}{12(\pi\hbar c)^2}\left[\frac{2}{3}\frac{d^2E}{dk^2}+\frac{1}{3k}\frac{dE}{dk}\right]_{k=k_0}. \tag{1·1}$$

The effect of the long-range part of the Coulomb interactions including the effect of subsidiary conditions was investigated by Kanazawa in the scheme of Bohm-Pines theory. All these works show that there is a small correction to the diamagnetic susceptibility due to the Coulomb interactions.

Wentzel[5] used an equivalent Hamiltonian which gives the correct high density value for the correlation energy and calculated the diamagnetic susceptibility. His conclusion is that there is no correction to the Landau value of non-interacting electron gas. His argument, however, is valid only in so far as the exchange effects are omitted. If we take the exchange effects into account, there remains a finite correction,[6] and in this case the equivalent Hamiltonian formalism of Wentzel cannot be applied. The diagrams which were taken into account by Wentzel are shown in Fig. 1a and Fig. 1b. The contribution from the process shown in Fig. 1a gives the Landau diamagnetism and the contributions from the processes shown in Fig. 1b vanish. Wentzel did not consider the contributions from other processes which are shown, for example, by Fig. 1c or Fig. 3c. In this paper we investigate the contributions from these processes and derive the exact high density formula for the correction to the Landau diamagnetism, using the Green function method.



(a) (b) (c)

Fig. 1. Diagrams contributing to susceptibility
Wavy line and dotted line represent magnetic perturbations and Coulomb interactions respectively.

In § 2 we express the diamagnetic susceptibility in terms of the two-particle Green function, which is calculated in a consistent approximation in § 3 and § 4.

Since temperature dependence of the diamagnetism is expected to be small, we calculate the susceptibility at zero temperature. The interaction Hamiltonian with the magnetic field is treated as a small perturbation, and consequently our formulation is not applicable to the case of strong magnetic field (de-Haas van Alphen effect).

§ 2. Magnetic susceptibility in terms of Green function

We consider an N-electron system in a box of unit volume. As usual it is embedded in the uniform positive charge. We apply a static magnetic field, which is expressed in terms of the vector potential $\boldsymbol{A}(\boldsymbol{r})=\sum_q \boldsymbol{A}(\boldsymbol{q}) \exp(i\boldsymbol{q}\cdot\boldsymbol{r})$. Then the Hamiltonian and the current operators are: $(\hbar=1)$

$$H=H_0+H_c+H'+H'' \tag{2·1}$$

$$H_0=\sum_p \varepsilon_p{}^0 a_p^+ a_p,\quad \varepsilon_p{}^0=p^2/2m \tag{2·2a}$$

$$H_c=\frac{1}{2}\sum_{\substack{p,p',k\\k\neq 0}} V(k)\, a_{p+k}^+ a_{p'-k}^+ a_{p'} a_p \tag{2·2b}$$

$$H'=-\frac{1}{c}\int d\boldsymbol{r}\, \boldsymbol{j}_0(\boldsymbol{r})\cdot\boldsymbol{A}(\boldsymbol{r}) \tag{2·2c}$$

$$H''=-\frac{1}{2c}\int d\boldsymbol{r}\, \boldsymbol{j}_1(\boldsymbol{r})\cdot\boldsymbol{A}(\boldsymbol{r}) \tag{2·2d}$$

$$\boldsymbol{j}_0(\boldsymbol{r})=-\frac{ie}{2m}\{\nabla\psi^+(\boldsymbol{r})\psi(\boldsymbol{r})-\psi^+(\boldsymbol{r})\nabla\psi(\boldsymbol{r})\} \tag{2·3}$$

$$\boldsymbol{j}_1(\boldsymbol{r})=-\frac{e^2}{mc}\boldsymbol{A}(\boldsymbol{r})\psi^+(\boldsymbol{r})\psi(\boldsymbol{r}) \tag{2·4}$$

where $\psi(\boldsymbol{r})=\sum_p a_p \exp(i\boldsymbol{p}\cdot\boldsymbol{r})$, $V(k)=4\pi e^2/k^2$, a_p and a_p^+ are the annihilation and creation operators of electrons. We have omitted spin indices for simplicity. The expectation value of the current $\boldsymbol{j}_0(\boldsymbol{q})+\boldsymbol{j}_1(\boldsymbol{q})$, which are the Fourier components of the current operators (2·3) and (2·4), is written in the form:

$$i_\alpha(\boldsymbol{q})=\langle\Psi(t)|j_\alpha(\boldsymbol{q},t)|\Psi(t)\rangle=\sum_\beta K^{\alpha\beta}(\boldsymbol{q})A_\beta(\boldsymbol{q})+\mathrm{O}(A^2) \tag{2·5}$$

where we have referred to the interaction representation with $H'+H''$ as the interaction Hamiltonian which is switched on adiabatically in the infinite past. $\Psi(t)$ is the Schroedinger function in this representation which is obtained adiabatically from Ψ_0, the ground state of H_0+H_c, and

$$\boldsymbol{j}(\boldsymbol{q},t)=\exp[i(H_0+H_c)t]\boldsymbol{j}(\boldsymbol{q})\exp[-i(H_0+H_c)t].$$

Gauge invariance and the condition of continuity require that[7]

$$K^{\alpha\beta}(\boldsymbol{q})=(q^2\delta_{\alpha\beta}-q_\alpha q_\beta)K(q). \tag{2·6}$$

Then the susceptibility is given by

$$\chi=\frac{1}{c}\lim_{q\to0}K(q). \tag{2·7}$$

Thus our problem is to calculate the expectation value of the current of our system.

As is seen from (2·5) and (2·7), we need to calculate $\boldsymbol{i}(\boldsymbol{q})$ only to the first order of A. Therefore in the calculation of $\boldsymbol{i}_1(\boldsymbol{q})=\langle\Psi(t)|\boldsymbol{j}_1(\boldsymbol{q},t)|\Psi(t)\rangle$ we may replace $\Psi(t)$ by Ψ_0 and we have

$$\boldsymbol{i}_1(\boldsymbol{r},t)=\langle\Psi_0|\boldsymbol{j}_1(\boldsymbol{r},t)|\Psi_0\rangle=-\frac{e^2}{mc}\boldsymbol{A}(\boldsymbol{r})\langle\Psi_0|\psi^+(\boldsymbol{r})\psi(\boldsymbol{r})|\Psi_0\rangle=-\frac{ne^2}{mc}\boldsymbol{A}(\boldsymbol{r}).$$

Therefore

$$\boldsymbol{i}_1(\boldsymbol{q},t)=-\frac{ne^2}{mc}\boldsymbol{A}(\boldsymbol{q}),\quad K_1^{\alpha\beta}=-\frac{ne^2}{mc}\delta_{\alpha\beta}. \tag{2·8}$$

This is the so-called London diamagnetic term, which is almost cancelled by the paramagnetic part.

Next we consider the paramagnetic current $\boldsymbol{i}_0$:

$$\begin{aligned}i_0^\alpha(\boldsymbol{r},t)&=\langle\Psi(t)|j_0^\alpha(\boldsymbol{r},t)|\Psi(t)\rangle\\&=-i\int_{-\infty}^t dt'\langle\Psi_0|[j_0^\alpha(\boldsymbol{r},t),\ H'(t')]|\Psi_0\rangle\\&=\frac{i}{c}\int d\boldsymbol{r}'\int_{-\infty}^t dt'\langle\Psi_0|[j_0^\alpha(\boldsymbol{r},t),\ j_0^\beta(\boldsymbol{r}',t')]|\Psi_0\rangle A_\beta(\boldsymbol{r}'),\end{aligned} \tag{2·9}$$

since

$$\Psi(t)=T\exp\left[-i\int_{-\infty}^t dt'(H'(t')+H''(t'))\right]\Psi_0$$

and higher order terms in A are neglected. From (2·3),

$$\begin{aligned}\boldsymbol{j}_0(x)\boldsymbol{j}_0(x')=\frac{e^2}{4m^2}\{&-\nabla\psi^+(x)\psi(x)\nabla'\psi^+(x')\psi(x')\\&-\psi^+(x)\nabla\psi(x)\psi^+(x')\nabla'\psi(x')\end{aligned}$$

$$+\Gamma\psi^+(x)\psi(x)\psi^+(x')\Gamma'\psi(x')$$
$$+\psi^+(x)\Gamma\psi(x)\Gamma'\psi^+(x')\psi(x')\}, \qquad (2\cdot 10)$$
$$(x=(\boldsymbol{r},\ t)).$$

Introducing the two-particle Green function

$$G_2(1,\ 2;\ 3,\ 4)=i\langle\Psi_0|T\psi(1)\psi(2)\psi^+(3)\psi^+(4)|\Psi_0\rangle$$

where $\psi(1)=\psi(\boldsymbol{r}_1,\ t_1)$, we get $(t_1=t>t'=t_2)$

$$\langle\Psi_0|j_0{}^\alpha(x_1)j_0{}^\beta(x_2)|\Psi_0\rangle$$
$$=\frac{-ie^2}{4m^2}\lim_{\substack{r'_{1,2}\to r_{1,2}\\ t'_{1,2}\to t_{1,2}+0}}(\Gamma_1{}^\alpha-\Gamma'_1{}^\alpha)(\Gamma_2{}^\beta-\Gamma'_2{}^\beta)G_2(x_1,\ x_2;\ x_1',\ x_2') \qquad (2\cdot 11)$$

and

$$\langle\Psi_0|j_0{}^\beta(x_2)j_0{}^\alpha(x_1)|\Psi_0\rangle=\langle\Psi_0|j_0{}^\alpha(x_1)j_0{}^\beta(x_2)|\Psi_0\rangle^*. \qquad (2\cdot 12)$$

From $(2\cdot 9)$ to $(2\cdot 12)$ we get the final expression of $\boldsymbol{i}_0$ in terms of G_2:

$$i_0{}^\alpha(\boldsymbol{r}_1,\ t_1)=\frac{e^2}{4m^2c}\int_{-\infty}^{t}dx_2\lim(\Gamma_1{}^\alpha-\Gamma'_1{}^\alpha)(\Gamma_2{}^\beta-\Gamma'_2{}^\beta)G_2(x_1,\ x_2;\ x_1',\ x_2')$$
$$\times A_\beta(\boldsymbol{r}_2)+\text{c.c.} \qquad (2\cdot 13)$$

Thus the whole information of diamagnetism is contained in the two-particle Green function for the system.

§ 3. Pair theory approximation

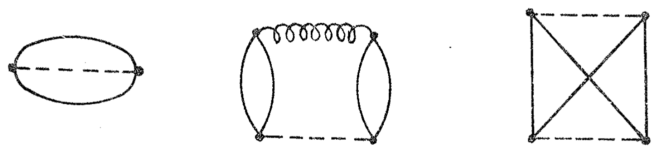
For a high-density electron gas the two-particle Green function, which gives the correct high density value for the correlation energy, has been obtained in I:

$$G_2(1,\ 2;\ 3,\ 4)=-iG_0(1,\ 4)G_0(2,\ 3)$$
$$-\int dx_5dx_6G_0(1,\ 5)G_0(2,\ 6)\mathcal{V}(5,\ 6)G_0(5,\ 3)G_0(6,\ 4)$$
$$+\int dx_5dx_6G_0(1,\ 5)G_0(2,\ 6)V(5,\ 6)G_0(5,\ 4)G_0(6,\ 3), \qquad (3\cdot 1)$$

where $\mathcal{V}(x,\ x')$ is the effective interaction, the Fourier transform of which is $\mathcal{V}(k,\ \omega)=V(k)/\varepsilon(k,\ \omega)$, $\varepsilon(k,\ \omega)$ being the complex dielectric constant and $V(x,\ x')=V(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t')$. G_0 is the unperturbed one-particle Green function and is given by

$$G_0(x,\ x')=\sum_p\int\frac{d\varepsilon}{2\pi}G_0(\boldsymbol{p},\ \varepsilon)\exp i(\boldsymbol{p}\cdot\boldsymbol{r}-\varepsilon t), \qquad (3\cdot 2)$$

$$G_0(\boldsymbol{p},\,\varepsilon) = -[\varepsilon - \varepsilon_p{}^0 + i\delta(1-2n_p{}^0)]^{-1} \tag{3·3}$$



(a) (b) (c)

Fig. 2. Diagrams for correlation energy
Helical line repesents the effective interaction.

where $n_p{}^0$ is the occupation number of the unperturbed state. The contribution of each term of (3·1) to the correlation energy is shown graphically in Fig. 2a, 2b and 2c. In this section we will use (3·1) for G_2. Inserting (3·2) and (3·3) into (3·1) we get

$$\begin{aligned}
&\lim_{r_{1,2}\to r_{1,2}} (\nabla_1{}^\alpha - \nabla'_1{}^\alpha)(\nabla_2{}^\beta - \nabla'_2{}^\beta) G_2(\boldsymbol{r}_1 t_1,\, \boldsymbol{r}_2 t_2;\, \boldsymbol{r}'_1 t_1{}^+,\, \boldsymbol{r}'_2 t_2{}^+) \\
&= +i\sum_{p_1 p_2}\int \frac{d\varepsilon_1 d\varepsilon_2}{(2\pi)^2} G_0(\boldsymbol{p}_1\varepsilon_1) G_0(\boldsymbol{p}_2\varepsilon_2) \\
&\quad \times (p_1+p_2)_\alpha (p_1+p_2)_\beta \exp[i(\boldsymbol{p}_1-\boldsymbol{p}_2)\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2) - i(\varepsilon_1-\varepsilon_2)(t_1-t_2)] \\
&\quad + \sum_{p_1 p_2 q}\int \frac{d\varepsilon d\varepsilon' d\omega}{(2\pi)^3} G_0(\boldsymbol{p}_1\varepsilon) G_0(\boldsymbol{p}_2\varepsilon')\, \mathcal{V}(\boldsymbol{q},\,\omega)\, G_0(\boldsymbol{p}_1-\boldsymbol{q},\,\varepsilon-\omega) \\
&\quad \times G_0(\boldsymbol{p}_2+\boldsymbol{q},\,\varepsilon'+\omega)(2p_1-q)_\alpha(2p_2+q)_\beta \exp[i\boldsymbol{q}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2) - i\omega(t_1-t_2)] \\
&\quad - \sum_{p_1 p_2 q}\int \frac{d\varepsilon d\varepsilon' d\omega}{(2\pi)^3} G_0(\boldsymbol{p}_1\varepsilon) G_0(\boldsymbol{p}_2\varepsilon')\, V(q)\, G_0(\boldsymbol{p}_1-\boldsymbol{q},\,\varepsilon'+\omega) \\
&\quad \times G_0(\boldsymbol{p}_2+\boldsymbol{q},\,\varepsilon-\omega)(p_1+p_2+q)_\alpha(p_1+p_2-q)_\beta \\
&\quad \times \exp[i(\boldsymbol{p}_1-\boldsymbol{p}_2-\boldsymbol{q})\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2) - i\omega(t_1-t_2)].
\end{aligned} \tag{3·4}$$

From (3·4) and (2·13) we obtain

$$i_0{}^\alpha(\boldsymbol{q}) = \frac{1}{c}\int\frac{d\omega}{2\pi}\frac{1}{\omega - i\delta} F^{\alpha\beta}(\boldsymbol{q},\,\omega) A_\beta(\boldsymbol{q}) + \text{c.c.}\ . \tag{3·5}$$

Therefore

$$K_0{}^{\alpha\beta}(\boldsymbol{q}) = \frac{2}{c}\int\frac{d\omega}{2\pi}\left[\mathrm{P}\frac{1}{\omega}\mathrm{Re}\,F^{\alpha\beta}(\boldsymbol{q},\,\omega) - \pi\delta(\omega)\,\mathrm{Im}F^{\alpha\beta}(\boldsymbol{q},\,\omega)\right]. \tag{3·6}$$

Here

$$F^{\alpha\beta}(\boldsymbol{q},\,\omega) = F_0{}^{\alpha\beta}(\boldsymbol{q},\,\omega) + F_1{}^{\alpha\beta}(\boldsymbol{q},\,\omega) + F_2{}^{\alpha\beta}(\boldsymbol{q},\,\omega) \tag{3·7}$$

with

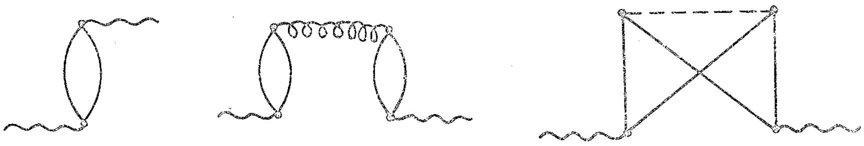
$$F_0^{\alpha\beta}(\boldsymbol{q},\omega)=\frac{e^2}{4m^2}\sum_p\int\frac{d\mathcal{E}}{2\pi}(2p-q)_\alpha(2p-q)_\beta G_0(\boldsymbol{p},\mathcal{E})G_0(\boldsymbol{p}-\boldsymbol{q},\mathcal{E}-\omega) \tag{3·8}$$

$$F_1^{\alpha\beta}(\boldsymbol{q},\omega)=-i\frac{e^2}{4m^2}\sum_{p_1p_2}\int\frac{d\mathcal{E}d\mathcal{E}'}{(2\pi)^2}\mathcal{V}(\boldsymbol{q},\omega)(2p_1-q)_\alpha(2p_2+q)_\beta$$
$$\times G_0(\boldsymbol{p}_1,\mathcal{E})G_0(\boldsymbol{p}_1-\boldsymbol{q},\mathcal{E}-\omega)G_0(\boldsymbol{p}_2,\mathcal{E}')G_0(\boldsymbol{p}_2+\boldsymbol{q},\mathcal{E}'+\omega) \tag{3·9}$$

$$F_2^{\alpha\beta}(\boldsymbol{q},\omega)=i\frac{e^2}{4m^2}\sum_{p_1p_2}\int\frac{d\mathcal{E}d\mathcal{E}'}{(2\pi)^2}V(\boldsymbol{p}_1-\boldsymbol{p}_2-\boldsymbol{q})(2p_1-q)_\alpha(2p_2+q)_\beta$$
$$\times G_0(\boldsymbol{p}_1,\mathcal{E})G_0(\boldsymbol{p}_1-\boldsymbol{q},\mathcal{E}-\omega)G_0(\boldsymbol{p}_2,\mathcal{E}')G_0(\boldsymbol{p}_2+\boldsymbol{q},\mathcal{E}'+\omega). \tag{3·10}$$

Here we notice that the terms $F_0^{\alpha\beta}$, $F_1^{\alpha\beta}$ and $F_2^{\alpha\beta}$ come from the first, the second and the third term of (3·1) respectively, and so it is evident that their contributions to $K_0^{\alpha\beta}$ are represented diagramatically as in Fig. 3a, 3b and 3c.* We write $K_0^{\alpha\beta}$ as

$$K_0^{\alpha\beta}(q)=K_{(0)}^{\alpha\beta}+K_{(1)}^{\alpha\beta}+K_{(2)}^{\alpha\beta}. \tag{3·11}$$



(a) (b) (c)

Fig. 3. Contribution from (3·1) or (3·11)

If we put $V(k)\to 0$ for the moment, then the second and the third terms of (3·11) vanish. Therefore $K_{(0)}^{\alpha\beta}$ must give, when combined with $K_1^{\alpha\beta}$ of (2·8), the usual Landau diamagnetism. This is actually the case, as is shown in Appendix I.

Next we consider $K_{(1)}^{\alpha\beta}$. Comparing Fig. 3b with Fig. 1b, we see at once that this is the term investigated by Wentzel. In other words, to take into account only the first and the second terms in (3·1) corresponds to Wentzel's approximation, in which H' is reduced to the parts involving only pair creation and annihilation terms. In our formulation the proof that $K_{(1)}^{\alpha\beta}$ vanishes is quite easy, if we rewrite (3·9) as follows:

$$F_1^{\alpha\beta}(\boldsymbol{q},\omega)=-i\mathcal{V}(\boldsymbol{q},\omega)L_\alpha(\boldsymbol{q},\omega)L_\beta(\boldsymbol{q},\omega)(e/2m)^2,$$
$$L_\alpha(\boldsymbol{q},\omega)=\sum_p\int\frac{d\mathcal{E}}{2\pi}(2p+q)_\alpha G_0(\boldsymbol{p},\mathcal{E})G_0(\boldsymbol{p}+\boldsymbol{q},\mathcal{E}+\omega). \tag{3·12}$$

Using

$$\int\frac{d\mathcal{E}}{2\pi}G_0(\boldsymbol{p},\mathcal{E})G_0(\boldsymbol{p}+\boldsymbol{q},\mathcal{E}+\omega)=i\left[\frac{n_{p+q}^0(1-n_p^0)}{\omega_{p,q}-\omega+i\delta}-\frac{n_p^0(1-n_{p+q}^0)}{\omega_{p,q}-\omega-i\delta}\right] \tag{3·13}$$

* $\boldsymbol{i}(\boldsymbol{q})=-(1/c)\partial E(A)/\partial A(-\boldsymbol{q})$, where $E(A)=E_0+\frac{1}{2}\chi\Sigma(\boldsymbol{q}\times A(\boldsymbol{q}))\cdot(\boldsymbol{q}\times A(-\boldsymbol{q}))$. Fig. 3 represents the diagrams which contribute to the second term.

we get

$$L_\alpha(\boldsymbol{q}, \omega) = i\sum_p n_p{}^0(1-n_{p+q}^0)(2p+q)_\alpha\left[\frac{-1}{\omega_{p,q}-\omega-i\delta}+\frac{-1}{\omega_{p,q}+\omega-i\delta}\right]$$

where $\omega_{p,q}=\mathcal{E}_{p+q}^0-\mathcal{E}_p{}^0$. Thus $L(\boldsymbol{q}, \omega)=L(\boldsymbol{q}, -\omega)$. Returning to $(3\cdot12)$ and changing the integration variables as $\boldsymbol{p}\to-\boldsymbol{p}-\boldsymbol{q}$, $\mathcal{E}\to\mathcal{E}-\omega$, we find that $L(\boldsymbol{q}, \omega) = -L(\boldsymbol{q}, -\omega) = -L(\boldsymbol{q}, \omega) = 0$.

Therefore in our approximation $(3\cdot1)$, the term which gives a correction to the Landau diamagnetism is only $K_{(2)}^{\alpha\beta}$, which corresponds to the diagram shown in Fig. 3c. The calculation is performed in Appendix II and the result is:

$$K_{(2)}^{\alpha\beta}=\frac{1}{c}\left(\frac{e}{m}\right)^2\sum_{pp'}V(\boldsymbol{p}-\boldsymbol{p}')(p+\tfrac{1}{2}q)_\alpha(p'+\tfrac{1}{2}q)_\beta\frac{n_{p+q}^0-n_p{}^0}{\omega_{p,q}}\cdot\frac{n_{p'+q}^0-n_{p'}^0}{\omega_{p',q}}. \tag{3·14}$$

Here we encounter with two difficulties. Firstly, $(3\cdot14)$ is not gauge-invariant. From the form of $(2\cdot6)$, gauge-invariance is guaranteed if $\sum_{\alpha,\beta}q_\alpha q_\beta K^{\alpha\beta}(\boldsymbol{q})=0$, which does not hold. Secondly the integral of $(3\cdot14)$ diverges.

These difficulties indicate clearly that our approximation of G_2 is not sufficient for the problem of diamagnetism. We must improve the two-particle Green function $(3\cdot1)$ by taking into account the higher order effects. This, however, is not surprising. The difficulty of gauge-invariance is rather evident at the beginning, because in the case of diamagnetism there is another term besides $(3\cdot14)$ which is linear in $V(k)$. From perturbation theoretic point of view, they together form the correct first order correction to the ideal gas value. Therefore it is not surprising that a part thereof alone, $(3\cdot14)$, is not gauge-invariant. In the case of correlation energy, in contrast to our case, all terms which are in the same order in the r_s expansion are all contained in $(3\cdot1)$. But now this is not the case. Thus we must include, besides $(3\cdot14)$, all terms that are of the same order in r_s. To this purpose we first replace G_0 in the first term of $(3\cdot1)$ by G_1, which we define as the one-particle Green function including exchange self-energy:

$$G_1(\boldsymbol{p}, \mathcal{E})^{-1}=G_0(\boldsymbol{p}, \mathcal{E})^{-1}-\Sigma_{ex}(\boldsymbol{p})$$

$$\Sigma_{ex}(\boldsymbol{p})=\sum_k V(k)\,n_{p+k}^0. \tag{3·15}$$

In other words, we replace, in the expression for the Landau diamagnetism (A2), $\mathcal{E}_p{}^0$ by $E_p=\mathcal{E}_p{}^0-\Sigma_{ex}(\boldsymbol{p})$. Next we expand it in $V(k)$ and retain only the first order. Then we get

$$K_{(2)}^{\prime\alpha\beta}=-\frac{1}{c}\left(\frac{e}{m}\right)^2\sum_{pp'}V(\boldsymbol{p}-\boldsymbol{p}')(p+\tfrac{1}{2}q)_\alpha(p'+\tfrac{1}{2}q)_\beta\frac{(n_{p+q}^0-n_p{}^0)\,(n_{p'+q}^0-n_{p'}^0)}{\omega_{p,q}^2}. \tag{3·16}$$

Combining $(3\cdot14)$ and $(3\cdot16)$ we obtain

$$K_2^{\alpha\beta}=K_{(2)}^{\alpha\beta}+K_{(2)}^{\prime\alpha\beta}=\frac{1}{c}\left(\frac{e}{m}\right)^2\sum_{pp'}V(\boldsymbol{p}-\boldsymbol{p}')\frac{(n_{p+q}^0-n_p{}^0)(n_{p'+q}^0-n_{p'}^0)}{\omega_{p,q}}$$

$$\times(p+\tfrac{1}{2}q)_\alpha\left[\frac{(p'+\tfrac{1}{2}q)_\beta}{\omega_{p',q}}-\frac{(p+\tfrac{1}{2}q)_\beta}{\omega_{p,q}}\right]. \tag{3·17}$$

This expression is evidently gauge-invariant as expected and thus the first difficulty has been removed. But the second difficulty still remains. We will investigate it in the next section.

§ 4. Elimination of divergence

In the preceding section we have looked for the correction which is linear in $V(k)$ and we have found it to be divergent. This is rather an expected result, since if we calculate the diamagnetic susceptibility in a simple manner using (1·1), it diverges in the Hartree-Fock approximation. As is well known in the calculation of the correlation energy, these divergences are removed by replacing $V(k)$ by the effective interaction $\mathcal{V}(\boldsymbol{k},\omega)$. Physically it means to take into account the correlation effect, or the screening of Coulomb potential, which removes the unnatural distribution of the energy level on the Fermi surface. In our calculation this effect is taken into account by replacing $G_0(x-x')$ in the first term of (3·1) by $G(x-x')$, which includes the polarization part besides the exchange energy, and replacing $V(x-x')$ in the third term of (3·1) by $\mathcal{V}(x-x')$: i.e.,

$$G_2(1,2;3,4)=-iG(1,4)G(2,3) \tag{4·1a}$$

$$+\int dx_5dx_6G_0(1,5)G_0(2,6)\mathcal{V}(5,6)G_0(5,4)G_0(6,3), \tag{4·1b}$$

where we have omitted the second term of (3·1) which gives no contribution. The Fourier transform of $G(x-x')$ in our case is, as is well known,

$$G(\boldsymbol{p},\varepsilon)^{-1}=G^0(\boldsymbol{p},\varepsilon)^{-1}-\Sigma_{ex}(\boldsymbol{p})-\Sigma_C(\boldsymbol{p},\varepsilon). \tag{4·2}$$

$\Sigma_{ex}(\boldsymbol{p})$ is given in (3·15), and

$$\Sigma_C(\boldsymbol{p},\varepsilon)=\sum_k\int\frac{d\omega}{2\pi i}V(k)\,G_0(\boldsymbol{p}+\boldsymbol{k},\varepsilon+\omega)\frac{Q(k,\omega)}{1+Q(k,\omega)} \tag{4·3}$$

where $Q(k,\omega)=\varepsilon(k,\omega)-1$.

Here we make a symplifying assumption:

$$\mathcal{V}(k,\omega)\longrightarrow\mathcal{V}(k,0), \tag{4·4}$$

then (4·3) is integrated straightforwardly and we get

$$\Sigma_{ex}(\boldsymbol{p})+\Sigma_C(\boldsymbol{p},\varepsilon)=\sum_k V(k)n_{p+k}^0\left\{1-\frac{Q(k,0)}{1+Q(k,0)}\right\}=\sum_k\mathcal{V}(k,0)n_{p+k}^0 \tag{4·5}$$

which is independent of ε. Comparing (4·2) with (3·15) we see at once that the contribution of the first term of (4·1) is $K_{(0)}^{\alpha\beta}+$(3·16), except that $V(p-p')$ is replaced by $\mathcal{V}(p-p', 0)$. Contribution of (4·1b) is calculated in the same fashion as Appendix II, and the result is just (3·14) where also $V(p-p')$ is replaced by $\mathcal{V}(p-p', 0)$. Thus we come to the final result:

$$K^{\alpha\beta}(\boldsymbol{q})=K_L{}^{\alpha\beta}(\boldsymbol{q})+K_C{}^{\alpha\beta}(\boldsymbol{q}), \tag{4·6}$$

$$K_C{}^{\alpha\beta}(\boldsymbol{q})=\frac{1}{c}\left(\frac{e}{m}\right)^2\sum_{pp'}\mathcal{V}(\boldsymbol{p}-\boldsymbol{p}', 0)\,(n_{p+q}^0-n_p{}^0)\,(n_{p'+q}^0-n_{p'}^0)$$

$$\times\frac{(p+\frac{1}{2}q)_\alpha}{\omega_{p,q}}\left[\frac{(p'+\frac{1}{2}q)_\beta}{\omega_{p',q}}-\frac{(p+\frac{1}{2}q)_\beta}{\omega_{p,q}}\right]. \tag{4·7}$$

Expression (4·7) is gauge-invariant and finite. Its calculation is elementary but somewhat lengthy, which we give in Appendix III.

In Appendix III we use a further approximation of replacing $\mathcal{V}(k, 0)$ by $\mathcal{V}'(k)$, where ($\boldsymbol{q}=\boldsymbol{k}/k_0$)

$$\mathcal{V}(k, 0)=\frac{4\pi e^2}{k_0{}^2}\left\{q^2+\frac{2\alpha r_s}{\pi}\left[1-\frac{q^2}{12}+O(q^4)\right]\right\}^{-1}, \tag{4·8a}$$

$$\mathcal{V}'(k)=\frac{4\pi e^2}{k_0{}^2}(q^2+2\mathcal{E})^{-1},\quad \mathcal{E}=\frac{\alpha r_s}{\pi}. \tag{4·8b}$$

Then the result is:

$$K_C^{\alpha\beta}(\boldsymbol{q})=(q^2\delta_{\alpha\beta}-q_\alpha q_\beta)\,K_C(q), \tag{4·9a}$$

$$K_C(q)=\frac{4\pi e^4}{(2\pi)^6 c}\left[q^{-2}I-\frac{1}{8}J\right] \tag{4·9b}$$

where I vanishes independent of $\mathcal{E}$, and

$$J=A\log\mathcal{E}+B+C\mathcal{E}\log\mathcal{E}+\cdots, \tag{4·9c}$$

$$A=\frac{8\pi^2}{9},\quad B=\frac{8\pi^2}{9}(4-\log 2). \tag{4·9d}$$

§ 5. Discussion

In our calculation we have made four approximations:

(i) approximation (4·1)

(ii) the approximation made in deriving the second term of (4·7) which originates from (4·1a)

(iii) neglect of retardation, i.e. the approximation (4·4)

(iv) replacement of $\mathcal{V}$ by $\mathcal{V}'$.

These approximations are justified as follows.

(i) In § 3 and § 4 we considered the processes that are represented diagramatically in Fig. 4. In other words, we considered the correction to Fig. 3a, which are of first order in H_c, and replaced $V(k)$ by the effective interaction (elimination of divergence). All other corrections may in principle be calculated by the prescription:

(a) write down the processes in diagrams (e.g. Fig. 5)
(b) construct the Green function G_2 which contribute to that diagram
(c) insert it into (2·13) and perform the calculation
(d) if divergences appear, they are always treated by the principle of elimination of divergence.

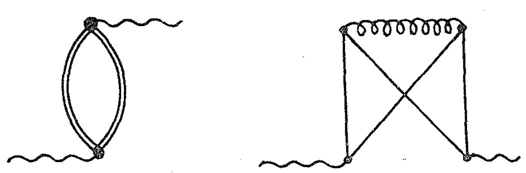


Fig. 4. Processes representing each term of (4·2) Double line is the propagator of electron and hole including self energy.

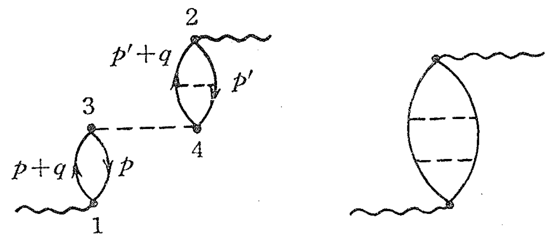


Fig. 5. Diagrams representing higher order corrections

For example, we will briefly investigate the processes represented in Fig. 5. Fig. 5a gives no contribution, just as in the case of Fig. 3b. This is the consequence of the situation that the matrix element at the point (1) or (2) in Fig. 5a is of the form $(\boldsymbol{p}+\frac{1}{2}\boldsymbol{q})\boldsymbol{A}(\boldsymbol{q})$, which changes sign by the replacement $\boldsymbol{p}\rightarrow-\boldsymbol{p}-\boldsymbol{q}$, and the integration variables $\boldsymbol{p}$ and $\boldsymbol{p}'$ are independent of each other. Thus in general diagrams of this type, i.e., diagrams which are composed of two parts each of which has one perturbation line H' and which are both connected by single interaction line H_c, give no contribution. The contribution from Fig. 5b does not vanish. However, it is of second order in H_c, and if we compare the result with that of Fig. 4b, it contains a factor e^2, or r_s. Thus the contribution is of higher order.

(ii) Approximation (ii) is justified in the same fashion. The contribution from (4·1a) (Fig. 4a) is just (A2), except that $\omega_{p,q}$ is replaced by $W(p,q)=E(p+q)-E(p)$, where $E(p)$ is the energy of the quasi-particle

$$E(p)=\varepsilon_p^{\,0}-\Sigma(p).$$

Our approximation is to replace

$$W(p,q)^{-1}-\omega_{p,q}^{-1}=\frac{\Sigma(p+q)-\Sigma(p)}{W(p,q)\,\omega_{p,q}} \tag{5·1}$$

by

$$\frac{\Sigma(p+q)-\Sigma(p)}{\omega_{p,q}^{\;2}}, \tag{5·2}$$

so the correction to our approximation is

$$(5\cdot1)-(5\cdot2)=\frac{[\Sigma(p+q)-\Sigma(p)]^2}{W(p,\ q)\,\omega^2_{p,q}},$$

which is also of the higher order in r_s.

(iii) Properties of the approximations of (iii) and (iv) are also of the same type as before, because $\tilde{\mathcal{V}}(k,\ \omega)-\tilde{\mathcal{V}}(k,\ 0)$ and $\tilde{\mathcal{V}}(k,\ 0)-\tilde{\mathcal{V}}'(k)$ are proportional to e^6 times integrals which do not diverge.

Finally we note that I in $(4\cdot9\text{b})$ vanishes independent of $\mathcal{E}$, as is seen in (A9). This means that our original form $(3\cdot17)$ does not contain the constant term, although the coefficient of q^2 is infinite. Therefore, our procedure of § 4, that is, the approximation mentioned above, does not affect the vanishing of I in $(4\cdot9\text{b})$.

Thus we conclude that our result $(4\cdot9)$ is exact up to the second term of $(4\cdot9\text{c})$.

It is interesting to compare our result with that obtained by Donovan and March. They give

$$(\chi/\chi_0)=1+\frac{\alpha r_s}{6\pi}[\log r_s+2(2+\log 0.417-\log 2)+\cdots]$$

while $(4\cdot9)$ gives

$$(\chi/\chi_0)=1+\frac{\alpha r_s}{6\pi}\left[\log r_s+4+\log\frac{\alpha}{2\pi}\right].$$

Numerically,

$$2(2+\log 0.417-\log 2)=1.12$$

$$4+\log(\alpha/2\pi)=1.51.$$

We find that the correction is finite but very small.

We are indebted to Prof. T. Usui, Miss E. Fujita and other members of the group of many-body problem for helpful discussions.

Appendix I

Landau diamagnetism

$(3\cdot8)$ can be readily integrated with respect to $\mathcal{E}$, using $(3\cdot3)$:

$$F_0^{\alpha\beta}(\boldsymbol{q},\ \omega)=-i\left(\frac{e}{m}\right)^2\sum_p(p+\tfrac{1}{2}q)_\alpha(p+\tfrac{1}{2}q)_\beta n_p^0(1-n^0_{p+q})$$

$$\times\left[\frac{1}{\omega_{p,q}-\omega-i\delta}+\frac{1}{\omega_{p,q}+\omega-i\delta}\right]. \tag{A1}$$

(A1) is put in $(3\cdot6)$, where we notice that (A1) is symmetrical with respect to ω, so that

$$K^{\alpha\beta}_{(0)}=-(1/c)\,\mathrm{Im}F_0^{\alpha\beta}(\boldsymbol{q},\ 0)$$

$$=\frac{2e^2}{m^2c}\sum_p (p+\tfrac{1}{2}q)_\alpha(p+\tfrac{1}{2}q)_\beta\frac{n_p{}^0(1-n^0_{p+q})}{\omega_{p,q}}. \tag{A2}$$

Now we transform the coordinate system from $(\alpha\beta\gamma)$ to (xyz), where we take z-axis pararell to $\boldsymbol{q}$. Thus

$$p_\alpha=\boldsymbol{p}\cdot\boldsymbol{\alpha}=\sum_i p_i\alpha_i,\ \text{etc.},$$

then the integration of (A2) over $\boldsymbol{p}$ is straightforward and yields

$$K^{\alpha\beta}_{(0)}=\frac{ne^2}{mc}q_\alpha q_\beta+\left(\delta_{\alpha\beta}-\frac{q_\alpha q_\beta}{q^2}\right)\frac{e^2}{4\pi^2 mc}\left\{\frac{5}{12}k_0{}^3-\frac{1}{16}q^2k_0{}^2\right.$$
$$\left.+\frac{1}{4q}\left(k_0{}^2-\frac{q^2}{4}\right)^2\log\left|\frac{k_0+\frac{1}{2}q}{k_0-\frac{1}{2}q}\right|\right\}.$$

Expanding logarithm in power series of q and adding (2·8),

$$K_L{}^{\alpha\beta}(\boldsymbol{q})=K_1{}^{\alpha\beta}+K^{\alpha\beta}_{(0)}=-(q^2\delta_{\alpha\beta}-q_\alpha q_\beta)\left[\frac{ne^2}{mc}\cdot\frac{1}{4k_0}+\cdots\right].$$

So that

$$\chi_0=-\frac{e^2k_0}{12\pi^2mc^2}=-\frac{1}{12\pi^2\alpha r_s}(1/137)^2 \tag{A3}$$

where we have put $n=k_0{}^3/3\pi^2$, taking spin into consideration.

Appendix II

Derivation of (3·14)

From (3·10) and (3·13),

$$F_2{}^{\alpha\beta}=i\left(\frac{e}{m}\right)^2\sum_{pp'}\int\frac{d\varepsilon d\varepsilon'}{(2\pi)^2}(p+\tfrac{1}{2}q)_\alpha(p'+\tfrac{1}{2}q)_\beta V(\boldsymbol{p}-\boldsymbol{p}')$$
$$\times G_0(\boldsymbol{p},\varepsilon)G_0(\boldsymbol{p}+\boldsymbol{q},\varepsilon+\omega)G_0(\boldsymbol{p}',\varepsilon')G_0(\boldsymbol{p}'+\boldsymbol{q},\varepsilon'+\omega)$$
$$=-i\left(\frac{e}{m}\right)^2\sum_{pp'}(p+\tfrac{1}{2}q)_\alpha(p'+\tfrac{1}{2}q)_\beta V(\boldsymbol{p}-\boldsymbol{p}')\left[\frac{n^0_{p+q}(1-n_p{}^0)}{\omega_{pq}-\omega+i\delta}\right.$$
$$\left.-\frac{n_p{}^0(1-n^0_{p+q})}{\omega_{p,q}-\omega-i\delta}\right]\times\left[\frac{n^0_{p'+q}(1-n^0_{p'})}{\omega_{p'q}-\omega+i\delta}-\frac{n^0_{p'}(1-n^0_{p'+q})}{\omega_{p'q}-\omega-i\delta}\right]. \tag{A4}$$

Here we note that $F_2{}^{\alpha\beta}(q,-\omega)=F_2{}^{\alpha\beta}(q,\omega)$, because in (A4) if we change the variable from $\boldsymbol{p}$, $\boldsymbol{p}'$ to $-\boldsymbol{p}-\boldsymbol{q}$, $-\boldsymbol{p}'-q$, nothing is changed except the sign of ω. Thus in (3·6) the first term of the integrand vanishes. So that

$$K^{\alpha\beta}_{(2)}=-\frac{1}{c}\mathrm{Im}F_2{}^{\alpha\beta}(\boldsymbol{q},0), \tag{A5}$$

which gives at once the result (3·14), since $\delta(\omega_{p,q})=0$ everywhere in the range of integration.

Appendix III

Calculation of $K_C^{\alpha\beta}(q)$

In the calculation of (4·7) we can choose, because of gauge-invariance, a special coordinate system where the z-axis is parallel to $\boldsymbol{q}$. As was stated in § 4, we make an approximation of replacing (4·8a) by (4·8b). (4·7) then becomes

$$K_C^{xx}(\boldsymbol{q})=q^2K_C(q)$$

or

$$K_C(q)=\frac{1}{c}\left(\frac{e}{m}\right)^2\frac{1}{q^2}\sum_{pp'}\mathcal{V}'(p-p')\,(n_{p+q}^0-n_p^0)\,(n_{p'+q}^0-n_{p'}^0)$$
$$\times\frac{p_x}{\omega_{p,q}}\cdot\left[\frac{p'_x}{\omega_{p',q}}-\frac{p_x}{\omega_{p,q}}\right]. \tag{A6}$$

Since we seek for the value of $K_C(q)$ in the limit of small q, we expand $(n_{p+q}^0-n_p^0)$ and $(n_{p'+q}^0-n_{p'}^0)$ in power series of q. Changing the variable in (A6) from $\boldsymbol{p}$, $\boldsymbol{p}'$ to $\boldsymbol{p}-\frac{1}{2}\boldsymbol{q}$, $\boldsymbol{p}'-\frac{1}{2}\boldsymbol{q}$ for convenience, we get

$$n_{p+q/2}^0-n_{p-q/2}^0=-\frac{(\boldsymbol{p}\cdot\boldsymbol{q})}{p}\delta(p-k_0)+\frac{1}{8}\left\{\left[\frac{q^2(\boldsymbol{p}\cdot\boldsymbol{q})}{p^3}-\frac{(\boldsymbol{p}\cdot\boldsymbol{q})^3}{p^5}\right]\delta(p-k_0)\right.$$
$$\left.+\left[\frac{(\boldsymbol{p}\cdot\boldsymbol{q})^3}{p^4}-\frac{q^2(\boldsymbol{p}\cdot\boldsymbol{q})}{p^2}\right]\delta'(p-k_0)-\frac{(\boldsymbol{p}\cdot\boldsymbol{q})^3}{3p^3}\delta''(p-k_0)\right\}+O(q^5), \tag{A7}$$

thus

$$K_C(q)=\frac{4\pi e^4}{(2\pi)^6cq^4}\int_0^\infty dpdp'\int_{-1}^1dxdx'\int_0^{2\pi}d\varphi d\varphi'\frac{1}{(\boldsymbol{p}-\boldsymbol{p}')^2+2\mathcal{E}k_0^2}$$
$$\times\frac{y\cos\varphi}{x}\left[\frac{y'\cos\varphi'}{x'}-\frac{y\cos\varphi}{x}\right]\left\{q^2xx'\delta(p-k_0)\delta(p'-k_0)\right.$$
$$-\frac{q^4}{8}x\delta(p-k_0)\left[\frac{x'}{k_0^2}y'^2\delta(p'-k_0)-\frac{x'}{p'}y'^2\delta'(p'-k_0)-\frac{x'^3}{3}\delta''(p'-k_0)\right]$$
$$\left.-\frac{q^4}{8}x'\delta(p'-k_0)\left[\frac{x}{k_0^2}y^2\delta(p-k_0)-\frac{x}{p}y^2\delta'(p-k_0)-\frac{x^3}{3}\delta''(p-k_0)\right]\right\}$$
$$=(4\cdot 9\mathrm{b}), \tag{A8}$$

where $x=\cos\vartheta$, $x'=\cos\vartheta'$,

$y^2=1-x^2$, $y'^2=1-x'^2$;

$$I=\int d\boldsymbol{p}d\boldsymbol{p}'\frac{xx'}{(\boldsymbol{p}-\boldsymbol{p}')^2+2\mathcal{E}k_0^2}\cdot\frac{y\cos\varphi}{x}\left[\frac{y'\cos\varphi'}{x'}-\frac{y\cos\varphi}{x}\right]$$
$$\times\delta(p-k_0)\delta(p'-k_0),$$

$$J=\int d\boldsymbol{p}\,d\boldsymbol{p}'\frac{1}{(\boldsymbol{p}-\boldsymbol{p}')^2+2\mathcal{E}k_0^2}\frac{y\cos\varphi}{x}\left[\frac{y'\cos\varphi'}{x'}-\frac{y\cos\varphi}{x}\right]$$

$$\times\left\{x\delta(p-k_0)\left[\frac{x'}{k_0^2}y'^2\delta(p'-k_0)-\frac{x'}{p'}y'^2\delta'(p'-k_0)-\frac{x'^3}{3}\delta''(p'-k_0)\right]\right.$$

$$\left.+x'\delta(p'-k_0)\left[\frac{x}{k_0^2}y^2\delta(p-k_0)-\frac{x}{p}y^2\delta'(p-k_0)-\frac{x^3}{3}\delta''(p-k_0)\right]\right\}.$$

In order to compute the integrals I and J, we use the following formulas:

$$(\boldsymbol{p}-\boldsymbol{p}')^2+2\varepsilon k_0^2=p^2+p'^2+2\varepsilon k_0^2-2pp'(xx'+yy'\cos\varphi''),\quad \varphi''=\varphi-\varphi'$$

$$\int_0^{2\pi}\frac{d\varphi d\varphi'}{\alpha-\beta\cos\varphi''}xy\cos\varphi\left[\frac{y'\cos\varphi'}{x'}-\frac{y\cos\varphi}{x}\right]$$

$$=\pi\int_0^{2\pi}d\varphi''\frac{xy}{\alpha-\beta\cos\varphi''}\left[\frac{y'\cos\varphi''}{x'}-\frac{y}{x}\right].$$

Then the integrations over p, p' and φ' are performed to obtain

$$I=(\pi/2)k_0^2J_1,$$

$$(1/\pi)J=J_1-\tfrac{1}{2}J_1'+\varepsilon J_2+\tfrac{1}{2}\left(\frac{1}{3}-\varepsilon\right)J_2'-\frac{\varepsilon^2}{3}J_3'$$

where

$$J_n=\int_{-1}^{1}dxdx'\int_0^{2\pi}d\varphi\frac{yy'\cos\varphi-(x'/x)y^2}{(\alpha-\beta\cos\varphi)^n},$$

$$J_n'=\int_{-1}^{1}dxdx'\int_0^{2\pi}d\varphi\frac{yy'\cos\varphi-(x'/x)y^2}{(\alpha-\beta\cos\varphi)^n}(x^2+x'^2),$$

$$\alpha=1+\varepsilon-xx',\qquad \beta=yy'.$$

Integrations over φ, x and x' are calculated straightforwardly. Here we write only the result:

$$J_1=J_2=0$$

$$J_1'=(8\pi/3)[-\tfrac{2}{3}-2\varepsilon(2+\varepsilon)+\varepsilon(1+\varepsilon)(2+\varepsilon)\gamma]$$

$$J_2'=(8\pi/3)[6(1+\varepsilon)-(2+6\varepsilon+3\varepsilon^2)\gamma]$$

where

$$\gamma=\log((2+\varepsilon)/\varepsilon),$$

and

$$\varepsilon^2J_3'\to 0\ \text{as}\ \varepsilon\to 0.$$

Thus we finally get

$$I=0, \tag{A9}$$

$$J=(8\pi^2/9)[\log(\varepsilon/2)+4]+\text{terms which vanish with }\varepsilon.$$

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