

## Correlation energy and its temperature dependence

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The correlation energy due to the ring diagrams of an electron gas is evaluated analytically at low temperatures. We emphasize an important correction term that was neglected in the previous calculation. This correction comes from the difference between the frequency summation and the corresponding integral of the zero-temperature limit. The correction contains a  $t^2 \ln t$  term, which cancels out the  $t^2 \ln t$  term in the exchange energy, and a large contribution to the  $t^2$  term. The coefficient of  $t^2$  in the exchange-correlation energy is thus obtained exactly in the standard random-phase approximation.

### I. INTRODUCTION

The correlation energy of an electron gas is one of the most fundamental quantities in electron theory of metals. The general exchange-correlation energy is given by a coupling constant integration,<sup>1</sup>

$$\Omega_{xc} = \frac{1}{\beta} \sum_{\mathbf{p}, i p_n} \int_0^1 \frac{d\eta}{\eta} \Sigma(\eta, p) \mathcal{G}(\eta, p), \quad (1)$$

where  $\mathcal{G}$  is the temperature Green's function with the self-energy  $\Sigma$ :  $\mathcal{G}(p) = \{i p_n - [\varepsilon_{\mathbf{p}} - \mu + \Sigma(p)]\}^{-1}$ , and  $\eta$  is the coupling constant. Here  $\mu$  is the chemical potential,  $\varepsilon_{\mathbf{p}} = \hbar^2 p^2 / 2m$ , and  $\beta = 1/k_B T$ . Equation (1) is an exact expression. In practice, it is necessary to make a suitable approximation to  $\mathcal{G}$  and  $\Sigma$  in order to evaluate  $\Omega_{xc}$ . The exchange-only scheme using the exchange self-energy  $\Sigma_x$  and the corresponding Green's function  $\mathcal{G}^{(x)}$  in Eq. (1) was studied in detail at nonzero temperatures by the present authors.<sup>2-5</sup> Here we wish to consider the temperature dependence of the correlation energy. The method we employ is to include the first-order exchange and the sum of a ring-diagram contribution to consider the screened exchange effects. The screened exchange self-energy is given by replacing the bare Coulomb interaction by the screened one in the usual exchange self-energy:

$$\Sigma_{sx}^{(0)}(p) = -\frac{1}{\beta\nu} \sum_{\mathbf{q}, i q_n} \frac{v_{\mathbf{q}}}{\varepsilon(q)} \mathcal{G}^{(0)}(p+q), \quad (2)$$

$$\varepsilon(q) = 1 - v_{\mathbf{q}} P_0(q), \quad (3)$$

where  $\mathcal{G}^{(0)}(p) = [i p_n - (\varepsilon_{\mathbf{p}} - \mu)]^{-1}$  is the unperturbed Green's function, and  $\varepsilon(q)$  is the RPA dielectric function, where RPA is the random-phase approximation. The RPA polarization  $P_0(q)$  is given by

$$\begin{aligned} P_0(q) &= \frac{2}{\beta\nu} \sum_{\mathbf{p}, i p_n} \mathcal{G}^{(0)}(p) \mathcal{G}^{(0)}(p+q) \\ &= \frac{2}{\nu} \sum_{\mathbf{p}} \frac{n_{\mathbf{p}} - n_{\mathbf{p}+\mathbf{q}}}{i q_n + \varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}+\mathbf{q}}}. \end{aligned} \quad (4)$$

By using  $\Sigma_{sx}^{(0)}$  and  $\mathcal{G}^{(0)}$  in Eq. (1) we obtain the exchange-correlation energy

$$\Omega_{xc} = \frac{1}{\beta} \sum_{\mathbf{p}, i p_n} \int_0^1 \frac{d\eta}{\eta} \Sigma_{sx}^{(0)}(\eta, p) \mathcal{G}^{(0)}(p) \quad (5)$$

$$= \frac{1}{2\beta} \sum_{\mathbf{q}, i q_n} \ln[1 - v_{\mathbf{q}} P_0(q)]. \quad (6)$$

For reasons that will be clarified in Appendix A, we divide  $\Omega_{xc}$  into the exchange energy  $\Omega_x$  and the ring-diagram contribution to correlation energy  $\Omega_r$ :

$$\Omega_x = -\frac{1}{2\beta} \sum_{\mathbf{q}, i q_n} v_{\mathbf{q}} P_0(q) = -\frac{1}{\nu} \sum_{\mathbf{p}, \mathbf{q}} v_{\mathbf{q}} n_{\mathbf{p}} n_{\mathbf{p}+\mathbf{q}}, \quad (7)$$

$$\Omega_r = \frac{1}{2\beta} \sum_{\mathbf{q}, i q_n} \{\ln[1 - v_{\mathbf{q}} P_0(q)] + v_{\mathbf{q}} P_0(q)\}. \quad (8)$$

The temperature dependence of the exchange energy was studied previously,<sup>2,6</sup> and now we evaluate the ring-diagram contribution  $\Omega_r$  at low temperatures. The latter will be called the RPA correlation energy.

The RPA correlation energy has previously been evaluated (i) analytically at low temperatures,<sup>7</sup> and (ii) numerically at all temperatures.<sup>8</sup> The aim of this paper is to investigate the small- $T$  region again, because the previous calculation by Isihara and Kojima<sup>7</sup> (to be referred to as IK) neglected an important correction term. They calculated the ring diagrams by replacing the frequency summation by the corresponding frequency integral while

expanding the integrand by the Sommerfeld expansion. Their results were given in a series in  $r_s$ , which is determined by  $n^{-1} = 4\pi(r_s a_B)^3/3$ , where  $n$  is the number density, and  $a_B$  is the Bohr radius. We show that to obtain the exact small- $T$  behavior one should note that the frequency summation also gives a  $T^2$  dependence.<sup>9</sup>

In Sec. II, the calculations of the RPA correlation energy are given at both  $T=0$  and  $T \neq 0$ . In Sec. III, the zero-temperature piece is compared with the previous calculations, and the temperature corrections are obtained and compared with those by IK. The coefficients of  $t^2$  of the correlation energy and its derivatives are considered, where  $t$  will be defined below. In the Appendices, the comment on the RPA correlation energy [Eq. (8)] and another formula using the structure factor  $S(q)$  is given, and the detailed calculations related to Secs. II and III are given.

## II. CALCULATIONS

Letting

$$i(\mathbf{q}, iq_n) = \ln[1 - v_{\mathbf{q}} P_0(\mathbf{q}, iq_n)] + v_{\mathbf{q}} P_0(\mathbf{q}, iq_n), \quad (9)$$

we consider the following decompositions by the Sommerfeld expansion

$$P_0(\mathbf{q}, iq_n) = P_0^{(0)}(\mathbf{q}, iq_n) + t^2 P_0^{(1)}(\mathbf{q}, iq_n), \quad (10)$$

$$i(\mathbf{q}, iq_n) = i^{(0)}(\mathbf{q}, iq_n) + t^2 i^{(1)}(\mathbf{q}, iq_n), \quad (11)$$

where  $t$  is the normalized temperature to the Fermi energy  $\mu^0 = \hbar^2 k_F^2/2m$ ,

$$t = k_B T / \mu^0. \quad (12)$$

Then we obtain  $i^{(0)}$  and  $i^{(1)}$  in terms of  $P_0^{(0)}$  and  $P_0^{(1)}$ ,

$$i^{(0)}(\mathbf{q}, iq_n) = \ln[1 - v_{\mathbf{q}} P_0^{(0)}] + v_{\mathbf{q}} P_0^{(0)}, \quad (13)$$

$$i^{(1)}(\mathbf{q}, iq_n) = \frac{-v_{\mathbf{q}}^2 P_0^{(0)} P_0^{(1)}}{1 - v_{\mathbf{q}} P_0^{(0)}}, \quad (14)$$

where the detailed forms of  $P_0^{(0)}$  and  $P_0^{(1)}$  are given in Appendix B. There,  $i\omega$  is used instead of  $iq_n$ . Note that since  $P_0(\mathbf{q}, iq_n)$  is a symmetric function of frequency, we have  $i^{(0)}(\mathbf{q}, -iq_n) = i^{(0)}(\mathbf{q}, iq_n)$  and  $i^{(1)}(\mathbf{q}, -iq_n) = i^{(1)}(\mathbf{q}, iq_n)$ .

If we just change the frequency summation into the frequency integration, we obtain

$$\Omega_r = \frac{1}{2} \sum_{\mathbf{q}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} [i^{(0)}(\mathbf{q}, i\omega) + t^2 i^{(1)}(\mathbf{q}, i\omega)], \quad (15)$$

where the second term is the temperature correction. This correlation energy  $\Omega_r$  was calculated by IK.<sup>7</sup> However, when changing the frequency summation into the integration, there is another important temperature correction term, which they neglected and will be considered below. They calculated Eq. (15) in a little different form: Equation (8) was their starting point. They evaluated

Eq. (8), (i) by expressing the logarithm in a power series, and applying the Mellin transformation to the power series, (ii) by applying the Sommerfeld expansion to the RPA polarization and expressing  $P_0^{(0)}$  and  $P_0^{(1)}$  to the order of  $(q/k_F)^4$ , and after that, (iii) by changing the frequency summation to the frequency integral by assuming its temperature correction to be small. Thus they obtained their results to the order of  $T^2$  in a series in  $r_s$ .

Here we will evaluate Eq. (15) directly without expanding  $P_0^{(0)}$  and  $P_0^{(1)}$ , and furthermore, evaluate another temperature correction coming when the frequency summation is changed into the frequency integral. The latter is the main aim of this paper. To get the correction term we let

$$\mathcal{I}(\mathbf{q}) \equiv \frac{1}{\beta} \sum_{iq_n} i(\mathbf{q}, iq_n), \quad (16)$$

$$i(\mathbf{q}, iq_n) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{I(\mathbf{q}, \omega)}{iq_n - \omega}, \quad (17)$$

where  $I(\mathbf{q}, \omega)$  is the spectral function of  $i(\mathbf{q}, iq_n)$ ,

$$I(\mathbf{q}, \omega) = -2\Im i_{\text{ret}}(\mathbf{q}, \omega), \quad (18)$$

$$i_{\text{ret}}(\mathbf{q}, \omega) = i(\mathbf{q}, iq_n)|_{iq_n \rightarrow \omega + i\delta}. \quad (19)$$

Here we have the summation  $\frac{1}{\beta} \sum_{iq_n} \frac{1}{iq_n - \omega}$ , which is equal to  $-[n_B(\omega) + 1/2]$ , where  $n_B(\omega)$  is the Bose function  $1/[e^{\beta\omega} - 1]$ . Then

$$\begin{aligned} \mathcal{I}(\mathbf{q}) &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} I(\mathbf{q}, \omega) \frac{1}{\beta} \sum_{iq_n} \frac{1}{iq_n - \omega} \\ &= - \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} I(\mathbf{q}, \omega) [n_B(\omega) + 1/2] \\ &= - \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} I(\mathbf{q}, \omega) n_B(\omega) \\ &= - \int_0^{\infty} \frac{d\omega}{2\pi} I(\mathbf{q}, \omega) [2n_B(\omega) + 1], \end{aligned} \quad (20)$$

where the third and fourth lines were obtained by using the relation  $I(\mathbf{q}, -\omega) = -I(\mathbf{q}, \omega)$ ,<sup>10</sup> which can be confirmed at  $T=0$  by doing direct calculations using the relation  $\varepsilon_2(\mathbf{q}, -\omega) = -\varepsilon_2(\mathbf{q}, \omega)$ , where  $\varepsilon_2(\mathbf{q}, \omega)$  is the imaginary part of the RPA retarded dielectric function at  $T=0$ . Thus we obtain for  $\Omega_r = \frac{1}{2} \sum_{\mathbf{q}} \mathcal{I}(\mathbf{q})$

$$\Omega_r = -\frac{1}{2} \sum_{\mathbf{q}} \int_0^{\infty} \frac{d\omega}{2\pi} I(\mathbf{q}, \omega) - \sum_{\mathbf{q}} \int_0^{\infty} \frac{d\omega}{2\pi} I(\mathbf{q}, \omega) n_B(\omega). \quad (21)$$

This result can be also obtained by using the relation  $I(\mathbf{q}, -\omega) = -I(\mathbf{q}, \omega)$  before doing the frequency summation. Using this relation, we have

$$i(\mathbf{q}, iq_n) = \int_0^{\infty} \frac{d\omega}{2\pi} \frac{2\omega I(\mathbf{q}, \omega)}{(iq_n)^2 - \omega^2}, \quad (22)$$

and thus

$$\begin{aligned} \mathcal{I}(\mathbf{q}) &= \int_0^\infty \frac{d\omega}{2\pi} 2\omega I(\mathbf{q}, \omega) \frac{1}{\beta} \sum_{iq_n} \frac{1}{(iq_n)^2 - \omega^2} \\ &= - \int_0^\infty \frac{d\omega}{2\pi} I(\mathbf{q}, \omega) [2n_B(\omega) + 1], \end{aligned} \quad (23)$$

where we used  $\frac{1}{\beta} \sum_{iq_n} \frac{1}{(iq_n)^2 - \omega^2} = \frac{-1}{2\omega} [2n_B(\omega) + 1]$ . This is the same as Eq. (20).

Note that the first term in Eq. (21) is the same as two terms in Eq. (15) and its second term is a new correction term, which will be shown to be  $O(T^2)$  below. Considering the decomposition

$$I(\mathbf{q}, \omega) = I^{(0)}(\mathbf{q}, \omega) + t^2 I^{(1)}(\mathbf{q}, \omega), \quad (24)$$

we replace  $I(\mathbf{q}, \omega)$  by  $I^{(0)}(\mathbf{q}, \omega)$  to the order of  $T^2$  in the second term in Eq. (21). In summary, we obtain at zero temperature

$$\Omega_r^{(0)} = \sum_{\mathbf{q}} \int_0^\infty \frac{d\omega}{2\pi} i^{(0)}(\mathbf{q}, i\omega), \quad (25)$$

which was evaluated previously using another formula containing the structure factor  $S(q)$ . The comment on the relation between Eq. (25), i.e., the  $T=0$  limit of Eq. (8), and the formula containing  $S(q)$  is given in Appendix A. The temperature corrections to the order of  $T^2$  are given by

$$\Omega_r^{(1)} = \Omega_{r,1}^{(1)} + \Omega_{r,2}^{(1)}, \quad (26)$$

$$\Omega_{r,1}^{(1)} = t^2 \sum_{\mathbf{q}} \int_0^\infty \frac{d\omega}{2\pi} i^{(1)}(\mathbf{q}, i\omega), \quad (27)$$

$$\Omega_{r,2}^{(1)} = - \sum_{\mathbf{q}} \int_0^\infty \frac{d\omega}{2\pi} I^{(0)}(\mathbf{q}, \omega) n_B(\omega). \quad (28)$$

In obtaining Eqs. (25) and (27) from Eq. (15), we used the fact that  $i^{(0)}(\mathbf{q}, i\omega)$  and  $i^{(1)}(\mathbf{q}, i\omega)$  are even functions of frequency.

Now we show that  $\Omega_{r,2}^{(1)}$  also gives  $\beta^{-2}$  (i.e.,  $t^2$ ) dependence. Let

$$A(\mathbf{q}) = \int_0^\infty \frac{d\omega}{2\pi} I^{(0)}(\mathbf{q}, \omega) n_B(\omega). \quad (29)$$

By partial integration, we obtain

$$\begin{aligned} A(\mathbf{q}) &= - \int_0^\infty \frac{d\omega}{2\pi} \frac{dI^{(0)}}{d\omega} \frac{1}{\beta} \ln |1 - e^{-\beta\omega}| \\ &= - \frac{1}{\beta^2} \int_0^\infty \frac{dx}{2\pi} \frac{dI^{(0)}}{d\omega} \Big|_{\omega=x/\beta} \ln |1 - e^{-x}|. \end{aligned} \quad (30)$$

Thus we find  $\beta^{-2}$  dependence, if  $\frac{dI^{(0)}}{d\omega} \Big|_{\omega=x/\beta}$  is of  $O(\beta^{-n})$ ,  $n$  being zero or a positive integer. Note that the integrand  $\ln |1 - e^{-x}|$  in Eq. (30) has a dominant contribution around  $x \sim 0$ , so we may consider only the small- $x$  region. Roughly speaking, since  $I^{(0)}(\mathbf{q}, -\omega) = -I^{(0)}(\mathbf{q}, \omega)$ , we can set  $I^{(0)}(\mathbf{q}, \omega) \sim g(\mathbf{q})\omega$  for the small- $\omega$  region, and then  $\frac{dI^{(0)}}{d\omega} \sim g(\mathbf{q})$ . Thus  $A(\mathbf{q}) \sim \beta^{-2}g(\mathbf{q})$ . However, a detailed calculation will show that when

$\frac{dI^{(0)}}{d\omega} \Big|_{\omega=x/\beta}$  is integrated over  $q$ , it gives a  $t^2 \ln t$  dependence in addition to a  $t^2$  dependence.

Consider the RPA retarded dielectric function  $\varepsilon_{\text{RPA}}(\mathbf{q}, \omega) = \varepsilon_{\text{ret}}(\mathbf{q}, \omega)$  at  $T=0$ . The retarded function is obtained by taking the analytical continuation  $iq_n \rightarrow \omega + i\delta$ . From the definition

$$\begin{aligned} \varepsilon_{\text{RPA}}(\mathbf{q}, \omega) &= 1 - v_{\mathbf{q}} P_{0,\text{ret}}^{(0)}(\mathbf{q}, \omega) \\ &= \varepsilon_1(\mathbf{q}, \omega) + i\varepsilon_2(\mathbf{q}, \omega), \end{aligned} \quad (31)$$

where  $P_{0,\text{ret}}^{(0)}(\mathbf{q}, \omega) = P_0^{(0)}(q, iq_n)|_{iq_n \rightarrow \omega + i\delta}$ , and  $\varepsilon_1$  and  $\varepsilon_2$  are the real and imaginary parts of  $\varepsilon_{\text{RPA}}(\mathbf{q}, \omega)$ , respectively, then  $I^{(0)}$  is given by

$$I^{(0)} = -2\Im i_{\text{ret}}^{(0)} = -2\Im [\ln(\varepsilon_1 + i\varepsilon_2) + 1 - \varepsilon_1 - i\varepsilon_2], \quad (32)$$

where the detailed forms of  $\varepsilon_1$  and  $\varepsilon_2$  are given in Appendix B. Exchanging the orders of differentiation and taking the imaginary part, we obtain for  $\frac{dI^{(0)}}{d\omega}$

$$\frac{dI^{(0)}}{d\omega} = \frac{-2}{\varepsilon_1^2 + \varepsilon_2^2} \left[ -\frac{d\varepsilon_1}{d\omega} \varepsilon_2 + \frac{d\varepsilon_2}{d\omega} [\varepsilon_1(1 - \varepsilon_1) - \varepsilon_2^2] \right]. \quad (33)$$

In the above expression of  $\frac{dI^{(0)}}{d\omega}$ , we see that terms having  $\omega^n$ ,  $n$  being a positive integer, contribute to higher orders than  $T^2$  when  $\omega$  is replaced by  $\omega = x/\beta$ . So, to the order of  $T^2$ , we may put 0 instead of  $x/\beta$  in the limit of  $\beta \rightarrow \infty$ . In this limit we see that the main contribution comes from  $\frac{dI^{(0)}}{d\omega} = -2\frac{d\varepsilon_2}{d\omega} \frac{1 - \varepsilon_1}{\varepsilon_1}$  in the limit of  $\beta \rightarrow \infty$  with  $\omega = x/\beta$ .

If we would just take the  $\beta \rightarrow \infty$  limit in  $\frac{dI^{(0)}}{d\omega} \Big|_{\omega=x/\beta}$ , we would find that it is independent of  $x$ , and would obtain

$$\begin{aligned} \Omega_{r,2}^{(1)} &= - \sum_{\mathbf{q}} A(\mathbf{q}) \\ &= \frac{1}{\beta^2} \sum_{\mathbf{q}} \int_0^\infty \frac{dx}{2\pi} \frac{dI^{(0)}}{d\omega} \Big|_{\omega=x/\beta=0} \ln |1 - e^{-x}| \\ &= \frac{-2}{\beta^2} \sum_{\mathbf{q}} \frac{d\varepsilon_2}{d\omega} \Big|_{\omega=0} \frac{1 - \tilde{\varepsilon}_1}{\tilde{\varepsilon}_1} \int_0^\infty \frac{dx}{2\pi} \ln |1 - e^{-x}|, \end{aligned} \quad (34)$$

where  $\tilde{\varepsilon}_1 = \varepsilon_1(\mathbf{q}, \omega = 0)$ . Using  $\int_0^\infty dx \ln |1 - e^{-x}| = -\frac{\pi^2}{6}$  and the relation (B14) of  $\frac{d\varepsilon_2}{d\omega} \Big|_{\omega=0}$  in Appendix B, we would obtain

$$\Omega_{r,2}^{(1)} = t^2 \frac{k_F^4 e^2}{24\pi} \int_0^{2k_F} \frac{dq}{q} \frac{1 - \tilde{\varepsilon}_1}{\tilde{\varepsilon}_1}. \quad (35)$$

The  $q \rightarrow 0$  limit gives  $(1 - \tilde{\varepsilon}_1)/\tilde{\varepsilon}_1 \rightarrow -1$ . Thus the integral in the above expression becomes divergent for  $q \rightarrow 0$ . This is an undesirable and wrong result. This happened because we considered the  $x$ -independent  $\frac{dI^{(0)}}{d\omega} \Big|_{\omega=x/\beta=0}$  by using the relation (B14) for  $\frac{d\varepsilon_2}{d\omega} \Big|_{\omega=0}$ . To avoid this divergence, we turn to the expression (B15): That is,

as before, we will take the limit  $\beta \rightarrow \infty$  of  $\frac{dI^{(0)}}{d\omega}\Big|_{\omega=x/\beta}$ , except for the most dominant term containing the expression (B15)

$$\frac{d\varepsilon_2}{d\omega}\Big|_{\omega=x/\beta} = \frac{2e^2 m^2}{q^3} \theta(2k_F - q) \theta(-Y - x/\beta), \quad (36)$$

where  $Y = \varepsilon_{\mathbf{q}} + qv_F$ , and the theta functions restrict the integral range over  $q$  to  $\frac{m\pi}{k_F\beta} < q < 2k_F$ . Then

$$\begin{aligned} \Omega_{r,2}^{(1)} &= \frac{-2}{\beta^2} \int_0^\infty \frac{dx}{2\pi} \ln|1 - e^{-x}| \sum_{\mathbf{q}} \frac{d\varepsilon_2}{d\omega}\Big|_{\omega=x/\beta} \frac{1 - \tilde{\varepsilon}_1}{\tilde{\varepsilon}_1} \\ &= -t^2 \frac{\nu e^2 k_F^4}{2\pi^2} \int_0^\infty \frac{dx}{2\pi} \ln|1 - e^{-x}| \int_{\frac{m\pi}{k_F\beta}}^{2k_F} \frac{dq}{q} \frac{1 - \varepsilon_1}{\varepsilon_1}. \end{aligned} \quad (37)$$

Considering the  $q \rightarrow 0$  limit, we obtain for the  $q$  integration

$$\int_{\frac{m\pi}{k_F\beta}}^{2k_F} \frac{dq}{q} (-1) = \ln(xt/4). \quad (38)$$

Extracting only the term containing  $t^2 \ln t$ , we obtain

$$-t^2 \frac{\nu e^2 k_F^4}{2\pi^2} \int_0^\infty \frac{dx}{2\pi} \ln|1 - e^{-x}| \ln t = \frac{\nu e^2 k_F^4}{4\pi^3} \frac{\pi^2}{6} t^2 \ln t. \quad (39)$$

We now see that this  $t^2 \ln t$  dependence gave the divergence in Eq. (35) when  $q \rightarrow 0$ . Note that the exchange energy is given by<sup>2</sup>

$$\Omega_x = -\frac{\nu e^2 k_F^4}{4\pi^3} \left( 1 + \frac{\pi^2}{6} t^2 \ln t + At^2 \right), \quad (40)$$

where  $A = -0.877525$ . It is very interesting to note that the  $t^2 \ln t$  term in the exchange energy is exactly canceled out by the  $t^2 \ln t$  term from the correlation energy shown in Eq. (39). This cancellation has been expected by the argument that if the screening effects are included, the singularity from the Fermi surface becomes smoothed out, and thus the logarithmic dependence in the exchange energy disappears.

Now we evaluate the temperature dependence of  $\Omega_{r,2}^{(1)}$  using

$$\begin{aligned} \int_{\frac{m\pi}{k_F\beta}}^{2k_F} \frac{dq}{q} \frac{1 - \tilde{\varepsilon}_1}{\tilde{\varepsilon}_1} &= -\int_{\frac{m\pi}{k_F\beta}}^{2k_F} \frac{dq}{q} + \int_{\frac{m\pi}{k_F\beta}}^{2k_F} \frac{dq}{q} \frac{1}{\tilde{\varepsilon}_1} \\ &\approx -\int_{\frac{m\pi}{k_F\beta}}^{2k_F} \frac{dq}{q} + \int_0^{2k_F} \frac{dq}{q} \frac{1}{\tilde{\varepsilon}_1}, \end{aligned} \quad (41)$$

where the second term, which will be denoted as  $J$ , does not contain any divergence when  $q \rightarrow 0$ . Thus we obtain

$$\begin{aligned} \Omega_{r,2}^{(1)} &= -\frac{\nu e^2 k_F^4}{2\pi^2} t^2 \int_0^\infty \frac{dx}{2\pi} \ln|1 - e^{-x}| [\ln(xt/4) + J] \\ &= \frac{\nu e^2 k_F^4}{24\pi} \left[ t^2 \ln t + t^2 \left( J - 2 \ln 2 - \frac{6}{\pi^2} C \right) \right] \\ &= \frac{\nu e^2 k_F^4}{24\pi} [t^2 \ln t + t^2 (J - 2.53347)], \end{aligned} \quad (42)$$

where we used  $C = \int_0^\infty \frac{dx}{2\pi} \ln|1 - e^{-x}| \ln x = 1.88703$ . Note that the temperature correction when the frequency summation is changed into the frequency integral is not small. This procedure to obtain the temperature dependence can be used in other problems containing the frequency summations.

Note that there is another term giving  $t^2$  dependence, which comes from the temperature dependence of the chemical potential  $\mu$ :  $\mu = \mu^0 (1 - \frac{\pi^2}{12} t^2)$ . Letting  $K_F^2 = 2m\mu$  and  $k_F^2 = 2m\mu^0$ , we have  $K_F = k_F (1 - \frac{\pi^2}{6} t^2)$ . If we decompose

$$P_0^{(0)}(\mathbf{q}, i\omega; K_F) = \bar{P}_0^{(0)}(\mathbf{q}, i\omega; k_F) + t^2 \bar{P}_{0,1}^{(0)}(\mathbf{q}, i\omega; k_F), \quad (43)$$

where  $P_0^{(0)}(\mathbf{q}, i\omega; K_F)$  is the same as Eq. (B2) with the replacement of  $k_F$  by  $K_F$ , so  $\bar{P}_0^{(0)}$  is the same as Eq. (B2) and the form of  $\bar{P}_{0,1}^{(0)}$  is given in Appendix B. Similarly, we obtain

$$i^{(0)}(\mathbf{q}, i\omega; K_F) = i_0^{(0)}(\mathbf{q}, i\omega; k_F) + t^2 i_1^{(0)}(\mathbf{q}, i\omega; k_F), \quad (44)$$

where  $i^{(0)}(\mathbf{q}, i\omega; K_F)$  is the same as Eq. (13) with  $K_F$ , and

$$i_0^{(0)} = \ln[1 - v_{\mathbf{q}} \bar{P}_0^{(0)}] + v_{\mathbf{q}} \bar{P}_0^{(0)}, \quad (45)$$

$$i_1^{(0)} = -\frac{v_{\mathbf{q}}^2 \bar{P}_0^{(0)} \bar{P}_{0,1}^{(0)}}{1 - v_{\mathbf{q}} \bar{P}_0^{(0)}}. \quad (46)$$

We denote the contribution of  $i_1^{(0)}$  to the  $t^2$  corrections by  $\Omega_{r,3}^{(1)}$

$$\Omega_{r,3}^{(1)} = t^2 \sum_{\mathbf{q}} \int_0^\infty \frac{d\omega}{2\pi} i_1^{(0)}(\mathbf{q}, i\omega). \quad (47)$$

Now we summarize the formulas for numerical calculations in units of  $N \times \text{Rydberg} = N \frac{e^2}{2a_B}$ , where  $N$  is the number of electrons. With  $z = q/k_F$  and  $\tilde{\omega} = \omega/\mu^0$ ,

$$\Omega_r^{(0)} = \frac{3}{4\pi^3} \frac{1}{\alpha^2} \int_0^\infty z^2 dz \int_0^\infty d\tilde{\omega} i^{(0)}(z, \tilde{\omega}), \quad (48)$$

$$\Omega_{r,1}^{(1)} = t^2 \frac{3}{4\pi^3} \frac{1}{\alpha^2} \int_0^\infty z^2 dz \int_0^\infty d\tilde{\omega} i^{(1)}(z, \tilde{\omega}), \quad (49)$$

$$\Omega_{r,2}^{(1)} = \frac{1}{4\alpha} t^2 \ln t + \frac{t^2}{4\alpha} \left[ \int_0^2 \frac{dz}{z} \frac{1}{\tilde{\varepsilon}_1(z)} - 2.53347 \right], \quad (50)$$

$$\Omega_{r,3}^{(1)} = t^2 \frac{3}{2\pi^3} \frac{1}{\alpha^2} \int_0^\infty z^2 dz \int_0^\infty d\tilde{\omega} i_1^{(0)}(z, \tilde{\omega}), \quad (51)$$

where

$$\alpha = \frac{1}{\pi a_B k_F} = \frac{r_s}{(9\pi^4/4)^{1/3}} = \frac{r_s}{6.029}. \quad (52)$$

Here we will denote the coefficients of  $t^2$  in Eqs. (49)–(51) as  $C_{r,1}$ ,  $C_{r,2}$ , and  $C_{r,3}$ , respectively. Then the temperature correction  $\Omega_r^{(1)}$  is written as

$$\Omega_r^{(1)} = \frac{1}{4\alpha} t^2 \ln t + (C_{r,1} + C_{r,2} + C_{r,3}) t^2. \quad (53)$$

### III. RESULTS AND DISCUSSION

For comparison, we summarize the results by IK in their notations: With  $\beta\Omega_r = -\ln \Xi_r$

$$\ln \Xi_r = \frac{\nu\beta p_F^2 e^4}{2\pi^5} \{C_1(\xi) - a_{11}(2) \ln \Lambda + O(e^2)\} - \frac{\pi^2}{12\eta^2} [C_2(\xi) + a_{21} \ln \Lambda + O(e^2)] + \dots, \quad (54)$$

where  $\eta = t$ , and they used  $2m \equiv 1$ , and  $\Lambda = \frac{2e^2}{\pi p_F}$ . They used the parameter  $\xi$  as cutoff in integration over  $q$ , and let  $\xi = 1, 2$ , and so obtained  $C_1(1) = 0.27325$ ,  $C_1(2) = 0.53873$ ,  $C_2(1) = 0.07169$ ,  $C_2(2) = 0.49229$ ,  $a_{11}(2) = \frac{\pi}{3}(1 - \ln 2)$ , and  $a_{21} = \frac{\pi}{4}(1 - \ln 4)$ . In units of  $N \times \text{Rydberg}$ , their results are given by

$$\Omega_r = \frac{2}{\pi^2} (1 - \ln 2) \ln r_s - D_1(\xi) + \frac{t^2}{8} [(1 - \ln 4) \ln r_s + D_2(\xi)], \quad (55)$$

where  $\frac{2}{\pi^2}(1 - \ln 2) = 0.0622$ , and

$$D_1(\xi) = -\frac{6}{\pi^3} C_1(\xi) + \frac{2}{\pi^2} (1 - \ln 2) \ln(4\alpha/r_s), \quad (56)$$

$$D_2(\xi) = \frac{4}{\pi} C_2(\xi) + (1 - \ln 4) \ln(4\alpha/r_s). \quad (57)$$

Our results are compared with those by IK. They considered two cases depending on the values of  $\xi$ . The results corresponding to  $\xi = 1, 2$  are denoted as “IK1” and “IK2”, respectively, in Figs. 1 and 2.

In Fig. 1, we plot the results obtained by Eq. (48) (dashed line), and Eq. (A14) (line with circles), along with those by IK (dotted and dot-dashed lines). Equation (48) is the  $T=0$  limit of Eq. (8). The data of circles come from Ref. 11. Our result using Eq. (48) is exactly the same as using Eq. (A14), the formula containing the structure factor  $S(q)$ . Note that the comment on these two formulas [Eqs. (8) and (A14)] is given in Appendix A. The result “IK2” (dot-dashed) is closer to our result than is “IK1” (dotted).

The coefficient  $C_{r,1}$  of  $t^2$  in  $\Omega_{r,1}^{(1)}$  [Eq. (49)] is compared with results of IK (dotted and dot-dashed lines) in Fig. 2. Only this coefficient can be compared since they calculated only the coefficient for temperature corrections.

The temperature corrections given by Eqs. (49)–(51) are given in Fig. 3. There, the coefficients of  $t^2$  in

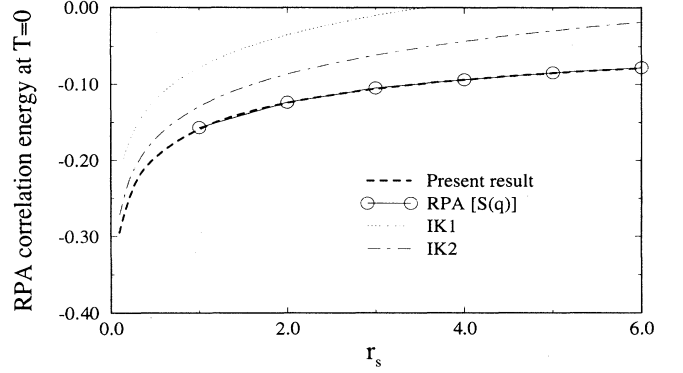


FIG. 1. Plot of Eqs. (48) and (A14) as a function of  $r_s$ , along with those by IK. The dashed line represents our result using Eq. (48), and the line with circles is obtained by Eq. (A14), while the results by IK are given by dotted and dot-dashed lines. Our result is exactly the same as those using the formula containing  $S(q)$ .

Eqs. (49)–(51) are shown as the dotted, dot-dashed, and dashed lines, respectively. Their sum  $C_r = C_{r,1} + C_{r,2} + C_{r,3}$  is also shown as the solid line. These coefficients were evaluated numerically. Note that two other results (dot-dashed and dashed lines) are much larger, compared with the dotted line, which was shown as a dashed line in Fig. 2. Especially, it is interesting to note that the result represented by the dot-dashed line, which IK assumed to be small, is quite big.

We consider the coefficient  $C_E(r_s)$  of  $t^2$  in the exchange-correlation energy  $\Omega_{xc}$ :

$$\Omega_{xc} = \Omega_{xc}^{(0)} [1 + C_E(r_s) t^2 + \dots], \quad (58)$$

$$\Omega_{xc}^{(0)} = \Omega_x^{(0)} + \Omega_r^{(0)}, \quad (59)$$

where  $\Omega_r^{(0)}$  is given by Eq. (48). Considering the exchange energy Eq. (40) in units of  $N \times \text{Rydberg}$

$$\Omega_x = -\frac{1}{4\alpha} t^2 \ln t - \frac{3}{2\pi^2 \alpha} (1 + At^2), \quad (60)$$

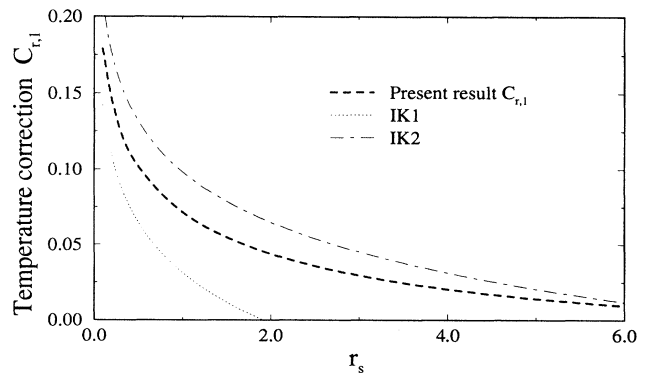


FIG. 2. Plot of the coefficient  $C_{r,1}$  of  $t^2$  in Eq. (49), as a function of  $r_s$ , along with the corresponding result by IK.

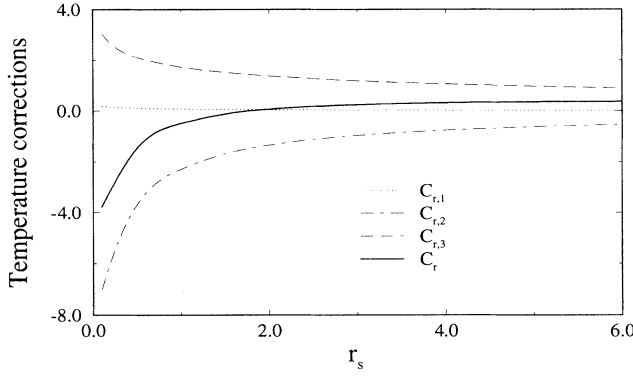


FIG. 3. Plot of the coefficients of  $t^2$  in  $\Omega_r^{(1)}$  [Eqs. (49)–(51)]. The dotted, dot-dashed, and dashed lines correspond to  $C_{r,1}$ ,  $C_{r,2}$ , and  $C_{r,3}$ , respectively. The solid line represents the sum  $C_r$  of three coefficients.

then we obtain  $\Omega_x^{(0)} = -\frac{3}{2\pi^2\alpha} = -\frac{0.9163}{r_s}$ . Thus  $C_E(r_s)$  is given by

$$C_E(r_s) = \frac{A + C_r/\Omega_x^{(0)}}{1 + \Omega_r^{(0)}/\Omega_x^{(0)}}. \quad (61)$$

The coefficient  $C_E(r_s)$  is shown in Fig. 4 as a function of  $r_s$ , along with two ratios,  $\Omega_r^{(0)}/\Omega_x^{(0)}$  and  $C_r/\Omega_x^{(0)}$ . As  $r_s \rightarrow 0$ ,  $\Omega_x^{(0)}$  becomes dominant, the two ratios will go to zero, and thus  $C_E(r_s)$  will approach  $A = -0.877525$ .

Finally, the exchange-correlation potential  $V_{xc}$  and the “interaction function”  $K_{xc}$  are considered, which appears in the calculation of response functions.<sup>13</sup> Here we wish to find the coefficients  $C_V(r_s)$ ,  $C_K(r_s)$  of  $t^2$  in  $V_{xc}$  and  $K_{xc}$ , respectively: With the exchange-correlation energy per volume  $E_{xc} = \Omega_{xc}/\nu$ , we obtain

$$V_{xc} = \frac{dE_{xc}}{dn} = V_{xc}^{(0)}[1 + C_V(r_s)t^2 + \dots], \quad (62)$$

$$V_{xc}^{(0)} = V_x^{(0)} + V_r^{(0)}, \quad (63)$$

$$K_{xc} = \frac{d^2E_{xc}}{dn^2} = K_{xc}^{(0)}[1 + C_K(r_s)t^2 + \dots], \quad (64)$$

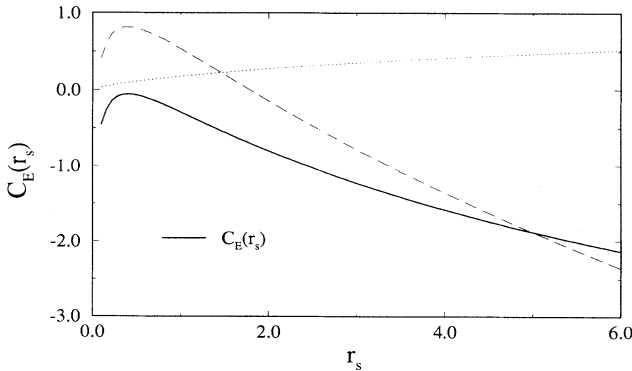


FIG. 4. Plot of the coefficient  $C_E(r_s)$  of  $t^2$  in the exchange-correlation energy  $\Omega_{xc}$  as a function of  $r_s$ . The solid line represents  $C_E(r_s)$ , while the dotted and dashed lines represent  $\Omega_r^{(0)}/\Omega_x^{(0)}$  and  $C_r/\Omega_x^{(0)}$ , respectively.

$$K_{xc}^{(0)} = K_x^{(0)} + K_r^{(0)}. \quad (65)$$

The exchange pieces were previously obtained:

$$V_x^{(0)} = -e^2 k_F / \pi, \quad (66)$$

$$K_x^{(0)} = -e^2 \pi / k_F^2. \quad (67)$$

Using these values as the normalization factors, we obtain for the coefficients

$$C_V(r_s) = \frac{V_r^{(1)}/V_x^{(0)}}{1 + V_r^{(0)}/V_x^{(0)}}, \quad (68)$$

$$C_K(r_s) = \frac{K_r^{(1)}/K_x^{(0)}}{1 + K_r^{(0)}/K_x^{(0)}}, \quad (69)$$

where  $V_r^{(1)}$ ,  $K_r^{(1)}$  are coefficients of  $t^2$  in  $V_r$ ,  $K_r$ , respectively:

$$V_r = \frac{d\tilde{E}_r}{dn} = V_r^{(0)} + V_r^{(1)}t^2, \quad (70)$$

$$K_r = \frac{d^2\tilde{E}_r}{dn^2} = K_r^{(0)} + K_r^{(1)}t^2, \quad (71)$$

where  $\tilde{E}_r = [\Omega_r^{(0)} + C_r t^2]/\nu$  is the correlation part of  $E_{xc}$ . In Appendix B, the detailed forms of  $V_r^{(0)}$ ,  $V_r^{(1)}$ ,  $K_r^{(0)}$ , and  $K_r^{(1)}$  are given. The behavior of  $C_V(r_s)$  and  $C_K(r_s)$  is shown in Figs. 5 and 6, respectively.

In conclusion, we calculated the RPA correlation energy at both  $T=0$  and  $T \neq 0$ . The zero-temperature result was compared with the previous ones. For nonzero temperatures, we found that a temperature correction [Eq. (50)], which was assumed small by IK, is actually large. It has a  $t^2 \ln t$  correction and also a very large coefficient of  $t^2$ , compared with the coefficient IK calculated. The  $t^2 \ln t$  correction in the RPA correlation energy was found to cancel out the corresponding term in the exchange energy. From the calculation of correlation energy, we evaluated the exact coefficient of  $t^2$  in the exchange-correlation energy, and also obtained the coefficients of  $t^2$  in  $V_{xc}$  and  $K_{xc}$ .

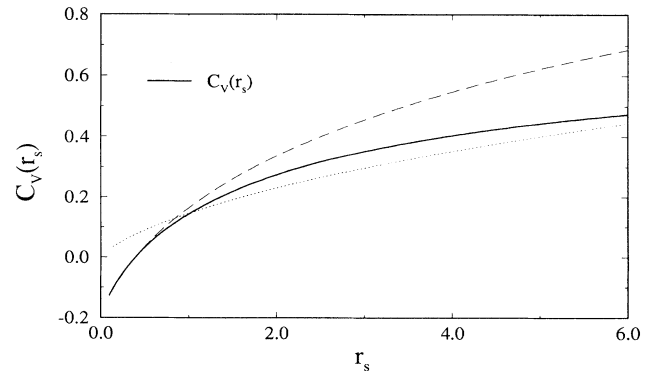


FIG. 5. Plot of the coefficient  $C_V(r_s)$  of  $t^2$  in  $V_{xc}$  as a function of  $r_s$ . The solid line represents  $C_V(r_s)$ , while the dotted and dashed lines represent  $V_r^{(0)}/V_x^{(0)}$  and  $V_r^{(1)}/V_x^{(0)}$ , respectively.

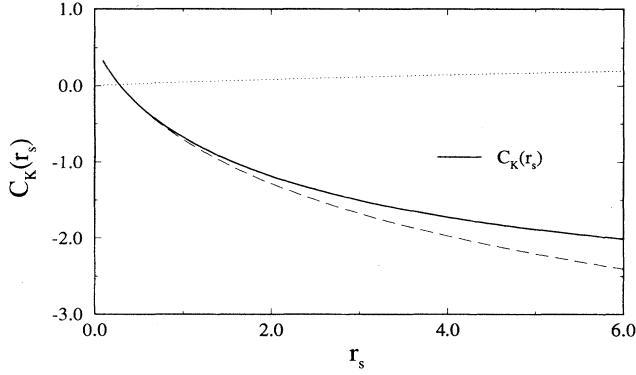


FIG. 6. Plot of the coefficient  $C_K(r_s)$  of  $t^2$  in  $K_{xc}$  as a function of  $r_s$ . The solid line represents  $C_K(r_s)$ , while the dotted and dashed lines represent  $K_r^{(0)}/K_x^{(0)}$  and  $K_r^{(1)}/K_x^{(0)}$ , respectively.

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### APPENDIX A: NOTE ON THE EXCHANGE-CORRELATION ENERGY

The exchange-correlation energy is given by

$$\begin{aligned} \Omega_{xc} &= \frac{1}{2\beta} \sum_{\mathbf{q}, iq_n} \ln[1 - v_{\mathbf{q}} P_0(\mathbf{q}, iq_n)] \\ &= - \int_0^1 \frac{d\eta}{\eta} \frac{1}{2\beta} \sum_{\mathbf{q}, iq_n} \frac{\eta v_{\mathbf{q}} P_0(\mathbf{q}, iq_n)}{1 - \eta v_{\mathbf{q}} P_0(\mathbf{q}, iq_n)} \\ &= - \int_0^1 \frac{d\eta}{\eta} \frac{1}{2\beta} \sum_{\mathbf{q}, iq_n} \left[ \frac{1}{\varepsilon_{\eta}(\mathbf{q}, iq_n)} - 1 \right], \end{aligned} \quad (\text{A1})$$

where  $\varepsilon_{\eta}(\mathbf{q}, iq_n) = 1 - \eta v_{\mathbf{q}} P_0(\mathbf{q}, iq_n)$ . Letting

$$h(\mathbf{q}, iq_n) = \frac{1}{\varepsilon_{\eta}(\mathbf{q}, iq_n)} - 1, \quad (\text{A2})$$

$$H(\mathbf{q}, \omega) = -2\mathfrak{S}h_{\text{ret}}(\mathbf{q}, \omega), \quad (\text{A3})$$

then

$$\Omega_{xc} = - \int_0^1 \frac{d\eta}{\eta} \frac{1}{2\beta} \sum_{\mathbf{q}, iq_n} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{H(\mathbf{q}, \omega)}{iq_n - \omega}. \quad (\text{A4})$$

Since  $H(k, -\omega) = -H(k, \omega)$ , we have

$$\begin{aligned} \frac{-1}{\beta} \sum_{iq_n} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{H(\mathbf{q}, \omega)}{iq_n - \omega} &= \frac{-1}{\beta} \sum_{iq_n} \int_0^{\infty} \frac{d\omega}{2\pi} \frac{2\omega H(\mathbf{q}, \omega)}{(iq_n)^2 - \omega^2} \\ &= \int_0^{\infty} \frac{d\omega}{2\pi} H(\mathbf{q}, \omega) [2n_B(\omega) + 1] \\ &\rightarrow \int_0^{\infty} \frac{d\omega}{2\pi} H(\mathbf{q}, \omega), \end{aligned} \quad (\text{A5})$$

where the last line was obtained when  $T \rightarrow 0$ . Then the exchange-correlation energy is at  $T=0$

$$\begin{aligned} \Omega_{xc} &= \frac{1}{2} \int_0^1 \frac{d\eta}{\eta} \sum_{\mathbf{q}} \int_0^{\infty} \frac{d\omega}{2\pi} H(\mathbf{q}, \omega) \\ &= - \frac{1}{2} \int_0^1 \frac{d\eta}{\eta} \sum_{\mathbf{q}} \int_0^{\infty} \frac{d\omega}{\pi} \mathfrak{S} \left[ \frac{1}{\varepsilon_{\eta, \text{ret}}(\mathbf{q}, \omega)} \right] \\ &= \frac{1}{2} \int_0^1 d\eta \sum_{\mathbf{q}} n v_{\mathbf{q}} S_{\eta}(\mathbf{q}), \end{aligned} \quad (\text{A6})$$

where in the last line we used the definition of the structure factor

$$S(\mathbf{q}) = - \frac{1}{n v_{\mathbf{q}}} \int_0^{\infty} \frac{d\omega}{\pi} \mathfrak{S} \left[ \frac{1}{\varepsilon_{\text{ret}}(\mathbf{q}, \omega)} \right], \quad (\text{A7})$$

$$S_{\eta}(\mathbf{q}) = - \frac{1}{\eta n v_{\mathbf{q}}} \int_0^{\infty} \frac{d\omega}{\pi} \mathfrak{S} \left[ \frac{1}{\varepsilon_{\eta, \text{ret}}(\mathbf{q}, \omega)} \right], \quad (\text{A8})$$

where at  $T=0$   $\varepsilon_{\text{ret}}(\mathbf{q}, \omega) = \varepsilon_{\text{RPA}}(\mathbf{q}, \omega)$ . In Rydberg units, the exchange-correlation energy per particle  $E_{xc}$  is

$$E_{xc} = - \frac{4}{\pi r_s} \left( \frac{9\pi}{4} \right)^{1/3} \int_0^1 d\eta \left[ \frac{-1}{2k_F} \int_0^{\infty} dq S_{\eta}(q) \right]. \quad (\text{A9})$$

We define

$$\gamma^* = - \frac{1}{2k_F} \int_0^{\infty} dq S(q), \quad (\text{A10})$$

then

$$E_{xc} = - \frac{4}{\pi r_s} \left( \frac{9\pi}{4} \right)^{1/3} \int_0^1 d\eta \gamma^*(\eta r_s), \quad (\text{A11})$$

which should be compared with a similar expression<sup>11,12</sup>

$$E_{xc} = - \frac{4}{\pi r_s} \left( \frac{9\pi}{4} \right)^{1/3} \int_0^1 d\eta \gamma(\eta r_s), \quad (\text{A12})$$

$$\gamma = - \frac{1}{2k_F} \int_0^{\infty} dq [S(q) - 1], \quad (\text{A13})$$

$$E_c = \frac{0.9163}{r_s} - \frac{4}{\pi r_s} \left( \frac{9\pi}{4} \right)^{1/3} \int_0^1 d\eta \gamma(\eta r_s). \quad (\text{A14})$$

Note that  $[S(q) - 1]$  in Eq. (A13) comes from the consideration of the average value of  $\rho(\mathbf{q})\rho(-\mathbf{q})$ ,  $\rho(\mathbf{q})$  being the density operator,

$$\langle \rho(\mathbf{q})\rho(-\mathbf{q}) \rangle' = N[N\delta_{\mathbf{q}=0} + S(q) - 1]. \quad (\text{A15})$$

The prime on the bracket means one is to omit the particle interacting with itself. This explains why this differs by  $-1$  from the similar average  $\langle \rho(\mathbf{q})\rho(-\mathbf{q}) \rangle$ .

The expression (A12) is correct rather than (A11), which will be shown below. Consider the expression

$$\begin{aligned}\Omega_x &= -\frac{1}{2\beta} \sum_{\mathbf{q}, iq_n} v_{\mathbf{q}} P_0(\mathbf{q}, iq_n) \\ &= -\frac{1}{2\beta} \sum_{\mathbf{q}, iq_n} v_{\mathbf{q}} \frac{2}{\beta\nu} \sum_{\mathbf{p}, ip_n} \mathcal{G}^{(0)}(p) \mathcal{G}^{(0)}(p+q).\end{aligned}\quad (\text{A16})$$

Here we give two ways of calculating  $\Omega_x$ : (i) Evaluate the frequency summation over  $iq_n$  before doing the summation over  $ip_n$ , and (ii) do the frequency summations in reverse order.

The procedure (i) gives the usual exchange energy

$$\Omega_x = -\frac{1}{\nu} \sum_{\mathbf{p}\mathbf{q}} v_{\mathbf{q}} n_{\mathbf{p}} n_{\mathbf{p}+\mathbf{q}}, \quad (\text{A17})$$

where we used

$$\frac{1}{\beta} \sum_{ip_n} \mathcal{G}^{(0)}(p) = n_{\mathbf{p}}. \quad (\text{A18})$$

On the other hand, the procedure (ii) gives

$$\begin{aligned}\Omega_x &= -\frac{1}{2\beta} \sum_{\mathbf{q}, iq_n} v_{\mathbf{q}} \frac{2}{\nu} \sum_{\mathbf{p}} \frac{n_{\mathbf{p}} - n_{\mathbf{p}+\mathbf{q}}}{iq_n + \varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}+\mathbf{q}}} \\ &= \frac{1}{\nu} \sum_{\mathbf{p}\mathbf{q}} v_{\mathbf{q}} [n_{\mathbf{p}} - n_{\mathbf{p}+\mathbf{q}}] n_B(\varepsilon_{\mathbf{p}+\mathbf{q}} - \varepsilon_{\mathbf{p}}) \\ &= \frac{1}{\nu} \sum_{\mathbf{p}\mathbf{q}} v_{\mathbf{q}} n_{\mathbf{p}+\mathbf{q}} (1 - n_{\mathbf{p}}) \\ &= -\frac{1}{\nu} \sum_{\mathbf{p}\mathbf{q}} v_{\mathbf{q}} n_{\mathbf{p}} n_{\mathbf{p}+\mathbf{q}} + \frac{1}{2} \sum_{\mathbf{q}} n v_{\mathbf{q}},\end{aligned}\quad (\text{A19})$$

where first we did the frequency summation over  $ip_n$  in Eq. (A16) to get the first line, and we used in the second equality  $\frac{1}{\beta} \sum_{iq_n} \frac{1}{iq_n - \omega} = -[n_B(\omega) + 1/2]$ , of which use gives the next line since  $\sum_{\mathbf{p}} [n_{\mathbf{p}} - n_{\mathbf{p}+\mathbf{q}}] = 0$ .

The above expression (A19) consists of the usual exchange energy and the interaction energy at zero separation. The latter quantity is independent of temperature. Thus if we use the following expression as the RPA correlation energy

$$\Omega_r = \Omega_{xc} + \frac{1}{2\beta} \sum_{\mathbf{q}, iq_n} v_{\mathbf{q}} P_0(\mathbf{q}, iq_n), \quad (\text{A20})$$

with keeping the procedure (ii) in mind, we obtain the correct Eq. (A14); that is, at  $T \rightarrow 0$  with Eqs. (A6) and (A19),

$$\Omega_r = \frac{1}{2} \int_0^1 d\eta \sum_{\mathbf{q}} n v_{\mathbf{q}} [S_{\eta}(q) - 1] + \frac{1}{\nu} \sum_{\mathbf{p}\mathbf{q}} v_{\mathbf{q}} n_{\mathbf{p}} n_{\mathbf{p}+\mathbf{q}}, \quad (\text{A21})$$

which at  $T=0$  is the same as Eq. (A14) in units of  $N \times \text{Rydberg}$ . If we evaluate this expression of  $\Omega_r$ , as we have already done in text, we should obtain the same result as the previous one given by Eq. (A14). Since we

used Eq. (8) in text, i.e., we used the RPA polarization, and then evaluated the frequency integral at  $T=0$ , we have actually considered the procedure (ii) in evaluating Eq. (A16): That is, we evaluated Eq. (48), which is the  $T=0$  limit of Eq. (8) and is the same as Eq. (A21) at  $T=0$ . Thus we obtained the same result as the previous one, which was shown in Fig. 1.

## APPENDIX B: DETAILED CALCULATIONS

In this part, we will give detailed formulas used in Secs. II and III. By Sommerfeld expansion the RPA polarization  $P_0(\mathbf{q}, i\omega)$  is given by

$$P_0(\mathbf{q}, i\omega) = P_0^{(0)}(\mathbf{q}, i\omega) + t^2 P_0^{(1)}(\mathbf{q}, i\omega), \quad (\text{B1})$$

where

$$\begin{aligned}P_0^{(0)} &= -\frac{mk_F}{2\pi^2} \left\{ 1 + \frac{m^2}{2k_F q^3} (-XY + \omega^2) \ln \left[ \frac{X^2 + \omega^2}{Y^2 + \omega^2} \right] \right. \\ &\quad \left. - \frac{\omega}{qv_F} \left[ \tan^{-1} \left( \frac{X}{\omega} \right) - \tan^{-1} \left( \frac{Y}{\omega} \right) \right] \right\},\end{aligned}\quad (\text{B2})$$

$$P_0^{(1)} = -\frac{k_F^3}{24} \left[ \frac{X}{X^2 + \omega^2} + \frac{Y}{Y^2 + \omega^2} \right], \quad (\text{B3})$$

with

$$X = \varepsilon_{\mathbf{q}} - qv_F, \quad (\text{B4})$$

$$Y = \varepsilon_{\mathbf{q}} + qv_F. \quad (\text{B5})$$

From the  $T=0$  part  $P_0^{(0)}$  of the polarization  $P_0$ , we obtain the retarded dielectric function  $\varepsilon_{\text{RPA}}$  at  $T=0$ :

$$\varepsilon_{\text{RPA}}(\mathbf{q}, \omega) = \varepsilon_1(\mathbf{q}, \omega) + \varepsilon_2(\mathbf{q}, \omega), \quad (\text{B6})$$

where

$$\begin{aligned}\varepsilon_1 &= 1 + \frac{1}{2} \frac{q_{\text{TF}}^2}{q^2} \left\{ 1 - \frac{m^2}{2k_F q^3} (X + \omega)(Y + \omega) \ln \left| \frac{X + \omega}{Y + \omega} \right| \right. \\ &\quad \left. + \frac{m^2}{2k_F q^3} (X - \omega)(\omega - Y) \ln \left| \frac{X - \omega}{Y - \omega} \right| \right\},\end{aligned}\quad (\text{B7})$$

$$\varepsilon_2 = \frac{e^2 m}{q^3} [\theta(k_F - p_1)(k_F^2 - p_1^2) - \theta(k_F - p_2)(k_F^2 - p_2^2)], \quad (\text{B8})$$

where  $p_1 = (m/q)|\omega - \varepsilon_{\mathbf{q}}|$ , and  $p_2 = (m/q)|\omega + \varepsilon_{\mathbf{q}}|$ . Note that  $\varepsilon_2(\mathbf{q}, -\omega) = -\varepsilon_2(\mathbf{q}, \omega)$ . Using this relation, we find that  $I^{(0)}(\mathbf{q}, -\omega) = -I^{(0)}(\mathbf{q}, \omega)$ . Expanding the theta functions in  $\varepsilon_2(\mathbf{q}, \omega)$ , we obtain

$$\varepsilon_2 = \frac{e^2 m}{q^3} [\theta(2k_F - q)A(\omega) + \theta(q - 2k_F)B(\omega)], \quad (\text{B9})$$

where

$$\begin{aligned}A(\omega) &= 2m\omega\theta(-Y - \omega) \\ &\quad + \left[ k_F^2 - \left( \frac{m}{q} \right)^2 (\omega - \varepsilon_{\mathbf{q}})^2 \right] \theta(X - \omega)\theta(\omega + Y),\end{aligned}\quad (\text{B10})$$



$$B(\omega) = \left[ k_F^2 - \left( \frac{m}{q} \right)^2 (\omega - \varepsilon_{\mathbf{q}})^2 \right] \theta(X - \omega) \theta(\omega - Y), \quad (\text{B11})$$

Differentiating  $A(\omega)$ ,  $B(\omega)$  with respect to  $\omega$ , we obtain

$$\begin{aligned} \frac{dA(\omega)}{d\omega} &= 2m\theta(-Y - \omega) - 2m\omega\delta(-Y - \omega) \\ &\quad - 2 \left( \frac{m}{q} \right)^2 (\omega - \varepsilon_{\mathbf{q}}) \theta(X - \omega) \theta(\omega + Y) \\ &\quad + \left[ k_F^2 - \left( \frac{m}{q} \right)^2 (\omega - \varepsilon_{\mathbf{q}})^2 \right] \theta(X - \omega) \delta(\omega + Y), \end{aligned} \quad (\text{B12})$$

$$\frac{dB(\omega)}{d\omega} = -2 \left( \frac{m}{q} \right)^2 (\omega - \varepsilon_{\mathbf{q}}) \theta(X - \omega) \theta(\omega - Y), \quad (\text{B13})$$

where we neglected several  $\delta$  functions that are zero. Also, two other  $\delta$  functions in  $\frac{dA(\omega)}{d\omega}$  cancel each other. Then when  $\omega$  is replaced by  $x/\beta$  and the  $\beta \rightarrow \infty$  limit is taken, all the quantities in  $\frac{dA(\omega)}{d\omega}$  and  $\frac{dB(\omega)}{d\omega}$  except  $2m\theta(-Y - \omega)$  vanish. So in the  $\beta \rightarrow \infty$  limit with  $\omega = x/\beta$ ,

$$\begin{aligned} \left. \frac{d\varepsilon_2}{d\omega} \right|_{\omega=x/\beta=0} &= \frac{e^2 m}{q^3} \theta(2k_F - q) [2m\theta(-Y)] \\ &= \frac{2e^2 m^2}{q^3} \theta(2k_F - q). \end{aligned} \quad (\text{B14})$$

Instead of using the above expression, we used a little different expression to obtain the exact temperature dependence in text,

$$\left. \frac{d\varepsilon_2}{d\omega} \right|_{\omega=x/\beta} = \frac{2e^2 m^2}{q^3} \theta(2k_F - q) \theta(-Y - x/\beta), \quad (\text{B15})$$

which gives  $\frac{m\alpha}{k_F\beta} < q < 2k_F$  as the integral range over  $q$ . Note that the third term in  $\frac{dA(\omega)}{d\omega}$  gives the range  $0 < q < \frac{m\alpha}{k_F\beta}$ , which reduces to null range when  $\beta \rightarrow \infty$ . For  $\varepsilon_1(\mathbf{q}, \omega)$ ,  $\varepsilon_2(\mathbf{q}, \omega)$ , with  $\omega = x/\beta$ , we obtain in the limit  $\beta \rightarrow \infty$

$$\varepsilon_1(\mathbf{q}, \omega = 0) = 1 + \frac{1}{2} \frac{q_{\text{TF}}^2}{q^2} \left[ 1 - \frac{m^2}{k_F q^3} XY \ln \left| \frac{X}{Y} \right| \right], \quad (\text{B16})$$

$$\varepsilon_2(\mathbf{q}, \omega = 0) = 0, \quad (\text{B17})$$

where  $\varepsilon_1(\mathbf{q}, \omega = 0)$  was denoted as  $\tilde{\varepsilon}_1$  in text. Thus we obtain

$$\left. \frac{dI^{(0)}}{d\omega} \right|_{\omega=x/\beta} = -2 \left. \frac{d\varepsilon_2}{d\omega} \right|_{\omega=x/\beta} \frac{(1 - \tilde{\varepsilon}_1)}{\tilde{\varepsilon}_1}, \quad (\text{B18})$$

in the limit of  $\beta \rightarrow \infty$  with  $\omega = x/\beta$ , but with  $\left. \frac{d\varepsilon_2}{d\omega} \right|_{\omega=x/\beta}$  of Eq. (B15). The expression (B18) was used in Eq. (37).

Next we consider  $\bar{P}_{0,1}^{(0)}$ , a correction term due to the temperature deviation in the chemical potential. Letting

$$\bar{P}_0^{(0)} = P_0^{(0)}(\mathbf{q}, i\omega; k_F) \equiv -\frac{m}{2\pi^2} k_F Q(k_F), \quad (\text{B19})$$

then  $\bar{P}_{0,1}^{(0)}$  is given by

$$\begin{aligned} t^2 \bar{P}_{0,1}^{(0)} &= -\frac{m}{2\pi^2} \left( -\frac{\pi^2}{6} k_F t^2 \right) \left[ Q(k_F) + k_F \frac{dQ}{dk_F} \right] \\ &= \frac{mk_F}{12} t^2 R(k_F), \end{aligned} \quad (\text{B20})$$

where

$$\begin{aligned} R &= 1 + \frac{k_F}{q} \ln \left[ \frac{X^2 + \omega^2}{Y^2 + \omega^2} \right] - \left[ \frac{\omega^2}{X^2 + \omega^2} + \frac{\omega^2}{Y^2 + \omega^2} \right] \\ &\quad + \frac{m}{q^2} (-XY + \omega^2) \left[ \frac{X}{X^2 + \omega^2} + \frac{Y}{Y^2 + \omega^2} \right]. \end{aligned} \quad (\text{B21})$$

Finally, we give the detailed forms of some quantities that were used in the calculation of  $C_V(r_s)$  and  $C_K(r_s)$  in Sec. III. With  $\varepsilon^{(0)}(\mathbf{q}, i\omega) = 1 - v_{\mathbf{q}} P_0^{(0)}(\mathbf{q}, i\omega)$ , define

$$j^{(0)}(\mathbf{q}, i\omega) = \ln[\varepsilon^{(0)}(\mathbf{q}, i\omega)] + \frac{4}{5} v_{\mathbf{q}} P_0^{(0)} + \frac{1}{5} \frac{v_{\mathbf{q}} P_0^{(0)}}{\varepsilon^{(0)}(\mathbf{q}, i\omega)}, \quad (\text{B22})$$

$$\begin{aligned} l^{(0)}(\mathbf{q}, i\omega) &= \ln[\varepsilon^{(0)}(\mathbf{q}, i\omega)] + \frac{2}{5} v_{\mathbf{q}} P_0^{(0)} \\ &\quad + \frac{7}{10} \frac{v_{\mathbf{q}} P_0^{(0)}}{\varepsilon^{(0)}(\mathbf{q}, i\omega)} - \frac{1}{10} \frac{v_{\mathbf{q}} P_0^{(0)}}{\varepsilon^{(0)}(\mathbf{q}, i\omega)^2}. \end{aligned} \quad (\text{B23})$$

Then with  $z = q/k_F$  and  $\tilde{\omega} = \omega/\mu^0$ ,

$$V_r^{(0)}/V_x^{(0)} = -\frac{5}{8\pi\alpha} \int_0^\infty z^2 dz \int_0^\infty d\tilde{\omega} j^{(0)}(z, i\tilde{\omega}), \quad (\text{B24})$$

$$K_r^{(0)}/K_x^{(0)} = -\frac{5}{4\pi\alpha} \int_0^\infty z^2 dz \int_0^\infty d\tilde{\omega} l^{(0)}(z, i\tilde{\omega}). \quad (\text{B25})$$

For temperature correction parts, if we define

$$j^{(1)}(\mathbf{q}, i\omega) = -\frac{i^{(1)}(\mathbf{q}, i\omega)}{\varepsilon^{(0)}(\mathbf{q}, i\omega)}, \quad (\text{B26})$$

$$l^{(1)}(\mathbf{q}, i\omega) = j^{(1)}(\mathbf{q}, i\omega) - \frac{i^{(1)}(\mathbf{q}, i\omega)}{\varepsilon^{(0)}(\mathbf{q}, i\omega)^2}, \quad (\text{B27})$$

we have

$$V_{r,1}^{(1)}/V_x^{(0)} = \frac{1}{8\pi\alpha} \int_0^\infty z^2 dz \int_0^\infty d\tilde{\omega} j^{(1)}(z, i\tilde{\omega}), \quad (\text{B28})$$

$$K_{r,1}^{(1)}/K_x^{(0)} = -\frac{1}{4\pi\alpha} \int_0^\infty z^2 dz \int_0^\infty d\tilde{\omega} l^{(1)}(z, i\tilde{\omega}). \quad (\text{B29})$$

Here if replacing  $i^{(1)}(\mathbf{q}, i\omega)$  [Eq. (14)] by  $i_1^{(0)}(\mathbf{q}, i\omega)$  [Eq. (46)], we obtain  $V_{r,3}^{(1)}/V_x^{(0)}$  and  $K_{r,3}^{(1)}/K_x^{(0)}$  corresponding to  $\Omega_{r,3}^{(1)}$ . Also, we obtain

$$V_{r,2}^{(1)}/V_x^{(0)} = -\frac{\pi^2}{24} \int_0^2 \frac{dz}{z} \frac{\tilde{\varepsilon}_1 - 1}{\tilde{\varepsilon}_1^2}, \quad (\text{B30})$$

$$K_{r,2}^{(1)}/K_x^{(0)} = \frac{\pi^2}{12} \int_0^2 \frac{dz \tilde{\epsilon}_1^2 - 1}{z \tilde{\epsilon}_1^3}. \quad (\text{B31})$$

Thus we obtain the coefficients  $V_r^{(1)}$ ,  $K_r^{(1)}$  of  $t^2$  in  $V_r$ ,  $K_r$ ,

respectively:

$$V_r^{(1)}/V_x^{(0)} = [V_{r,1}^{(1)} + V_{r,2}^{(1)} + V_{r,3}^{(1)}]/V_x^{(0)}, \quad (\text{B32})$$

$$K_r^{(1)}/K_x^{(0)} = [K_{r,1}^{(1)} + K_{r,2}^{(1)} + K_{r,3}^{(1)}]/K_x^{(0)}. \quad (\text{B33})$$

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<sup>8</sup> U. Gupta and A.K. Rajagopal, Phys. Rev. A **22**, 2792 (1980).

<sup>9</sup> Here when we are saying  $T^2$  dependence, we imply that it could be interpreted as either  $T^2$  or as  $T^2 \ln T$  terms.

<sup>10</sup> Note that the RPA dielectric function is related to (the average of product of) the density operators, which have boson properties. Thus  $I(\mathbf{q}, \omega)$  can be considered a spectral function for boson operators, so it satisfies the relation  $I(\mathbf{q}, -\omega) = -I(\mathbf{q}, \omega)$ , which is the general property for boson spectral functions.

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