

## Diamagnetic susceptibility of an interacting electron gas\*

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The effects of exchange and correlations on the diamagnetic susceptibility of an interacting electron gas are investigated using the double-time Green's-function method. The equation of motion of the appropriate Green's function is linearized using a moment-conserving decoupling approximation. The many-body corrections to the diamagnetic susceptibility at metallic densities are found to be small. The present expression reduces to the exact result in the high-density limit. Many of the results of earlier calculations also follow from our expression for the diamagnetic susceptibility.

### I. INTRODUCTION

The diamagnetic susceptibility of an interacting electron gas has received lesser attention<sup>1</sup> than the spin susceptibility. The problem here is to calculate the effect of electron-electron interactions on the free-electron diamagnetism (i. e., Landau diamagnetism). The first rigorous attempt in this direction was made by Kanazawa and Matsudaira<sup>2</sup> and Fujita and Usui.<sup>3</sup> The authors have obtained the result which is only valid in the high-density limit. Stephen<sup>4</sup> and Isihara and Tsai<sup>5</sup> have also calculated the orbital susceptibility using perturbation theory. Their<sup>5</sup> result is correct to  $O(r_s^2)$ , where  $r_s$  is the average interelectronic distance. Rajagopal and Jain<sup>6</sup> have obtained an expression for the diamagnetic susceptibility by solving the equation for the appropriate vertex function using the variational procedure. A moment-conserving method has also been used by Rajagopal and Rath<sup>7</sup> to calculate the orbital susceptibility. But apart from other approximations, the moment relation used by them is an approximate one. Philippas and McClure<sup>8</sup> have given the proof of the Sampson-Seitz prescription for calculating the diamagnetic susceptibility, using the Green's-function method. Their result for the many-body effects on the diamagnetism of free electrons is the same as obtained by Rajagopal and Jain.<sup>6</sup> All these calculations give the exact result<sup>9</sup> in the high-density limit. However, most of the above<sup>4-6,8</sup> results for the diamagnetic susceptibility are not expected to be good at metallic densities.

In this paper, we present a calculation of the diamagnetism of an electron liquid at metallic densities. Recently, we have derived<sup>10</sup> an exact moment sum rule for the transverse-current-density response function. This function is directly related<sup>6,11</sup> to the diamagnetic susceptibility of the system. The sum rule is used to decouple the equation of motion of the appropriate double-time Green's function. In the high-density limit, our expression for the diamagnetic susceptibility reduces to the exact result.<sup>2,3</sup> Further, if we completely neglect the potential con-

tribution to the first-moment sum rule, the present result exactly agrees with the result of Rajagopal and Jain<sup>6</sup> and Philippas and McClure.<sup>8</sup> The result of Rajagopal and Rath<sup>7</sup> can also be obtained, provided we calculate the potential contribution to the first-moment sum rule in the Hartree-Fock approximation.

The general formulation of the problem is given in Sec. II. The calculation of the diamagnetic susceptibility is also described there. The results are presented in Sec. III and various special cases are discussed. Section IV contains the discussion and the conclusions.

### II. GENERAL THEORY

The linear response of the system to a space- and time-dependent external transverse probe which couples to the current-density fluctuations in the system is described<sup>11</sup> through the transverse-current-density response function. It is defined in terms of retarded Green's function as<sup>12</sup>

$$\chi_{\perp}(\vec{q}, t) = \langle\langle J_{\perp}(\vec{q}, t); J_{\perp}^{\dagger}(\vec{q}, 0) \rangle\rangle \\ = -i\Theta(t)\langle\langle [J_{\perp}(\vec{q}, t), J_{\perp}^{\dagger}(\vec{q}, 0)] \rangle\rangle, \quad (1)$$

where  $\Theta(t)$  and  $J_{\perp}(\vec{q})$  are the unit step function and the component of the current density perpendicular to  $\vec{q}$ , respectively. In the second-quantized form,  $J_{\perp}(\vec{q})$  is given by

$$J_{\perp}(\vec{q}) = \frac{1}{m} \sum_{\vec{k}_1} k_{1y} a_{\vec{k}_1}^{\dagger} a_{\vec{k}_1+\vec{q}} \\ = \frac{1}{m} \sum_{\vec{k}_1} k_{1y} \rho_{\vec{k}_1}(\vec{q}), \quad (2)$$

where  $\vec{q}$  is chosen along the  $x$  axis and  $a_{\vec{k}_1}^{\dagger}$ ,  $a_{\vec{k}_1}$  are the electron creation and annihilation operators, respectively. The single angular brackets in Eq. (1) denotes the equilibrium ensemble average, appropriate to the system Hamiltonian:

$$H = H_0 + H_1 = \sum_{\vec{k}} \omega_{\vec{k}} a_{\vec{k}}^{\dagger} a_{\vec{k}} \\ + \frac{1}{2} \sum_{\vec{k} \neq 0} \phi(\vec{k}) [\rho(\vec{k}) \rho^{\dagger}(\vec{k}) - n], \quad (3)$$

where  $\omega_{\vec{k}} = k^2/2m$ ,  $\phi(\vec{k}) = 4\pi e^2/k^2$ ,  $n$  is the uniform electron density, and

$$\rho(\vec{k}) = \sum_{\vec{k}_1} \rho_{\vec{k}_1}(\vec{k})$$

is the electron-density-fluctuation operator. For simplicity, we omit the spin indices and take them to be included in the suffixes  $k$ 's.

In the static and long-wavelength limit, the Fourier transform of the transverse-current-density response function is related<sup>6,11</sup> to the diamagnetic susceptibility of the system through the relation

$$\chi_{\text{dia}}(q, 0) = -(e^2/c^2 q^2)(\chi_{\perp}(q, 0) + n/m). \quad (4)$$

It follows from Eqs. (1) and (2) that

$$\chi_{\perp}(\vec{q}, t) = \frac{1}{m^2} \sum_{\vec{k}_1, \vec{k}_2} k_{1y} k_{2y} G_{\vec{k}_1, \vec{k}_2}(\vec{q}, t), \quad (5)$$

where

$$G_{\vec{k}_1, \vec{k}_2}(\vec{q}, t) = \langle\langle \rho_{\vec{k}_1}(\vec{q}, t); \rho_{\vec{k}_2}^{\dagger}(\vec{q}, 0) \rangle\rangle \quad (6)$$

is the two-particle Green's function. The Fourier transform of its equation of motion is given by

$$G_{\vec{k}_1, \vec{k}_2}(\vec{q}, \omega) = \frac{n_{\vec{k}_1} - n_{\vec{k}_1 + \vec{q}}}{\omega - \omega(\vec{k}_1, \vec{q})} \delta_{\vec{k}_1, \vec{k}_2} + \frac{\langle\langle [\rho_{\vec{k}_1}(\vec{q}), H_1]; \rho_{\vec{k}_2}^{\dagger}(\vec{q}) \rangle\rangle_{\omega}}{\omega - \omega(\vec{k}_1, \vec{q})}, \quad (7)$$

where  $\omega(\vec{k}_1, \vec{q}) = \omega_{\vec{k}_1 + \vec{q}} - \omega_{\vec{k}_1}$ . Finally, the equation for the transverse-current-density response function can be seen to be

$$\chi_{\perp}(\vec{q}, \omega) = \chi_{\perp}^0(\vec{q}, \omega) + \frac{1}{m^2} \sum_{\vec{k}_1} \frac{1}{\omega - \omega(\vec{k}_1, \vec{q})} \times \sum_{\vec{k}_2} k_{1y} k_{2y} \langle\langle [\rho_{\vec{k}_1}(\vec{q}), H_1]; \rho_{\vec{k}_2}^{\dagger}(\vec{q}) \rangle\rangle_{\omega}, \quad (8)$$

where

$$\chi_{\perp}^0(\vec{q}, \omega) = \frac{1}{m^2} \sum_{\vec{k}_1} k_{1y}^2 \frac{n_{\vec{k}_1} - n_{\vec{k}_1 + \vec{q}}}{\omega - \omega(\vec{k}_1, \vec{q})}, \quad (9)$$

is the transverse-current-density response function of the noninteracting electron gas. Equation (7) for the two-particle Green's function involves, in turn, the three-particle Green's function, and so on. We now proceed to terminate this infinite hierarchy of equations using the approximations described below

#### A. Random-phase approximation (RPA)

If we linearize the second term on the right-hand side of Eq. (7) in the RPA and pair off the equal momentum operators by setting  $\langle a_{\vec{k}_1}^{\dagger} a_{\vec{k}_1} \rangle = n_{\vec{k}_1}$ . The result obtained is

$$G_{\vec{k}_1, \vec{k}_2}(\vec{q}, \omega) = G_{\vec{k}_1}^0(\vec{q}, \omega) \times \left( \delta_{\vec{k}_1, \vec{k}_2} + \phi(\vec{q}) \sum_{\vec{k}_3} G_{\vec{k}_3, \vec{k}_2}(\vec{q}, \omega) \right), \quad (10)$$

where  $G_{\vec{k}_1}^0(\vec{q}, \omega) = (n_{\vec{k}_1} - n_{\vec{k}_1 + \vec{q}})/[\omega - \omega(\vec{k}_1, \vec{q})]$ , is the free-electron Green's function. Using Eq. (10) in the Fourier transform of Eq. (5), we obtain

$$\chi_{\perp}(\vec{q}, \omega) = \chi_{\perp}^0(\vec{q}, \omega) + \frac{\phi(\vec{q})}{m^2} \sum_{\vec{k}_1} k_{1y} G_{\vec{k}_1}^0(\vec{q}, \omega) \times \sum_{\vec{k}_2, \vec{k}_3} k_{2y} G_{\vec{k}_3, \vec{k}_2}(\vec{q}, \omega). \quad (11)$$

This equation can be solved exactly by iteration, using Eq. (10), and the result is

$$\chi_{\perp}(\vec{q}, \omega) = \chi_{\perp}^0(\vec{q}, \omega) + \phi(\vec{q}) \frac{[\chi_{J\rho}^0(\vec{q}, \omega)]^2}{1 - \phi(\vec{q})\chi^0(\vec{q}, \omega)}, \quad (12)$$

where

$$\chi^0(\vec{q}, \omega) = \sum_{\vec{k}_1} G_{\vec{k}_1}^0(\vec{q}, \omega)$$

is the density-density response function in the noninteracting case and

$$\chi_{J\rho}^0(\vec{q}, \omega) = \frac{1}{m} \sum_{\vec{k}_1} k_{1y} G_{\vec{k}_1}^0(\vec{q}, \omega) \quad (13)$$

is the transverse-current and density-response function of the noninteracting system. It is interesting to note that Eq. (12) involves three different response functions of the system. The second term in this equation can be seen to be zero only in the static case, so that the diamagnetic susceptibility in the RPA is the same as for the noninteracting system.

One can also linearize Eq. (7) using the Hartree-Fock-like decoupling approximation (i. e., the RPA including exchange). The resulting equation is

$$G_{\vec{k}_1, \vec{k}_2}(\vec{q}, \omega) = \frac{n_{\vec{k}_1} - n_{\vec{k}_1 + \vec{q}}}{\omega - \tilde{\omega}(\vec{k}_1, \vec{q})} \times \left( \delta_{\vec{k}_1, \vec{k}_2} + \sum_{\vec{k}_3} [\phi(\vec{q}) - \phi(\vec{k}_1 - \vec{k}_3)] G_{\vec{k}_3, \vec{k}_2}(\vec{q}, \omega) \right), \quad (14)$$

where we have  $\tilde{\omega}(\vec{k}_1, \vec{q}) = \tilde{\omega}_{\vec{k}_1 + \vec{q}} - \tilde{\omega}_{\vec{k}_1}$  and

$$\tilde{\omega}_{\vec{k}_1} = \omega_{\vec{k}_1} - \sum_{\vec{k}' \neq 0} \phi(\vec{k}') n_{\vec{k}_1 + \vec{k}'}. \quad (15)$$

is the one-particle energy including the exchange self-energy. Equation (14) has been solved by Rajagopal<sup>13,6</sup> using the variational procedure.

#### B. Moment-conserving-decoupling approximation

We shall now linearize Eq. (8) using the moment-conserving-decoupling approximation.<sup>14-17</sup> We make use of an *Ansatz* proposed by Rajagopal *et al.*<sup>7</sup>:

$$\sum_{\vec{k}_2} k_{1y} k_{2y} \langle\langle [\rho_{\vec{k}_1}(\vec{q}), H_1]; \rho_{\vec{k}_2}^{\dagger}(\vec{q}) \rangle\rangle_{\omega} = [A_{\vec{k}_1}(\vec{q}) + \omega B_{\vec{k}_1}(\vec{q})]$$

$$\sum_{\vec{k}_1, \vec{k}_2} k_{1y} k_{2y} \langle \langle \rho_{\vec{k}_1}(\vec{q}); \rho_{\vec{k}_2}^\dagger(\vec{q}) \rangle \rangle_\omega \quad (16)$$

It is necessary here to retain both the coefficients  $A_{\vec{k}_1}(\vec{q})$  and  $B_{\vec{k}_1}(\vec{q})$ . If either of them is taken to be zero, one obtains a nonzero coefficient of the  $1/\omega^3$  term in the high-frequency expansion of the transverse-current-density response function. This kind of term is not present in the exact asymptotic expansion of  $\chi_{\perp}(\vec{q}, \omega)$ .<sup>10</sup> Further, it is also found that the transverse-current-density response function obtained by using only a single coefficient in Eq. (16) does not even formally satisfy its exact first frequency moment. Therefore, the reason for the chosen form of the coefficients in Eq. (16) is that it formally gives the exact expression for the first frequency moment and also yields the correct asymptotic behavior of the transverse-current-density response function.

We now substitute Eq. (16) into Eq. (8) and obtain

$$\chi_{\perp}(\vec{q}, \omega) = \chi_{\perp}^0(\vec{q}, \omega) / [1 - F(\vec{q}, \omega)], \quad (17)$$

where

$$F(\vec{q}, \omega) = \sum_{\vec{k}_1} \frac{A_{\vec{k}_1}(\vec{q}) + \omega B_{\vec{k}_1}(\vec{q})}{\omega - \omega(\vec{k}_1, \vec{q})} \quad (18)$$

is the function which takes into account the effect of exchange and correlations on the transverse-current-density response function of the system.

The coefficients  $B_{\vec{k}_1}(\vec{q})$  and  $A_{\vec{k}_1}(\vec{q})$  in  $F(\vec{q}, \omega)$  are determined, respectively, from the conditions that the zeroth and the first frequency moments of both sides of Eq. (16) must be equal. As the even moments of  $\chi_{\perp}(\vec{q}, \omega)$  are zero, we obtain

$$A_{\vec{k}_1}(\vec{q}) = \sum_{\vec{k}_2} \frac{k_{1y} k_{2y} \langle [ [\rho_{\vec{k}_1}(\vec{q}), H_1], H ], \rho_{\vec{k}_2}^\dagger(\vec{q}) \rangle}{\langle \omega_{\perp}^1 \rangle} \quad (19)$$

and

$$B_{\vec{k}_1}(\vec{q}) = \sum_{\vec{k}_2} \frac{k_{1y} k_{2y} \langle [ [\rho_{\vec{k}_1}(\vec{q}), H_1], \rho_{\vec{k}_2}^\dagger(\vec{q}) \rangle ]}{\langle \omega_{\perp}^1 \rangle} \quad (20)$$

Here

$$\langle \omega_{\perp}^1 \rangle = \sum_{\vec{k}_1, \vec{k}_2} k_{1y} k_{2y} \langle [ [\rho_{\vec{k}_1}(\vec{q}), H ], \rho_{\vec{k}_2}^\dagger(\vec{q}) \rangle ] \rangle \quad (21)$$

is the first frequency moment of the transverse-current-density response function for which we have recently obtained an exact expression<sup>10</sup>:

$$\langle \omega_{\perp}^1 \rangle = nm \left( \frac{4}{3} \omega_{\vec{q}} \langle T_{\text{KE}} \rangle + \frac{1}{2m} \sum_{\vec{k}} \phi(\vec{k}) (\hat{q} \times \vec{k})^2 \times [S(\vec{q} - \vec{k}) - S(\vec{k})] \right). \quad (22)$$

In Eq. (22),  $S(k)$  is the static structure factor and  $\langle T_{\text{KE}} \rangle$  is the exact kinetic energy per electron of the system. The various commutators in Eqs. (19) and (20) can be handled easily. The only complicated commutator<sup>18</sup> is

$$\begin{aligned} [ [\rho_{\vec{k}_1}(\vec{q}), H_1], H_0 ], H_0 ] = \sum_{\vec{q}_1} \phi(\vec{q}_1) [ \{ a_{\vec{k}_1}^\dagger \rho(\vec{q}_1) a_{\vec{k}_1 + \vec{q} - \vec{q}_1} - a_{\vec{k}_1 + \vec{q}_1}^\dagger \rho(\vec{q}_1) a_{\vec{k}_1 + \vec{q}} \}, H_0 ] = \sum_{\vec{q}_1} \phi(\vec{q}_1) \left( [ \omega(\vec{k}_1, \vec{q} - \vec{q}_1) a_{\vec{k}_1}^\dagger \rho(\vec{q}_1) a_{\vec{k}_1 + \vec{q} - \vec{q}_1} \right. \\ \left. - \omega(\vec{k}_1 + \vec{q}_1, \vec{q} - \vec{q}_1) a_{\vec{k}_1 + \vec{q}_1}^\dagger \rho(\vec{q}_1) a_{\vec{k}_1 + \vec{q}} \right] + \sum_{\vec{q}_2} \omega(\vec{q}_2, \vec{q}_1) [ a_{\vec{k}_1}^\dagger \rho(\vec{q}_1) a_{\vec{k}_1 + \vec{q} - \vec{q}_1} - a_{\vec{k}_1 + \vec{q}_1}^\dagger \rho(\vec{q}_1) a_{\vec{k}_1 + \vec{q}} \right]. \quad (23) \end{aligned}$$

The averages of the product of four operators are decoupled in the usual Hartree-Fock-like approximation, as has mostly been done in the past.<sup>7, 15-17</sup> (In Appendix A, we present a method<sup>19</sup> of calculating the lowest-order corrections to the Hartree-Fock-like decoupling.) After a lengthy calculation we find

$$F(\vec{q}, \omega) = \sum_{\vec{k}_1, \vec{k}_2} \phi(\vec{k}_2) \frac{(n_{\vec{k}_1 + \vec{q}} - n_{\vec{k}_1})(n_{\vec{k}_1 + \vec{k}_2 + \vec{q}} - n_{\vec{k}_1 + \vec{k}_2})}{[\omega - \omega(\vec{k}_1, \vec{q})] \langle \omega_{\perp}^1 \rangle} [k_{1y} \omega(\vec{k}_1, \vec{q}) + k_{1y} k_{2y} \omega - (k_{1y}^2 + k_{1y} k_{2y}) \omega(\vec{k}_1 + \vec{k}_2, \vec{q})]. \quad (24)$$

This expression reduces to that obtained by Rajagopal and Rath,<sup>7</sup> provided we use the Hartree-Fock structure factor in the evaluation of  $\langle \omega_{\perp}^1 \rangle$ .

In the static and long-wavelength limit, the integrals involved in Eq. (24) can be done exactly by following Rajagopal.<sup>13</sup> The result is

$$F(q, 0) = \frac{q^2 k_F^4}{1800 \pi^4} \left[ \left( \frac{d^2}{dx^2} - \frac{d}{dx} \right) \left\{ x^4 \left[ \frac{1}{7} \phi^{(3)}(k_F, k_F x) - \frac{1}{3} \phi^{(1)}(k_F, k_F x) \right] \right\} \right]_{x=1} \left[ nm \left( \frac{2}{3} \frac{\langle T_{\text{KE}} \rangle}{m} + \frac{\omega_p^2}{5 k_F^2} \gamma \right) \right]^{-1} \quad (25)$$

where  $\omega_p^2 = 4\pi n e^2 / m$ ,  $k_F$  is the Fermi wave vector, and

$$\gamma = -\frac{1}{2k_F} \int_0^\infty dk (S(k) - 1). \quad (26)$$

In Eq. (25),  $\phi^{(3)}(k_F, k_F x)$  and  $\phi^{(1)}(k_F, k_F x)$  are the various expansion coefficients when one expands the Coulomb potential in the terms of spherical harmonics and are given by

$$\phi^{(l)}(k_1, k_2) = (l + \frac{1}{2}) \int_{-1}^1 d\mu P_l(\mu) \phi(\vec{k}_1 - \vec{k}_2). \quad (27)$$

Here  $P_l(\mu)$  denotes a Legendre polynomial of  $l$ th order and  $\mu$  is the cosine of the angle between the vectors  $\vec{k}_1$  and  $\vec{k}_2$ . Equation (25) simplifies to

$$F(q, 0) = \frac{mq^2}{120\pi^2 k_F} \left[ \left( \frac{d^2}{dx^2} - \frac{d}{dx} \right) \left\{ x^4 \left[ \frac{1}{7} \phi^{(3)}(k_F, k_F x) - \frac{1}{3} \phi^{(1)}(k_F, k_F x) \right] \right\} \right]_{x=1} \left( 1 + \frac{4}{3} \frac{\alpha r_s \gamma}{\pi} \right)^{-1}, \quad (28)$$

where  $\alpha r_s = me^2/k_F$ , so that  $\alpha = (4/9\pi)^{1/3}$ .

It can be seen that  $F(q, 0)$  is divergent for the bare Coulomb potential, as in the case of earlier calculations.<sup>2-8</sup> This divergence might have been expected also due to the fact that all the averages in  $F(\vec{q}, \omega)$  were calculated in the lowest-order approximation. Thus the screening of the Coulomb potential is essential to get a finite result, as has already been emphasized.<sup>6</sup> Kanazawa and Matsudaira<sup>2</sup> gave a phenomenological way to screen the Coulomb potential in the Green's-function formalism. In general, the potential should be screened by the frequency and wave-vector dependent dielectric function. But to make contact with earlier calculations<sup>2-8</sup> on diamagnetism, we take the Coulomb potential to be screened by the Thomas-Fermi screening function.<sup>11</sup> Therefore, we use

$$\phi(\vec{k}) = 4\pi e^2 / (k^2 + \xi^2 k_F^2), \quad (29)$$

where we have the dimensionless parameter  $\xi^2 = 4\alpha r_s/\pi$ . Making use of Eq. (29) in (28) and carrying out the integrations, we obtain

$$F(q, 0) = -\frac{q^2}{4k_F^2} \frac{\alpha r_s}{\pi} \left[ \frac{2}{3} + \frac{1}{3} \frac{\xi^2}{4 + \xi^2} \right] - \left( \frac{1}{6} + \frac{\xi^2}{4} \right) \ln \left( \frac{4 + \xi^2}{\xi^2} \right) \times \left( 1 + \frac{4}{3} \frac{\alpha r_s \gamma}{\pi} \right)^{-1} \quad (30)$$

In order to see the effect of screening the Coulomb potential by a different dielectric function, we have also carried out the calculations by using the RPA screening function. The integrations involved are very complicated and have been done numerically.

### III. RESULTS

The expression for the diamagnetic susceptibility of the electron liquid is obtained by using Eqs. (30) and (17) in Eq. (4) and then taking the  $q \rightarrow 0$  limit. The result is

$$\chi_{\text{dia}} = \chi_L (1 + \beta), \quad (31)$$

where  $\chi_L = -e^2 k_F / 12\pi^2 m c^2$  is the Landau diamagnetism and

$$\beta = \frac{\alpha r_s}{\pi} \frac{\frac{2}{3} + \frac{1}{3} \frac{\xi^2}{4 + \xi^2} - \left( \frac{1}{6} + \frac{1}{4} \frac{\xi^2}{\xi^2} \right) \ln(1 + 4/\xi^2)}{1 + \frac{4}{3} (\alpha r_s/\pi) \gamma} \quad (32)$$

gives the corrections due to the exchange and correlation effects. Now we proceed to discuss our results in the following special cases: (i) In the high-density limit (i. e.,  $r_s < 1$ ), we obtain

$$\chi_{\text{dia}} = \chi_L \left\{ 1 + (\alpha r_s/6\pi) [4 + \ln(\alpha r_s/\pi)] \right\}, \quad (33)$$

which coincides with the exact high-density result.<sup>2,3</sup>

(ii) If we entirely neglect the effect of Coulomb potential on the first frequency moment of  $\chi_L(\vec{q}, \omega)$ , then  $\gamma = 0$ , and it can be easily seen that

$$\chi_{\text{dia}} = \chi_L \left\{ 1 + \frac{\alpha r_s}{6\pi} \left[ 4 + \frac{2\xi^2}{4 + \xi^2} - \left( 1 + \frac{3}{2} \xi^2 \right) \ln \left( 1 + \frac{4}{\xi^2} \right) \right] \right\}. \quad (34)$$

This result is exactly the same as that of Rajagopal and Jain<sup>6</sup> and Philippas and McClure.<sup>8</sup> (iii) When one treats the effects of the Coulomb potential on  $\langle \omega_1^1 \rangle$  in the Hartree-Fock approximation, then  $S(k) = S_0(k)$ , where  $S_0(k)$  is the Hartree-Fock structure factor of the system. We then obtain

$$\chi_{\text{dia}} = \chi_L \times \frac{1 + (\alpha r_s/6\pi) [4 + 2\xi^2/(4 + \xi^2) - (1 + \frac{3}{2} \xi^2) \ln(1 + 4/\xi^2)]}{1 + \frac{1}{2} \alpha r_s/\pi}. \quad (35)$$

This result coincides with that obtained after simplifying the expression of Rajagopal and Rath.<sup>7</sup> (iv) We now calculate the orbital susceptibility from our expression (31). The only unknown input in this expression is  $\gamma$ . This is calculated using our<sup>20</sup> self-consistent values of the structure factor. It is relevant here to use these values of the structure factor because they are obtained by solving an integral equation, derived also by using the moment sum rules. The values of  $\gamma$  thus obtained are presented in Table I. These values are quite close to those obtained by Vashishta and Singwi.<sup>21</sup> We now estimate the diamagnetic susceptibility of the electron liquid over the entire metallic density range and present the results in Fig. 1. The results of Kanazawa and Matsudaira<sup>2</sup> (KM) and Ishihara and Tsai<sup>5</sup> (IT) are also plotted for the sake of comparison. It is interesting to note that the effects of exchange and correlations due to electron-electron interactions are very small, so that the present results are quite close to the results for Landau diamagnetism. The results of Rajagopal and Jain<sup>6</sup> [i. e., Eq.

TABLE I. Values of  $\gamma$ .

$r_s$	1	2	3	4	5	6
$\gamma$	0.46386	0.50624	0.53580	0.55845	0.57666	0.59172

(34)] are not plotted because they are also very close to the present results. Although the results for the diamagnetic susceptibility in some of the above calculations are quite close, the exchange and correlation correction is appreciably different. To make this apparent, the results for the exchange and correlation correction factor  $\beta$  are presented in Table II. We have also calculated  $\beta$  numerically by screening the Coulomb potential with the RPA dielectric function and the results are given in Table II. The values of  $\beta$ , thus obtained, can be seen to be the smallest of all. Thus, while the exchange and correlation are crucial for the proper treatment of diamagnetism, their numerical effect on the diamagnetic susceptibility seems to be small.

#### IV. DISCUSSION AND CONCLUSIONS

In this paper, we have confined ourselves to the calculation of the steady diamagnetic susceptibility of an interacting electron system in the ground state. It is proved explicitly that the susceptibility in the RPA (excluding exchange) is the same as for the noninteracting system. This is expected physically also<sup>11</sup> because in the static case there is no

dielectric screening of the transverse field, and further the single-particle excitations in the RPA are unchanged from their free-particle values. The exact first frequency moment sum rule<sup>10</sup> is then used to calculate the diamagnetic susceptibility using the moment-conserving decoupling approximation. The particular form of the decoupling *Ansatz*, Eq. (16), is chosen to get formally exact first frequency moment and the correct asymptotic behavior of the transverse-current-density response function.

The important conclusion of the present work is that the exchange and correlation correction to the Landau diamagnetism is numerically small. This is in contrast to the Pauli paramagnetism which is appreciably enhanced<sup>22</sup> due to the effect of electron correlations. Our result for the diamagnetic susceptibility does give the exact high-density result.<sup>2,3</sup> Further, the results of the other earlier calculations<sup>6-8</sup> also follow from the present results, if we treat the effect of Coulomb correlations on the first frequency moment in various approximations. Therefore, it is hoped that the present results will be good for metallic densities. It is also known that the moment-conserving decoupling approximation<sup>15</sup> yields a positive pair-correlation function up to  $r_s \lesssim 3$ . Thus validity of our results in the metallic density range may be believed to be good.

The averages of the product of four operators in Eqs. (19) and (20) have been evaluated in the simplest approximation, as has also been done in the past by others. Such a decoupling approximation neglects altogether the effect of electron-electron interactions. We have given a method for finding lowest-order corrections to such a decoupling approximation in the Appendix. An explicit result is derived for the corrections to the average of the product of four operators. It is hoped that this result can be useful in estimating the corrections to the present as well as earlier results.

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#### APPENDIX: LOWEST-ORDER CORRECTIONS TO THE DECOUPLING APPROXIMATION

On solving the commutators in Eqs. (19) and (20), one can see that they involve the averages over the

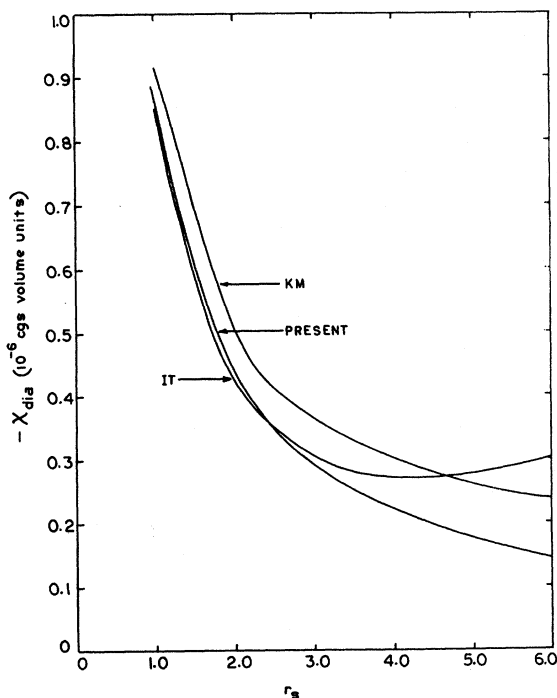


FIG. 1. Diamagnetic susceptibility vs  $r_s$ .

TABLE II. Exchange and correlation correction factor  $\beta$  for simple metals.

	Li	Na	K	Rb	Cs
$r_s$	3.22	3.96	4.87	5.18	5.57
Present results	0.017	0.016	0.015	0.015	0.014
Present results <sup>a</sup>	0.014	0.012	0.010	0.009	0.008
Rajagopal and Jain	0.023	0.024	0.025	0.025	0.025
Ishihara and Tsai	0.101	0.256	0.554	0.687	0.874
Kanazawa and Matsudaira	0.300	0.392	0.510	0.551	0.604

<sup>a</sup>These results are obtained when the Coulomb potential is screened by the RPA (instead of Thomas-Fermi) dielectric function.

product of four operators. Such averages have usually been evaluated<sup>7,15-17,23</sup> in the Hartree-Fock-like decoupling

$$\langle a_{\vec{k}_1}^\dagger a_{\vec{k}_2}^\dagger a_{\vec{k}_3} a_{\vec{k}_4} \rangle = \langle a_{\vec{k}_1}^\dagger a_{\vec{k}_4} \rangle \langle a_{\vec{k}_2}^\dagger a_{\vec{k}_3} \rangle - \langle a_{\vec{k}_1}^\dagger a_{\vec{k}_3} \rangle \langle a_{\vec{k}_2}^\dagger a_{\vec{k}_4} \rangle. \quad (A1)$$

This decoupling is true only when the average is assumed to be taken with respect to the noninteracting part of the Hamiltonian. It altogether neglects the effects of interactions. It is clear that when the above equation is used in evaluating the various averages in Eqs. (19) and (20), all those terms are retained in the summations for which the pair of subscripts of the operators are equal and the remaining terms are neglected. We shall now find

the lowest-order corrections<sup>19</sup> to Eq. (A1) in which none of the subscripts are equal.

It is known that the equal-time correlation functions are independent of time, which implies that

$$i \frac{d}{dt} \langle a_{\vec{k}_1}^\dagger(t) a_{\vec{k}_2}^\dagger(t) a_{\vec{k}_3}(t) a_{\vec{k}_4}(t) \rangle' = 0, \quad (A2)$$

where the prime on the average reminds us that the terms for which any pair of subscripts of the operators involved are equal, are not allowed. Making use of the Heisenberg equation of motion, we obtain

$$\langle [a_{\vec{k}_1}^\dagger, H] a_{\vec{k}_2}^\dagger a_{\vec{k}_3} a_{\vec{k}_4} \rangle + \langle a_{\vec{k}_1}^\dagger [a_{\vec{k}_2}^\dagger, H] a_{\vec{k}_3} a_{\vec{k}_4} \rangle + \langle a_{\vec{k}_1}^\dagger a_{\vec{k}_2}^\dagger [a_{\vec{k}_3}, H] a_{\vec{k}_4} \rangle + \langle a_{\vec{k}_1}^\dagger a_{\vec{k}_2}^\dagger a_{\vec{k}_3} [a_{\vec{k}_4}, H] \rangle = 0. \quad (A3)$$

After solving for the trivial commutators, the above equation reduces to

$$(\omega_{\vec{k}_1} + \omega_{\vec{k}_2} - \omega_{\vec{k}_3} - \omega_{\vec{k}_4}) \langle a_{\vec{k}_1}^\dagger a_{\vec{k}_2}^\dagger a_{\vec{k}_3} a_{\vec{k}_4} \rangle' = \sum_{\vec{q}_1, \vec{q}_2} \phi(\vec{q}_1) (\langle a_{\vec{k}_1}^\dagger a_{\vec{k}_2}^\dagger a_{\vec{k}_3} a_{\vec{k}_4} a_{\vec{q}_2}^\dagger a_{\vec{q}_2+\vec{q}_1} a_{\vec{k}_4-\vec{q}_1} \rangle + \langle a_{\vec{k}_1}^\dagger a_{\vec{k}_2}^\dagger a_{\vec{q}_2}^\dagger a_{\vec{q}_2+\vec{q}_1} a_{\vec{k}_3-\vec{q}_1} a_{\vec{k}_4} \rangle - \langle a_{\vec{k}_1}^\dagger a_{\vec{k}_2}^\dagger a_{\vec{q}_2}^\dagger a_{\vec{q}_2+\vec{q}_1} a_{\vec{k}_3} a_{\vec{k}_4} \rangle - \langle a_{\vec{k}_1}^\dagger a_{\vec{q}_2}^\dagger a_{\vec{q}_2+\vec{q}_1} a_{\vec{k}_2}^\dagger a_{\vec{k}_3} a_{\vec{k}_4} \rangle). \quad (A4)$$

In this equation the averages of the product of six operators are evaluated by making a decoupling approximation of the type given by Eq. (A1). The final result obtained is

$$\langle a_{\vec{k}_1}^\dagger a_{\vec{k}_2}^\dagger a_{\vec{k}_3} a_{\vec{k}_4} \rangle' = [\delta_{\vec{k}_4, \vec{k}_1+\vec{k}_2-\vec{k}_3} / (\omega_{\vec{k}_1} + \omega_{\vec{k}_2} - \omega_{\vec{k}_3} - \omega_{\vec{k}_4})] [\phi(\vec{k}_2 - \vec{k}_3) - \phi(\vec{k}_3 - \vec{k}_1)] [n_{\vec{k}_1} n_{\vec{k}_2} (1 - n_{\vec{k}_3} - n_{\vec{k}_4}) - n_{\vec{k}_3} n_{\vec{k}_4} (1 - n_{\vec{k}_1} - n_{\vec{k}_2})], \quad (A5)$$

which gives the corrections to the average value of the product of four equal time operators and should be added to the right-hand side of Eq. (A1). By taking into account these corrections one can hope to modify the present as well as earlier results.

The method given is quite simple and general and can be extended to a larger number of operators. It is equally applicable to Boson operators as well, though to be specific we have confined ourselves to Fermi operators only.

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