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Wave-vector dependence of the exchange contribution to the electron-gas response functions: An analytic derivation

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We present an analytic procedure for evaluating the wave-vector, q, dependence of the lowest-order exchange contribution to the density and spin-density response functions for the homogeneous electron gas. The two types of contributing diagrams are calculated seperately by different methods. The simpler one based on the lowest-order self-energy insertion can be integrated directly. To obtain the analytic form of the more complex "vertex correction" diagram a differential equation is derived from the original integral representation and then integrated. The derivative of the result has a $(\ln|q-2k_F|)^3$ divergence at $q=2k_F$, which is stronger than that of the Lindhard function. Some consequences of this singularity are discussed, e.g., the asymptotic structure of the statically screened potential of an impurity in a metal and the density fluctuation induced by it. Furthermore, from the low-q expansion of the result we obtain higher-order gradient corrections to the exchange energy functional within linear response.

I. INTRODUCTION

For more than 30 years there have been many attempts to evaluate the effect of the electron-electron interaction on the wave-vector and frequency dependence of the proper density response function $\Pi(\mathbf{q},\omega)$ of the homogeneous electron gas, i.e., to go beyond the Lindhard function.[1] A formal expression for the lowest order correction, $\Pi^1(\mathbf{q},\omega)$, in terms of Feynman integrals was written down in 1959 by DuBois.[2] The first calculation of its q dependence was reported in 1970 and was restricted to the static response function $\Pi^1(\mathbf{q},\omega=0)$ (Geldart and Taylor[3,4]—in the following referred to as GT). It took almost 10 more years until the complete frequency dependence had been examined (Brosens *et al.* and subsequent publications,[5] Holas *et al.*,[6] and Rao *et al.*[7]). $\Pi^1(\mathbf{q},0)$ and variants of it have been recalculated several times (e.g., by Tripathy and Mandal,[8] Toigo and Woodruff,[9] and Alvarellos and Flores[10]). All of the above work on Π^1 required substantial numerical integrations due to the complexity of the Feynman integrals involved. Recently, there has been renewed interest in $\Pi^1(\mathbf{q},0)$ (Kleinman and collaborators,[11] and Chevary and Vosko[12]), especially for the region near $|\mathbf{q}|=q=0$. Again all of these works were left with very complex two-dimensional integrals, which had to be evaluated numerically. However, numerical calculations can approach the origin only up to a small but finite value of q depending on the quality of the numerical integration (compare Refs. 11 and 12). Also the region near $q=2k_F$ is difficult to treat numerically. In particular, the analytic form of the derivative of $\Pi^1(\mathbf{q},0)$, which is expected to diverge at this point, cannot be extracted directly. It is the objective of this paper to present the first completely analytic derivation of $\Pi^1(\mathbf{q},0)$. The novel technique that made this derivation possible is described since it may be useful for related problems. Special attention is paid to the region around $q=2k_F$. In particular, the singularity in the derivative of $\Pi^1(\mathbf{q},0)$ at $q=2k_F$ is found to be $(\ln|q-2k_F|)^3$. If the strength of this singularity is not damped by higher-order corrections, its effect on a number of phenomena, e.g., Kohn anomalies, will be important. We indicate consequences of this property and those of $\Pi^1(\mathbf{q},0)$ at $q=0$. It is worth noting that $\Pi^1(\mathbf{q},0)$ also determines the exchange contribution to the spin response function.[13]

Diagrammatically $\Pi^1(\mathbf{q},\omega)$ (we shall refer to Π^1 as the exchange contribution to Π in distinction to the Hartree-Fock series of which Π^1 is the lowest-order term) is given by the graphs shown in Fig. 1.[14] In the following we shall use the notation introduced by Geldart and Vosko,[15] who call the first diagram in Fig. 1 Π_A, whereas the sum of the latter two diagrams is denoted by Π_B. The frequency integrations in these diagrams are simple contour integrals. In terms of the dimensionless function

$$I(\mathbf{q}) = \frac{\pi^3}{m^2e^2}\Pi^1(\mathbf{q},0) = A(\mathbf{q}) + B(\mathbf{q}) \qquad (1)$$

one finds, for the A and B graphs, respectively,

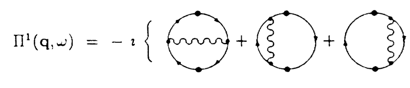

FIG. 1. Feynman diagrams for $\Pi^1(\mathbf{q},\omega)$, which for $\omega=0$ give rise to Eqs. (2) and (3).

$$A(\mathbf{q}) \equiv -16\pi^4 \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} \frac{\Theta(k_F - |\mathbf{p} - \frac{1}{2}\mathbf{q}|)\Theta(k_F - |\mathbf{k} - \frac{1}{2}\mathbf{q}|)}{(\mathbf{q}\cdot\mathbf{p})\,(\mathbf{q}\cdot\mathbf{k})} \left(\frac{+1}{(\mathbf{p}+\mathbf{k})^2} + \frac{+1}{(\mathbf{p}-\mathbf{k})^2} \right)$$
$$\equiv A_+(\mathbf{q}) + A_-(\mathbf{q}) \,, \qquad (2)$$

$$B(\mathbf{q}) \equiv -16\pi^4 \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} \frac{\Theta(k_F - |\mathbf{p} - \frac{1}{2}\mathbf{q}|)\Theta(k_F - |\mathbf{k} - \frac{1}{2}\mathbf{q}|)}{(\mathbf{q}\cdot\mathbf{p})^2} \left(\frac{+1}{(\mathbf{p}+\mathbf{k})^2} - \frac{1}{(\mathbf{p}-\mathbf{k})^2} \right)$$
$$\equiv B_+(\mathbf{q}) + B_-(\mathbf{q}) \,, \qquad (3)$$

where the $\pm$ signs in $A_\pm(\mathbf{q})$ and $B_\pm(\mathbf{q})$ refer to the relative sign between $\mathbf{p}$ and $\mathbf{k}$ in the Coulomb denominator inside the large parentheses [note that these formulas differ from the corresponding ones of GT by a factor of -2, where the minus sign is due to the different definitions of $\Pi(\mathbf{q},\omega)$]. These "symmetric" (in $\mathbf{p}$ and $\mathbf{k}$) forms for $A_\pm(\mathbf{q})$ and $B_\pm(\mathbf{q})$ are deceptive, in that they make it appear that the $+$ and the $-$ terms are very similar. In fact they are not, the $+$ type of term being much more complicated to evaluate, as will be seen below.

Chevary and Vosko[12] emphasize the importance of Pauli-principle restrictions for the numerical calculation of $I(\mathbf{q})$. This shows up in additional step functions in the integrands of Eqs. (2) and (3) without changing the value of these integrals. In this way one avoids terms involving principal-part integrals that do not exist in the final result. For an analytic evaluation, however, principal-part integrals pose no problems. We thus use the above simple form of $A(\mathbf{q})$ and $B(\mathbf{q})$.

The symmetric forms for $A(\mathbf{q})$ and $B(\mathbf{q})$, Eqs. (2) and (3), have been useful for numerical work in that they allow the $\ln|q|$ singularities present in the individual terms to be cancelled on a point by point basis. Furthermore, in evaluating integrals of this type there has been a tendency towards using spherical coordinates. For example, GT utilized them and, after performing the two azimuthal angle integrations analytically, were left with a four-dimensional integral which they had to calculate numerically. Brosens *et al.*[5] appreciated that in cylindrical coordinates with the z axis in $\mathbf{q}$ direction four of the variables only enter the interaction part of the integrand and can be integrated analytically. However, the resulting expression is very complicated and no way has been found to evaluate the remaining two integrals analytically. On the other hand it is well known that the B type of graph is based on the self-energy which can be evaluated analytically for a static interaction. Thus the B diagram is easily reduced to a two-dimensional integral. Using cylindrical coordinates again this integral can be performed. We outline the main steps in Appendix A. Unfortunately, for the A type of graph an unsymmetric choice for the coordinates does not allow for a straightforward integration due to the inherent symmetries in the integral. To evaluate this integral we utilized a new technique. Basically, we transform the original integral (2) into a differential equation for $A(\mathbf{q})$ (again applying cylindrical coordinates) which can be solved easily. The boundary conditions in this context are given by low-order terms of the large-q expansion of the original integral. This method turns out to be very powerful in the present case and consequently could be very useful for similar problems. We demonstrate this point in Appendix B by applying our method also to $B(\mathbf{q})$, which makes its evaluation very simple.

The organization of the paper is as follows. In Sec. II we evaluate and discuss the analytic form of $I(\mathbf{q})$, Eq. (1), refering to the various Appendixes for details. In Sec. III the effect of $I(\mathbf{q})$ on screening of impurities in the homogeneous electron gas is presented, with the surprising result that for very large distances r from the impurity the screening charge falls off as $[\cos(2k_Fr)(\ln|4k_Fr|)^2]/r^3$ in distinction to $\cos(2k_Fr)/r^3$ for the noninteracting situation. Furthermore, in Appendix E we use our $I(\mathbf{q})$ to obtain low-order gradient corrections to the exchange-energy functional.

II. EVALUATION OF $I(\mathbf{Q})$

We start with a direct integration of $B(\mathbf{q})$. For the evaluation of the integral (3) one rewrites it in terms of the lowest-order self-energy,[14]

$$B_+(\mathbf{q}) = \frac{2}{e^2} \int d^3p \frac{\Theta(k_F - p)}{(q^2 + 2\mathbf{q}\cdot\mathbf{p})^2} \Sigma(|\mathbf{p}+\mathbf{q}|) \,, \qquad (4)$$

$$B_-(\mathbf{q}) = -\frac{2}{e^2} \int d^3p \frac{\Theta(k_F - p)}{(q^2 + 2\mathbf{q}\cdot\mathbf{p})^2} \Sigma(p) \,, \qquad (5)$$

$$\Sigma(p) = -\frac{e^2}{2\pi} \left(2k_F + \frac{k_F^2 - p^2}{p} \ln\left|\frac{p+k_F}{p-k_F}\right| \right) . \qquad (6)$$

The subsequent integrations are elementary. They are summarized in Appendix A. In terms of the characteristic dimensionless variable $Q = q/2k_F$ the results are

$$B_+(Q) = \frac{1-Q^2}{16Q^2} \left(\ln\left|\frac{1+Q}{1-Q}\right| \right)^2 - \ln|Q| + \frac{1}{4Q^2} + \frac{1+2Q}{4Q} \ln|1+Q| - \frac{1-2Q}{4Q} \ln|1-Q| \,, \qquad (7)$$

$$B_-(Q) = \frac{1-Q^2}{16Q^2} \left(\ln\left|\frac{1+Q}{1-Q}\right| \right)^2 + \frac{1}{4Q} \ln\left|\frac{1+Q}{1-Q}\right| - \frac{1}{4Q^2} \,. \qquad (8)$$

It is interesting to note that $B_{\pm}(Q)$ diverge like $\pm 1/4Q^2$ for small Q. On the other hand the combined result $B(Q)$,

$$B(Q) = \frac{1-Q^2}{8Q^2}\left(\ln\left|\frac{1+Q}{1-Q}\right|\right)^2 + \frac{1+Q}{2Q}\ln|1+Q| - \frac{1-Q}{2Q}\ln|1-Q| - \ln|Q| \, , \tag{9}$$

only diverges logarithmically, as has been shown previously by GT and is finite elsewhere. Note that the singularity of its derivative at $Q = 1$ is stronger than that of the static Lindhard function; however, we will see that the singularity in $A(Q)$ is even stronger.

Using the identity

$$\left(\ln\left|\frac{1+x}{1-x}\right|\right)^2 = 4\left(\sum_{n=0}^{\infty}\frac{x^{2n+1}}{2n+1}\right)^2 = 4\sum_{n=0}^{\infty}\left(\frac{1}{n+1}\sum_{l=0}^{n}\frac{1}{2l+1}x^{2n+2}\right) \, ,$$

one can expand this function for small and large Q,

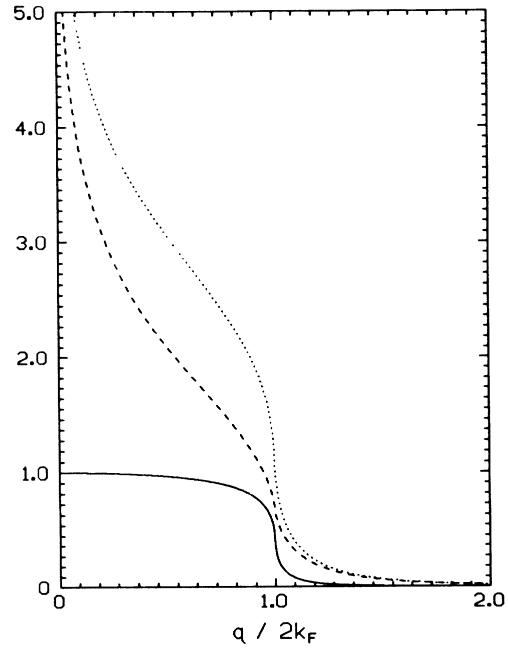

FIG. 2. Wave-vector dependence of the "vertex-correction" diagram, $-A(q)$ (dotted line), the "self-energy insertion" diagrams, $B(q)$ (dashed line), and their sum, $-I(q)$ (solid line).

$$B(Q) = \begin{cases} -\ln|Q| + \frac{3}{2} - \frac{1}{2}\sum_{n=1}^{\infty}\left(\frac{1}{n(n+1)}\sum_{k=0}^{n}\frac{1}{2k+1}Q^{2n}\right) = -\ln|Q| + \frac{3}{2} - \frac{1}{3}Q^2 - \frac{23}{180}Q^4 - \cdots, & Q \le 1 \quad (10) \\ \frac{1}{2}\sum_{n=0}^{\infty}\left(\frac{1}{(n+1)(n+2)}\sum_{k=0}^{n}\frac{1}{2k+1}\frac{1}{Q^{2n+4}}\right) = \frac{1}{4}\frac{1}{Q^4} + \frac{1}{9}\frac{1}{Q^6} + \frac{23}{360}\frac{1}{Q^8} + \cdots, & Q \ge 1 \, . \quad (11) \end{cases}$$

The small-Q expansion agrees with the result of GT, who evaluated the logarithm and the constant of $\frac{3}{2}$. The large-Q expansion agrees with their result in the leading term (compare Eq. 5 of Ref. 4) but differs for the $1/Q^6$ contribution, which is the highest order they present, by a factor of $\frac{8}{7}$. However, the sum of the large-Q expansion of $B(Q)$ and $A(Q)$ is given correctly by GT. Note the similarity between the small-Q and the large-Q expansion. The basic ingredient in both cases is the sum

$$\sum_{k=0}^{n}\frac{1}{2k+1} = \tfrac{1}{2}[\psi(n+\tfrac{3}{2}) + C] + \ln(2) \equiv \Psi(n) \, , \tag{12}$$

where $\psi(n)$ is Euler's psi function. In the following we abbreviate this sum by $\Psi(n)$. As can be seen best from Fig. 2, $B(Q)$ is positive for all Q (and monotonically decreasing).

As already mentioned in the Introduction, we are not able to find $A(Q)$ by direct integration. We thus have to rely on a different technique. In the following we use the fact that there are several ways of defining a function. First, one can represent it in terms of elementary or special functions. A Taylor-series expansion of the function contains the same information. Equivalent to these two possibilities are integral representations (which is the starting point in our case). Finally, a differential equation plus boundary conditions gives a function uniquely. We shall combine the various representations to derive $A(Q)$. As an illustration of its power and validity, the same method is applied to $B(Q)$ in Appendix B.

We start with the discussion of $A_-(Q)$. After scaling $\mathbf{p}$ and $\mathbf{k}$ in the corresponding integral (2) by $\mathbf{q}/2$, one obtains

$$A_-(K^{-1}) = -4\pi^4\int\frac{d^3p}{(2\pi)^3}\int\frac{d^3k}{(2\pi)^3}\frac{\Theta(K-|\mathbf{p}-\hat{\mathbf{q}}|)\,\Theta(K-|\mathbf{k}-\hat{\mathbf{q}}|)}{(\hat{\mathbf{q}}\cdot\mathbf{p})(\hat{\mathbf{q}}\cdot\mathbf{k})(\mathbf{p}-\mathbf{k})^2} \, , \tag{13}$$

where $K = 1/Q = 2k_F/q$ and $\hat{\mathbf{q}} = \mathbf{q}/q$. The variable K is most useful for the following discussion as it enters only in the boundaries of the above integral. In other words, as the first step of our scheme we transform the original integral in such a way as to make the external momentum only appear in the limits, which is easily achieved in the present case. We now first shift both the $\mathbf{p}$ and $\mathbf{k}$ integrations by $\hat{\mathbf{q}}$,

$$A_-(K^{-1}) = -4\pi^4 \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} \frac{\Theta(K-p)\,\Theta(K-k)}{(1+\hat{\mathbf{q}}\cdot\mathbf{p})(1+\hat{\mathbf{q}}\cdot\mathbf{k})(\mathbf{p}-\mathbf{k})^2} \,. \tag{14}$$

Using cylindrical coordinates[5] and carrying through the ϕ integrations, one arrives at

$$A_-(K^{-1}) = -\tfrac{1}{16} \int_{-K}^{K} dz \int_{-K}^{K} dz' \int_0^{K^2-z^2} dx \int_0^{K^2-z'^2} dy \frac{1}{(1+z)(1+z')} \frac{1}{\{[(z-z')^2+x+y]^2-4xy\}^{1/2}} \,. \tag{15}$$

The crucial observation now is that a differentiation with respect to K automatically reduces the number of integrations by one. Actually, only the derivative of the inner integrals gives a nonzero result. In this way one starts to transform the integral representation (14) into a differential equation which will turn out to be easier to solve than the initial integral. This transformation represents the second step of our method. The details of this process are given in Appendix C. The result is

$$\frac{d}{dK}(1-K^2)\frac{d}{dK}\frac{1}{K}\frac{d}{dK}A_-(K^{-1}) = -\frac{1}{K(1-K^2)} \ln\left|\frac{1+K}{1-K}\right| \,, \tag{16}$$

which can easily be rewritten in terms of Q,

$$\frac{d}{dQ}(1-Q^2)\frac{d}{dQ}Q^3\frac{d}{dQ}A_-(Q) = \frac{Q}{1-Q^2} \ln\left|\frac{1+Q}{1-Q}\right| \,. \tag{17}$$

The solution of this differential equation is the third step of our scheme. In the present case it can be integrated directly twice using the fact that

$$\int_0^Q dx \left(f(x) \int_0^x dy\, g(y)\right) = F(Q) \int_0^Q dy\, g(y) - \int_0^Q dx\, F(x)\, g(x) \,,$$

where

$$\frac{d}{dx}F(x) = f(x) \,,$$

by virtue of a partial integration in which the y integral is used as one x-dependent function, $f(x)$ as the other. One finally ends up with

$$\begin{aligned} A_-(Q) = {} & -\frac{1-Q^2}{48Q}\left(\ln\left|\frac{1+Q}{1-Q}\right|\right)^3 - \frac{1-Q^2}{24Q^2}\int_0^Q dx \left(\ln\left|\frac{1+x}{1-x}\right|\right)^3 \\ & + \left(\frac{1}{8Q} + \frac{1-Q^2}{16Q^2}\ln\left|\frac{1+Q}{1-Q}\right|\right)\int_0^Q dx \left(\ln\left|\frac{1+x}{1-x}\right|\right)^2 + a\left(\frac{1-Q^2}{Q^2}\ln\left|\frac{1+Q}{1-Q}\right| + \frac{2}{Q}\right) + \frac{b}{Q^2} + c \,. \end{aligned} \tag{18}$$

The terms containing the constants a, b, and c represent the solution of the homogeneous differential equation corresponding to Eq. (17). As one knows that $A_-(Q)$ has to vanish like $1/Q^4$ for large Q (see GT or Appendix D) and is an even function of Q, the coefficients a, b, and c have to be identically zero.

We proceed with the discussion of $A_+(Q)$. If one attempts to find $A_+(Q)$ in the same way as we obtained $A_-(Q)$, one has to start with the scaled and shifted integral

$$A_+(K^{-1}) = -4\pi^4 \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} \frac{\Theta(K-p)\,\Theta(K-k)}{(1+\hat{\mathbf{q}}\cdot\mathbf{p})(1+\hat{\mathbf{q}}\cdot\mathbf{k})(2\hat{\mathbf{q}}+\mathbf{p}+\mathbf{k})^2} \,. \tag{19}$$

In the shifted form of the integral the difference between $A_-(Q)$, Eq. (14), and $A_+(Q)$, Eq. (19), is apparent. The additional $2\hat{\mathbf{q}}$ in the denominator leads to substantial complications. Again the angular integrations can be carried through directly,

$$A_+(K^{-1}) = -\tfrac{1}{16} \int_{-K}^{K} dz \int_{-K}^{K} dz' \int_0^{K^2-z^2} dx \int_0^{K^2-z'^2} dy \frac{1}{(1+z)(1+z')} \frac{1}{\{[(2+z+z')^2+x+y]^2-4xy\}^{1/2}} \,.$$

Differentiating once and carrying through the remaining x integration, one ends up with

$$\frac{d}{dK}A_+(K^{-1}) = -\frac{K}{4} \int_{-K}^{K} dz \int_{-K}^{K} dz' \frac{1}{(1+z)(1+z')} \ln\left|\frac{W(z,z',K) + z(2+z+z') + 2(1+z')}{(2+z+z')^2}\right| \,,$$

where $W(p,k,K)$ is given by

$$W(p,k,K) \;=\; [K^2(2+z+z')^2+4(1+z)(1+z')(1+z+z')]^{1/2} \; . \tag{20}$$

In contrast to the case of $A_-(Q)$ the second differentiation does not simplify the expression sufficiently to perform further integrations. Thus the second step of our scheme cannot be carried through in full generality for the case of $A_+(Q)$.

To circumvent this difficulty we resort to a power-series expansion in $1/Q$ (i.e., K). We have calculated the first five terms of $A_+(Q)$ (see Appendix D). After applying the same differential operator on these lowest five orders as we found useful for $A_-(K^{-1})$, one obtains the small-K expansion of the differential equation for $A_+(Q)$,

$$\frac{d}{dK}(1-K^2)\frac{d}{dK}\frac{1}{K}\frac{d}{dK}A_+(K^{-1}) = -2K^2(1+\tfrac{4}{3}K^2+\tfrac{23}{15}K^4+\tfrac{176}{105}K^6+\tfrac{563}{315}K^8+\cdots) \; . \tag{21}$$

This can be compared to the corresponding expansion of the inhomogeneity in the differential equation of $A_-(K^{-1})$,

$$\frac{d}{dK}(1-K^2)\frac{d}{dK}\frac{1}{K}\frac{d}{dK}A_-(K^{-1}) = -2\sum_{n=0}^{\infty}\Psi(n)\,K^{2n} = -2(1+\tfrac{4}{3}K^2+\tfrac{23}{15}K^4+\tfrac{176}{105}K^6+\tfrac{563}{315}K^8+\cdots) \; . \tag{22}$$

The difference between both expansions is simply a factor of K^2. The similarity of $A_-(Q)$ and $A_+(Q)$ is only evident after the above differential operator has been applied and does not occur in $A_-(Q)$ and $A_+(Q)$ themselves. We thus presume

$$\frac{d}{dK}(1-K^2)\frac{d}{dK}\frac{1}{K}\frac{d}{dK}A_+(K^{-1}) \;=\; -\frac{K}{(1-K^2)}\,\ln\left|\frac{1+K}{1-K}\right| \tag{23}$$

and consequently

$$\frac{d}{dQ}(1-Q^2)\frac{d}{dQ}Q^3\frac{d}{dQ}A_+(Q) \;=\; \frac{1}{Q(1-Q^2)}\,\ln\left|\frac{1+Q}{1-Q}\right| \tag{24}$$

to be the correct differential equation for $A_+(K^{-1})$. Again we note that the difference between Eqs. (24) and (17) is only a factor of Q^2, the form of the differential operator being an essential ingredient in illustrating the relation between both functions. At the moment we have no completely general proof for Eq. (24). It is based on the above-shown lowest five orders of the small-K expansion. However, we have no doubt about the correctness of Eqs. (23) and (24). We shall comment on this point below.

As for $A_-(Q)$ the differential equation (24) can be integrated directly, with the result (the homogeneous terms have already been dropped)

$$\begin{aligned} A_+(Q) = &-\frac{1-Q^2}{48Q^3}\left(\ln\left|\frac{1+Q}{1-Q}\right|\right)^3+\frac{1-Q^2}{24Q^2}\int_0^Q dx\,\frac{1}{x^2}\left(\ln\left|\frac{1+x}{1-x}\right|\right)^3 \\ &-\left(\frac{1}{8Q}+\frac{1-Q^2}{16Q^2}\ln\left|\frac{1+Q}{1-Q}\right|\right)\int_0^Q dx\,\frac{1}{x^2}\left(\ln\left|\frac{1+x}{1-x}\right|\right)^2 \\ &-\frac{1-Q^2}{8Q^2}\left(\ln\left|\frac{1+Q}{1-Q}\right|\right)^2-\frac{1+Q}{2Q}\ln|1+Q|+\frac{1-Q}{2Q}\ln|1-Q|+\ln|Q| \; . \end{aligned} \tag{25}$$

$A_+(Q)$ has been written in this particular form in order to emphasize that the last line exactly represents $-B(Q)$, showing the large degree of cancellation between $A(Q)$ and $B(Q)$ first noted by DuBois.[2]

Combining the results (18) and (25) leads to the complete $A(Q)$,

$$\begin{aligned} A(Q) = &-\frac{1-Q^4}{48Q^3}\left(\ln\left|\frac{1+Q}{1-Q}\right|\right)^3+\frac{1-Q^2}{24Q^2}\int_0^Q dx\,\frac{1-x^2}{x^2}\left(\ln\left|\frac{1+x}{1-x}\right|\right)^3 \\ &-\left(\frac{1}{8Q}+\frac{1-Q^2}{16Q^2}\ln\left|\frac{1+Q}{1-Q}\right|\right)\int_0^Q dx\,\frac{1-x^2}{x^2}\left(\ln\left|\frac{1+x}{1-x}\right|\right)^2-B(Q) \; . \end{aligned} \tag{26}$$

This result, of course, satisfies the combined differential equations (17) and (24). We did not find a representation for $A(Q)$ in terms of elementary functions. However, there are several ways of representing $A(Q)$ via simple integrals or special functions. The version chosen here exhibits the finite value of $A(Q)$ and the strength of the singularity of its first derivative at $Q=1$ most clearly.

For completeness we present the expansions of $A(Q)$ for small and large Q,

$$A(Q) = \begin{cases} \ln|Q| - \frac{5}{2} + \frac{1}{2}\sum_{n=1}^{\infty}\left(\frac{\Psi(n)^2}{n(n+1)}Q^{2n}\right) = \ln|Q| - \frac{5}{2} + \frac{4}{9}Q^2 + \frac{529}{2700}Q^4 + \cdots, \quad Q \le 1 & (27) \\ -\frac{1}{2}\sum_{n=0}^{\infty}\left(\frac{\Psi(n)^2}{(n+1)(n+2)}\,\frac{1}{Q^{2n+4}}\right) & \\ = -\left[\frac{1}{4}\frac{1}{Q^4} + \frac{1}{12}\left(\frac{4}{3}\right)^2\frac{1}{Q^6} + \frac{1}{24}\left(\frac{23}{15}\right)^2\frac{1}{Q^8} + \frac{1}{40}\left(\frac{176}{105}\right)^2\frac{1}{Q^{10}} + \cdots\right], \quad Q \ge 1\,. & (28) \end{cases}$$

As for $B(Q)$ the large-Q expansion agrees with the work of GT for the leading $1/Q^4$ term. The coefficient of the $1/Q^6$ contribution (which is the highest order that they present) differs from their result (Eq. 3 of Ref. 4) by a factor of $\frac{32}{29}$. As already mentioned for the expansion of $B(Q)$, GT's expansion of the sum of $A(Q)$ and $B(Q)$ is correct. Note, that the coefficients of both expansions of $A(Q)$ differ from the corresponding ones of $B(Q)$ just by an additional $\Psi(n)$, Eq. (12), in $A(Q)$.

In Fig. 2 $A(Q)$ is compared with $B(Q)$. $A(Q)$ is negative for all Q and one has

$$|A(Q)| > |B(Q)|\,.$$

Furthermore, Fig. 2 indicates the large degree of cancellation between the diagrams.

With the results for $B(Q)$, Eq. (9), and $A(Q)$, Eq. (26), it is straightforward to write down the exchange contribution to the response function at zero frequency, $I(Q)$,

$$I(Q) = -\frac{1-Q^4}{48Q^3}\left(\ln\left|\frac{1+Q}{1-Q}\right|\right)^3 + \frac{1-Q^2}{24Q^2}\int_0^Q dx\,\frac{1-x^2}{x^2}\left(\ln\left|\frac{1+x}{1-x}\right|\right)^3$$
$$-\frac{1}{8}\left(\frac{1}{Q} + \frac{1-Q^2}{2Q^2}\ln\left|\frac{1+Q}{1-Q}\right|\right)\int_0^Q dx\,\frac{1-x^2}{x^2}\left(\ln\left|\frac{1+x}{1-x}\right|\right)^2\,. \tag{29}$$

Equation (29) represents the main result of the present paper. The above form exhibits most obviously the structure of $I(Q)$ and its first derivative at $Q=1$. To allow for comparison we furthermore show the Taylor expansions of $I(Q)$ for small and large Q,

$$I(Q) = \begin{cases} -1 + \frac{1}{2}\sum_{n=1}^{\infty}\left(\frac{\Psi(n)[\Psi(n)-1]}{n(n+1)}Q^{2n}\right) = -1 + \frac{1}{9}Q^2 + \frac{46}{675}Q^4 + \frac{1562}{33\,075}Q^6 + \frac{17\,453}{496\,125}Q^8 + \cdots, \quad Q \le 1 & (30) \\ \frac{1}{2}\sum_{n=1}^{\infty}\left(\frac{\Psi(n)[\Psi(n)-1]}{(n+1)(n+2)}\,\frac{1}{Q^{2n+4}}\right) = -\left(\frac{1}{27}\frac{1}{Q^6} + \frac{23}{675}\frac{1}{Q^8} + \frac{1562}{55\,125}\frac{1}{Q^{10}} + \frac{34\,906}{1\,488\,375}\frac{1}{Q^{12}} + \cdots\right), \quad Q \ge 1\,, & (31) \end{cases}$$

where $\Psi(n)$ is given by Eq. (12). Both expansions agree with all existing work[2,15,4,16] to the orders that were already known (the coefficients of the second and third terms in the large-Q expansion have been evaluated by Chevary and Vosko[16]). For the large-Q expansion this is in no way surprising as our calculation is based on this expansion. On the other hand it is a strong confirmation of our result that the value of $I(Q)$ at $Q=0$ is identical with DuBois's calculation.[2]

The values for $I(Q)$ from our analytic function are identical with those of the numerical calculation of Chevary and Vosko.[12] The agreement between both results depends only on the accuracy of the numerical integration they used. The two regions of Q that are numerically difficult to treat are near $Q=0$ and $Q=1$. Consequently one finds at $Q=0.001$ a relative accuracy of 10^{-8} and at $Q=0.5$ less than 10^{-10}. The point $Q=1$ represents the numerically most subtle case. So the agreement reduces to 1.5×10^{-7} at $Q=0.999$ and finally to 3×10^{-5} at $Q=1$. For values of Q greater than 1 the agreement is even better ($Q=1.001{:}10^{-8}$). Also Chevary and Vosko fitted the first four coefficients of the small-Q expansion from their numerical results (without knowledge of the analytic form presented here). The coefficients of Q^2 and Q^4 that they obtained are identical to our result; the Q^6 coefficient is off by no more than 0.36%. This comparison definitively establishes the correctness of our analytic $I(Q)$ in spite of the missing general proof for the differential equation for $A_+(Q)$.

One can also directly calculate the leading terms of an expansion of $I(Q)$ around $Q=1$. Defining $\tilde{Q} = Q-1$ one finds

$$I(1+\tilde{Q}) = \frac{1}{8}\Bigg\{ -\frac{\pi^2}{3} - \tilde{Q}\left[\frac{2}{3}\left(\ln\left|\frac{\tilde{Q}}{2}\right|\right)^3 + \frac{\pi^2}{3}\ln\left|\frac{\tilde{Q}}{2}\right| + \frac{2}{3}J - \frac{\pi^2}{3}\right]$$
$$+\tilde{Q}^2\left[\left(\ln\left|\frac{\tilde{Q}}{2}\right|\right)^3 + 2\left(\ln\left|\frac{\tilde{Q}}{2}\right|\right)^2 + \left(\frac{\pi^2}{2}-1\right)\ln\left|\frac{\tilde{Q}}{2}\right| + J - \frac{\pi^2}{6} + \frac{1}{2}\right]$$
$$-\tilde{Q}^3\left[\frac{4}{3}\left(\ln\left|\frac{\tilde{Q}}{2}\right|\right)^3 + \frac{15}{4}\left(\ln\left|\frac{\tilde{Q}}{2}\right|\right)^2 + \frac{2\pi^2}{3}\ln\left|\frac{\tilde{Q}}{2}\right| + \frac{4}{3}J - \frac{\pi^2}{24}\right]$$
$$+\tilde{Q}^4\left[\frac{5}{3}\left(\ln\left|\frac{\tilde{Q}}{2}\right|\right)^3 + \frac{131}{24}\left(\ln\left|\frac{\tilde{Q}}{2}\right|\right)^2 + \left(\frac{5\pi^2}{6}+\frac{13}{8}\right)\ln\left|\frac{\tilde{Q}}{2}\right| + \frac{5}{3}J + \frac{11\pi^2}{144} - \frac{37}{96}\right]$$
$$-\tilde{Q}^5\left[2\left(\ln\left|\frac{\tilde{Q}}{2}\right|\right)^3 + \frac{229}{32}\left(\ln\left|\frac{\tilde{Q}}{2}\right|\right)^2 + \left(\pi^2+\frac{173}{48}\right)\ln\left|\frac{\tilde{Q}}{2}\right| + 2J + \frac{37\pi^2}{192} - \frac{125}{192}\right]$$
$$+O(\tilde{Q}^6(\ln|\tilde{Q}|)^3)\Bigg\}\,. \qquad (32)$$

where

$$J = \int_0^1 dx\,\frac{1-x^2}{x^2}\left(\ln\left|\frac{1+x}{1-x}\right|\right)^3 = 3.606\,170\,709\,7\cdots\,.$$

The relative accuracy of Eq. (32) is 4×10^{-6} at $Q=0.9$ and 4×10^{-5} at $Q=1.1$. $I(Q)$ is plotted in Fig. 2. Note that the value at $Q=1$ can be evaluated analytically by using

$$\int_0^1 dx\frac{1-x^2}{x^2}\left(\ln\left|\frac{1+x}{1-x}\right|\right)^2 = \frac{\pi^2}{3}\,.$$

The value of $|I(Q=1)| = \pi^2/24 = 0.411\,233\,517\ldots$ may be compared to the numerical results of GT (0.4089), Antoniewicz and Kleinman[11] (0.4098), and Chevary and Vosko[12] (0.411 221) confirming the accuracy Chevary and Vosko are claiming to reach ($0.411\,22 \pm 0.000\,02$).

The strength of the singularity of the derivative of $I(Q)$ at $Q=1$ is

$$\left.\frac{d}{dQ}I(Q)\right|_{Q\approx1} \approx -\frac{1}{24}\left[2\left(\ln\left|\frac{1-Q}{2}\right|\right)^3 + \pi^2\ln\left|\frac{1-Q}{2}\right| + \text{finite terms}\right],$$

which is stronger than that of the static Lindhard function. Assuming this result to be characteristic for the exact screening function leads to interesting consequences, the most basic of which is discussed in Sec. III. It is, however, not clear to what extent dynamic screening will alter this behavior. Thus any use of this result for real physical phenomena has to be regarded as tentative.

So far we have discussed only the spin-unpolarized case. Noting that for a spin-polarized system the spin-up and spin-down electrons respond seperately for all one electron-hole pair processes, we can write

$$I_{SP}(Q) = \tfrac{1}{2}[I(Q_\uparrow) + I(Q_\downarrow)]\,. \qquad (33)$$

Here $Q_\uparrow$ and $Q_\downarrow$ differ by their scale given by the spin-up and spin-down Fermi momenta,

$$Q_\uparrow = \frac{q}{2k_{F\uparrow}}\,, \qquad (34)$$

$$Q_\downarrow = \frac{q}{2k_{F\downarrow}}\,. \qquad (35)$$

III. STATIC SCREENING IN THE HOMOGENEOUS ELECTRON GAS

One of the most important consequences of the structure of the response function is the screening of impurities in the homogeneous electron gas. To lowest order this leads to the well-known long-range oscillations in the density deviation $\delta n(r)$ (induced by a localized charge) which, e.g., are responsible for the Friedel oscillations due to impurities in metals.[17,18] In the following we want to show that the exchange contribution to the response function qualitatively changes the large-r behaviour of $\delta n(r)$.

In linear response the density deviation induced by a point charge of strength Ze is given by

$$\delta n(r) = \frac{Zi}{4\pi^2 r}\int_{-\infty}^{\infty} dq\, q e^{iqr}\left(\frac{q^2}{q^2 - 4\pi e^2\Pi(q,0)} - 1\right)\,. \qquad (36)$$

In order to show the asymptotic behaviour of $\delta n(r)$, this integral has to be evaluated for large r. A standard procedure (compare Ref. 14) is to rewrite Eq. (36) as a contour integral. Noting that due to their origin all logarithms in $\Pi^1(Q,0)$ can be interpreted as

$$\ln|1\pm Q| = \tfrac{1}{2}\lim_{\eta\to0}\ln[(1\pm Q)^2+\eta^2]\,, \qquad (37)$$

one can write Eq. (36) (to first order),

$$\delta n(r) = \frac{Zi}{4\pi^2 r} \lim_{\eta\to 0} \int_{-\infty}^{\infty} dq\, q e^{iqr} \left(\frac{q^2}{q^2 - 4\pi e^2[\Pi_\eta^0(q,0) + \Pi_\eta^1(q,0)]} - 1 \right) , \tag{38}$$

where the subscript η indicates that all logarithmic terms have to be replaced by Eq. (37). Choosing the branch cuts of $\ln|(1 \pm Q)^2 + \eta^2|$ to extend from $\pm 1 \pm i\eta$ to $\pm 1 \pm i\infty$ and deforming the integration contour to go along these branch cuts as shown in Fig. 3, the integral (38) is essentially determined by the phase shift of the logarithms in $\Pi_\eta(q,0)$. The new feature of $\Pi^1(q,0)$, Eqs. (1) and (29), is the occurrence of squares and cubes of the logarithm whose associated phase shifts along $C_{1,2}$ (where $Q = \pm 1 + iv$) are

$$\lim_{\epsilon\to 0}\{[\ln|(\epsilon + iv)^2 + \eta^2|]^2 - [\ln|(-\epsilon + iv)^2 + \eta^2|]^2\} = 4\pi i \ln|v^2 - \eta^2| ,$$

$$\lim_{\epsilon\to 0}\{[\ln|(\epsilon + iv)^2 + \eta^2|]^3 - [\ln|(-\epsilon + iv)^2 + \eta^2|]^3\} = 6\pi i(\ln|v^2 - \eta^2|)^2 - 2\pi^3 i .$$

For the asymptotically dominant terms one finds (including the lowest order[17])

$$\delta n(r) \sim -\frac{Z\alpha r_s}{\pi^2\left(2 + \frac{\alpha r_s}{\pi} + \frac{\alpha^2 r_s^2}{12}\right)^2} \frac{\cos(2k_F r)}{r^3} \left[1 + \frac{\alpha r_s}{2\pi}\left(\frac{\pi^2}{4} - 1 + (1 - C - \ln|4k_F r|)^2\right)\right] \quad \text{as } r \to \infty , \tag{39}$$

where $\alpha = (4/9\pi)^{1/3}$ and $C = 0.5772\ldots$ is the Euler-Mascheroni constant. Note that the integrated asymptotic density remains finite.

Thus for very high density and not too large r the lowest order in e^2, i.e., r_s, dominates. But with increasing r the $\ln|4k_F r|$ term from the exchange contribution becomes more important than the lowest-order term for all densities. This effect sets in for smaller r the lower the density. As an example one finds at the nearest-neighbor distance in aluminum, $r_{\rm NN} = 8.58/2k_F$, that the exchange term changes $\delta n(r_{\rm NN})$ by a factor of 1.5, whereas in sodium, $r_{\rm NN} = 6.73/2k_F$, it is already a factor of 3. Similar modifications to the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction will occur since $\Pi^1(q,0)$ is also the exchange contribution to the spin response function.

Of course, dynamic screening of the bare Coulomb interaction may affect the singularity of the derivative of $\Pi^1(q,0)$ at $q = 2k_F$. If screening alters the singularity this can only lead to a reduction of its strength, and even in this case it is not clear whether the reduction would soften the singularity so much as to let $\Pi^0(q,0)$ dominate for all r. Furthermore, as one could expect higher-order contributions to $\Pi(q,0)$ to contain still higher powers of the relevant logarithm, this result is only an indication that the lowest-order term $\Pi^0(q,0)$ might not represent the final answer. The complete response function could lead to a qualitatively different asymptotic behavior than the Lindhard function.

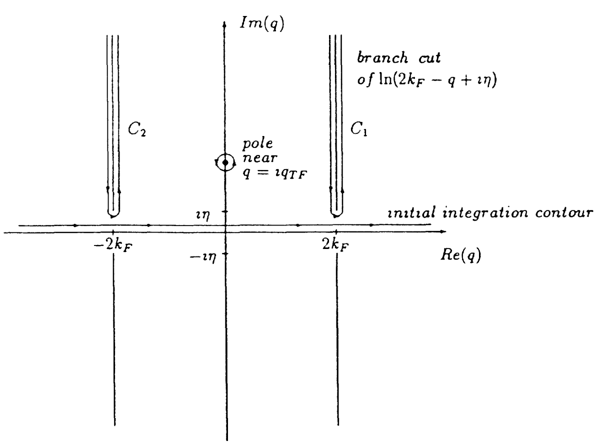

FIG. 3. C_1 and C_2 are the deformed contours for the asymptotic evaluation of Eq. (38).

IV. CONCLUSIONS

We have derived the analytic form of the first-order proper response function, Eqs. (1) and (29). Although for one part of this function a completely general proof is still lacking, there can be no doubt that the part of the result obtained by generalizing a large-q expansion, Eq. (25), is correct (especially in view of the identity of our analytic result with the numerical calculation of Chevary and Vosko). The most interesting feature of the analytic $\Pi^1(q,0)$ certainly is its structure near $q = 2k_F$. The cubic logarithmic divergence of its derivative at this point dominates over the single logarithmic divergence of the Lindhard function. We demonstrated the qualitative change in the density deviation induced by an impurity in a homogeneous electron gas. If this result is unaffected by dynamic screening, important consequences would emerge due to the effect of screening on various physical phenomena. The so-called Kohn anomalies in phonon dispersion curves may serve as an example.

As a by-product of our analytic result for $\Pi^1(\mathbf{q},0)$ we also obtained (in Appendix E) low-order gradient contributions to the exchange-energy functional within linear response beyond the corrected Sham term.[19]

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APPENDIX A: DIRECT ANALYTIC INTEGRATION OF $B(\mathbf{q})$

Starting with Eqs. (4) and (5) and using cylindrical coordinates one has to evaluate

$$B_+(q) = \frac{4\pi}{e^2q^2}\int_{-k_F}^{k_F} dz \int_0^{\sqrt{k_F^2-z^2}} d\rho \, \frac{\rho}{(q+2z)^2}\Sigma(\sqrt{\rho^2+z^2+2zq+q^2}) , \tag{A1}$$

$$B_-(q) = -\frac{4\pi}{e^2q^2}\int_{-k_F}^{k_F} dz \int_0^{\sqrt{k_F^2-z^2}} d\rho \, \frac{\rho}{(q+2z)^2}\Sigma(\sqrt{\rho^2+z^2}) . \tag{A2}$$

With the transformations

$$G = \sqrt{\rho^2+q^2+2qz+z^2}, \qquad E = \sqrt{\rho^2+z^2} ,$$

for $B_+(q)$ and $B_-(q)$, respectively, one can perform the ρ integration directly,

$$B_+(q) = \frac{2}{3q^2}\int_{-k_F}^{k_F} dz \frac{1}{(q+2z)^2}[F(\sqrt{q^2+2qz+k_F^2}) - F(q+z) - 3k_F(k_F^2-z^2)] , \tag{A3}$$

$$B_-(q) = \frac{2}{3q^2}\int_{-k_F}^{k_F} dz \frac{1}{(q+2z)^2}[F(z) - F(k_F) + 3k_F(k_F^2-z^2)] , \tag{A4}$$

$$F(x) = (x^3-3k_F^2x-2k_F^3)\ln\left|1+\frac{x}{k_F}\right| - (x^3-3k_F^2x+2k_F^3)\ln\left|1-\frac{x}{k_F}\right| + k_Fx^2 . \tag{A5}$$

Note that these integrals are well defined for all values of q [apart form the point $q = 2k_F$ where only the sum of $B_+(q)$ and $B_-(q)$ is finite]. Singularities of individual terms cancel each other. Apart from the first term in $B_+(q)$ the integration is straightforward after a shift in the integration variable, $2z = y - q$. For the first term the transformation $u = \sqrt{q^2+2qz+k_F^2}$ is applied. Finally one uses the fact that

$$\int_{\frac{2k_F-q}{2k_F+q}}^{1} dt \frac{\ln|1-t^2|}{t} + \int_{\frac{2k_F+q}{2k_F-q}}^{1} dt \frac{\ln|1-t^2|}{t} = 2\int_{\frac{2k_F-q}{2k_F+q}}^{1} dz \frac{\ln|z|}{z} = \left(\ln\left|\frac{2k_F+q}{2k_F-q}\right|\right)^2 \tag{A6}$$

by virtue of the transformation $z = 1/t$ in one of the terms. After some algebraic manipulations one finds Eqs. (7) and (8).

APPENDIX B: ALTERNATIVE EVALUATION OF $B(q)$

As shown in Appendix A, $B(Q)$ can be obtained by direct integration. The problem is that the same is not possible for $A(Q)$. However, we can derive an ordinary differential equation for $A_-(Q)$ and infer one from the large-Q expansion for $A_+(Q)$. These differential equations are easily solved. In this Appendix we want to demonstrate this procedure for $B(Q)$ in order to establish the method.

The scheme we shall use can be summarized as follows. We first derive an ordinary differential equation for $B_-(Q)$ from the integral representation (3), i.e., with symmetric integration momenta $\mathbf{p}$ and $\mathbf{k}$. We show that this procedure is no more difficult than the direct integration in the more appropriate unsymmetric coordinates. However, we cannot find the differential equation for $B_+(Q)$ using the symmetric coordinates. Instead of applying the same unsymmetric coordinates as for the direct integration (which we know to solve this problem) we shall simulate the situation where one does not have this possibility [as for $A_+(Q)$]. We shall resort to a power-series expansion for large Q, calculating its lowest five orders. We then construct the differential equation for $B_+(Q)$ from this expansion. It turns out to be very similar to that of $B_-(Q)$ and thus allows for a much easier integration than the original integral.

As first step in this alternative evaluation of $B(Q)$ we rewrite the original integral such that the external momentum Q only enters in the boundaries of the integral. After scaling all momenta in Eq. (3) by $q/2$ one finds the equivalent of Eq. (13),

$$B_-(K^{-1}) = 4\pi^4\int\frac{d^3p}{(2\pi)^3}\int\frac{d^3k}{(2\pi)^3}\frac{\Theta(K-|\mathbf{p}-\hat{\mathbf{q}}|)\,\Theta(K-|\mathbf{k}-\hat{\mathbf{q}}|)}{(\hat{\mathbf{q}}\cdot\mathbf{p})^2\,(\mathbf{p}-\mathbf{k})^2} ,$$

where $\hat{\mathbf{q}} = \mathbf{q}/q$ and $K = 1/Q$. In cylindrical coordinates the angular integrations are easily carried through,

$$B_-(K^{-1}) = \tfrac{1}{16}\int_{-K}^{K}dz\int_0^{K^2-z^2}dx\int_{-K}^{K}dz'\int_0^{K^2-z'^2}dy\,\frac{1}{(1+z)^2}\frac{1}{\{[(z-z')^2+x+y]^2-4xy\}^{1/2}}\,. \tag{B1}$$

The x and y integrations can also be performed.[5] However, the result is a rather complex two-dimensional integral that has not been evaluated analytically up to now. By the method we want to illustrate in this Appendix, one obtains simple integrals even for the above symmetric coordinates.

As second step we derive a differential equation for $B_-(Q)$. Differentiating Eq. (B1) by K and carrying through the remaining x and y integrations yields

$$\begin{aligned}\frac{1}{K}\frac{d}{dK}B_-(K^{-1}) &= \tfrac{1}{8}\int_{-K}^{K}dz\frac{1}{(1+z)^2}\Bigg(\int_{-K}^{z}dz'(\ln|z'-K|+\ln|z+K|)\\ &\qquad +\int_{z}^{K}dz'(\ln|z'+K|+\ln|z-K|)-2\int_{-K}^{K}dz'\ln|z-z'|\Bigg)\\ &= \tfrac{1}{4}\int_{-K}^{K}dz\frac{1}{(1+z)^2}[(z-K)\ln|z-K|-(z+K)\ln|z+K|+2K\ln|2K|+K]\,.\end{aligned}$$

There are several ways to proceed from this point. In anticipation of a transformation that is useful for $A_-(Q)$, we substitute $y=(1+z)/(1\pm K)$ and find

$$\begin{aligned}\frac{1}{K}\frac{d}{dK}B_-(K^{-1}) = \frac{1}{4}\Bigg[&-\frac{2K}{1-K}\ln|1+K|+\frac{2K}{1+K}\ln|1-K|+\frac{2K^2}{1-K^2}(2\ln|2K|+1)+\left(\ln\left|\frac{1+K}{1-K}\right|\right)^2\\ &+\int_1^{\frac{1-K}{1+K}}dy\frac{1-y}{y^2}\ln|1-y|+\int_1^{\frac{1+K}{1-K}}dy\frac{1-y}{y^2}\ln|1-y|\Bigg]\,.\end{aligned}$$

Of course, one could perform the remaining integral by use of the substition $x=1/y$. But we want to show that our method does not require "refined" transformations. We thus take one more derivative and find the differential equation

$$\frac{d}{dK}\frac{1}{K}\frac{d}{dK}B_-(K^{-1}) = \frac{1}{2}\frac{1}{1-K^2}\ln\left|\frac{1+K}{1-K}\right| + \frac{K}{(1-K^2)^2}\,. \tag{B2}$$

In terms of Q this means

$$\frac{d}{dQ}Q^3\frac{d}{dQ}B_-(Q) = -\frac{1}{2}\frac{1}{1-Q^2}\ln\left|\frac{1+Q}{1-Q}\right| + \frac{Q}{(1-Q^2)^2}\,. \tag{B3}$$

This differential equation can be integrated much easier than the original integral,

$$B_-(Q) = \frac{1-Q^2}{16Q^2}\left(\ln\left|\frac{1+Q}{1-Q}\right|\right)^2 + \frac{1}{4Q}\ln\left|\frac{1+Q}{1-Q}\right| - \frac{1}{4Q^2} + \frac{a}{Q^2} + b\,. \tag{B4}$$

Finally, as one sees from the original integral after the shift $\mathbf{p}\to\mathbf{p}+\frac{1}{2}\mathbf{q}$, $\mathbf{k}\to\mathbf{k}+\frac{1}{2}\mathbf{q}$,

$$B_-(\mathbf{q}) = 64\pi^4\int\frac{d^3p}{(2\pi)^3}\int\frac{d^3k}{(2\pi)^3}\frac{\Theta(k_F-p)\,\Theta(k_F-k)}{(q^2+2\mathbf{q}\cdot\mathbf{p})^2(\mathbf{p}-\mathbf{k})^2}\,, \tag{B5}$$

$B_-(Q)$ falls off like $1/Q^4$ for large Q. This leads to the conclusion that $a=b=0$.

If one now tries the same procedure for $B_+(K^{-1})$ using symmetric coordinates, one ends up with

$$\frac{1}{K}\frac{d}{dK}B_+(K^{-1}) = -\tfrac{1}{8}\int_{-K}^{K}dz\int_{-K}^{K}dz'\left(\frac{1}{(1+z)^2}+\frac{1}{(1+z')^2}\right)\ln\left|\frac{W(z,z',K)+z(2+z+z')+2(1+z')}{(2+z+z')^2}\right|\,,$$

where $W(z,z',K)$ is given by Eq. (20). This integral seems to be prohibitively complex. Further differentiation does not simplify the problem. The symmetric coordinates are not appropriate for the discussion of $B_+(K^{-1})$. Of course, we know from the direct integration that an unsymmetric choice for the coordinates solves this difficulty. However, assuming that this would not be possible, we can find the differential equation for $B_+(Q)$ by a large-Q expansion.

To this aim we first calculate this expansion of $B_+(Q)$ from the integral (3) shifted by $\mathbf{q}/2$ and scaled by k_F,

$$B_+(\mathbf{q}) = -4\frac{\pi^4}{Q^2}\int\frac{d^3p}{(2\pi)^3}\int\frac{d^3k}{(2\pi)^3}\frac{\Theta(1-p)\,\Theta(1-k)}{(Q+\hat{\mathbf{q}}\cdot\mathbf{p})^2(2Q\hat{\mathbf{q}}+\mathbf{p}+\mathbf{k})^2}\,. \tag{B6}$$

Again, instead of using a partially integrated version of this integral for expansion we attack it by a "brute-force" expansion, thus simulating a more complicated integrand. Its general expansion reads

$$B_+(Q) = -\frac{\pi^4}{Q^6}\sum_{n=0}^{\infty}\frac{1}{Q^{2n}}\int\frac{d^3p}{(2\pi)^3}\int\frac{d^3k}{(2\pi)^3}\Theta(1-p)\Theta(1-k)\sum_{m=0}^{n}\left(a_{n-m}b_m+\frac{1}{Q^2}c_{n-m}d_m\right) , \tag{B7}$$

$$a_m = (2m+1)(\hat{\mathbf{q}}\cdot\mathbf{p})^{2m} , \tag{B8}$$

$$b_m = \frac{1}{2^{2m}}\sum_{l=0}^{m}\left(\frac{(m+l)!\,(-1)^{m+l}}{(m-l)!\,(2l)!}[2\hat{\mathbf{q}}\cdot(\mathbf{p}+\mathbf{k})]^{2l}[(\mathbf{p}+\mathbf{k})^2]^{m-l}\right) , \tag{B9}$$

$$c_m = (2m+2)(\hat{\mathbf{q}}\cdot\mathbf{p})^{2m+1} , \tag{B10}$$

$$d_m = \frac{1}{2^{2m+1}}\sum_{l=0}^{m}\left(\frac{(m+l+1)!\,(-1)^{m+l}}{(m-l)!\,(2l+1)!}[2\hat{\mathbf{q}}\cdot(\mathbf{p}+\mathbf{k})]^{2l+1}[(\mathbf{p}+\mathbf{k})^2]^{m-l}\right) . \tag{B11}$$

The resulting integrals are elementary, but become very lengthy for higher orders. We thus restrict ourselves to presenting the result of the lowest five orders,

$$B_+(Q) = -\frac{1}{36}\frac{1}{Q^6}\left(1+\frac{11}{10}\frac{1}{Q^2}+\frac{183}{175}\frac{1}{Q^4}+\frac{506}{525}\frac{1}{Q^6}+\frac{7141}{8085}\frac{1}{Q^8}+\cdots\right) . \tag{B12}$$

In order to derive a differential equation from this expansion, we act on it with the same differential operator that we found in the differential equation of $B_-(Q)$,

$$\frac{d}{dQ}Q^3\frac{d}{dQ}B_+(Q) = -\left(\frac{2}{3}\frac{1}{Q^5}+\frac{22}{15}\frac{1}{Q^7}+\frac{244}{105}\frac{1}{Q^9}+\frac{1012}{315}\frac{1}{Q^{11}}+\frac{14\,282}{3465}\frac{1}{Q^{13}}+\cdots\right) . \tag{B13}$$

We now compare this with the expansion of the differential equation (B3) for $B_-(Q)$,

$$\frac{d}{dQ}Q^3\frac{d}{dQ}B_-(Q) = \left(\frac{1}{Q^3}+\frac{4}{3}\frac{1}{Q^5}+\frac{23}{15}\frac{1}{Q^7}+\frac{176}{105}\frac{1}{Q^9}+\frac{563}{315}\frac{1}{Q^{11}}+\frac{6508}{3465}\frac{1}{Q^{13}}+\cdots\right) + \left(\frac{1}{Q^3}+\frac{2}{Q^5}+\frac{3}{Q^7}+\frac{4}{Q^9}+\frac{5}{Q^{11}}+\frac{6}{Q^{13}}+\cdots\right) ,$$

where we have seperated the expansions of both contributing terms. Looking carefully at both expansions, one recognizes that the coefficients of the $B_+(Q)$ equation are just the difference of the above two series instead of their sum as for $B_-(Q)$. One thus concludes that $B_+(Q)$ should obey the differential equation

$$\frac{d}{dQ}Q^3\frac{d}{dQ}B_+(Q) = -\frac{1}{2}\frac{1}{1-Q^2}\ln\left|\frac{1+Q}{1-Q}\right| - \frac{Q}{(1-Q^2)^2} . \tag{B14}$$

In fact, this equation is satisfied by the exact result (7). We thus have found the correct differential equation by use of the large-Q expansion. A straightforward integration of Eq. (B14) as for $B_-(Q)$ consequently gives exactly Eq. (7).

Of course, all results of this scheme are identical with those of the direct integration presented in Appendix A. It has the particular advantage that it can be used when a direct integration is not possible, while some kind of expansion is (almost) always available.

APPENDIX C: DIFFERENTIAL EQUATION FOR $A_-(K^{-1})$

In this Appendix we derive Eq. (16). To this aim we differentiate Eq. (15) with respect to K,

$$\frac{d}{dK}A_-(K^{-1}) = -\frac{K}{4}\int_{-K}^{K}dz\int_{-K}^{K}dz'\int_0^{K^2-z^2}dx\,\frac{1}{(1+z)(1+z')} \times\frac{1}{\{[(z-z')^2+x+K^2-z'^2]^2-4x(K^2-z'^2)\}^{1/2}} .$$

Carrying through the remaining x integration, one arrives at

$$\frac{1}{K}\frac{d}{dK}A_-(K^{-1}) = -\frac{K}{4}\int_{-K}^{K}dz\int_{-K}^{K}dz'\frac{1}{(1+z)(1+z')}\ln\left|\frac{K|z-z'|+z'(z'-z)}{(z'-z)^2}\right| .$$

A second differentiation,

$$\frac{d}{dK}\frac{1}{K}\frac{d}{dK}A_-(K^{-1}) = -\tfrac{1}{4}\int_{-K}^{K} dz \frac{1}{(1+z)}\left(\frac{1}{1+K}\ln\left|\frac{2K}{K-z}\right| + \frac{1}{1-K}\ln\left|\frac{2K}{K+z}\right|\right)$$
$$-\tfrac{1}{4}\int_{-K}^{K} dz \int_{-K}^{z} dz' \frac{1}{(1+z)(1+z')(K-z')} - \tfrac{1}{4}\int_{-K}^{K} dz \int_{z}^{K} dz' \frac{1}{(1+z)(1+z')(K+z')} ,$$

and evaluating the z' integration gives

$$(1-K^2)\frac{d}{dK}\frac{1}{K}\frac{d}{dK}A_-(K^{-1}) = -\tfrac{1}{4}\int_{-K}^{K} dz \frac{1}{1+z}\left[(1-K)\left(\ln\left|\frac{1+z}{1-K}\right| + 2\ln\left|\frac{2K}{K-z}\right|\right)\right.$$
$$\left. +(1+K)\left(\ln\left|\frac{1+z}{1+K}\right| + 2\ln\left|\frac{2K}{K+z}\right|\right)\right] .$$

Using the transformations $y=(1+z)/(1\pm K)$ for the more complicated second and fourth terms one obtains

$$(1-K^2)\frac{d}{dK}\frac{1}{K}\frac{d}{dK}A_-(K^{-1}) = -\frac{1}{4}\left(\ln\left|\frac{1+K}{1-K}\right|\right)^2 + \tfrac{1}{2}\ln\left|\frac{1-K^2}{4K^2}\right|\ln\left|\frac{1+K}{1-K}\right| + \int_1^{\frac{1+K}{1-K}} dy \frac{\ln|1-y|}{y} .$$

Finally one can carry through the last K differentiation. This leads to the differential equation (16).

APPENDIX D: LARGE-Q EXPANSION OF $A(Q)$

A suitable starting point for an evaluation of $A(Q)$ for large Q is found in Eq. (2) after the transformations $\mathbf{p}\to\mathbf{p}+\frac{1}{2}\mathbf{q}$, $\mathbf{k}\to\mathbf{k}+\frac{1}{2}\mathbf{q}$ and scaling of both momenta by k_F,

$$A_+(Q) = -\frac{4\pi^4}{Q^2}\int\frac{d^3p}{(2\pi)^3}\int\frac{d^3k}{(2\pi)^3}\frac{\Theta(1-p)\,\Theta(1-k)}{(Q+\hat{\mathbf{q}}\cdot\mathbf{p})(Q+\hat{\mathbf{q}}\cdot\mathbf{k})(2Q\hat{\mathbf{q}}+\mathbf{p}+\mathbf{k})^2} ,$$

$$A_-(Q) = -\frac{4\pi^4}{Q^2}\int\frac{d^3p}{(2\pi)^3}\int\frac{d^3k}{(2\pi)^3}\frac{\Theta(1-p)\,\Theta(1-k)}{(Q+\hat{\mathbf{q}}\cdot\mathbf{p})(Q+\hat{\mathbf{q}}\cdot\mathbf{k})(\mathbf{p}-\mathbf{k})^2} ,$$

where $\hat{\mathbf{q}}$ is the unit vector in the $\mathbf{q}$ direction. Both integrals can be expanded to all orders in $Q^{-2}=4k_F^2/q^2$,

$$A_-(Q) = -\frac{\pi^4}{Q^4}\sum_{n=0}^{\infty}\frac{1}{Q^{2n}}\int\frac{d^3p}{(2\pi)^3}\int\frac{d^3k}{(2\pi)^3}\frac{\Theta(1-p)\Theta(1-k)}{(\mathbf{p}-\mathbf{k})^2}\sum_{m=0}^{2n}(\hat{\mathbf{q}}\cdot\mathbf{k})^{2n-m}(\hat{\mathbf{q}}\cdot\mathbf{p})^m , \tag{D1}$$

$$A_+(Q) = -\frac{\pi^4}{Q^6}\sum_{n=0}^{\infty}\frac{1}{Q^{2n}}\int\frac{d^3p}{(2\pi)^3}\int\frac{d^3k}{(2\pi)^3}\,\Theta(1-p)\Theta(1-k)\sum_{m=0}^{n}\left(e_{n-m}b_m + \frac{1}{Q^2}f_{n-m}d_m\right) , \tag{D2}$$

$$e_m = \sum_{l=0}^{2m}(\hat{\mathbf{q}}\cdot\mathbf{k})^{2m-l}(\hat{\mathbf{q}}\cdot\mathbf{p})^l , \tag{D3}$$

$$f_m = \sum_{l=0}^{2m+1}(\hat{\mathbf{q}}\cdot\mathbf{k})^{2m+1-l}(\hat{\mathbf{q}}\cdot\mathbf{p})^l , \tag{D4}$$

where b_n and d_n are given by Eqs. (B9) and (B11). We would like to mention that using the standard Feynman trick to combine denominators turns out to simplify the expansion considerably for $A_-(Q)$ (where one has only two polynomials to combine), but does not help for the more interesting case of $A_+(Q)$. The above integrals can be solved completely. One finds five coupled sums for the coefficient of order n. At the moment we are not able to simplify these results in order to allow for further manipulations. Instead we show the lowest five orders. Using

$$\int_{-1}^{1} dy\frac{y^{2n}}{k^2+p^2-2pky} = -2\left(\sum_{l=0}^{n-1}\frac{(k^2+p^2)^{2l+1}}{(2n-2l-1)(2pk)^{2l+2}} + \frac{(k^2+p^2)^{2n}}{(2pk)^{2n+1}}\ln\left|\frac{k-p}{k+p}\right|\right) ,$$

$$\int_{-1}^{1} dy \frac{y^{2n-1}}{k^2+p^2-2pky} = \frac{2pk}{k^2+p^2} \int_{-1}^{1} dy \frac{y^{2n}}{k^2+p^2-2pky} ,$$

and

$$\int_0^1 dp \int_0^1 dk p^{2n+1} \, k^{2m+1} \ln \left|\frac{p+k}{p-k}\right| = \frac{1}{2(n+m+2)} \left(\frac{1}{n+1} \sum_{l=0}^{n} \frac{1}{2l+1} + \frac{1}{m+1} \sum_{l=0}^{m} \frac{1}{2l+1} \right) ,$$

one arrives after a considerable amount of algebraic manipulations at

$$A_-(Q) = -\left(\frac{1}{4}\frac{1}{Q^4} + \frac{1}{12}\frac{13}{(3)^2}\frac{1}{Q^6} + \frac{1}{24}\frac{394}{(15)^2}\frac{1}{Q^8} + \frac{1}{40}\frac{21\,946}{(105)^2}\frac{1}{Q^{10}} + \frac{1}{60}\frac{217\,219}{(315)^2}\frac{1}{Q^{12}} + \frac{1}{84}\frac{28\,333\,519}{(3465)^2}\frac{1}{Q^{14}} + \cdots \right) , \tag{D5}$$

$$A_+(Q) = -\left(\frac{1}{36}\frac{1}{Q^6} + \frac{1}{40}\frac{1}{Q^8} + \frac{43}{2100}\frac{1}{Q^{10}} + \frac{19}{1134}\frac{1}{Q^{12}} + \frac{12\,139}{873\,180}\frac{1}{Q^{14}} + \cdots \right) . \tag{D6}$$

The expansion (D6) is used to derive Eq. (21). Adding up $A_-(Q)$ and $A_+(Q)$ leads to

$$A(Q) = -\left[\frac{1}{4}\frac{1}{Q^4} + \frac{1}{12}\left(\frac{4}{3}\right)^2 \frac{1}{Q^6} + \frac{1}{24}\left(\frac{23}{15}\right)^2 \frac{1}{Q^8} + \frac{1}{40}\left(\frac{176}{105}\right)^2 \frac{1}{Q^{10}} + \frac{1}{60}\left(\frac{563}{315}\right)^2 \frac{1}{Q^{12}} + \frac{1}{84}\left(\frac{6508}{3465}\right)^2 \frac{1}{Q^{14}} + \cdots \right] . \tag{D7}$$

APPENDIX E: GRADIENT CORRECTIONS TO THE EXCHANGE FUNCTIONAL IN LINEAR RESPONSE

Within linear response, i.e., for a slightly disturbed system with density deviation $\delta n(\mathbf{r})$ from the density n_0 of the unperturbed homogeneous system, the change of the exchange-correlation functional from the homogeneous system is

$$\Delta E_{\mathrm{xc}}[n_0,\delta n] = -\tfrac{1}{2} \int \frac{d^3q}{(2\pi)^3} \delta n(\mathbf{q}) \times \left(\frac{1}{\Pi(\mathbf{q},0)} - \frac{1}{\Pi^0(\mathbf{q},0)} \right) \delta n(-\mathbf{q}) . \tag{E1}$$

The contribution of order e^2 to the functional (E1),

$$\Delta E_x^{(1)}[n_0,\delta n] = \tfrac{1}{2} \int \frac{d^3q}{(2\pi)^3} \, \delta n(\mathbf{q}) \frac{\Pi^1(\mathbf{q},0)}{[\Pi^0(\mathbf{q},0)]^2} \delta n(-\mathbf{q}) , \tag{E2}$$

represents the lowest-order correction to the exchange functional of a homogeneous system.

For the lowest-order gradient contribution to this exchange functional, only the two lowest coefficients of the Taylor expansion of $\Pi^1(\mathbf{q},0)$ and $\Pi^0(\mathbf{q},0)$ for small $\mathbf{q}$ are necessary. This lowest-order gradient contribution to the functional (E2) was first evaluated by Sham.[19] As the analytic form of $\Pi^1(\mathbf{q},0)$ was unknown, he expanded the integrands of Eqs. (2) and (3) in powers of q^2 in the spirit of the related work of Ma and Brueckner[20] on the correlation energy functional. As this expansion does not exist for small q^2, he had to introduce a finite screening parameter into the Coulomb interaction which serves as a regularization to keep all integrals finite for low momentum. After carrying through the integration, the limit of vanishing screening parameter is taken. Even with that prescription only the sum of both integrals remains finite as individual divergencies due to the leading logarithms in both $A(\mathbf{q})$ and $B(\mathbf{q})$ have to cancel. This procedure leads to the well-known exchange functional

$$\delta E_x^{(1)}[n] = -\frac{7e^2}{432\pi(3\pi^2)^{1/3}} \int d^3r \, \frac{[\nabla n(\mathbf{r})]^2}{[n(\mathbf{r})]^{4/3}} . \tag{E3}$$

The prefactor of this functional, however, has been questioned by Kleinman and collaborators in a series of publications.[11] Their numerical evaluation of the q^2 coefficient of $\Pi^1(\mathbf{q},0)$ led roughly to a relative prefactor of $\frac{10}{7}$ for the lowest-order exchange functional compared to Sham's coefficient. In their highly accurate numerical treatment of $\Pi^1(\mathbf{q},0)$, Chevary and Vosko[12] come to the same conclusion with an accuracy of about 10^{-6}. They also could show numerically that the order of taking the limits $q \to 0$ and $q_{\mathrm{screening}} \to 0$ is crucial for that result.

With our analytic result it is easy to obtain low-order gradient corrections to the exchange functional within linear response. After transformation into r space, one ends up with the exchange-energy density

$$\Delta\epsilon_x^{(1)} = \frac{-5e^2}{216\pi(3\pi^2)^{1/3}} \left(\frac{[\nabla n(\mathbf{r})]^2}{n(\mathbf{r})^{4/3}} + \frac{73}{500}\frac{[\Delta n(\mathbf{r})]^2}{[n(\mathbf{r})]^2} + \frac{19\,261}{882\,000}\frac{[\nabla\Delta n(\mathbf{r})]^2}{[n(\mathbf{r})]^{8/3}} + \cdots \right) . \tag{E4}$$

As is obvious from the identity of our analytic result for $\Pi^1(Q,0)$ with the numerical evaluation of Chevary and Vosko,[12] we find the same prefactor as these authors and Kleinman and collaborators.

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