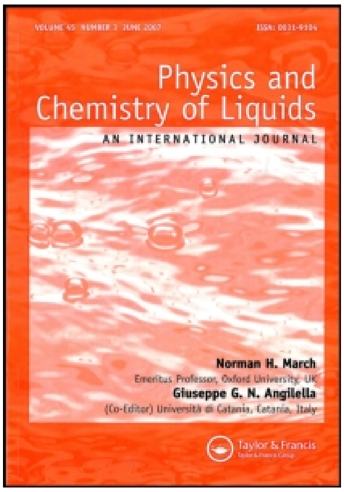

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Long-range Behaviour of the Pair-correlation Function of a Dense Electron Liquid

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The large r expansion of the pair-correlation function $g(r)$ is calculated by first-order perturbation theory in the dense metallic electron liquid regime of jellium. The non-oscillatory terms in $g(r) - 1$ at large r are completely changed from the Hartree–Fock (HF) case, the leading term being $\propto r^{-8}$, not r^{-4} as in the HF result. But the oscillatory terms arising from the sharp Fermi surface, though changed quantitatively from the HF predictions, remain largely intact. These terms, in fact, dominate the large r behaviour.

KEY WORDS: Structure factor, plasmon, proper polarizability, pair correlation function.

I INTRODUCTION

Though qualitatively accurate treatments of the structure factor $S(k)$ and the corresponding pair function $g(r)$ now exist, the behaviour of both quantities remains of interest for analytic theory in the jellium model of a metal. Specifically we tackle here the problem of the long-range behaviour of $g(r)$ in the dense electron liquid regime.

In Section II, we set out briefly the mathematics of asymptotic expansion of a Fourier transform. Section III concerns the application of this technique to the singularities in $S(k)$ at $k = 0$ and the way these determine long-range contributions to $g(r)$, first-order many-body perturbation theory being used explicitly. Section IV then treats the Fermi surface non-analyticities in $S(k)$, which are assumed to occur solely at $2k_F$, the diameter of the Fermi sphere. Section V consists of a discussion and summary. Some details concerning the mathematics involved in the calculation of present results are given in the nine Appendices.

As to the microscopic theory of $g(r)$, which we shall invoke below, the pair-correlation function $g(r)$ of the uniform electron liquid may be expressed[1,2] in terms of the proper polarizability $\Pi(k, \omega)$ via the dynamic structure factor $S(k, \omega)$ and its integral over all energy transfer—the static structure factor, namely $S(k)$:

$$g(r) - 1 = \frac{3}{8\pi} \int \mathrm{d}^3k \, [S(k) - 1] \exp(i\mathbf{k} \cdot \mathbf{r})$$

$$= \frac{3}{2r} \int_0^\infty \mathrm{d}k \, \sin(kr)\{k[S(k) - 1]\}, \tag{1.1}$$

$$S(k) = \int_{-\infty}^{\infty} \mathrm{d}\omega \, S(k, \omega), \tag{1.2}$$

$$S(k, \omega) = \frac{-\hbar}{\pi n} \operatorname{Im} \chi(k, \omega)\theta(\omega) \tag{1.3}$$

while the dynamical susceptibility (response function) χ is related to Π by

$$\chi(k, \omega) = \Pi(k, \omega)/[1 - v_k\Pi(k, \omega)], \tag{1.4}$$

v_k being the bare Coulomb interaction

$$v_k = \frac{4\pi e^2}{k^2}. \tag{1.5}$$

It is in fact convenient to work with the dimensionless proper polarizability

$$Q(k, \omega)) = \varepsilon(k, \omega) - 1 = -v_k\Pi(k, \omega) \tag{1.6}$$

in terms of which the density-density response function (1.4) is given by

$$\chi(k, \omega) = \frac{-1}{v_k} \frac{Q(k, \omega)}{1 + Q(k, \omega)} \tag{1.7}$$

and then one finds

$$S(k, \omega) = \theta(\omega) \frac{3k^2}{4\alpha r_s} \operatorname{Im}\left[\frac{-1}{1 + Q(k, \omega)}\right]. \qquad (1.8)$$

Throughout this paper, $k_F^{-1} = \alpha a_B r_s$ is used as the unit of length, wave vectors k and q being measured in units of k_F, while $2E_F\hbar^{-1} = \hbar m^{-1}k_F^2$ is the unit of frequency ω, $\alpha = (\frac{4}{9}\pi)^{1/3} \approx 0.521$.

II ASYMPTOTIC EXPANSION OF A FOURIER TRANSFORM

Since $g(r)$ is the Fourier transform (FT) of a function involving $S(k)$ as in Eq. (1.1) we will require the technique given by Lighthill[3]. The large y properties of $f_{\mathrm{FT}}(y)$ defined as

$$f(x) \underset{\mathrm{FT}}{\rightarrow} f_{\mathrm{FT}}(y) = \int_{-\infty}^{\infty} dx \exp(ixy) f(x) \qquad (2.1)$$

are thereby determined solely by the number and nature of singularities of the function $f(x)$. If $x_1, x_2, \ldots, x_M$ denote these points of non-analyticity, such that in the vicinity of each of them

$$f(x) = F_m(x - x_m) + \text{small remainder} \qquad (2.2)$$

where $F_m(\xi)$ involves $\operatorname{sgn}(\xi)$, $\theta(\xi)$, $\ln|\xi|$ etc. then

$$f_{\mathrm{FT}}(y) = \sum_{m=1}^{M} \exp(ix_m y) F_{m,\mathrm{FT}}(y)$$

$$+ \text{contribution from remainder.} \qquad (2.3)$$

A table of FT of a variety of non-analytic functions $F_m(\xi)$ is given in Ref. 3 and in Appendix 9. As an example, following from (A9.7) and (A9.11) we have

$$x^n \operatorname{sgn}(x) \underset{\mathrm{FT}}{\rightarrow} n!2\left(\frac{i}{y}\right)^{n+1}. \qquad (2.4)$$

III NON-OSCILLATORY ASYMPTOTIC CONTRIBUTIONS TO *g(r)*

The function $g(r)$ may be expressed in the standard form (2.1) if we rewrite (1.1) as

$$g(r) - 1 = \frac{3}{2r} \operatorname{Im} \int_{-\infty}^{\infty} dk \exp(ikr)\{\theta(k)[S(k) - 1]k\}. \qquad (3.1)$$

The presence of $\theta(k)$ in Eq. (3.1) means that $k = 0$ is one of the points of non-analyticity. Applying Lighthill's formalism, we arrive at the following contribution to $g(r)$:

$$[g(r) - 1]_{\text{non-osc}} = \frac{3}{2} \sum_{m=0}^{\infty} \frac{(-1)^m D_{2m}}{r^{2m+2}} \tag{3.2}$$

where

$$D_l = \left(\frac{\mathrm{d}}{\mathrm{d}k}\right)^l \{[S(k) - 1]k\}_{k=0}. \tag{3.3}$$

From Eqs (3.2) and (3.3) it follows that only odd terms in the power series expansion of $S(k)$ for small k contribute to asymptotics of $g(r)$, namely $S(k) \propto k^{2m+1}$ leads to $[g(r) - 1] \propto 1/r^{2m+4}$. Besides this, contributions due to non-analyticity at some $k_0 \neq 0$ are expected. While $[g(r) - 1]_{\text{non-osc}}$ has a form of power series in r^{-1}, Eq. (3.2), the second contribution to $[g(r) - 1]$, depends on r in a more complicated way, involving, among others, oscillatory factors $\cos(k_0 r)$ and $\sin(k_0 r)$ as in Eq. (2.3).

A Example of Hartree–Fock structure factor

We immediately illustrate the general result (2.3) and (3.2) by using the Hartree–Fock structure factor $S_{\text{HF}}(k)$, which has the well known form

$$S_{\text{HF}}(k) = \begin{cases} 3k/4 - k^3/16 & \text{for } k \leqslant 2 \\ 1 & \text{for } k > 2 \end{cases}. \tag{3.4}$$

In the vicinity of $k_0 = 2$ it may be rewritten as

$$S_{\text{HF}}(2 + \xi) = 1 - [(\tfrac{3}{16})\xi^2 + (\tfrac{1}{32})\xi^3] + \text{sgn}(\xi)[(\tfrac{3}{16})\xi^2 + (\tfrac{1}{32})\xi^3]. \tag{3.5}$$

We see that there are two points of non-analyticity: $k = 0$ and $k = 2$. The asymptotic form of $g(r)$, corresponding to them, is

$$\begin{aligned} g_{\text{HF}}(r) - 1 &= [g_{\text{HF}}(r) - 1]_{\text{non-osc}} + [g_{\text{HF}}(r) - 1]_{\text{osc}} \\ &= -(\tfrac{9}{4})(1/r^4 + 1/r^6) \\ &\quad - (\tfrac{9}{4})[\cos(2r)/r^4 - 2\sin(2r)/r^5 - \cos(2r)/r^6]. \end{aligned} \tag{3.6}$$

Because expansions (3.4) and (3.5) have a finite number of terms, the expression (3.6) is exact (not only asymptotic).

B Non-oscillatory terms in many-body perturbation theory

In turning from the Hartree–Fock result, exact at $r_s = 0$ (i.e. for the non-interacting electron gas) to non-zero r_s, one must recognize that two additional physical parameters enter the theory, namely the plasma frequency ω_p and the Thomas–Fermi wave vector k_{TF}. These quantities are small for a dense electron liquid (i.e. small r_s) according to

$$\omega_p = \left(\frac{4\alpha r_s}{3\pi}\right)^{1/2} \tag{3.7}$$

and

$$k_{\mathrm{TF}} = \left(\frac{4\alpha r_s}{\pi}\right)^{1/2} = 3^{1/2}\omega_p \tag{3.8}$$

in the units defined above.

Therefore, in seeking the small k expansion of $S(k)$, one must consider the range of $k \ll k_{\mathrm{TF}}$. In this region the dynamical structure factor $S(k, \omega)$ has the following form: (i) there is a small "bump" in the frequency range

$$0 \leqslant \omega < \omega_+(k) = 3^{1/2}\omega_p\left(\frac{k}{k_{\mathrm{TF}}}\right)\left[1 + \frac{3^{1/2}}{2}\omega_p\left(\frac{k}{k_{\mathrm{TF}}}\right)\right]$$

and (ii) for higher frequencies a weak tail, with a narrow plasmon peak imposed on it at frequencies close to ω_p.

This general picture simplifies in the approximation of first-order perturbation theory[2], namely there is no tail for $\omega > \omega_+(k)$ and the plasmon, being now undamped, becomes a delta-function peak. This is because $\mathrm{Im}\{Q^0(k, \omega) + Q^1(k, \omega)] = 0$ for $\omega > \omega_+(k)$. Therefore in first-order perturbation theory the dynamical structure factor may be split unambiguously into the sum of two parts:

$$S(k, \omega) = S_{\mathrm{inc}}(k, \omega) + S_{\mathrm{pl}}(k, \omega) \tag{3.9}$$

where the first part is the incoherent contribution from the electron-hole continuum while the second arises from the plasmon peak.

C Plasmon contribution

The first-order perturbation theory of the plasmon dispersion is known to yield[2]

$$\omega_{\mathrm{pl}}(k) = \omega_p\left[1 + \frac{9}{10}\left(1 - \frac{\alpha r_s}{3\pi}\right)\left(\frac{k}{k_{\mathrm{TF}}}\right) + O\left(\left(\frac{k}{k_{\mathrm{TF}}}\right)^4\right)\right]. \tag{3.10}$$

Therefore it follows from Eq. (1.8) that

$$S_{\rm pl}(k,\omega)$$

$$=\frac{3}{\pi}\left(\frac{k}{k_{\rm TF}}\right)^2 \operatorname{Im}\frac{-1}{\left[\left.\frac{\partial\varepsilon(k,\omega)}{\partial\omega}\right|_{\omega=\omega_{\rm pl}(k)}+O(\omega-\omega_{\rm pl}(k))\right][\omega+i0^+-\omega_{\rm pl}(k)]}$$

$$=3\left(\frac{k}{k_{\rm TF}}\right)^2\frac{\partial(\omega-\omega_{\rm pl}(k))}{\partial\varepsilon(k,\omega)/\partial\omega}, \tag{3.11}$$

an expansion of the dielectric function $\varepsilon(k, \omega)$, Eq. (1.6), in being made about the plasmon frequency.

The derivative of ε appearing in Eq. (3.11) can be readily calculated in the region of small k from the known expansions for $Q^0(k, \omega)$ and $Q^1(k, \omega)$ given in Ref. 2. The result is

$$\left.\frac{\partial\varepsilon(k,\omega)}{\partial\omega}\right|_{\omega=\omega_{\rm pl}(k)}=\frac{1}{2\omega_p^2}\left[\omega_{\rm pl}(k)+O\left(\left(\frac{k}{k_{\rm TF}}\right)^4\right)\right]. \tag{3.12}$$

Therefore one has finally the result

$$S_{\rm pl}(k,\omega)=\frac{3}{2}\omega_p\left(\frac{k}{k_{\rm TF}}\right)^2\left[1-\frac{9}{10}\left(1-\frac{\alpha r_s}{3\pi}\right)\left(\frac{k}{k_{\rm TF}}\right)^2+O\left(\left(\frac{k}{k_{\rm TF}}\right)^4\right)\right]\delta(\omega-\omega_{\rm pl}(k)) \tag{3.13}$$

which deals with the plasmon contribution to $S(k, \omega)$. To obtain the desired contribution to the static structure factor $S(k)$, Eq. (1.2) is used to yield

$$S_{\rm pl}(k)=\int_{\omega_+(k)}^{\infty}{\rm d}\omega\, S_{\rm pl}(k,\omega)$$

$$=\frac{3}{2}\omega_p\left(\frac{k}{k_{\rm TF}}\right)^2\left[1-\frac{9}{10}\left(1-\frac{\alpha r_s}{3\pi}\right)\left(\frac{k}{k_{\rm TF}}\right)^2+O\left(\left(\frac{k}{k_{\rm TF}}\right)^4\right)\right]. \tag{3.14}$$

D Incoherent contribution

To deal with the incoherent part $S_{\rm inc}(k, \omega)$, it is first to be noted that

$$Q(k,\omega)=\varepsilon(k,\omega)-1=\left(\frac{k}{k_{\rm TF}}\right)^2\tilde{\Pi}(k,\omega) \tag{3.15}$$

where the proper polarizability $|\tilde{\Pi}(k, \omega)| \sim 1$ in the frequency range $0 \leqslant \omega \leqslant \omega_+(k)$. Therefore in this range, and for $k \ll k_{TF}$, one has

$$S_{inc}(k, \omega) = \frac{3}{\pi}\left(\frac{k}{k_{TF}}\right)^2 \operatorname{Im}\left[\frac{-1}{1 + \left(\frac{k_{TF}}{k}\right)^2 \tilde{\Pi}(k, \omega)}\right]$$
$$= \frac{3}{\pi}\left(\frac{k}{k_{TF}}\right)^4 \operatorname{Im}\left\{\frac{-1}{\tilde{\Pi}(k, \omega)}\right\}\left[1 + O\left(\left(\frac{k}{k_{TF}}\right)^2\right)\right]. \quad (3.16)$$

In first-order perturbation theory,

$$\frac{1}{\tilde{\Pi}(k, \omega)} \simeq \frac{1}{\tilde{\Pi}^0 + \tilde{\Pi}^1} = \frac{1}{\tilde{\Pi}^0} - \frac{\tilde{\Pi}^1}{(\tilde{\Pi}^0)^2} + O(r_s^2). \quad (3.17)$$

Separating S_{inc} into zeroth- and first-order parts then leads to:

$$S_{inc}(k, \omega) = S_{inc}^0 + S_{inc}^1 + \cdots \quad (3.18)$$

where

$$S_{inc}^0(k, \omega) = \frac{3}{\pi}\left(\frac{k}{k_{TF}}\right)^4 \operatorname{Im}\left[\frac{-1}{P^0(\omega/k)}\right]\left[1 + 0\left(\left(\frac{k}{k_{TF}}\right)^0\right)\right] \quad (3.19)$$

while

$$S_{inc}^1(k, \omega) = \frac{3}{\pi}\left(\frac{k}{k_{TF}}\right)^4\left(\frac{\alpha r_s}{4\pi}\right)\operatorname{Im}\left\{\frac{P^1(\omega/k)}{[P^0(\omega/k)]^2}\right\}\left[1 + o\left(\left(\frac{k}{k_{TF}}\right)^0\right)\right] \quad (3.20)$$

Here P^0 and P^1 are defined by:

$$P^0(x) = \lim_{k \to 0}\left(\frac{k}{k_{TF}}\right)^2 Q^0(k, kx)$$
$$= \lim_{k \to 0} \tilde{\Pi}^0(k, kx) \quad (3.21)$$

and

$$P^1(x) = \frac{4\pi}{\alpha r_s} \lim_{k \to 0} \tilde{\Pi}^1(k, kx). \quad (3.22)$$

It is to be noted that both $S_{inc}^0(k, kx)$ and $S_{inc}^1(k, kx)$ are zero for $x > 1 (= \lim_{k \to 0}(\omega_+(k)/k))$.

To obtain the desired contribution to the static structure factor $S(k)$, Eq. (1.2) is used to yield

$$S_{\rm inc}(k) = \int_0^1 dx\, kS_{\rm inc}(k, kx)$$
$$= \frac{3^{3/2}}{2}\omega_p\left(\frac{k}{k_{\rm TF}}\right)^5\left[I_0^0 + \frac{\alpha r_s}{4\pi}I_0^1\right]\left[1 + o\left(\left(\frac{k}{k_{\rm TF}}\right)^0\right)\right] \tag{3.23}$$

where

$$I_0^0 = \frac{2}{\pi}\,{\rm Im}\int_0^1 dx\,\frac{(-1)}{P^0(x)} = 0.3447085 \tag{3.24}$$

and

$$I_0^1 = \frac{2}{\pi}\,{\rm Im}\int_0^1 dx\,\frac{P^1(x)}{[P^0(x)]^2} = 1.547067. \tag{3.25}$$

The details of these evaluations are given in the Appendices 2 and 3.

Equation (3.23) demonstrates that the leading term of $S_{\rm inc}(k)$ is of the order of k^5.

E Comparison with the predictions of Nozières and Pines

This is the point at which to compare the present results with the predictions made by Pines and Nozières[1], namely

$$S(k) = \frac{k^2}{2\omega_p} + c_{\rm mp}k^4 + c_{\rm sp}k^5 + \cdots \tag{3.26}$$

where the three terms exhibited are the leading ones from (i) plasmon excitation, (ii) multipair excitations and (iii) single-pair excitations.

The result (3.14) derived above contains the first term in Eq. (3.26) exactly (using Eq. (3.8)), and corrections involving higher even powers of k. Our leading term from the incoherent contribution (Eq. (3.23)), $\sim k^5$, corresponds to the single-pair term in Eq. (3.26). However, it is entirely possible that higher order terms contribute to the term proportional to k^5 in Eq. (3.26). It is clear from our analysis that $c_{\rm mp}$ is zero to the order in r_s to which we have worked. This in no way denies the possibility that $c_{\rm mp} \neq 0$ in higher orders of perturbation theory (i.e. it must arise from $Q^2 + Q^3 + \cdots$).

F The form of non-oscillatory part of $g(r)$

The above result for the small k expansion of the static structure factor $S(k)$ may be used, in conjunction with Eqs (3.2) and (3.3) to yield long-range non-oscillatory contributions to the pair function $g(r)$ as

$$[g(r) - 1]_{\text{non-osc}} = -245.79 r_s^2 \left\{ [1 + 0.18609 r_s + \cdots] \left(\frac{r_{\text{TF}}}{r}\right)^8 + O\left(\left(\frac{r_{\text{TF}}}{r}\right)^{10}\right) \right\} \tag{3.27}$$

where $r_{\text{TF}} = k_{\text{TF}}^{-1} = (\pi/4\alpha r_s)^{1/2}$.

IV OSCILLATORY TERMS IN LONG-RANGE BEHAVIOUR OF $g(r)$

We know, from the structure factor for non-interacting electrons $S_{\text{HF}}(k)$, Eqs (3.4), (3.5), that there is non-analyticity at $k = 2$, i.e. at the wave vector equal to the diameter of the Fermi sphere. The fact that the sharp Fermi sphere remains after switching on the electron-electron interaction means that one must expect that $k = 2$ is the point of non-analyticity at finite r_s also. As will be shown, within the 1st-order perturbation theory there are no more points of non analyticity $k \neq 0$ and we expect this to be true in general.

For $k > k_{\text{TF}}$ (i.e. in the range where plasmon excitations do not occur) and for small r_s ($r_s \lesssim 2$) we have $|Q(k, \omega)| \ll 1$, e.g. at $k = 2$, $|Q(k, 0)| \approx |Q^0(k, 0)| = 0.08\, r_s$. Therefore the following expansion of the dynamical structure factor (1.8) is possible:

$$S(k, \omega) = \theta(\omega) \frac{3}{\pi} \left(\frac{k}{k_{\text{TF}}}\right)^2 \operatorname{Im}[Q - (Q)^2 + (Q)^3 - \cdots]. \tag{4.1}$$

Taking into account that the subsequent terms of the perturbation series $Q = Q^0 + Q^1 + \cdots$ are of the order of $\sim r_s^1, r_s^2, r_s^3 \ln r_s$, respectively, we arrive at the following series for $S(k, \omega)$:

$$S(k, \omega) = S^0(k, \omega) + S^1(k, \omega) + \cdots \tag{4.2}$$

where the zeroth-order term is obviously the Hartree–Fock dynamical structure factor:

$$S^0(k, \omega) = S_{\text{HF}}(k, \omega) = \theta(\omega) \frac{3}{\pi} \left(\frac{k}{k_{\text{TF}}}\right)^2 \operatorname{Im} Q^0(k, \omega). \tag{4.3}$$

The first-order term comes from two sources:

$$S^1(k, \omega) = \theta(\omega)\frac{3}{\pi}\left(\frac{k}{k_{TF}}\right)^2 \text{Im}\{Q^1(k, \omega) - [Q^0(k, \omega)]^2\}; \tag{4.4}$$

one due to the first-order part Q^1 of the proper polarizability, which may be usefully divided further into the exchange and self-energy parts[2]:

$$Q^1(k, \omega) = Q^{Ex}(k, \omega) + Q^{SE}(k, \omega) \tag{4.5}$$

and the other, due to screening effects (improper polarizability consisting of two zeroth-order proper polarizabilities, so this contribution occurs in RPA):

$$Q^{Sc}(k, \omega) = -[Q^0(k, \omega)]^2. \tag{4.6}$$

By integration over frequencies according to Eq. (1.2), we obtain the contributions to the static structure factor, corresponding to them.

It is interesting that the self-energy diagram does not contribute to asymptotics of $g(r)$ because

$$S^{SE}(k) = 0 \tag{4.7}$$

for any $k > 0$; see Appendix 5.

The remaining terms: $S^0(k)$, $S^{Ex}(k)$ and $S^{Sc}(k)$ exhibit non-analyticity at $k = 2$, which produces the following asymptotics of the pair-correlation function:

$$\begin{aligned}[g(r) - 1]_{osc} = &-\frac{9}{4}\frac{\cos 2r}{r^4}\left\{1 + \frac{\alpha r_s}{2\pi}\left[-2 - \ln 2 - \frac{\pi^2}{6} + (\gamma + \ln 2r)^2\right]\right\} \\ &+\frac{9}{2}\frac{\sin 2r}{r^5}\left\{1 + \frac{\alpha r_s}{2\pi}\left[-\frac{1}{2} - \frac{\ln 2}{2} + \frac{3}{2}(\gamma + \ln 2r) + \cdots\right]\right\} \\ &+\frac{9}{2}\frac{\cos 2r}{r^5}\left\{0 + \frac{\alpha r_s}{2\pi}\left[\frac{-\pi}{4} + \cdots\right]\right\} + 0\left(\frac{(\ln r)^n}{r^6}\right)\end{aligned} \tag{4.8}$$

where dots represent (not calculated yet) "Ex" contributions to the term αr^{-5}. Here $\gamma \simeq 0.5772$ is the Euler constant. The details leading to this result are recorded in Appendices 4 and 6.

V DISCUSSION AND SUMMARY

Equation (4.8) giving the oscillatory terms in the long-range behaviour of $g(r)$, and the non-oscillatory terms in Eq. (3.27) constitute the main results of this work. We emphasize again that these formulae are valid precisely to first order in perturbation theory.

It follows then that the asymptotic expansion of the pair-correlation function is the sum:

$$g(r) - 1 = [g(r) - 1]_{\text{non-osc}} + [g(r) - 1]_{\text{osc}} \tag{5.1}$$

in the metallic regime of jellium, i.e. $r_s < \sim 80$. Naturally the explicit results for the two contributions in Eq. (5.1) presented in this paper are only quantitatively valid[2] $r_s \lesssim 2$.

However, in spite of this quantitative limitation on our expansions, we can draw some more general conclusions as to the switching on of electron-electron interactions in jellium:

a) among non-oscillatory terms, those of the form r^{-4} and r^{-6} predicted by the Hartree-Fock case are annulled by the Coulomb interactions, while a new term of the form $r_s^2(r_{\text{TF}}/r)^8$ arises from single-particle excitations.

b) among oscillatory terms, all those from the Hartree-Fock case remain. However, the leading Hartree-Fock term $\cos(2k_F r)/r^4$ is multiplied by a factor which is 1 plus a first-order correction which has a weak r dependence of the form $(\gamma + \ln 2r)^2$.*

The major conclusion therefore is that while the non-oscillatory terms in $g(r)$ at large r are crucially changed by switching on the electron-electron interactions, the oscillatory terms arising from the sharp Fermi surface are altered in a quantitative rather than a qualitative way.

Note added in proof

Using the relation $x \simeq 1 - \exp(-x)$, one can write for this small correction

$$\frac{\alpha r_s}{2\pi}(\gamma + \ln 2r)^2 \simeq \left[1 - \left(\frac{r_0}{r}\right)^{\mu}\right]^2,$$

where $\mu = (\alpha r_s/2\pi)^{1/2} \simeq (r_s/12)^{1/2}$ and $r_0 = (2\exp\gamma)^{-1} \simeq 0.3$. This term may herald a change in the long-range behaviour, namely by a fractional (μ) inverse power of r.

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Appendix 1 Integral Representation of $Q^1(k, \omega)$

The first-order contribution $Q^1(k, \omega)$ to the proper polarizability $Q(k, \omega)$ was obtained in Ref. 2 directly from the appropriate diagrams as

$$Q^1(k, \omega) = Q^{\mathrm{Ex}}(k, \omega) + Q^{\mathrm{SE}}(k, \omega) = \left(\frac{\alpha r_s}{\pi^2 k}\right)^2 F^1(k, \omega) \qquad \text{(A1.1)}$$

with

$$F^1(k, \omega) = F^{\mathrm{Ex}}(k, \omega) + F^{\mathrm{SE}}(k, \omega)$$

$$= \frac{1}{2} \int \frac{d^3\mathbf{p}_1 d^3\mathbf{p}_2}{(\mathbf{p}_1 - \mathbf{p}_2)^2} (n^0_{\mathbf{p}_1} - n^0_{\mathbf{p}_1+\mathbf{k}})(n^0_{\mathbf{p}_2} - n^0_{\mathbf{p}_2+\mathbf{k}}) \qquad \text{(A1.2)}$$

$$\times \left\{ \left[\frac{1}{(\omega + i0^+ + \omega_{\mathbf{p}_1} - \omega_{\mathbf{p}_1+\mathbf{k}})(\omega + i0^+ + \omega_{\mathbf{p}_2} - \omega_{\mathbf{p}_2+\mathbf{k}})} \right]_{\mathrm{Ex}} + \left[\frac{-1}{2(\omega + i0^+ + \omega_{\mathbf{p}_1} - \omega_{\mathbf{p}_1+\mathbf{k}})^2} + \frac{-1}{2(\omega + i0^+ + \omega_{\mathbf{p}_2} - \omega_{\mathbf{p}_2+\mathbf{k}})^2} \right]_{\mathrm{SE}} \right\} \qquad \text{(A1.3)}$$

where

$$n^0_{\mathbf{q}} = \theta(1 - \mathbf{q}^2)$$
$$\omega_{\mathbf{q}} = \tfrac{1}{2}\mathbf{q}^2. \qquad \text{(A1.4)}$$

The imaginary part of the six-dimensional integral (A1.2) was subsequently evaluated in the form of a combination of elementary functions ("SE" diagram) and a one-dimensional integral of a combination of elementary functions ("Ex" diagram). The real part was obtained numerically by evaluation of the Hilbert transform of the imaginary part. Unfortunately, this representation of $Q^1(k, \omega)$ is not suitable for the analytical investigation of its properties as $k \to 0$ or as $k \to 2$, which are of interest in the present paper. Therefore we shall transform Eq. (A1.2) in such a manner, that its dependence of k will be easy to manipulate.

In the first step we introduce new variables of integration, $\mathbf{q}_i$, shifting the origin of the coordinate system:

$$\mathbf{p}_i = \mathbf{q}_i - \tfrac{1}{2}\mathbf{k}, \qquad \text{(A1.5)}$$

which simplifies the denominators

$$\omega_{\mathbf{p}_i} - \omega_{\mathbf{p}_i+\mathbf{k}} = \frac{1}{2}\left[\left(\mathbf{q}_i - \frac{\mathbf{k}}{2}\right)^2 - \left(\mathbf{q}_i + \frac{\mathbf{k}}{2}\right)^2\right] = -\mathbf{k}\cdot\mathbf{q}_i. \quad \text{(A1.6)}$$

Then Eq. (A1.2) may be rewritten as

$$F^1(k,\omega) = \frac{1}{2}\int \frac{d^3\mathbf{q}_1 d^3\mathbf{q}_2}{(\mathbf{q}_1 - \mathbf{q}_2)^2}(n^0_{\mathbf{q}_1-\mathbf{k}/2} - n^0_{\mathbf{q}_1+\mathbf{k}/2})(n^0_{\mathbf{q}_2-\mathbf{k}/2} - n^0_{\mathbf{q}2+\mathbf{k}/2})$$
$$\times\left\{\left[\frac{1}{(\omega + i0^+ - \mathbf{k}\cdot\mathbf{q}_1)(\omega + i0^+ - \mathbf{k}\cdot\mathbf{q}_2)}\right] + \left[\frac{-1}{2(\omega + i0^+ - \mathbf{k}\cdot\mathbf{q}_1)^2} + \frac{-1}{2(\omega + i0^+ - \mathbf{k}\cdot\mathbf{q}_2)^2}\right]\right\}. \quad \text{(A1.7)}$$

Now cylindrical coordinates are introduced, with z-axis parallel to $\mathbf{k} = (0, 0, k)$:

$$\mathbf{q}_i = (\rho_i \cos\phi_i, \rho_i \sin\phi_i, z_i) \quad \text{(A1.8)}$$

so

$$(\mathbf{q}_i \pm \tfrac{1}{2}\mathbf{k})^2 = \rho_i^2 + (z_i \pm \tfrac{1}{2}k)^2 \quad \text{(A1.9)}$$

and

$$\int d^3\mathbf{q}_i = \pi\int_{-\infty}^{\infty} dz_i \int_0^{\infty} 2\rho_i\, d\rho_i \oint \frac{d\phi_i}{2\pi}. \quad \text{(A1.10)}$$

The dependence of the integrand in (A1.7) on variables φ_i enters via $1/(\mathbf{q}_1 - \mathbf{q}_2)^2$, i.e. the Coulomb potential only. It may be integrated out immediately to give

$$\beta((z_1 - z_2)^2, \rho_1^2, \rho_2^2) = \oint\frac{d\phi_1}{2\pi}\oint\frac{d\phi_2}{2\pi}[(z_1 - z_2)^2 + \rho_1^2 + \rho_2^2 - 2\rho_1\rho_2\cos(\phi_1 - \phi_2)]^{-1}$$
$$= [(z_1 - z_2)^4 + 2(z_1 - z_2)^2(\rho_1^2 + \rho_2^2) + (\rho_1^2 - \rho_2^2)^2]^{-1/2} \quad \text{(A1.11)}$$

We see that new variables

$$s_i = \rho_i^2 \quad \text{(A1.12)}$$

may be introduced. It is convenient also to represent the frequency as

$$\omega = kx \quad \text{(A1.13)}$$

Finally, we arrive at the following integral representation of the first-order diagram

$$F^{\mathrm{Ex,SE}}(k, kx) = \frac{\pi^2}{2}\int_{-\infty}^{\infty} \mathrm{d}z_1 \int_0^{\infty} \mathrm{d}s_1 \frac{N(z_1, s_1, k)}{k} \times \int_{-\infty}^{\infty} \mathrm{d}z_2 \int_0^{\infty} \mathrm{d}s_2 \frac{N(z_2, s_2, k)}{k} \times \beta((z_1 - z_2)^2, s_1, s_2)\gamma^{\mathrm{Ex,SE}}(x + i0^+, z_1, z_2) \tag{A1.14}$$

where

$$\gamma^{\mathrm{Ex}}(z, z_1, z_2) = \frac{1}{(z - z_1)(z - z_2)}, \tag{A1.15}$$

$$\gamma^{\mathrm{SE}}(z, z_1, z_2) = \frac{-1}{2(z - z_1)^2} + \frac{-1}{2(z - z_2)^2}, \tag{A1.16}$$

$$N(z_i, s_i, k) = \theta(1 - (s_i + (z_i - \tfrac{1}{2}k)^2)) - \theta(1 - (s_i + (z_i + \tfrac{1}{2}k)^2)) \tag{A1.17}$$

and β was defined by Eq. (A1.11). Note that $N(z_i, s_i, k)$ is odd in z_i

$$N(-z_i, s_i, k) = -N(z_i, s_i, k) \tag{A1.18}$$

and odd in k

$$N(z_i, s_i, -k) = -N(z_i, s_i, k). \tag{A1.19}$$

We see that the dependence on k enters the integrand of Eq. (A1.14) via two factors $[N(z_i, s_i, k)/k]$, $i = 1, 2$, only, while the dependence on the frequency (x) occurs via the factor $\gamma(x + i0^+, z_1, z_2)$.

Appendix 2 Evaluation of I_0^0

This quantity is defined according to Eq. (3.24) as

$$I_0^0 = \frac{2}{\pi}\,\mathrm{Im}\int_0^1 \mathrm{d}x[-P^0(x)]^{-1} \tag{A2.1}$$

where $P^0(x)$ is related to $Q^0(k, \omega)$—the 0th-order proper polarizability (Lindhard's function), Eq. (3.21), by

$$P^0(x) = \lim_{k\to 0}\left(\frac{k}{k_{\mathrm{TF}}}\right)^2 Q^0(k, kx) \tag{A2.2}$$

Because the Lindhard function is well known[1], Eq. (A4.4), this limit may be found analytically, leading to the result

$$\operatorname{Im} P^0(x) = \frac{\pi}{2} x\theta(1 - x^2), \tag{A2.3}$$

$$\operatorname{Re} P^0(x) = 1 - \tfrac{1}{2}x \ln\left|\frac{1 + x}{1 - x}\right|. \tag{A2.4}$$

Writing I_0^0 in terms of the above explicit functions one finds

$$I_0^0 = \frac{2}{\pi}\int_0^1 dx[\operatorname{Im} P^0(x)]\{[\operatorname{Re} P^0(x)]^2 + [\operatorname{Im} P^0(x)]^2\}^{-1} \tag{A2.5}$$

which is a form suitable for numerical evaluation. The term diverging logarithmically for $x \to 1$, Re $P^0(x)$, happens to be in the denominator, so the integrand is finite. Nevertheless, because of it, the region close to $x = 1$ needs special attention (increased density of integration points) in order to ensure desired accuracy of the numerical quadrature. The result thus obtained is

$$I_0^0 = 0.3447085. \tag{A2.6}$$

Appendix 3 Evaluation of I_0^1

This quantity is defined according to (3.25) as

$$I_0^1 = \frac{2}{\pi} \operatorname{Im} \int_0^1 dx P^1(x)[P^0(x)]^{-2} \tag{A3.1}$$

where $P^1(x)$ is related to $Q^1(k, \omega)$—the first-order proper polarizability diagram, Eqs (3.22), (3.15)

$$P^1(x) = \frac{\pi^2}{\alpha^2 r_s^2} \lim_{k\to 0} k^2 Q^1(k, kx) \tag{A3.2}$$

or, using Eq. (A1.1), to the function $F^1(k, \omega)$

$$P^1(x) = \frac{1}{\pi} \lim_{k\to 0} F^1(k, kx). \tag{A3.3}$$

The form (A1.14) of $F^1(k, kx)$ is very suitable to perform the required limit. Let us expand $N(z_i, s_i, k)$ Eq. (A1.17), in a power series in k:

$$N(z_i, s_i, k) = N(z_i, s_i, 0) + \left.\frac{\partial N}{\partial k}\right|_{k=0} k + O(k^2)$$
$$= 0 + 2z_i\delta(1 - s_i - z_i^2)k + O(k^2). \qquad \text{(A3.4)}$$

After inserting this expansion into (A1.14), one gets immediately the limit (A3.3) as

$$P^1(x) = \frac{1}{2}\int_{-\infty}^{\infty} dz_1 \int_0^{\infty} ds_1 2z_1\delta(1 - s_1 - z_1^2)$$
$$\times \int_{-\infty}^{\infty} dz_2 \int_0^{\infty} ds_2 2z_2\delta(1 - s_2 - z_2^2)\beta\gamma^1$$
$$= 2\int_{-\infty}^{\infty} dz_1 z_1 \theta(1 - z_1^2) \int_{-\infty}^{\infty} dz_2 z_2 \theta(1 - z_2^2)$$
$$\times \beta((z_1 - z_2)^2, 1 - z_1^2, 1 - z_2^2)\gamma^1(x + i0^+, z_1, z_2). \qquad \text{(A3.5)}$$

The function β, Eq. (A1.11), with arguments given in Eq. (A3.5), simplifies to

$$\beta = [2|z_1 - z_2|]^{-1}$$

Therefore

$$P^1(x) = \int_{-1}^{1} dz_1 \int_{-1}^{1} dz_2 z_1 z_2 \gamma^1(x + iO^+, z_1, z_2)/|z_1 - z_2|. \qquad \text{(A3.6)}$$

The function $\gamma^1 = \gamma^{\text{Ex}} + \gamma^{\text{SE}}$, Eqs (A1.15), (A1.16), introduces singularities to the integrand, laying along the lines $z_1 = x$ and $z_2 = x$. Coincidence of the singularities at the point of intersection of these lines produces a new type of distribution which is difficult to handle. Therefore, in order to avoid this problem we transform the function γ using a well known Feynman identity

$$\frac{1}{(z - x_1)(z - x_2)} = \int_0^1 \frac{d\alpha}{[z - x_1 - \alpha(x_2 - x_1)]^2}$$
$$= \int_0^1 \frac{d\alpha}{[z - x_2 - \alpha(x_1 - x_2)]^2} \qquad \text{(A3.7)}$$

to rewrite its "Ex" part, and then an obvious identity

$$\frac{1}{(z - x_0)^2} = \frac{-\partial}{\partial z}\frac{1}{(z - x_0)} \qquad \text{(A3.8)}$$

to further transform both "Ex" and "SE" parts:

$$\gamma^1(z, z_1, z_2) = \frac{-\partial}{\partial z}\frac{1}{2}\int_0^1 \mathrm{d}\alpha \left\{\left[\frac{1}{z - z_1 - \alpha(z_2 - z_1)} - \frac{1}{z - z_1}\right] + [z_1 \rightleftarrows z_2]\right\}. \tag{A3.9}$$

Although $P^1(x)$ was defined originally for real x, Eq. (A3.6) shows that it is an analytical function of complex z in the upper half plan $\mathrm{Im}\, z > 0$, because poles, occurring in γ^1, are located on the real axis (z_1, z_2 are real).

Inserting (A3.9) into (A3.6) we arrive at

$$P^1(z) = \frac{\mathrm{d}}{\mathrm{d}z} R(z) \tag{A3.10}$$

where the function

$$R(z) = \int_{-1}^1 \mathrm{d}z_1 \int_{-1}^1 \mathrm{d}z_2 \frac{z_1 z_2}{|z_1 - z_2|}\left(-\frac{1}{2}\right) \times \int_0^1 \mathrm{d}\alpha \left\{\left[\frac{1}{z - z_1 - \alpha(z_2 - z_1)} - \frac{1}{z - z_1}\right] + [z_1 \rightleftarrows z_2]\right\} \tag{A3.11}$$

is also an analytical function of z in the $\mathrm{Im}\, z > 0$ half plane. From (A3.11) we can immediately calculate $\mathrm{Im}\, R(x)$ for real argument x as

$$\mathrm{Im}\, R(x) = \frac{\pi}{2}\int_0^1 \mathrm{d}\alpha \int_{-1}^1 \mathrm{d}z_1 \int_{-1}^1 \mathrm{d}z_2 \frac{z_1 z_2}{|z_1 - z_2|} \times [\delta(x - z_1 - \alpha(z_2 - z_1)) - \delta(x - z_1) + \delta(x - z_2 - \alpha(z_1 - z_2)) - \delta(x - z_2)]. \tag{A3.12}$$

To make further progress, notice that the integrand is symmetrical with respect to the interchange of z_1 and x_2. In such a case, for general $f(z_2, z_1) = f(z_1, z_2)$ we have

$$\int_{-1}^1 \mathrm{d}z_1 \int_{-1}^1 \mathrm{d}z_2 f(z_1, z_2) = 2\int_{-1}^1 \mathrm{d}z_1 \int_{z_1}^1 \mathrm{d}z_2 f(z_1, z_2) = 4\int_0^1 \mathrm{d}r_2 \int_{-(1-r_2)}^{(1-r_2)} \mathrm{d}r_1 f(r_1 - r_2, r_1 + r_2).$$

Applying this to (A3.11), after some algebra, we get ($r = r_2$)

$$\mathrm{Im}\, R(x) = \pi \int_0^1 \mathrm{d}\alpha \int_0^1 \frac{\mathrm{d}r}{r} [R_0(x, \alpha, r) + R_0(-x, \alpha, r)] \tag{A3.13}$$

where

$$R_0(x, \alpha, r) = \theta(1 - x - 2(1 - \alpha)r)\theta(1 + x - 2\alpha r) \times \{[r(1 - 2\alpha) + x]^2 - r^2\} - \theta(1 - x - 2r)\theta(1 + x)\{[r + x]^2 - r^2\}. \quad \text{(A3.14)}$$

The function R_0 represents a quadratic polynomial of r, extending over a restricted range of r, dictated by θ-functions. Because, a priori, we do not know if the integral is convergent, let us put for a moment a positive ε instead of 0 as a lower limit of integration over r. After performing these integrations we find that the coefficient at $\ln \varepsilon$ is exactly zero, so the integral is convergent. It must be stressed, however, that the last fact holds only in the case when the sum of the "Ex" and "SE" contributions appears as the integrand (the first and the second terms of Eq. (A3.14), respectively). If one attempts to calculate each one of these contributions separately, this would lead to divergent results. After some straightforward algebra the final result is obtained from (A3.13) as

$$\text{Im } R(x) = \pi\theta(1 - x^2)\left[1 + 3x^2 + \ln\left(\frac{1 - x^2}{4}\right)\right]. \quad \text{(A3.15)}$$

Coming back to the evaluation of (A3.1), we see that $P^0(x)$ is needed (but this function is known, Eqs (A2.3), (A2.4)), and $P^1(x)$—both its real and imaginary part. From the form (A3.10) it is clear that we need Re $R(x)$ besides Im $R(x)$, found in Eq. (A3.15). The function Re $R(x)$ may be calculated, in principle, from Im $R(x)$, using Kramers-Krönig relations. But in the case of Im $R(x)$ having a logarithmic singularity at $x \to \pm 1$, this approach is difficult because we do not know a ready prescription as to the way to handle a product of this singular function and the principal value $P(1/(x - x_0))$ distribution, when one point of singularity approaches the second one. Similar difficulties will arise during subsequent integration (A3.1).

Therefore we choose another way of calculating the integral (A3.1), namely by application of the methods of analytical functions, in the spirit of an example discussed in Appendix 7. Because for $x > 1$, Im $P(x) = 0$, see Eq. (A3.15), and Im $P^0(x) = 0$, Eq. (A2.3), therefore we may formally extend the upper limit of integration in (A3.1) and write

$$I_0^1 = \frac{2}{\pi} \text{Im} \int_0^\infty dx P^1(x)[P^0(x)]^{-2} \quad \text{(A3.16)}$$

and then integrate along a contour in the complex plane, starting from 0 and ending at ∞, but omitting the point of singularity $x = 1$.

We insert (A3.10) into (A3.16) and then integrate by parts

$$I_0^1 = \frac{2}{\pi} \operatorname{Im} \int_0^\infty dz [P^0(z)]^{-2} \frac{d}{dz} R(z)$$

$$= \frac{2}{\pi} \operatorname{Im}\{[P^0(\infty)]^{-2} R(\infty) - [P^0(0)]^{-2} R(0)\}$$

$$- \frac{2}{\pi} \operatorname{Im} \int_0^\infty dz R(z) \frac{d}{dz} [P(z)]^{-2}. \tag{A3.17}$$

Because for $|x| > 1$ both $P^0(x)$ and $R(x)$ are purely real, there is no contribution of the first term of the above result. From (A2.3) and (A2.4) we find $\operatorname{Re} P^0(0) = 1$, $\operatorname{Im} P^0(0) = 0$, while from (A3.15) $\operatorname{Im} R(0) = \pi(1 - \ln 4)$ and, as it will be shown in Eq. (A3.22), $\operatorname{Re} R(0) = 0$. Therefore Eq. (A3.17) may be rewritten as

$$I_0^1 = -\frac{2}{\pi} \pi(1 - \ln 4) - \frac{2}{\pi} \operatorname{Im} \int_0^\infty dz R(z) \frac{d}{dz} [P^0(z)]^{-2}. \tag{A3.18}$$

Now we are going to apply the results of Appendix 7. For that reason we must find the spectral representations for the functions occuring in the integral in (A3.18).

Concerning $R(z)$, we must check its behaviour at large $|x|$. We expand the integrand of (A3.11) in powers of $1/z$, and, after some algebra we find

$$R(z) = -\frac{4}{45z^3} + O\left(\frac{1}{z^4}\right). \tag{A3.19}$$

Therefore the spectral representation (A7.2) for the function R exists

$$R_{SR}(z) = \int_{-\infty}^\infty \frac{d\xi}{\pi} \frac{\operatorname{Im} R(\xi)}{\xi - z} \tag{A3.20}$$

and, for real argument,

$$R(x) = R_{SR}(x + i0^+). \tag{A3.21}$$

Note that because $\operatorname{Im} R(x)$, Eq. (A3.15), is an even function, then, according to (A3.21), (A3.20)

$$\operatorname{Re} R(-x) = -\operatorname{Re} R(x). \tag{A3.22}$$

Now let us investigate $d[P^0(z)]^{-2}/dz$. From (A2.3) and (A2.4) it is easy to obtain an analytical continuation of $P^0(x)$ from real x into the complex plane:

$$P^0(z) = 1 + \frac{z}{2} \ln\left(\frac{z-1}{z+1}\right) \tag{A3.23}$$

We see that this function is analytical on the whole complex plane except the poles at $z = \pm 1$. A cut, connecting these points, makes this function single-valued. By tracing countours of $|P^0(z)| = \text{const}$ on the complex plane we analyzed the behaviour of this function and found that $[P^0(z)]^{-1}$ has no poles, and it must be analytical function, as being a reciprocal of the analytical function. Therefore the function $\mathrm{d}[P^0(z)]^{-2}/\mathrm{d}z$ must be also analytical. Now we investigate it at large $|z|$. Expanding $P^0(z)$, Eq. (A3.23)

$$P^0(z) = -\frac{1}{3z^2}\left(1 + \frac{3}{5z^2} + \frac{3}{7z^4} + \cdots\right) \tag{A3.24}$$

and then performing differentiation and other manipulations on the series we get finally

$$\frac{\mathrm{d}}{\mathrm{d}z}[P^0(z)]^{-2} = 36z^3 - \frac{108}{5}z + \frac{0}{z} - \frac{192}{875z^3} - \frac{5184}{67375z^5} + \cdots \tag{A3.25}$$

Therefore the spectral representation is possible after subtracting the terms which are large for large $|z|$:

$$\frac{\mathrm{d}}{\mathrm{d}z}[P^0(z)]^{-2} = 36z^3 - \frac{108}{5}z + S_{\mathrm{SR}}(z), \tag{A3.26}$$

$$S_{\mathrm{SR}}(z) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\xi}{\pi} \frac{\mathrm{Im}\, S(\xi)}{\xi - z}, \tag{A3.27}$$

$$\mathrm{Im}\, S(x) = \mathrm{Im} \frac{\mathrm{d}}{\mathrm{d}x}[P^0(x)]^{-2}. \tag{A3.28}$$

The last quantity is obtained by direct differentiation of the known expressions (A2.3) and (A2.4).

In the final step we insert (A3.21) and (A3.26) into (A3.18) to get

$$\begin{aligned} I_0^1 &= 2(\ln 4 - 1) - \frac{2}{\pi} \mathrm{Im} \int_0^\infty \mathrm{d}x R_{\mathrm{SR}}(x + i0^+) \\ &\quad \times [36x^3 - \tfrac{108}{5}x + S_{\mathrm{SR}}(x + i0^+)] \\ &= 2(\ln 4 - 1) - \frac{2}{\pi}\int_0^1 \mathrm{d}x \left[1 + 3x^2 + \ln\left(\frac{1-x^2}{4}\right)\right] \\ &\quad \times [36x^3 - \tfrac{108}{5}x] - I[R, S] = 1.1819290 - I[R, S] \end{aligned} \tag{A3.29}$$

where $I[R, S]$ is to be calculated according to (A7.8). Because Im $S(x)$ and Im $R(x)$ are both even functions, therefore the result is not zero,

$$I[R, S] = -4 \int_0^1 \frac{dx_1}{\pi} \operatorname{Im} R(x_1) \int_0^1 \frac{dx_2}{\pi} \operatorname{Im} S(x_2) \frac{1}{x_1 + x_2}$$
$$= -0.3651376 \tag{A3.30}$$

by numerical integration. Therefore, finally

$$I_0^1 = 1.5470666. \tag{A3.31}$$

Some remarks concerning numerical integration (A3.30) may be useful. For small x_1 and x_2, the functions Im $R(x_1)$ and Im $S(x_2)$ tend to constant values. If polar coordinates are used in this region, the integrand becomes finite. In the regions $x_1 \to 1$ or $x_2 \to 1$ the integrand diverges, Im $R(1 - \xi) \propto \ln(\xi)$, Im $S(1 - \xi) \propto \{1/[\xi(\ln \xi)^4]\}$, but is integrable. Numerical quadratures must take into account this singular behaviour. Their quality and accuracy may be easily checked because similar integrals

$$S_{Ml} = \frac{2}{\pi} \int_0^1 dx \operatorname{Im} S(x) x^l \tag{A3.32}$$

are exactly known, e.g. $S_{M0} = 0$, $S_{M2} = 192/875$, $S_{M4} = 5184/67375$. This property is immediately established if the large-$|z|$ expansion of (A3.27) is inserted into (A3.26) and compared with the expansion (A3.25). A similar check exists for integration of Im $R(x)$.

Appendix 4 Evaluation of $S^{Sc}(k)$ and its contribution to $[g(r) - 1]_{osc}$

According to (1.4), (4.4) and (4.6), the screening-effect part of the static structure factor is given by

$$S^{Sc}(k) = \int_{-\infty}^{\infty} d\omega S^{Sc}(k, \omega) \tag{A4.1}$$

$$S^{Sc}(k, \omega) = \theta(\omega) \frac{3}{\pi} \left(\frac{k}{k_{TF}}\right)^2 \operatorname{Im} Q^{Sc}(k, \omega) \tag{A4.2}$$

$$Q^{Sc}(k, \omega) = -[Q^0(k, \omega)]^2 \tag{A4.3}$$

i.e. it is expressed in terms of the well known[1] Lindhard's function $Q^0(k, \omega)$. We recall its form (note $\omega = kx$)

$$Q^0(k, kx) = \frac{3\pi\omega_p^2}{4k^3}\left\{\frac{4}{\pi}\left[\left(\frac{k}{2} - x\right)f_L\left(\frac{k}{2} - x\right) + \left(\frac{k}{2} + x\right)f_L\left(\frac{k}{2} + x\right)\right]\right.$$
$$+ i\left[\theta\left(1 - \left(\frac{k}{2} - x\right)^2\right)\left(1 - \left(\frac{k}{2} - x\right)^2\right)\right.$$
$$\left.\left. - \theta\left(1 - \left(\frac{k}{2} + x\right)^2\right)\left(1 - \left(\frac{k}{2} + x\right)^2\right)\right]\right\} \quad \text{(A4.4)}$$

where $f_L(x)$ is the normalized static Lindhard's function

$$f_L(x) = \frac{1}{2} + \frac{1 - x^2}{4x} \ln\left|\frac{1 + x}{1 - x}\right|. \quad \text{(A4.5)}$$

So, according to (A4.3) and (A4.2)

$$\operatorname{Im} Q^{\mathrm{Sc}}(k, \omega) = -2 \operatorname{Re} Q^0(k, \omega) \operatorname{Im} Q^0(k, \omega) \quad \text{(A4.6)}$$

$$S^{\mathrm{Sc}}(k, kx) = \theta(x)C^{\mathrm{Sc}}(k)\left[\theta\left(1 - \left(\frac{k}{2} - x\right)^2\right)\Phi^{\mathrm{Sc}}\left(\frac{k}{2} - x, k\right)\right.$$
$$\left. - \theta\left(1 - \left(\frac{k}{2} + x\right)^2\right)\Phi^{\mathrm{Sc}}\left(\frac{k}{2} + x, k\right)\right] \quad \text{(A4.7)}$$

where

$$C^{\mathrm{Sc}}(k) = -\frac{8}{\pi}\left(\frac{3\pi}{4}\frac{\omega_p^2}{k^3}\right)^2 \frac{3}{\pi}\left(\frac{k}{k_{\mathrm{TF}}}\right)^2 = -\frac{9}{2}\frac{\omega_p^2}{k^4} \quad \text{(A4.8)}$$

$$\Phi^{\mathrm{Sc}}(v, k) = (1 - v^2)[vf_L(v) + (k - v)f_L(k - v)]. \quad \text{(A4.9)}$$

Now we integrate over frequencies, Eq. (A4.1), and obtain

$$S^{\mathrm{Sc}}(k) = kC^{\mathrm{Sc}}(k)[S_A(k) - 2\theta(2 - k)S_B(k)] \quad \text{(A4.10)}$$

where

$$S_A(k) = \int_{-1}^{1} dv\Phi^{\mathrm{Sc}}(v, k) \quad \text{(A4.11)}$$

$$S_B(k) = \int_0^{(2-k)/2} dx\Phi^{\mathrm{Sc}}(1 - x, k). \quad \text{(A4.12)}$$

The form (A4.10) is dictated by the presence of θ-functions in (A4.7).

The function $S^{\mathrm{Sc}}(k)$ is non-analytical at $k = 2$. In order to apply the Lighthill procedure (see Section II) we must expand it in powers of a small departure from the point of non-analyticity $\xi = k - 2$.

Inserting (A4.9) into (A4.11) we get

$$S_A(2 + \xi) = \int_{-1}^{1} \mathrm{d}v(1 - v^2)vf_L(v) + \int_{-1}^{1} \mathrm{d}v(1 - v^2)(2 + \xi - v)f_L(2 + \xi - v). \quad \text{(A4.13)}$$

Because $f_L(x)$, Eq. (A4.5), is even, the first integral vanishes. To analyze the second one, let us rewrite $xf_L(x)$ as $xf_L(x) = x/2 - \frac{1}{4}(x - 1)(x + 1)\ln|x + 1| + \frac{1}{4}(x + 1)(x - 1)\ln|x - 1|$. Proceeding to isolate the non-analytic (na) part, we see that the region of $x \approx 1$ will be involved. We find after some calculation the result

$$S_{A\mathrm{na}}(2 + \xi) = \tfrac{1}{6}[\xi^3 + O(\xi^4)]\ln|\xi|. \quad \text{(A4.14)}$$

Similarly, calculating the contribution B we find

$$S_B(2 + \xi) = \tfrac{1}{4}\xi^2 + [\tfrac{1}{16} - \tfrac{1}{12}\ln 2 + \tfrac{1}{8}\ln|\xi|]\xi^3 + O(\xi^4 \ln|\xi|). \quad \text{(A4.15)}$$

Here analytical terms must be also included, because the factor $\theta(-\xi)$ in (A4.10) provides the non-analyticity. So, combining both contributions in (4.10) and taking into acount the k-dependent prefactor, we get finally for the non-analytical part of $[S(k) - 1]k$ the contribution

$$[S^{\mathrm{Sc}}(2 + \xi)(2 + \xi)]_{\mathrm{na}} = \tfrac{9}{8}\omega_p^2\{-\tfrac{1}{4}\xi^2\,\mathrm{sgn}(\xi) + \xi^3[(\tfrac{3}{16} + \tfrac{1}{12}\ln 2)\,\mathrm{sgn}(\xi) - \tfrac{1}{24}\ln|\xi| - \tfrac{1}{8}\ln|\xi|\,\mathrm{sgn}(\xi)] + O(\xi^4\ln|\xi|)\}. \quad \text{(A4.16)}$$

Making use of the Fourier transform of $\xi^n\,\mathrm{sgn}(\xi)$, Eq. (2.4), and of $\xi^n \ln|\xi|$, $\xi^n \ln|\xi|\,\mathrm{sgn}(\xi)$, see Lighthill's[3] table or Eq. (A9.4)-(A9.11), and applying (2.1) with (2.3) to (3.1), we get

$$[g(r) - 1]^{\mathrm{Sc}}_{\mathrm{osc}} = \frac{9\alpha r_s}{4\pi}\left\{\frac{\cos(2r)}{r^4} - \frac{\pi}{4}\frac{\cos(2r)}{r^5} + [\tfrac{3}{2}(\gamma + \ln 2r) - \tfrac{1}{2}(1 + \ln 2)]\frac{\sin(2r)}{r^5} + O\left(\frac{\ln r}{r^6}\right)\right\} \quad \text{(A4.17)}$$

where $\gamma \simeq 0.5772$ is Euler's constant.

Appendix 5 Evaluation of $S^{SE}(k)$

According to (1.2), (4.4), (4.5) and (A1.1), the self-energy part of the static structure factor is given by

$$S^{SE}(k) = \int_{-\infty}^{\infty} d\omega S^{SE}(k, \omega) \tag{A5.1}$$

$$S^{SE}(k, \omega) = \theta(\omega) \frac{3}{\pi} \left(\frac{k}{k_{TF}} \right)^2 \operatorname{Im} Q^{SE}(k, \omega) \tag{A5.2}$$

$$Q^{SE}(k, \omega) = \left(\frac{\alpha r_s}{\pi^2 k} \right)^2 F^{SE}(k, \omega) \tag{A5.3}$$

where $F^{SE}(k, \omega)$ is defined by (A1.14). The dependence on the frequency $\omega = kx$ enters $F^{SE}(k, \omega)$ only via the function γ^{SE}, Eq. (1.16), being a factor of its integrand:

$$\gamma^{SE}(z, z_1, z_2) = -\frac{1}{2}\left[\frac{1}{(z - z_1)^2} + \frac{1}{(z - z_2)^2} \right], \tag{A5.4}$$

$z = x + iO^+$. Therefore the integration over frequencies, Eq. (A5.1), including $\theta(\omega)$ from Eq. (A5.2), will affect only Im γ^{SE}:

$$\begin{aligned} &\int_0^{\infty} k \, dx \operatorname{Im} \gamma^{SE}(x + i0^+, z_1, z_2) \\ &= \frac{k}{2} \operatorname{Im} \left[\frac{1}{x + i0^+ - z_1} + \frac{1}{x + i0^+ - z_2} \right]_{x=0}^{x=\infty} \\ &= \frac{k}{2} \operatorname{Im} \left[\frac{1}{z_1 + i0^+} + \frac{1}{z_2 + i0^+} \right] \\ &= \frac{k\pi}{2} [\delta(z_1) + \delta(z_2)]. \end{aligned} \tag{A5.5}$$

So, using (A1.14),

$$\begin{aligned} S^{SE}(k) &\propto \int dz_1 \, dz_2 \, ds_1 \, ds_2 N(z_1, s_1, k) N(z_2, s_2, k) \\ &\quad \times \beta((z_1 - z_2)^2, s_1, s_2)[\delta(z_1) + \delta(z_2)] \\ &= \int ds_1 \, ds_2 \left[N(0, s_1, k) \int dz_2 N(z_2, s_2, k) \beta(z_2^2, s_1, s_2) \right. \\ &\quad \left. + N(0, s_2, k) \int dz_1 N(z_1, s_1, k) \beta(z_1^2, s_1, s_2) \right] \end{aligned} \tag{A5.6}$$

But, according to (A1.17)

$$N(0, s_i, k) = 0 \tag{A5.7}$$

so, finally

$$S^{SE}(k) = 0 \tag{A5.8}$$

for any $k > 0$.

Appendix 6 Evaluation of $S^{Ex}(k)$ and its contribution to $[g(r) - 1]_{osc}$

According to Eqs (1.2), (4.4), (4.5) and (A1.1) the exchange part of the static structure factor for $k > 0$ is given by

$$S^{Ex}(k) = \int_{-\infty}^{\infty} d\omega S^{Ex}(k, \omega) \tag{A6.1}$$

$$S^{Ex}(k, \omega) = \theta(\omega) \frac{3}{\pi}\left(\frac{k}{k_{TF}}\right)^2 \operatorname{Im} Q^{Ex}(k, \omega) \tag{A6.2}$$

$$Q^{Ex}(k, \omega) = \left(\frac{\alpha r_s}{\pi^2 k}\right)^2 F^{Ex}(k, \omega) \tag{A6.3}$$

where $F^{Ex}(k, \omega)$ is defined by (A1.14) with (A1.15). The dependence on frequency $\omega = kx$ enters $F^{Ex}(k, \omega)$ only via the function $\gamma^{Ex}(x + i0^+, z_1, z_2)$, Eq. (A1.15), being a factor of its integrand. Therefore the integration over frequencies, Eq. (A6.1), including $\theta(\omega)$ from (A6.2), will affect only Im γ^{Ex}:

$$\int_0^{\infty} k \, dx \operatorname{Im} \gamma^{Ex}(x + i0^+, z_1, z_2) = \frac{\pi k}{2} \phi(z_1, z_2), \tag{A6.4}$$

see Eqs (A7.5)-(A7.7). Therefore

$$\begin{aligned} S^{Ex}(k) &= \frac{3\alpha r_s}{4\pi^4} \frac{\pi^2}{2} \frac{(-\pi)k}{k^2} \int_0^{\infty} ds_1 \int_0^{\infty} ds_2 \int_{-\infty}^{\infty} dz_1 \\ &\quad \times \int_{-\infty}^{\infty} dz_2 \frac{\theta(-z_1 z_2)}{|z_1| + |z_2|} NN\beta \\ &= \frac{3\alpha r_2}{4\pi k} \int_0^{\infty} ds_1 \int_0^{\infty} ds_2 \int_0^{\infty} dz_1 \int_0^{\infty} dz_2 \frac{\beta((z_1 + z_2)^2, s_1, s_2)}{z_1 + z_2} \\ &\quad \times N(z_1, s_1, k) N(z_2, s_2, k). \end{aligned} \tag{A6.5}$$

We tried to perform integrations in (A6.5), but it happened impossible to obtain a result in terms of elementary functions. Therefore we proceeed to calculate the contributions to the pair-correlation function, according to (1.1), keeping $S^{\mathrm{Ex}}(k)$ in its integral form

$$[g(r) - 1]^{\mathrm{Ex}}_{\mathrm{osc}} = \frac{3}{2r} \operatorname{Im} \int_0^\infty \mathrm{d}k \exp(ikr) S^{\mathrm{Ex}}(k) k. \tag{A6.6}$$

Here non-analyticity of $S^{\mathrm{Ex}}(k)$, at $k > 0$, must be taken into account. Using (A6.5), Eq. (A6.6) has been transformed into

$$[g(r) - 1]^{\mathrm{Ex}}_{\mathrm{osc}} = \frac{9\alpha r_s}{8\pi r} \int_0^\infty \mathrm{d}z_1 \int_0^\infty \mathrm{d}z_2 \int_0^\infty \mathrm{d}s_2 \int_0^\infty \mathrm{d}s_1 \times \frac{\beta((z_1 + z_2)^2, s_1, s_2)}{z_1 + z_2} \Xi(r, z_1, s_1, z_2, s_2) \tag{A6.7}$$

where

$$\Xi(r, z_1, s_1, z_2, s_2) = \operatorname{Im} \int_0^\infty \mathrm{d}k \exp(ikr) N(z_1, s_1, k) N(z_2, s_2, k). \tag{A6.8}$$

Let us investigate the dependence on k of the function $N(z_i, s_i, k)$, occurring above. For $z_i > 0$, according to Eq. (A1.17) we find

$$\begin{aligned} N(z_i, s_i, k = 2\kappa) &= \theta(1 - s_i - (\kappa - z_i)^2) - \theta(1 - s_i - (\kappa + z_i)^2) \\ &= \theta(1 - s_i) B(\kappa, |\sqrt{1 - s_i} - z_i|, \sqrt{1 - s_i} + z_i) \end{aligned} \tag{A6.9}$$

where the "gate" function is introduced

$$B(x, a, b) = \begin{cases} 1 & \text{for } a < x < b \\ 0 & \text{for remaining } x. \end{cases} \tag{A6.10}$$

The following identity will be useful

$$\begin{aligned} &B(x, a_1, b_1) B(x, a_2, b_2) \\ &\quad = [\theta(x - a_1) B(a_1, a_2, b_2) - \theta(x - b_1) B(b_1, a_2, b_2)] + [1 \rightleftarrows 2]. \end{aligned} \tag{A6.11}$$

Using this, integral (A6.8) is evaluated to be

$$\begin{aligned} \Xi(r, z_1, s_1, z_2, s_2) = \frac{1}{r} \theta(1 - s_1) \theta(1 - s_2) \{ &[\cos(2ra_1) B(a_1, a_2, b_2) \\ &- \cos(2rb_1) B(b_1, a_2, b_2)] + [1 \rightleftarrows 2] \} \end{aligned} \tag{A6.12}$$

where

$$a(z, s) = |\sqrt{1 - s} - z|; \qquad a_i = a(z_i, s_i) \tag{A6.13}$$

$$b(z, s) = \sqrt{1 - s} + z; \qquad b_i = b(z_i, s_i) \tag{A6.14}$$

Because of the symmetry of (A6.7), the contribution of the terms from the second square brackets in (A6.12) is exactly the same as of those from the first square bracket.

We see that the dependence on r of Eq. (A6.7) with (A6.12) is in the form of a prefactor $1/r^2$ and, within the integrand, as factors $\cos(2ra_1)$ and $\cos(2rb_1)$. So Lighthill's procedure may be applied, if the next integration, involving a variable present in a_1 or b_1, is performed. In doing this it is sufficient to keep only the leading terms in $1/r$ expansion, which simplifies substantially the resulting lengthy expressions.

It is impossible to give all details here of the calculation of integrals in (A6.7), so we will merely record the main steps. The variable s_1 is replaced by $\tau_1 = (1 - s_1)^{1/2}$. Note that $\cos(2ra_1) = \cos(2r(\tau_1 - z_1)) = \mathrm{Re}\exp(i2r(\tau_1 - z_1))$, and similarly with b_1. The nonanalyticity of the integrand, as a function of τ_1, is due to integration limits: $B(\tau_1, 0, 1)$ and the factors $B(|\tau_1 - z_1|, a_2, b_2)$ or $B(\tau_1 + z_1, a_2, b_2)$.

The following leading terms are obtained after the integration over τ_1 being performed

$$[g(r) - 1]^{\mathrm{Ex}}_{\mathrm{osc}} = -\frac{9\alpha r_s}{8\pi r^3}\,\mathrm{Im}[\exp(-i2r)A_{1\,\mathrm{FT}}(2r) + \exp(i2r)A_{2\,\mathrm{FT}}(2r)] \tag{A6.15}$$

where

$$A_{j\mathrm{FT}}(2r) = \int_{-\infty}^{\infty} \mathrm{d}z_1 \exp(i2rz_1)A_j(z_1) \tag{A6.16}$$

$$A_j(z_1) = \theta(z_1)\int_0^{\infty} \mathrm{d}z_2 \frac{2}{z_1 + z_2}C_j(z_1, z_2) \tag{A6.17}$$

$$C_j(z_1, z_2) = \int_0^1 \mathrm{d}s_2 \frac{1}{(z_1 + z_2)^2 + s_2}B_j(z_1, z_2, s_2) \tag{A6.18}$$

$$B_1(z_1, z_2, s_2) = B(|z_1 - 1|, a_2, b_2) \tag{A6.19}$$

$$B_2(z_1, z_2, s_2) = B(z_1 + 1, a_2, b_2). \tag{A6.20}$$

It is easy to evaluate C_j, Eq. (A6.18), because the only role of B_j is to change the limits of integration, depending on (z_1, z_2). In different regions of the (z_1, z_2)-plane, which are separated by straight lines, different expression for C_j are obtained, like a constant, $\ln(z_1 + z_2)$ or

$$C_j \propto \ln(2z_1 z_2 + z_1 - z_2). \tag{A6.21}$$

Then evaluation of A_j, Eq. (A6.17), with such C_j as in the first two examples, is straightforward. The case (A6.21) leads to the following integral

$$\begin{aligned}\tilde{A}(z_1) &= \int_{\alpha(z_1)}^{\beta(z_1)} \frac{dz_2}{z_1 + z_2} \ln(2z_1 z_2 + z_1 - z_2) \\ &= \int_{z_1+\alpha}^{z_1+\beta} \frac{dx}{x}\left[\ln|2z_1(1 - z_1)| + \ln\left|1 - \frac{(1-2z_1)x}{2z_1(1-z_1)}\right|\right] \\ &= \ln|2z_1(1 - z_1)| \cdot \ln\left|\frac{z_1 + \beta}{z_1 + \alpha}\right| - \operatorname{dilog}\left(\frac{(1-2z_1)(z_1+\beta)}{2z_1(1-z_1)}\right) \\ &\quad + \operatorname{dilog}\left(\frac{(1-2z_1)(z_1+\alpha)}{2z_1(1-z_1)}\right).\end{aligned} \tag{A6.22}$$

The special function dilog(x) is defined and some of its properties are listed in Appendix 8.

In the next step analytical properties of $A_j(z_1)$ are investigated. The function $A_2(z_1)$ exhibits one point of non-analyticity at $z_1 = 0$, where its non-analytical part is

$$[A_2(z_1)]_{\text{na}} = \theta(z_1)[(\ln|z_1|)^2 - \frac{\pi^2}{3} + O(z_1 \ln|z_1|)]. \tag{A6.23}$$

The function $A_1(z_1)$ is non-analytical at the same point

$$[A_1(z_1)]_{\text{na}} = \theta(z_1)[(\ln|z_1|)^2 + \frac{\pi^2}{6} - 2\ln 2 + O(z_1 \ln|z_1|)] \tag{A6.24}$$

and also at points $z_1 = 1$ and $z_1 = 2$. As follows from Eq. (2.3) in application to (A6.16), non-analyticity at $z_1 = 1$ would lead to $A_{1\,\text{FT}} \propto \exp(i2r)/r$, so, according to (A6.15), to $[g(r) - 1]^{\text{Ex}} \propto \exp(i0)/r^4$, i.e. non-oscillatory character ($k = 0$), which must be excluded, since the expansion (4.1) is valid for $k > 0$. Close to the point $z_1 = 2$, $A_1(z_1) = O((z_1 - 2)^2)$, so it leads to $[g(r) - 1] = O(\exp(i4r)/r^5)$, i.e. higher order contribution. This contribution probably cancels out with other terms $O(1/r^5)$, discarded during the earlier steps of calculation.

It should be mentioned that in order to obtain the results (A6.23) and (A6.24), the properties of the dilogarithm (A8.3)–(A8.7) must be used.

Now we are ready to calculate $A_{j\mathrm{FT}}(2r)$, Eq. (A6.16), from Eqs (A6.23) and (A6.24), using (A9.5), (A9.7) and (A9.9), and remembering that $\theta(x) = [1 + \mathrm{sgn}(x)]/2$. We obtain

$$A_{1\mathrm{FT}}(2r) = \frac{\pi}{2r}[\gamma + \ln 2r] + \frac{i}{2r}\left[\frac{\pi^2}{12} - 2\ln 2 + (\gamma + \ln 2r)^2\right], \quad \text{(A6.25)}$$

$$A_{2\mathrm{FT}}(2r) = \frac{\pi}{2r}[\gamma + \ln 2r] + \frac{i}{2r}\left[-\frac{\pi^2}{12} - \frac{\pi^2}{3} + (\gamma + \ln 2r)^2\right]. \quad \text{(A6.26)}$$

Combining above terms into Eq. (A6.15) we get finally

$$[g(r) - 1]^{\mathrm{Ex}}_{\mathrm{osc}} = -\frac{9\alpha r_s \cos(2r)}{8\pi r^4}\left[(\gamma + \ln 2r)^2 - \ln 2 - \frac{\pi^2}{6}\right] + O\left(\frac{(\ln r)^2}{r^5}\right) \quad \text{(A6.27)}$$

Here an estimate of the terms, neglected during early stages, is added.

Appendix 7 Integral of the product of analytical functions

Let us investigate the following integral

$$I[F_1, F_2] = \frac{2}{\pi}\,\mathrm{Im}\int_0^{\infty} \mathrm{d}x F_1(x)F_2(x) \quad \text{(A7.1)}$$

involving two analytical functions $F_1(x)$ and $F_2(x)$ which are given in the form of the spectral representations

$$F_{j\mathrm{SR}}(z) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\xi_j}{\pi}\frac{\mathrm{Im}\,F_j(\xi_j)}{\xi_j - z}. \quad \text{(A7.2)}$$

Let us recall that such representation is possible if (i) the function $F_j(z)$ is analytical in the half-plane $\mathrm{Im}\,z > 0$, and (ii) if for large $|z|$ it is of the order of $1/z^{\alpha}$, $\alpha > 1$. Then for real argument x one has

$$F_j(x) = F_{j\mathrm{SR}}(x + i0^+). \quad \text{(A7.3)}$$

Substituting (A7.3) and (A7.2) into (A7.1) and interchanging the order of integrations, we find

$$I[F_1, F_2] = \int_{-\infty}^{\infty} \frac{\mathrm{d}\xi_1}{\pi}\,\mathrm{Im}\,F_1(\xi_1)\int_{-\infty}^{\infty} \frac{\mathrm{d}\xi_2}{\pi}\,\mathrm{Im}\,F_2(\xi_2)\phi(\xi_1, \xi_2) \quad \text{(A7.4)}$$

where

$$\phi(\xi_1, \xi_2) = \frac{2}{\pi} \operatorname{Im} \int_0^\infty dx \frac{1}{(x + i0^+ - \xi_1)(x + i0^+ - \xi_2)}. \quad \text{(A7.5)}$$

But

$$\frac{1}{(z - \xi_1)(z - \xi_2)} = \frac{1}{(\xi_1 - \xi_2)} \left[\frac{1}{z - \xi_1} - \frac{1}{z - \xi_2} \right] \quad \text{(A7.6)}$$

so

$$\phi(\xi_1, \xi_2) = \frac{2}{\pi(\xi_1 - \xi_2)} \int_0^\infty dx[-\pi\delta(x - \xi_1) + \pi\delta(x - \xi_2)]$$

$$= -\frac{2[\theta(\xi_1) - \theta(\xi_2)]}{\xi_1 - \xi_2} = -2\theta(-\xi_1\xi_2)/(|\xi_1| + |\xi_2|). \quad \text{(A7.7)}$$

Therefore

$$I[F_1, F_2] = -\frac{2}{\pi^2} \left[\int_0^\infty d\xi_1 \int_{-\infty}^0 d\xi_2 + \int_{-\infty}^0 d\xi_1 \int_0^\infty d\xi_2 \right] \times \frac{\operatorname{Im} F_1(\xi_1) \operatorname{Im} F_2(\xi_2)}{|\xi_1| + |\xi_2|}$$

and finally

$$I[F_1, F_2] = \frac{-2}{\pi^2} \int_0^\infty d\xi_1 \int_0^\infty d\xi_2 \frac{1}{\xi_1 + \xi_2} [\operatorname{Im} F_1(\xi_1) \operatorname{Im} F_2(-\xi_2) + \operatorname{Im} F_1(-\xi_1) \operatorname{Im} F_2(\xi_2)] \quad \text{(A7.8)}$$

Note that $I[F_1, F_2]$ is zero if the parity of Im F_1 is different than that of Im F_2. We see from Eq. (A7.8) that for evaluation of the integral (A7.1) it is enough, in essence, to know only imaginary part of each of the functions involved in the integration.

Appendix 8 Dilogarithm

A special function of a real argument, defined as

$$\operatorname{dilog}(x) = \int_0^x \frac{-\ln|1 - t|}{t} dt \quad \text{(A8.1)}$$

and called dilogarithm is very useful for integration over dx of expressions like $\ln|a + bx|/(c + ex)$. The definition (A8.1) is a narrowed version of the definition introduced by Lewin[4] for $\mathrm{Li}_2(x)$—the logarithmic integral of the second order, namely

$$\mathrm{dilog}(x) = \mathrm{Re}\ \mathrm{Li}_2(x). \tag{A8.2}$$

We recall here from the Lewin's monograph[4] some useful properties of the dilogarithm. This function is continuous everywhere and it is analytical for all x except $x = 1$ and $x = \pm\infty$. Here are some particular values of it:

$$\mathrm{dilog}(-1) = -\pi^2/12 \tag{A8.3}$$

$$\mathrm{dilog}(1) = -\pi^2/6. \tag{A8.4}$$

The following identities are of interest

$$\mathrm{dilog}(x) + \mathrm{dilog}(1 - x) = \mathrm{dilog}(1) - \ln|x| \ln|1 - x| \tag{A8.5}$$

$$\mathrm{dilog}(x) + \mathrm{dilog}(1/x) = 2\ \mathrm{dilog}(\mathrm{sgn}(x)) - \tfrac{1}{2}(\ln|x|)^2 \tag{A8.6}$$

and the expansion, valid for $|x| \leqslant 1$:

$$\mathrm{dilog}(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^2}. \tag{A8.7}$$

From Eq. (A8.5) the expansion around $x = 1$ may be found or the value at $x = \frac{1}{2}$ and $x = 2$; from Eq. (A8.6)—behaviour at $|x| \to \infty$ established.

Appendix 9 Fourier transform of powers of the logarithm

We are going to use here the methods developed by Lighthill[3] to calculate the Fourier transform, Eq. (2.1), of the non-analytical functions, involving powers of the logarithm.

Because

$$\left(\frac{\partial}{\partial\alpha}\right)^n |x|^\alpha = \left(\frac{\partial}{\partial\alpha}\right)^n \exp(\alpha \ln|x|) = (\ln|x|)^n |x|^\alpha \tag{A9.1}$$

we can obtain the FT of $(\ln|x|)^n$ from the n-th derivatives over α of the FT of $|x|^\alpha$, and the FT of $\mathrm{sgn}(x)(\ln|x|)^n$ from the n-th derivative of the

FT of $\mathrm{sgn}(x)|x|^\alpha$, all in the limit $\alpha \to 0$. We use the following expressions, given by Lighthill:

$$|x|^\alpha \underset{\mathrm{FT}}{\to} \frac{2}{|y|} \cos\left(\frac{\pi(\alpha+1)}{2}\right)\Gamma(\alpha+1)|y|^{-\alpha} \quad \text{(A9.2)}$$

$$|x|^\alpha \,\mathrm{sgn}(x) \underset{\mathrm{FT}}{\to} \frac{2i}{y} \sin\left(\frac{\pi(\alpha+1)}{2}\right)\Gamma(\alpha+1)|y|^{-\alpha}. \quad \text{(A9.3)}$$

The following results are obtained

$$(\ln|x|)^1 \underset{\mathrm{FT}}{\to} 2|y|^{-1}\left[\frac{-\pi}{2}\right] \quad \text{(A9.4)}$$

$$(\ln|x|)^2 \underset{\mathrm{FT}}{\to} 2|y|^{-1}[\pi(\gamma + \ln|y|)] \quad \text{(A9.5)}$$

$$(\ln|x|)^3 \underset{\mathrm{FT}}{\to} 2|y|^{-1}\left[-\frac{\pi^3}{8} - \frac{3\pi}{2}(\gamma + \ln|y|)^2\right] \quad \text{(A9.6)}$$

$$\mathrm{sgn}(x) \underset{\mathrm{FT}}{\to} 2iy^{-1} \quad \text{(A9.7)}$$

$$(\ln|x|)^1 \,\mathrm{sgn}(x) \underset{\mathrm{FT}}{\to} 2iy^{-1}[-(\gamma + \ln|y|)] \quad \text{(A9.8)}$$

$$(\ln|x|)^2 \,\mathrm{sgn}(x) \underset{\mathrm{FT}}{\to} 2iy^{-1}\left[\frac{-\pi^2}{12} + (\gamma + \ln|y|)^2\right] \quad \text{(A9.9)}$$

$$(\ln|x|)^3 \,\mathrm{sgn}(x) \underset{\mathrm{FT}}{\to} 2iy^{-1}\left[-2\zeta(3) + \frac{\pi^2}{4}(\gamma + \ln|y|) - (\gamma + \ln|y|)^3\right] \quad \text{(A9.10)}$$

We recall also the useful relation

$$x^n f(x) \underset{\mathrm{FT}}{\to} \left(\frac{\mathrm{d}}{i\,\mathrm{d}y}\right)^n f_{\mathrm{FT}}(y). \quad \text{(A9.11)}$$

The Euler constant $\gamma \simeq 0.5772$ and Riemann's function $\zeta(3) \simeq 1.2021$ are involved above.