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Coordinate Space Form of Interacting Reference Response Function of d-Dimensional Jellium.

R. FANTONI and M. P. TOSI

Istituto Nazionale di Fisica della Materia and Classe di Scienze, Scuola Normale Superiore Piazza dei Cavalieri 7, I-56126 Pisa, Italy

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Summary. — The interacting reference response function $\chi_{\mathrm{I}}^{[3]}(k)$ of three-dimensional jellium in k space was defined by Niklasson in terms of the momentum distribution of the interacting electron assembly. Here the Fourier transform $F_{\mathrm{I}}^{[d]}(r)$ of $\chi_{\mathrm{I}}^{[d]}(k)$ is studied for the jellium model with e^2/r interactions in dimensionality $d = 1$, 2 and 3, in an extension of recent work by Holas, March and Tosi for the case $d = 3$. The small-r and large-r forms of $F_{\mathrm{I}}^{[d]}(r)$ are explicitly evaluated from the analytic behaviour of the momentum distribution $n_d(p)$. In the appendix, a model of $n_d(p)$ is constructed which interpolates between these limits.

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1. – Introduction.

The linear density response function $\chi^{[d]}(k, \omega)$ of the jellium model in dimensionality d is customarily written in the form of an RPA-like expression involving a single-particle reference susceptibility and a local field factor [1]. While the reference susceptibility is usually taken as the Lindhard function for the ideal Fermi gas, Niklasson [2] introduced for $d = 3$ an interacting reference susceptibility which is defined in a similar way as the Lindhard function but with the ideal Fermi momentum distribution replaced by the true momentum distribution of the interacting electron assembly. This involves, of course, a redefinition of the local field factor, which acquires the appealing feature of tending to a constant at large wave number k instead of being asymptotically proportional to k^2 [3, 4].

In recent work Holas, March and Tosi [5], hereafter referred to as HMT, have evaluated the r-dependence of the Fourier transform of Niklasson's interacting reference susceptibility in the static case for $d = 3$, using known analytic properties of the true momentum distribution. The present work extends their approach to lower dimensionalities ($d = 2$ and 1) and contrasts the results with those obtained for $d = 3$.

2. – Interacting reference susceptibility and local field factor.

2·1. *Definition of interacting reference susceptibility in* $\boldsymbol{k}$ *space.* – The interacting reference susceptibility in the static case ($\omega = 0$) is defined in $\boldsymbol{k}$ or reciprocal space as

$$\chi_{\mathrm{I}}^{[d]}(k) = -\frac{2^{(3-d)}m}{\pi^d} P \int \mathrm{d}^d p \frac{n_d(p)}{k^2 + 2\boldsymbol{k}\cdot\boldsymbol{p}}, \tag{2.1}$$

where m is the electronic mass and $n_d(p)$ is the momentum distribution function of the interacting electron fluid. Owing to the isotropy of the homogeneous phase of jellium, the angular integration in eq. (2.1) can be carried out to yield

$$\chi_{\mathrm{I}}^{[3]}(k) = -\frac{m}{\pi^2 k} \int_0^\infty \mathrm{d}p\, p\, n_3(p) \ln \left| \frac{k+2p}{k-2p} \right|, \tag{2.2}$$

$$\chi_{\mathrm{I}}^{[2]}(k) = -\frac{4m}{\pi k} \int_0^\infty \mathrm{d}p\, p\, n_2(p) \frac{\theta(k-2p)}{\sqrt{k^2-4p^2}} \tag{2.3}$$

and

$$\chi_{\mathrm{I}}^{[1]}(k) = -\frac{8m}{\pi} \int_0^\infty \mathrm{d}p\, n_1(p) \frac{1}{k^2-4p^2}. \tag{2.4}$$

When the true momentum distribution in eqs. (2.2)-(2.4) is replaced by the ideal Fermi distribution, one recovers the well-known Lindhard results:

$$\chi_0^{[3]}(k) = -\frac{m k_{\mathrm{F}}}{2\pi^2}\left[1 + \frac{(2k_{\mathrm{F}})^2 - k^2}{4k_{\mathrm{F}} k} \ln \left| \frac{k+2k_{\mathrm{F}}}{k-2k_{\mathrm{F}}} \right|\right], \tag{2.5}$$

$$\chi_0^{[2]}(k) = -\frac{m}{\pi}\left[1 - \theta(k-2k_{\mathrm{F}})\sqrt{1-\left(\frac{2k_{\mathrm{F}}}{k}\right)^2}\right] \tag{2.6}$$

and

$$\chi_0^{[1]}(k) = -\frac{4m}{\pi k} \ln \left| \frac{k+2k_{\mathrm{F}}}{k-2k_{\mathrm{F}}} \right|. \tag{2.7}$$

The Fermi momentum k_{F} is related to the particle number density ϱ_d by

$$k_{\mathrm{F}} = 2\pi^{1/2}\left[\frac{1}{4} d\, \Gamma\left(\frac{d}{2}\right) \varrho_d\right]^{1/d}. \tag{2.8}$$

2·2. *Local field factor.* – The density response function $\chi^{[d]}(k, \omega)$ is written in terms of the interacting reference susceptibility $\chi_{\mathrm{I}}^{[d]}(k, \omega)$ and of a local field factor

$\tilde{G}_d(k, \omega)$ as

$$\chi^{[d]}(k, \omega) = \frac{\chi_{\mathrm{I}}^{[d]}(k, \omega)}{1 - v_d(k)[1 - \tilde{G}_d(k, \omega)]\chi_{\mathrm{I}}^{[d]}(k, \omega)} . \tag{2.9}$$

Here, $v_d(k)$ is the d-dimensional Fourier transform of the e^2/r Coulomb repulsive interaction, given by $4\pi e^2/k^2$ for $d = 3$ and by $2\pi e^2/k$ for $d = 2$. In the jellium model for electrons in a quantum wire the Coulomb matrix element can be taken as

$$v_1(k) = e^2 h(kR_0) , \tag{2.10}$$

where R_0 is the effective radius of the wire and the function $h(x)$ can be of various forms depending on the type of transverse confinement. We shall take it to have the asymptotic behaviours

$$h(x \to 0) = C_-(R_0) \ln(x) \tag{2.11}$$

and

$$h(x \to \infty) = C_+(R_0) \frac{4\pi e^2}{x^2} , \tag{2.12}$$

the latter being valid when both transverse confinement lengths are finite [6]. $C_-(R_0)$ and $C_+(R_0)$ in eqs. (2.11) and (2.12) are confinement-dependent functions.

It was first shown by Niklasson [2] from the equations of motion for the single-particle and two-particle density matrices that, in regions of the (k, ω)-plane well outside the particle-hole continuum, the local field factor introduced in eq. (2.9) satisfies two exact relations in particular limits (see also [7]). These relations are easily expressed in terms of the following function:

$$G_d^{\mathrm{PV}}(k) = \frac{1}{N} \sum_{k'} \left\{ \left(\frac{\boldsymbol{k} \cdot \boldsymbol{k}'}{k^2} \right)^2 \frac{v_d(k')}{v_d(k)} - \left(\frac{\boldsymbol{k} \cdot (\boldsymbol{k} + \boldsymbol{k}')}{k^2} \right)^2 \frac{v_d(|\boldsymbol{k} + \boldsymbol{k}'|)}{v_d(k)} \right\} (S_d(k') - 1) . \tag{2.13}$$

Here, $S_d(k)$ is the static structure factor of d-dimensional jellium, related to the pair distribution function $g_d(r)$ by

$$1 - g_d(r) = \frac{1}{N} \sum_{\boldsymbol{k}} [1 - S_d(k)] \exp[i\boldsymbol{k} \cdot \boldsymbol{r}] . \tag{2.14}$$

$G_d^{\mathrm{PV}}(k)$ in eq. (2.13) is the form taken in d-dimensional jellium by the static local field factor first introduced by Pathak and Vashishta [8]. Precisely, for $|\omega \pm k^2/2m| \gg k_{\mathrm{F}}/2m$ one has

$$\lim_{k \to \infty} \tilde{G}_d(k, \omega) = G_d^{\mathrm{PV}}(\infty) \tag{2.15}$$

at finite ω and

$$\lim_{\omega \to \infty} \tilde{G}_d(k, \omega) = G_d^{\mathrm{PV}}(k) \tag{2.16}$$

at finite k.

2·3. *Asymptotic behaviour of local field factors for large k.* – Equations (2.13) and (2.15) yield the following exact asymptotic values of the local field factor for large

wave number and finite frequency:

$$(2.17)\qquad \tilde{G}_d(k\to\infty,\omega)=\begin{cases}\dfrac{2}{3}[1-g_3(0)] & \text{for } d=3\,,\\ 1-g_2(0) & \text{for } d=2\,,\\ 1-g_1(0)+(R_0^2/4\pi\varrho_1 C_+)\displaystyle\int \mathrm{d}\boldsymbol{q}\, q^2 h(qR_0)[S_1(q)-1] & \\ & \text{for } d=1\,.\end{cases}$$

An alternative form of the local field factor needs to be introduced when one replaces $\chi_{\mathrm{I}}^{[d]}(k,\omega)$ in eq. (2.9) with the Lindhard function $\chi_0^{[d]}(k,\omega)$, namely

$$(2.18)\qquad G_d(k,\omega)=1+[v_d(k)\chi^{[d]}(k,\omega)]^{-1}-[v_d(k)\chi_0^{[d]}(k,\omega)]^{-1}=$$
$$=\tilde{G}_d(k,\omega)+[v_d(k)\chi_{\mathrm{I}}^{[d]}(k,\omega)]^{-1}-[v_d(k)\chi_0^{[d]}(k,\omega)]^{-1}\,.$$

Following the analysis given by Holas [3], the static Lindhard function has the large-k expansion

$$(2.19)\qquad \chi_0^{[d]}(k)=-4m\varrho_d k^{-2}[1+4C_1^{[d]}\langle p^2\rangle_0^{[d]}k^{-2}+16C_2^{[d]}\langle p^4\rangle_0^{[d]}k^{-4}+\ldots],$$

where

$$(2.20)\qquad C_n^{[d]}=\begin{cases}(2n+1)^{-1} & \text{for } d=3\,,\\ (2n-1)!!/(2n)!! & \text{for } d=2\,,\\ 1 & \text{for } d=1\end{cases}$$

and the notation

$$(2.21)\qquad \langle f(\boldsymbol{p})\rangle_0^{[d]}=\frac{2}{N}\sum_{\boldsymbol{p}} n_d^0(p)f(\boldsymbol{p})$$

has been used, $n_d^0(p)$ being the ideal Fermi-momentum distribution. In particular,

$$(2.22)\qquad \langle p^{2n}\rangle_0^{[d]}=\frac{d}{2n+d}k_{\mathrm{F}}^{2n}\,.$$

With the notation $\langle\ldots\rangle_{\mathrm{I}}^{[d]}$ for the average in eq. (2.21) when $n_d^0(p)$ is replaced by $n_d(p)$, and using the normalization condition $\sum_{\boldsymbol{p}} n_d^0(p)=\sum_{\boldsymbol{p}} n_d(p)=N/2$, we reach the result

$$(2.23)\qquad G_d(k,0)=\tilde{G}_d(k,0)+\frac{1}{m\varrho_d v_d(k)}\{(\langle p^2\rangle_{\mathrm{I}}^{[d]}-\langle p^2\rangle_0^{[d]})C_1^{[d]}+$$
$$+\frac{4}{k^2}[(\langle p^4\rangle_{\mathrm{I}}^{[d]}-\langle p^4\rangle_0^{[d]})C_2^{[d]}-((\langle p^2\rangle_{\mathrm{I}}^{[d]})^2-(\langle p^2\rangle_0^{[d]})^2)(C_1^{[d]})^2]+O(k^{-4})\}\,.$$

Taking into account eq. (2.17), we conclude that the leading term in the high-k

expansion of $G_d(k, 0)$ is given by

$$G_d(k, 0) \xrightarrow[k \to \infty]{} \begin{cases} \Delta_T^{[3]} k^2/(6\pi \varrho_3 e^2) & \text{for } d = 3\,, \\ \Delta_T^{[2]} k/(2\pi \varrho_2 e^2) & \text{for } d = 2\,, \\ \Delta_T^{[1]} (R_0 k)^2/(2\pi \varrho_1 e^2 C_+) & \text{for } d = 1\,, \end{cases} \tag{2.24}$$

where $\Delta_T^{[d]} = \langle T \rangle_{\mathrm{I}}^{[d]} - \langle T \rangle_0^{[d]}$ and $T = p^2/2m$ is the kinetic energy operator.

2·4. *Asymptotic behaviour of $G_d(k, \omega)$ for large ω.* – Following Iwamoto [9], the asymptotic form of the Lindhard function at high frequency can be given in terms of the frequency-moment sum rules, namely

$$\lim_{\omega \to \infty} \chi_0^{[d]}(k, \omega) = \sum_{j=1}^{\infty} \frac{L_{2j+1}^{[d]}(k)}{\omega^{2j}}\,. \tag{2.25}$$

The first two moments in eq. (2.25) are

$$L_1^{[d]}(k) = \frac{\varrho_d k^2}{m} \tag{2.26}$$

and

$$L_3^{[d]}(k) = \frac{\varrho_d k^2}{m}\left[\left(\frac{k^2}{2m}\right)^2 + \frac{12}{d}\langle T \rangle_0^{[d]} \frac{k^2}{2m}\right]. \tag{2.27}$$

The analogous expansion for $\chi_{\mathrm{I}}^{[d]}(k, \omega)$ is obtained by replacing $\langle \ldots \rangle_{\mathrm{I}}^{[d]}$ with $\langle \ldots \rangle_0^{[d]}$ in the frequency moments. By substituting these expansions into eq. (2.18) we find

$$G_d(k, \omega = \infty) = G_d^{\mathrm{PV}}(k) - \frac{12}{d} \frac{\Delta_T^{[d]}}{2\varrho_d v_d(k)}\,. \tag{2.28}$$

Comparison of eqs. (2.23) and (2.28) shows that their leading terms differ only by a numerical factor.

3. – Coordinate space response function $F_{\mathrm{I}}^{[d]}(r)$.

The response function $F_{\mathrm{I}}^{[d]}(r)$ in coordinate space is defined as the d-dimensional Fourier transform of $\chi_{\mathrm{I}}^{[d]}(k)$. Angular integration yields

$$F_{\mathrm{I}}^{[3]}(r) = \frac{1}{2\pi^2 r} \int_0^{\infty} \mathrm{d}k\, k\, \chi_{\mathrm{I}}^{[3]}(k) \sin(kr)\,, \tag{3.1}$$

$$F_{\mathrm{I}}^{[2]}(r) = \frac{1}{2\pi} \int_0^{\infty} \mathrm{d}k\, k\, \chi_{\mathrm{I}}^{[2]}(k) J_0(kr) \tag{3.2}$$

and

$$F_{\mathrm{I}}^{[1]}(r) = \frac{1}{\pi}\int_0^\infty \mathrm{d}k\, k\, \chi_{\mathrm{I}}^{[1]}(k)\cos(kr)\,. \tag{3.3}$$

Using eqs. (2.2)-(2.4) in eqs. (3.1)-(3.3) and two definite integrals given by Gradshteyn and Ryzhik [10] we find

$$F_{\mathrm{I}}^{[3]}(r) = -\frac{m}{2\pi^3 r^2}\int_0^\infty \mathrm{d}p\, p\, n_3(p)\sin(2pr)\,, \tag{3.4}$$

$$F_{\mathrm{I}}^{[2]}(r) = \frac{m}{\pi^2 r}\int_0^\infty \mathrm{d}p\, n_2(p)[\pi p r J_0(pr)\, Y_0(pr)] \tag{3.5}$$

and

$$F_{\mathrm{I}}^{[1]}(r) = -\frac{2m}{\pi}\int_0^\infty \mathrm{d}p\, \frac{n_1(p)}{p}\sin(2pr)\,. \tag{3.6}$$

Upon inserting the ideal Fermi distribution in place of the true momentum distribution in eqs. (3.1)-(3.3), we recover results for the Lindhard function in r-space [11]:

$$F_0^{[3]}(r) = -\frac{m k_{\mathrm{F}}^2}{2\pi^3}\frac{j_1(2k_{\mathrm{F}} r)}{r^2}\,, \tag{3.7}$$

$$F_0^{[2]}(r) = -\frac{m k_{\mathrm{F}}^2}{2\pi}[J_0(k_{\mathrm{F}} r)\, Y_0(k_{\mathrm{F}} r) + J_1(k_{\mathrm{F}} r)\, Y_1(k_{\mathrm{F}} r)] \tag{3.8}$$

and

$$F_0^{[1]}(r) = -\frac{2m}{\pi}\mathrm{Si}(2k_{\mathrm{F}} r)\,. \tag{3.9}$$

In these equations $j_1(x)$ is the spherical Bessel function $[\sin(x) - x\cos(x)]/x^2$, $J_n(x)$ and $Y_n(x)$ are the n-th-order Bessel functions of the first and the second kind and $\mathrm{Si}(x)$ is the sine integral.

Of course, $n_d(p)$ tends to the ideal Fermi distribution in the limit of coupling strength tending to zero. However, at finite coupling strength the momentum distribution acquires a high-momentum tail and its discontinuous jump across the Fermi surface is reduced below unity. Numerical determinations of $n_d(p)$ by quantal simulation methods are available both for $d = 2$ [12] and $d = 3$ [13]. In the following sections we shall use the above-mentioned properties of $n_d(p)$ to determine the behaviours of $F_{\mathrm{I}}^{[d]}(r)$ at small and large r.

4. – Small-r expansion of interacting susceptibility.

The small-r properties of $F_{\mathrm{I}}^{[d]}(r)$ are determined by the behaviour of $n_d(p)$ at large momenta. This is known to be

$$n_3(p) = \left(\frac{4\pi\varrho_3}{a_0}\right)^2 g_3(0)\,p^{-8} + \ldots \tag{4.1}$$

for $d = 3$, from the work of Kimball [14, 15] and

$$n_2(p) = \left(\frac{2\pi\varrho_2}{a_0}\right)^2 g_2(0)\,p^{-6} + \ldots \tag{4.2}$$

for $d = 2$, from the work of Rajagopal and Kimball [16]. In these equations a_0 is the Bohr radius and $g_d(0)$ is the value of the pair distribution function $g_d(r)$ evaluated at separation $r = 0$. This value is related to the asymptotic behaviour of the structure factor $S_d(k)$ according to

$$g_3(0) = \frac{3\pi a_0}{8k_{\mathrm{F}}^3} \lim_{k\to\infty} k^4(1 - S_3(k)) \tag{4.3}$$

and

$$g_2(0) = \frac{a_0}{2k_{\mathrm{F}}^2} \lim_{k\to\infty} k^3(1 - S_2(k)). \tag{4.4}$$

The asymptotic behaviour of the momentum distribution for the case $d = 1$ has been evaluated in [6]. The result is

$$n_1(p) = \left(\frac{4\pi\varrho_1 C_+}{a_0 R_0^2}\right)^2 g_1(0)\,p^{-8} + \ldots, \tag{4.5}$$

where

$$g_1(0) = \frac{a_0 R_0^2}{4\pi k_{\mathrm{F}} C_+} \lim_{k\to\infty} k^4(1 - S_1(k)). \tag{4.6}$$

Using eq. (4.1) in eq. (3.4) HTM find

$$F_{\mathrm{I}}^{[3]}(r) = -\frac{m\varrho_3}{\pi r}\left\{1 - \frac{4}{3}\langle T\rangle_{\mathrm{I}}^{[3]} m r^2 + \frac{8}{15}\langle T^2\rangle_{\mathrm{I}}^{[3]} m^2 r^4 - \frac{a_8}{45\pi\varrho_3} r^5 + \ldots\right\}, \tag{4.7}$$

where a_8 is the coefficient of p^{-8} in eq. (4.1) and $\langle T^n\rangle_{\mathrm{I}}^{[d]}$ is the n-th moment of the kinetic energy T.

For the other dimensionalities we obtain the following expressions by the same

method. For $d = 2$ we get

$$(4.8)\qquad F_{\mathrm{I}}^{[2]}(r) = \frac{2m\varrho_2}{\pi}\Big\{\big[(\gamma - \ln(2)) + \langle \ln(p)\rangle_{\mathrm{I}}^{[2]}\big] + \\ + \ln(r) + \Big[\Big(\frac{1}{2} - \gamma + \ln(2)\Big) m\langle T\rangle_{\mathrm{I}}^{[2]} - \langle T\ln(p)\rangle_{\mathrm{I}}^{[2]}\Big] r^2 + m\langle T\rangle_{\mathrm{I}}^{[2]} r^2 \ln(r) + \ldots\Big\},$$

where $\gamma = 0.57721\ldots$ is Euler's constant. For $d = 1$ we find

$$(4.9)\qquad F_{\mathrm{I}}^{[1]}(r) = -2m\varrho_1 r\Big\{\sum_{n=0}^{3} \frac{(-8m)^n}{(2n+1)!}\langle T^n\rangle_{\mathrm{I}}^{[1]} r^{2n} + \frac{a_w}{8!\,\varrho_1}(2r)^7 + \ldots\Big\},$$

where a_w is the coefficient of p^{-8} in eq. (4.5).

It should be noticed that higher-order terms in the expansions given in eqs. (4.7)-(4.9) cannot be evaluated without knowledge of the high-momentum behaviour of $n_d(p)$ going beyond that explicitly shown in eqs. (4.1), (4.2) and (4.5). The coefficients of such higher-order terms may diverge for some forms of $n_d(p)$.

5. – Long-range behaviour of $F_{\mathrm{I}}^{[d]}(r)$.

In order to determine the behaviour of $F_{\mathrm{I}}^{[3]}(r)$ at large r, HMT rewrite the right-hand side of eq. (3.4) in the form of the one-dimensional Fourier transform of the function $\vartheta(p)\,p\,n_3(p)$ and apply the Lighthill technique for the asymptotic estimation of such Fourier transforms [17].

The momentum distribution in the homogeneous phase of d-dimensional jellium is known to have a discontinuity (reduction by a jump) of magnitude Z_{F} at $p = k_{\mathrm{F}}$ and most probably discontinuities in its derivatives there. One can thus express $n_d(p)$ as

$$(5.1)\qquad n_d(p) = \mathrm{sgn}(p - k_{\mathrm{F}}) \sum_{n=0}^{\infty} \frac{b_n^{[d]}}{n!}(p - k_{\mathrm{F}})^n + \text{analytical terms},$$

with $b_0^{[d]} = -Z_{\mathrm{F}}/2$. Moreover, we assume that the expansion

$$(5.2)\qquad n_d(p) = \sum_{n=0}^{\infty} \frac{c_n^{[d]}}{n!} p^n + \text{analytical terms}$$

holds for $n_d(p)$ near $p = 0$.

HMT conclude from such behaviours of $n_3(p)$ that the asymptotic large-r expansion for $F_{\mathrm{I}}^{[3]}(r)$ has an oscillatory part

$$(5.3)\qquad [F_{\mathrm{I}}^{[3]}(r)]^{\mathrm{osc}} = -\frac{m}{\pi^3 r^2}\,\mathrm{Im}\Big\{\exp[2ik_{\mathrm{F}} r] \sum_{n=0}^{\infty} (k_{\mathrm{F}} b_n^{[3]} + n b_{n-1}^{[3]})^{n+1}\Big\}$$

with leading term $-[mk_{\mathrm{F}} b_0^{[3]}/2\pi^3]\cos(2k_{\mathrm{F}} r)/r^3$, as well as a non-oscillatory contribution

$$(5.4)\qquad [F_{\mathrm{I}}^{[3]}(r)]^{\text{non-osc}} = -\frac{m}{2\pi^3 r^2} \sum_{n=1}^{\infty} (-1)^n \frac{2n c_{2n-1}^{[3]}}{(2r)^{2n+1}},$$

where only the odd terms in the power series expansion (5.2) contribute, with leading term $[mc_{\mathrm{I}}^{[3]}/(2\pi)^3]/r^3$.

In the following two subsections we shall apply these arguments to determine the long-range behaviour of $F_{\mathrm{I}}^{[2]}(r)$ and $F_{\mathrm{I}}^{[1]}(r)$.

5·1. *Two-dimensional jellium.* – The analysis of the large-r behaviour of $F_{\mathrm{I}}^{[2]}(r)$ on the basis of the behaviours of $n_2(p)$ in eqs. (5.1) and (5.2) is quite complex. There does not seem to be an asymptotic expansion for the product $J_0(x)\,Y_0(x)$ in eq. (3.5) having a simple expression for its coefficients.

We start by defining the function $f_0(x) = \pi x[J_0(x)\,Y_0(x)]$ for $x \geqslant 0$ and its successive integrals

$$f_1(x) = \int^x f_0(t)\,\mathrm{d}t = \frac{\pi}{2}x^2[J_0(x)\,Y_0(x) + J_1(x)\,Y_1(x)] = \int_0^x f_0(t)\,\mathrm{d}t \tag{5.5}$$

and

$$f_n(x) = \int^x f_{n-1}(t)\,\mathrm{d}t\,. \tag{5.6}$$

These functions possess an upper bound ($|f_n(x)| \leqslant$ constant) and have the following asymptotic expansions:

i) the large-x expansion

$$f_0(x) = \cos(2x)\left[-1 + \frac{20}{128\,x^2} + O(x^{-4})\right] + \sin(2x)\left[-\frac{1}{4x} - \frac{42}{256\,x^3} + O(x^{-5})\right] \tag{5.7}$$

and for any $n > 0$

$$f_n(x) \xrightarrow[x\to\infty]{} \begin{cases} \dfrac{(-)^{n/2+1}}{2^n}\cos(2x) + \ldots & \text{for even } n\,, \\[2ex] \dfrac{(-)^{(n-1)/2}}{2^n}\sin(2x) + \ldots & \text{for odd } n\,; \end{cases} \tag{5.8}$$

ii) the small-x expansion

$$f_0(x) = 2x\ln(2x) + O(x) \tag{5.9}$$

and for any $n > 0$

$$f_n(x) \xrightarrow[x\to 0]{} \frac{2}{(n+1)!}x^{n+1}\ln(x) + \sum_{i=1}^{n}\frac{d_i}{(n-i)!}x^{n-i}\,. \tag{5.10}$$

Here, the coeefficients d_i are the integration constants needed to connect with the large-x behaviour in eq. (5.8). For example, we have $d_1 = 0$ (see eq. (5.5)) and $d_2 \approx$

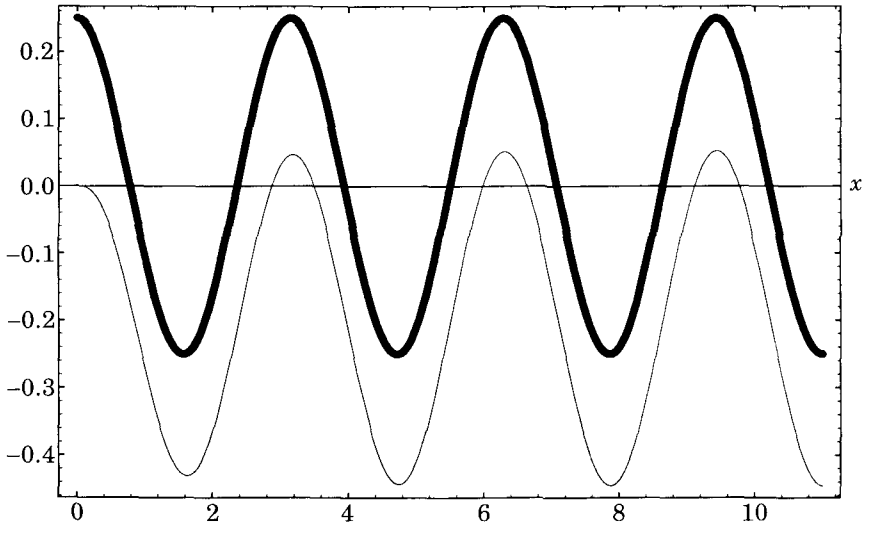

Fig. 1. – Plot of the function $(\pi/2)x^2\int_0^x[J_0(t)Y_0(t)+J_1(t)Y_1(t)]\,dt$ (lower curve) compared with $\cos(2x)/4$ (upper curve).

$\approx -0.196344\ldots$ (see fig. 1). In general d_n can be obtained by a limiting process,

$$d_n = \lim_{j\to\infty}\begin{cases}\displaystyle\int_0^{(2j+1)(\pi/4)} f_{n-1}(t)\,dt & \text{for even } n\,,\\ \displaystyle\int_0^{j(\pi/2)} f_{n-1}(t)\,dt & \text{for odd } n\,.\end{cases} \tag{5.11}$$

Given these definitions, the long-range behaviour of $F_{\mathrm{I}}^{[2]}(r)$ can be obtained by successive integration by parts on eq. (3.5). A first integration by parts yields

$$F_{\mathrm{I}}^{[2]}(r) = -\frac{m}{(\pi r)^2}\int_0^\infty (2b_0^{[2]}\delta(p-k_{\mathrm{F}}) + [D_{\mathrm{F}}^1 n_2](p))f_1(pr)\,dp = \tag{5.12}$$

$$= -\frac{m}{\pi^2 r}\left(\frac{2b_0^{[2]}f_1(k_{\mathrm{F}}r)}{r} + \frac{1}{r}\int_0^\infty [D_{\mathrm{F}}^1 n_2](p)f_1(pr)\,dp\right),$$

where we have introduced the notation $[D_{\mathrm{F}}n_2](p)$ for the derivative of $n_2(p)$ at $p>k_{\mathrm{F}}$ and $p<k_{\mathrm{F}}$ and have made use of the fact that $n_2(p)f_1(pr)$ vanishes both at infinity and in the origin. From eqs. (5.8) and (5.12) we thus find

$$F_{\mathrm{I}}^{[2]}(r) = \frac{mb_0^{[2]}\sin(2k_{\mathrm{F}}r)}{(\pi r)^2} + O\left(\frac{1}{r^2}\right). \tag{5.13}$$

After N integrations by parts, we obtain

$$F_{\mathrm{I}}^{[2]}(r) = -\frac{m}{\pi^2 r}\left[\sum_{n=1}^{N}(-)^n \frac{2b_{n-1}^{[2]} f_n(k_{\mathrm{F}} r)}{r^n} - \sum_{n=1}^{N}(-)^n \frac{d_n c_{n-1}^{[2]}}{r^n} + \ldots\right]. \tag{5.14}$$

Evidently, in analogy with the case $d = 3$ the large-r asymptotic expansion of $F_{\mathrm{I}}^{[2]}(r)$ can be divided into the sum of an oscillatory part and a non-oscillatory part. The former is given by the first term on the right-hand side of eq. (5.14) and its leading term is

$$[F_{\mathrm{I}}^{[2]}(r)]^{\mathrm{osc}} \approx \frac{m b_0^{[2]} \sin(2k_{\mathrm{F}} r)}{(\pi r)^2}. \tag{5.15}$$

The non-oscillatory part is given by the second term on the right-hand side of eq. (5.14) and its leading term is

$$[F_{\mathrm{I}}^{[2]}(r)]^{\text{non-osc}} \approx \frac{m d_2 c_1^{[2]}}{\pi^2 r^3}. \tag{5.16}$$

5·2. *One-dimensional jellium.* – In order to apply the Lighthill technique to determine the long-range behaviour of $F_{\mathrm{I}}^{[1]}(r)$, we first rewrite eq. (3.6) in the form of a one-dimensional Fourier transform,

$$F_{\mathrm{I}}^{[1]}(r) = -\frac{2m}{\pi}\,\mathrm{Im}\int_{-\infty}^{\infty} \mathrm{d}p\,\theta(p)\frac{n_1(p)}{p}\exp[2ipr]. \tag{5.17}$$

Because of the θ function the integrand in eq. (5.17) is non-analytic at $p = 0$. This may lead to a non-oscillatory contribution to the large-r expansion. From expansion (5.2) we obtain

$$[F_{\mathrm{I}}^{[1]}(r)]^{\text{non-osc}} = -\frac{2m}{\pi}\left[\frac{c_0^{[1]}\pi}{2} + \sum_{n=0}^{\infty}\frac{c_{2n+1}^{[1]}}{(2n+1)!}\left(\frac{-1}{2r}\right)^{2n+1}\right]. \tag{5.18}$$

The singularity of $n_1(p)$ at $p = k_{\mathrm{F}}$ is instead responsible for an oscillatory contribution, following from eq. (5.1) as

$$[F_{\mathrm{I}}^{[1]}(r)]^{\mathrm{osc}} = -\frac{2m}{\pi}\,\mathrm{Im}\sum_{n=0}^{\infty}\left\{\frac{b_n^{[1]}}{n!}\int_{-\infty}^{\infty}\mathrm{d}p\,\mathrm{sgn}(p)\frac{p^n}{p+k_{\mathrm{F}}}\exp[2ipr]\right\}\exp[-2ik_{\mathrm{F}} r]. \tag{5.19}$$

To leading order the result is

$$[F_{\mathrm{I}}^{[1]}(r)]^{\mathrm{osc}} = \frac{2m b_0^{[1]}\cos(2k_{\mathrm{F}} r)}{\pi k_{\mathrm{F}} r} + O\left(\frac{1}{r^2}\right). \tag{5.20}$$

5·3. *Comparison of results in various dimensionalities.* – In summary, table I compares the leading terms of the large-r asymptotic expansion of $F_{\mathrm{I}}^{[d]}(r)$ in the various dimensionalities. Evidently, the leading term in the asymptotic expansion

TABLE I. – *Leading terms of the large-r asymptotic expansion for the oscillating and non-oscillating parts of* $F_{\mathrm{I}}^{[d]}(r)$.

$F_{\mathrm{I}}^{[d]}(r \to \infty)$	Oscillating term	Non-oscillating term
$d = 3$	$-\dfrac{m k_{\mathrm{F}} b_0^{[3]} \cos(2k_{\mathrm{F}} r)}{2(\pi r)^3}$	$\dfrac{m c_1^{[3]}}{(2\pi)^3 r^5}$
$d = 2$	$\dfrac{m b_0^{[2]} \sin(2k_{\mathrm{F}} r)}{(\pi r)^2}$	$\dfrac{m d_2 c_1^{[2]}}{\pi^2 r^3}$
$d = 1$	$\dfrac{2m b_0^{[1]} \cos(2k_{\mathrm{F}} r)}{\pi k_{\mathrm{F}} r}$	$-m c_0^{[1]}$

is the oscillating one for $d = 3$ and $d = 2$, while in the quantum wire the non-oscillating term is dominant.

6. – Conclusions.

The main results of the present work concern i) the asymptotic behaviours of the local field factors $\tilde{G}_d(k, \omega)$ and $G_d(k, \omega)$ in eqs. (2.17), (2.24) and (2.28); ii) expressions (3.4)-(3.6) for the interacting reference susceptibility $F_{\mathrm{I}}^{[d]}(r)$ in the form of a single integral and iii) the small-r and large-r expansions of $F_{\mathrm{I}}^{[d]}(r)$ in eqs. (4.7)-(4.9), (5.3), (5.4), (5.14) and (5.18)-(5.20). These results were already known in the literature [3-5] for $d = 3$, but are mostly new for $d = 2$ and $d = 1$.

In the Appendix we have evaluated a model for the momentum distribution $n_d(r)$, which leads to a model for $F_{\mathrm{I}}^{[d]}(r)$ allowing an interpolation between the limiting behaviours discussed in sect. 4 and 5.

APPENDIX

Evaluation of $F_{\mathrm{I}}^{[d]}(r)$ using a model $n_d(r)$.

Following HMT we consider a model momentum distribution given for $d = 2$ and $d = 3$ by

$$n_d(p) = n_d^A(p) + n_d^B(p) = \vartheta(k_{\mathrm{F}} - p)(\alpha_d + \beta_d p^2) + \frac{a_{2(d+1)}}{(\zeta_d^2 + p^2)^{d+1}}, \tag{A.1}$$

and for $d = 1$ by

$$n_1(p) = \vartheta(k_{\mathrm{F}} - p)(\alpha_1 + \beta_1 p^2) + \frac{a_w}{(\zeta_1^2 + p^2)^4}; \tag{A.2}$$

eqs. (A.1) and (A.2) satisfy properties (4.1), (4.2) and (4.5). Of their five parameters,

k_F and a_8, a_6 and a_w have an obvious meaning, while α_d, β_d and ζ_d can be determined from three requirements on the momentum distribution:

i) it satisfies the normalization condition $2\sum_p n_d(p) = N$, leading to

$$1 = \begin{cases} \alpha_3 + \dfrac{3}{5}\beta_3 k_F^2 + \dfrac{3\pi}{32}\dfrac{a_8}{k_F^3\zeta_3^5} & \text{for } d = 3\,, \\ \alpha_2 + \dfrac{1}{2}\beta_2 k_F^2 + \dfrac{1}{2}\dfrac{a_6}{k_F^2\zeta_2^4} & \text{for } d = 2\,, \\ \alpha_1 + \dfrac{1}{3}\beta_1 k_F^2 + \dfrac{5\pi}{32}\dfrac{a_w}{k_F\zeta_1^7} & \text{for } d = 1\,; \end{cases} \tag{A.3}$$

ii) it reproduces the value of the mean kinetic energy $\langle T\rangle_I^{[d]}$, leading to

$$\frac{\langle T\rangle_I^{[d]}}{\langle T\rangle_0^{[d]}} = \begin{cases} \alpha_3 + \dfrac{5}{7}\beta_3 k_F^2 + \dfrac{5\pi}{32}\dfrac{a_8}{k_F^5\zeta_3^3} & \text{for } d = 3\,, \\ \alpha_2 + \dfrac{2}{3}\beta_2 k_F^2 + \dfrac{a_6}{k_F^4\zeta_2^2} & \text{for } d = 2\,, \\ \alpha_1 + \dfrac{3}{5}\beta_1 k_F^2 + \dfrac{3\pi}{32}\dfrac{a_w}{k_F^3\zeta_1^5} & \text{for } d = 1\,; \end{cases} \tag{A.4}$$

iii) it reproduces the discontinuity Z_F at $p = k_F$, leading to

$$\alpha_d + k_F^2\beta_d = Z_F\,. \tag{A.5}$$

After inserting the model $n_d(p)$ of eqs. (A.1) and (A.2) into eqs. (3.4)-(3.6), all integrations can be performed analytically. The results are reported in the following subsections.

A·1. *Three-dimensional jellium.* – HMT find for $d = 3$

$$F_I^{[3]^A}(r) = -\frac{m k_F}{4(\pi r)^3}\left\{\left[-(\alpha_3 + k_F^2\beta_3) + \frac{3\beta_3}{2r^2}\right]\cos(2k_F r) + \right. \\ \left. + \left[\frac{\alpha_3 + 3k_F^2\beta_3}{2k_F r} - \frac{3\beta_3}{4k_F r^3}\right]\sin(2k_F r)\right\} \tag{A.6}$$

and (assuming $\zeta_3 > 0$)

$$F_I^{[3]^B}(r) = -\frac{m a_8}{32\pi^2\zeta_3^5 r}\left(1 + 2\zeta_3 r + \frac{4}{3}(\zeta_3 r)^2\right)\exp[-2\zeta_3 r]\,. \tag{A.7}$$

The model reference susceptibility is the sum of the two contributions in eqs. (A.6) and (A.7).

The small-r and large-r expansions of this model $F_I^{[3]}(r)$ agree with those given in eq. (4.7) and in eqs. (5.3) and (5.4). The contribution due to $F_I^{[3]^B}(r)$

is exponentially small at large r and non-oscillatory terms are absent because even powers only enter the small-p expansion of the model $n_3(p)$ in eq. (A.1).

A·2. *Two-dimensional jellium.* – For $d = 2$ we obtain, from well-known properties of the Bessel functions [18],

$$\text{(A.8)}\quad F_{\mathrm{I}}^{[2]^A}(r) = -\frac{m\alpha_2}{\pi r^2}\left\{\frac{(k_{\mathrm{F}}r)^2}{2}[J_0(k_{\mathrm{F}}r)Y_0(k_{\mathrm{F}}r) + J_1(k_{\mathrm{F}}r)Y_1(k_{\mathrm{F}}r)]\right\} -$$

$$-\frac{m\beta_2}{\pi r^4}\left\{\frac{(k_{\mathrm{F}}r)^4}{12}[3J_0(k_{\mathrm{F}}r)Y_0(k_{\mathrm{F}}r) + 2J_1(k_{\mathrm{F}}r)Y_1(k_{\mathrm{F}}r) - J_2(k_{\mathrm{F}}r)Y_2(k_{\mathrm{F}}r)]\right\} \xrightarrow[r\to\infty]{}$$

$$\xrightarrow[r\to\infty]{} m(\alpha_2 + k_{\mathrm{F}}^2\beta_2)\frac{\sin(2k_{\mathrm{F}}r)}{2(\pi r)^2}$$

and (assuming $\zeta_2 > 0$)

$$\text{(A.9)}\qquad F_{\mathrm{I}}^{[2]^B}(r) = \frac{\pi^2 a_6}{2^5} r\left[\frac{1}{\zeta_2}\frac{\mathrm{d}}{\mathrm{d}\zeta_2}\right]^2 [H_0^{(1)}(i\zeta_2 r)]^2\,,$$

where $H_0^{(1)}(x) = J_0(x) + iY_0(x)$ is the zeroth-order Bessel function of the third kind. The asymptotic large-r behaviour of this function is

$$\text{(A.10)}\qquad [H_0^{(1)}(i\zeta_2 r)]^2 \to -\frac{2}{\pi\zeta_2 r}\exp[-2\zeta_2 r]\,.$$

Finally, we have the model reference susceptibility

$$\text{(A.11)}\qquad F_{\mathrm{I}}^{[2]}(r) = F_{\mathrm{I}}^{[2]^A}(r) + F_{\mathrm{I}}^{[2]^B}(r)\,.$$

It is readily verified that the small-r and large-r expansions of this function agree with those given in eq. (4.8) and in eqs. (5.15) and (5.16). As in the case $d = 3$, the contribution due to $F_{\mathrm{I}}^{[2]^B}(r)$ is exponentially small at large r.

A·3. *One-dimensional jellium.* – For $d = 1$ we obtain

$$\text{(A.12)}\quad F_{\mathrm{I}}^{[1]^A}(r) = -\frac{2m\alpha_1}{\pi}\,\mathrm{Si}(2k_{\mathrm{F}}r) + \frac{m\beta_1}{\pi}\left[\frac{k_{\mathrm{F}}\cos(2k_{\mathrm{F}}r)}{r} - \frac{\sin(2k_{\mathrm{F}}r)}{2r^2}\right]$$

and (assuming $\zeta_1 > 0$)

$$\text{(A.13)}\qquad F_{\mathrm{I}}^{[1]^B}(r) = -\frac{m a_w}{\zeta_1^8}\left[1 - \left(1 + \frac{11}{4}\zeta_1 r + \frac{3}{4}(\zeta_1 r)^2 + \frac{1}{6}(\zeta_1 r)^3\right)\exp[-2\zeta_1 r]\right].$$

Finally, we have the model response function

$$\text{(A.14)}\qquad F_{\mathrm{I}}^{[1]}(r) = F_{\mathrm{I}}^{[1]^A}(r) + F_{\mathrm{I}}^{[1]^B}(r)\,.$$

Again it is readily verified that the small-r and large-r expansions of this function agree with those in eq. (4.9) and in eqs. (5.18) and (5.20). Contrary

to the other cases the term $F_{\mathrm{I}}^{[1]^{\beta}}(r)$ contributes to the leading term in the large-r expansion of $F_{\mathrm{I}}^{[1]}(r)$, its magnitude being $-m\,c_0^{[1]}$ with $c_0^{[1]} = \alpha_1 + a_w/\zeta_1^8$.

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