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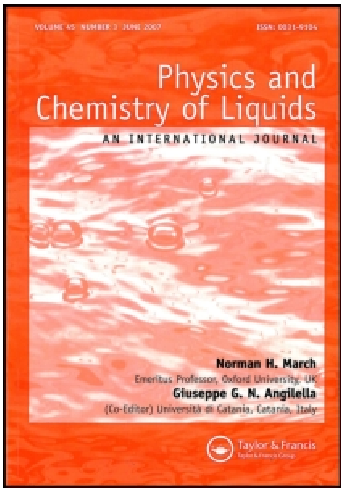

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Coordinate Space form of Interacting Reference Response Function of Jellium Model of an Electron Liquid

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COORDINATE SPACE FORM OF INTERACTING REFERENCE RESPONSE FUNCTION OF JELLIUM MODEL OF AN ELECTRON LIQUID

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The interacting reference response function $\chi_I(k)$ of jellium in **k** space is defined, according to Niklasson (1974), in terms of the momentum distribution $n(p)$ of the interacting electron liquid in a similar way as the Lindhard function $\chi_0(k)$ in terms of the Fermi distribution $n_0(p)$. Here the Fourier transform $F_I(r)$ of $\chi_I(k)$ is investigated. Using the known analytic behaviour of $n(p)$, the small and large r forms of F_I are exhibited explicitly. In an Appendix, it is shown that a suitable model of $n(p)$ can be constructed which interpolates between these limits. Some brief comments are added concerning the representation of $F_I(r)$ in terms of the Green function.

KEY WORDS: Momentum distribution, interacting electron liquid.

1. INTRODUCTION

The exact linear density response function $\chi(k,\omega)$ of the jellium model of an interacting electron liquid is customarily written in the form of an RPA-like expression modified by the presence of the local field factor for exchange and correlation. The non-interacting (Lindhard) response function $\chi_o(k,\omega)$ plays the role of a reference function in this expression. If, however, it is replaced by $\chi_I(k,\omega)$-the interacting reference response function (IRRF) defined by Niklasson[1] in a similar way as $\chi_o(k,\omega)$ but with the ideal Fermi momentum distribution $n_o(p)$ replaced by the true momentum distribution $n(p)$-then the accompanying local field factor is much weaker in the large-k region. It tends to a constant at large k, as compared with the local field factor accompanying the Lindhard function which, as shown by Holas,[2] is asymptotically proportional to k^2.

In a recent paper[3] the interacting linear response function of the jellium model has been studied in relation to the local field factor for exchange and correlation. The present work lies in the same general area.

1.1 *Definition of interacting reference response function in* **k** *space*

In **k** or reciprocal space, the IRRF (in the static limit $\omega = 0$ which is of interest only here) is defined[1] (see also Holas[2]) as

$$\chi_I(k) = \chi_I(k, \omega = 0) = -\frac{m}{\pi^3} P \int d^3p \frac{n(p)}{k^2 + 2\mathbf{k}\cdot\mathbf{p}}, \tag{1.1}$$

where $n(p)$ is the momentum distribution of the interacting electron fluid and we have set $\hbar = 1$. Owing to the isotropy of the homogeneous phase of jellium, the angular integration in eqn. (1.1) can be carried out to yield:

$$\chi_I(k) = -\frac{m}{\pi^2 k} \int_0^\infty dp\, p\, n(p) \ln\left|\frac{k+2p}{k-2p}\right|. \tag{1.2}$$

When the momentum distribution $n(p)$ is replaced by the non-interacting result-namely the Fermi distribution

$$n_O(p) = \theta(k_f - p), \tag{1.3}$$

with Fermi momentum k_f related to the electron density ρ by $k_f^3 = 3\pi^2\rho$, one obtains the well-known Lindhard result

$$\chi_O(k) = -\frac{mk_f}{\pi^2}\left[\frac{1}{2} + \frac{(2k_f)^2 - k^2}{8kk_f} \ln\left|\frac{k+2k_f}{k-2k_f}\right|\right]. \tag{1.4}$$

In the following section, we shall investigate the coordinate space response function, $F_I(r)$ say, which is the Fourier transform of $\chi_I(k)$, namely

$$F_I(r) = \frac{1}{(2\pi)^3} \int d^3k \exp(i\mathbf{k}\cdot\mathbf{r})\, \chi_I(k)$$

$$= \frac{1}{2\pi^2 r} \int_0^\infty dk\, k \sin(kr)\, \chi_I(k). \tag{1.5}$$

The second step in eqn. (1.5) follows readily after again performing the angular integration.

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2. COORDINATE-SPACE RESPONSE FUNCTION $F_I(r)$

Using eqn. (1.2) for $\chi_I(k)$ in eqn. (1.5) we can employ the definite integral

$$\int_0^\infty dk \sin(kr) \ln\left|\frac{k+2p}{k-2p}\right| = \frac{\pi}{r}\sin(2pr) \tag{2.1}$$

given by Gradshteyn and Ryzhik[4] to obtain the **r** space form of the IRRF, namely

$$F_I(r) = -\frac{m}{2\pi^3 r^2}\int_0^\infty dp\, p\, n(p)\sin(2pr). \tag{2.2}$$

Of course, $n(p)$ depends on the jellium density $\rho = 3/(4\pi r_s^3)$, where r_s is the mean interelectronic spacing. In the homogeneous phase $n(p)$ tends to $n_o(p)$ in eqn (1.3) as $r_s \to 0$ and Daniel and Vosko[5] have used many-body perturbation theory to study the form of $n(p)$ in the regime of small r_s. But in the density range corresponding to simple metals, with $2 < r_s < 6$ in units of the Bohr radius a_o, we cannot determine $n(p)$ analytically, though numerical data now exist from quantal Monte Carlo simulation.[6]

Inserting the Fermi distribution $n_o(p)$ in eqn. (2.2) the well known result of March and Murray[7] for free electrons follows:

$$F_o(r) = -\frac{mk_f^2}{2\pi^3}\frac{j_1(2k_f r)}{r^2} \tag{2.3}$$

where $j_1(x)$ is the first-order spherical Bessel function $[\sin(x) - x\cos(x)]/x^2$.

2.1 *Small-r expansion of response function $F_I(r)$*

It will be convenient in what follows to introduce the function $A_I(r)$ related to $F_I(r)$ by

$$\begin{aligned} A_I(r) &= -\frac{2\pi^3 r^2}{m}F_I(r) \\ &= \int_0^\infty dp\, p\, n(p)\sin(2pr). \end{aligned} \tag{2.4}$$

Evidently, the small-r properties of $A_I(r)$ are determined by the behaviour of $n(p)$ at large momenta, and this is known to be

$$n(p) = \frac{a_8}{p^8} + \text{higher-order terms} \tag{2.5}$$

with $a_8 = (m\omega_p)^4 g(0)$. Knowing the form (2.5) the derivatives of $A_I(r)$ at $r = 0$ can be calculated as far as the sixth derivative and the results are collected in Appendix 1.

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The seventh and higher derivatives cannot be evaluated without detailed knowledge of the large-p behaviour of $n(p)$ going beyond that explicitly shown in eqn (2.5). In particular, these derivatives may become infinite for some forms of $n(p)$. But in Appendix 2, a model for $n(p)$ is set up which is analytical as $p \to \infty$ and which satisfies the property (2.5). The corresponding $A_I(r)$ is analytical at $r = 0$.

Using eqns (A1.1)–(A1.8), the following asymptotic expansion is obtained:

$$F_I(r) = -\frac{m\rho}{\pi r}\left[1 - \frac{4}{3}m\langle T\rangle r^2 + \frac{8}{15}m^2\langle T^2\rangle r^4 - \frac{a_8}{45\pi\rho}r^5 + \cdots\right]. \tag{2.6}$$

The first three terms in the square brackets are as given by March and Tosi,[3] the term of $O(r^5)$ being evaluated beyond their study. The normalization condition $\int d^3p\, n(p) = \int d^3p\, n_o(p) = 4\pi^3\rho$ has been utilized above, and the average of the n^{th} power of the kinetic energy is given as

$$\langle T^n\rangle = (2m)^{-n}\frac{\int d^3p\, p^{2n} n(p)}{\int d^3p\, n(p)}. \tag{2.7}$$

We turn next to the large-r expansion of $F_I(r)$.

2.2 *Long-range behaviour of $F_I(r)$*

Since $A_I(r)$ in eqn.(2.4) can be readily rewritten in the form of a one-dimensional Fourier transform

$$A_I(r) = \mathrm{Im}\int_{-\infty}^{\infty} dp\,\theta(p)\, p\, n(p) \exp(2irp), \tag{2.8}$$

one can apply immediately the methods developed by Holas and March.[8] These were based on the Lighthill[9] technique and were used explicitly to analyze the long-range behaviour of the total correlation function $g(r) - 1$ in jellium, having a form analogous to that in eqn. (2.8).

The momentum distribution $n(p)$ is known in the homogeneous phase to have a discontinuity (reduction by a jump) Z_f at $p = k_f$ and, most probably, discontinuities in its derivatives there. The form of $n(p)$ may be expressed generally as

$$n(p) = \mathrm{sgn}(p - k_f)\left[\sum_{j=0}^{\infty}\frac{1}{j!}b_j(p - k_f)^j\right] + \text{analytical part} \tag{2.9}$$

where the coefficient $b_o = -Z_f/2$. Therefore the oscillatory part of the large-r asymptotic expansion is

$$A_I^{\text{osc}}(r) = 2\,\mathrm{Im}\left\{\left[\sum_{j=0}^{\infty}(k_f b_j + j b_{j-1})\left(\frac{i}{2r}\right)^{j+1}\right]\exp(2ik_f r)\right\}$$

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$$= 2\cos(2k_f r)\left[\frac{k_f b_o}{2r} - \frac{k_f b_2 + 2b_1}{(2r)^3} + O\left(\frac{1}{r^5}\right)\right]$$

$$- 2\sin(2k_f r)\left[\frac{k_f b_1 + b_o}{(2r)^2} - \frac{k_f b_3 + 3b_2}{(2r)^4} + O\left(\frac{1}{r^6}\right)\right]. \quad (2.10)$$

Because of the theta function present in eqn. (2.8), the integrand is non-analytic at $p = 0$. This may lead to a non-oscillatory contribution to the large-r expansion. Assuming the following expansion of $n(p)$ at $p = 0$,

$$n(p) = \sum_{j=0}^{\infty} \frac{1}{j!} c_j p^j \quad (2.11)$$

we obtain

$$A_I^{\text{non-osc}}(r) = \sum_{n=1}^{\infty} (-1)^n \frac{2nc_{2n-1}}{(2r)^{2n+1}}. \quad (2.12)$$

It should be noted that only the odd terms in the power series expansion (2.11) contribute to the long-range expansion (2.12), with the leading term being of order r^{-3} if the first derivative of $n(p)$ at $p = 0$ is non-zero.

Thus, one has the following asymptotic large-r expansion for the interacting response function:

$$F_I(r) = -\frac{m}{2\pi^3 r^2}[A_I^{\text{non-osc}}(r) + A_I^{\text{osc}}(r)]. \quad (2.13)$$

This has a leading term $\approx [\cos(2k_f r)]/r^3$, which is due to the discontinuity in $n(p)$ at $p = k_f$. This is the same type of behaviour as exhibited by the March-Murray non-interacting function $F_o(r)$ in eqn. (2.3), but one can expect the coefficient in that function multiplying the $[\cos(2k_f r)]/r^3$ term at large r to be reduced by the electron-electron interactions since the discontinuity in $n(p)$ at k_f is $Z_f < 1$ for $r_s > 0$.

3. DISCUSSION AND SUMMARY

In Appendix 1 of March and Tosi[3] the non-interacting response function F_o is written in terms of the Green function. Knowledge of the exact momentum distribution function $n(p)$ in the homogeneous phase of jellium determines the interacting reference response function completely because of eqn. (2.2). In Appendix 3, therefore, a brief summary is given of the way in which $n(p)$ can be expressed in terms of the Green function.

To summarize, the main results of the present work are the expression (2.2) for the interacting reference response function $F_I(r)$ in the form of a single integral, and the small-r and large-r expansions of this function given in eqns. (2.6) and (2.13)

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respectively. In addition, a model form of $n(p)$ has been set up in eqn. (A2.1) in Appendix 2, which leads to the model for $F_I(r)$ in eqn. (A2.7) interpolating between these two limiting forms.

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APPENDIX 1. LOW-ORDER DERIVATIVES OF $A_I(r)$ at $r = 0$

The following results are immediately found from eqn. (2.4):

$$\frac{d}{dr} A_I(r)|_{r=0} = 2\int_0^\infty dp\, p^2\, n(p), \tag{A1.1}$$

$$\left(\frac{d}{dr}\right)^2 A_I(r)|_{r=0} = 0, \tag{A1.2}$$

$$\left(\frac{d}{dr}\right)^3 A_I(r)|_{r=0} = -2^3\int_0^\infty dp\, p^4\, n(p), \tag{A1.3}$$

$$\left(\frac{d}{dr}\right)^4 A_I(r)|_{r=0} = 0 \tag{A1.4}$$

and

$$\left(\frac{d}{dr}\right)^5 A_I(r)|_{r=0} = 2^5\int_0^\infty dp\, p^6\, n(p). \tag{A1.5}$$

Evaluation of the sixth derivative needs some care. We can write

$$\left(\frac{d}{dr}\right)^6 A_I(r) = -2^6 \int_0^{\infty} dp\, p^7\, n(p) \sin(2rp)$$

$$= -2^6 \left[\int_0^{p_o} dp\, p^7\, n(p) \sin(2rp) + a_8 \int_{p_o}^{\infty} dp \frac{\sin(2rp)}{p} \right], \tag{A1.6}$$

where the momentum p_o has such a large value that $n(p)$ for $p > p_o$ is accurately represented by the leading term of the expansion (2.5). The second integral in the square brackets in eqn. (A1.6) is equal to $[Si(\infty) - Si(2rp_o)]$, where $Si(x)$ is the so-called integral sine function,

$$Si(x) = \int_0^x dt \frac{\sin(t)}{t} \tag{A1.7}$$

with $Si(\infty) = \pi/2$ and $Si(0) = 0$. Thus the limit of the result (A1.6) for $r \to 0$ is given by

$$\left(\frac{d}{dr}\right)^6 A_I(r)|_{r=0} = -2^5 \pi a_8. \tag{A1.8}$$

APPENDIX 2. EVALUATION OF $F_I(r)$ USING A MODEL $n(p)$

Let us consider the following model momentum distribution function,

$$n(p) = n_A(p) + n_B(p) = \theta(k_f - p)(\alpha + \beta p^2) + \frac{a_8}{(\gamma^2 + p^2)^4}. \tag{A2.1}$$

It obviously satisfies the property (2.5), being also analytical at $p = \infty$. Of its five parameters, k_f and a_8 have obvious meaning, while α, β and γ can be determined from three requirements on $n(p)$:

(i) it satisfies the normalization condition formulated under eqn. (2.6), which now takes the form

$$\alpha + \frac{3}{5} k_f^2 \beta + \frac{3\pi}{32} \frac{a_8}{k_f^3 \gamma^5} = 1; \tag{A2.2}$$

(ii) it reproduces the value of $\langle T \rangle$, which is quite accurately known from differentiation of the correlation energy of the interacting electron gas,

$$\alpha + \frac{5}{7} k_f^2 \beta + \frac{5\pi}{32} \frac{a_8}{k_f^5 \gamma^3} = \frac{\langle T \rangle}{\langle T_0 \rangle}; \tag{A2.3}$$

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(iii) it reproduces the discontinuity Z_f, also available with reasonable accuracy,

$$\alpha + k_f^2 \beta = Z_f. \tag{A2.4}$$

After inserting the model $n(p)$, eqn. (A2.1) into eqn. (2.4) all integrations can be performed analytically. The result is

$$A_I^A(r) = \frac{k_f}{2r}\left\{\left[-(\alpha + k_f^2\beta) + \frac{3\beta}{2r^2}\right]\cos(2k_f r) + \left[\frac{\alpha + 3k_f^2\beta}{2k_f r} - \frac{3\beta}{4k_f r^3}\right]\sin(2k_f r)\right\} \tag{A2.5}$$

and

$$A_I^B(r) = \frac{3\pi}{48}\frac{a_8}{\gamma^5} r\left(1 + 2\gamma r + \frac{4}{3}\gamma^2 r^2\right)\exp(-2\gamma r). \tag{A2.6}$$

The latter result was obtained with the help of tables[4] under the assumption that $\gamma > 0$. It should be noted that $A_I^B(r)$ is analytical at $r = 0$, in spite of the behaviour $n_B(p) \approx p^{-8} + O(p^{-10})$ at large p. Of course $A_I^A(r)$ is analytical at $r = 0$ too.

Finally, we have the following model response function,

$$F_I(r) = -\frac{m}{2\pi^3 r^2}[A_I^A(r) + A_I^B(r)]. \tag{A2.7}$$

It can be readily verified that the small-r expansion of this function (A2.7) agrees with the small-r expansion (2.6), while its large-r behaviour agrees with the expansion in eqn. (2.13). It should be noted that the contribution due to $A_I^B(r)$ is exponentially small at large r, and that non-oscillatory terms are absent because even powers only enter the small-p expansion of the model $n(p)$ in eqn (A2.1).

APPENDIX 3. REPRESENTATION OF $n(p)$ IN TERMS OF THE GREEN FUNCTION

Knowing the exact $n(p)$ we have the exact $F_I(r)$ through eqn. (2.2). But (see, for example, Ziesche and Lehmann[10]) the momentum distribution can be expressed in the form

$$n(p) = -iG(p, -\delta) = \frac{1}{2\pi i}\int_C d\omega\, G(p,\omega)\exp(i\omega\delta) \tag{A3.1}$$

with δ a positive infinitesimal. Here C is a contour in the upper half of the complex-ω plane and $G(p,t)$ is the one-particle propagator (Green function)

$$G(p,t) = -i \langle\langle \hat{T}[a_p(t)\, a_p^+(0)] \rangle\rangle. \tag{A3.2}$$

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$G(p, \omega)$ is simply the Fourier transform of $G(p, t)$, while $\hat{T}$ is the time ordering operator.

The interacting Green function $G(p, \omega)$ can be expressed by means of Dyson's equation in terms of the free-electron Green function $G_o(p, \omega)$ and the mass operator $\sum(p, \omega)$:

$$G(p, \omega) = \left[\omega - \omega_p^o - \sum(p, \omega) \right]^{-1}, \tag{A3.3}$$

from which the discontinuity Z_f is obtained as

$$Z_f = \left[1 - \frac{\partial Re \sum(p, \omega)}{\partial \omega} |_{p = k_f, \omega = \omega_f} \right]^{-1}.$$

Thus the Appendix in the work of March and Tosi[3] could be generalized to the many-body case.

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