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Some Implications of an Expression for the Response of the Electron Liquid*

Flavio Toigo† and Truman O. Woodruff
Department of Physics, Michigan State University, East Lansing, Michigan 48823

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The pair correlation function, the screening of a fixed impurity charge, the correlation energy, the cohesive energy of alkali metals, and the plasmon dispersion relation in the small-k limit are calculated using an expression for the dielectric function derived in a previous paper. Results are compared with those obtained from other theories.

I. INTRODUCTION

In a previous paper[1] hereafter referred to as I, we derived an expression [denoted henceforth by $\epsilon_I(k, \omega)$] for the dielectric response function of the electron liquid by means of a momentum-conserving decoupling for the Green's functions involved. (Decoupling by this method is equivalent to imposing the f sum rule on the response function.) This expression is of the form first suggested by Hubbard,[2]

$$\epsilon(\vec{k}, \omega) = 1 + \frac{Q_0(\vec{k}, \omega)}{1 - G(\vec{k}, \omega) Q_0(\vec{k}, \omega)} , \qquad (1.1)$$

where $Q_0(\vec{k}, \omega)$ is Lindhard's[3] function. For computational reasons we gave explicit results only for $G(\vec{k}, 0)$, on the assumption that the term (A3) in I can be neglected. The first noteworthy feature is that it satisfies the compressibility sum rule[4]

$$\lim_{k \to 0} k^2 \, \epsilon(\vec{k}, 0) = \frac{4\alpha r_s}{\pi} \frac{C}{C_0} , \qquad (1.2)$$

with $\alpha = (4/9\pi)^{1/3}$, and k in units of k_F (where C is the compressibility of the electron liquid and C_0 that of the gas) more accurately than do all other available approximations in which the sum rule is not explicitly imposed. This note summarizes the results of calculations based on ϵ_I for some other properties of the electron liquid (i.e., the degenerate gas of interacting electrons): the pair correlation function, the screening of a fixed impurity charge, the correlation energy, the cohesive energy of alkali metals, and the plasmon dispersion in the small-k limit. In addition we show that in the large-k limit, $\epsilon_I(k, \omega)$ includes the effect of a correction to the screening in the random-phase approximation (RPA) previously calculated by Geldart and Taylor.[5]

In the following it is assumed throughout that $G(k, \omega)$ is only weakly dependent on ω so that the dielectric function may be written as

$$\epsilon(\vec{k}, \omega) = 1 + Q_0(\vec{k}, \omega) / [1 - G(\vec{k}) Q_0(\vec{k}, \omega)] , \qquad (1.3)$$

with $G(\vec{k}) = G(\vec{k}, 0)$.

This approximation has been widely used in the literature[2,6,7] due to the mathematical difficulties inherent in the computation of the ω dependence of G. The complete expression for $G(k, \omega)$ is given in I.

II. CALCULATION AND RESULTS

A. Pair Correlation Function $g(r)$

It is well known that the pair correlation function

$$g(\vec{r}) = [1/N(N-1)] \, \langle \Psi_0 | \sum_{i \neq j} \delta \, (\vec{r} + \vec{r}_i - \vec{r}_j) | \Psi_0 \rangle \qquad (2.1)$$

is related to the static form factor

$$S(\vec{k}) = (1/N) \, \langle \Psi_0 | \rho_{\vec{k}}^{\dagger} \rho_{\vec{k}} | \Psi_0 \rangle \qquad (2.2)$$

as follows:

$$g(\vec{r}) = \frac{1}{N-1} \sum_{\vec{k} \neq 0} [S(\vec{k}) - 1] e^{i\vec{k} \cdot r} + 1 , \qquad (2.3)$$

that is, changing the sum into an integral,

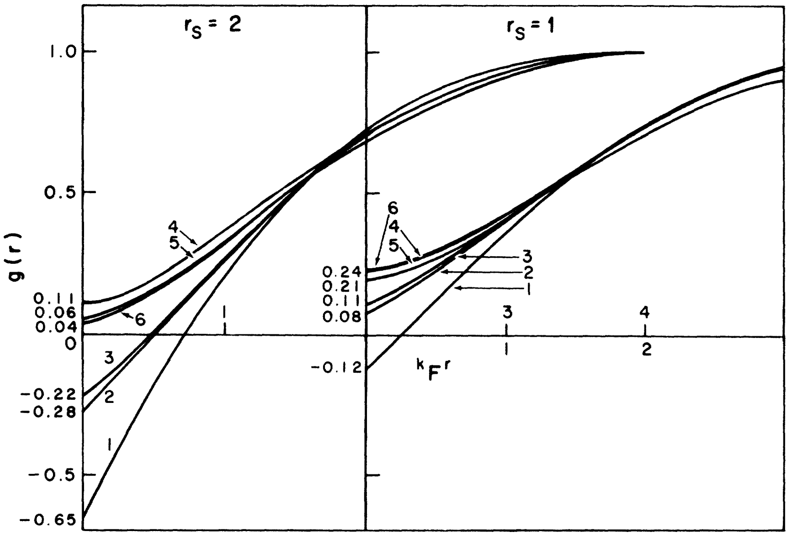

FIG. 1. Pair correlation function $g(r)$ vs $k_F r$ for $r_s = 1$ and $r_s = 2$. Curves 1, 2, 3, 4, 5, and 6 are, respectively, RPA, Hubbard, Antoniewicz and Kleinman, STLS I, STLS IV, and present theory. Curves 1 and 2 from Ref. 9.

$$g(r) = 1 + \frac{3}{2}\int_0^\infty k^2 \, [S(k) - 1] \, \frac{\sin kr}{kr} \, dk \, . \qquad (2.4)$$

Also familiar is the relation

$$S(\vec{k}) = (1/N) \int_0^\infty S(\vec{k}, \omega) d\omega \quad , \qquad (2.5)$$

where $S(k, \omega)$ is obtained from the dielectric function via

$$S(\vec{k}, \omega) = -\frac{\hbar k^2}{4\pi^2 e^2} \mathrm{Im}\left[\frac{1}{\epsilon(\vec{k}, \omega)}\right] \, . \qquad (2.6)$$

It is then easy to calculate the pair correlation function if $\epsilon(\vec{k}, \omega)$ is known. In Figs. 1–3 we compare our result with results obtained by other authors[6,8,9] using different dielectric functions. It will be noted that the present $g(r)$ becomes slightly negative at $r = 0$ for $r_s \simeq 3$, but is much less negative than the corresponding function in all other theories except that of Singwi *et al.*[6,8] It is worth remarking that in STLS I (Ref. 6) $g(0)$ was positive for r_s up to 5, but the compressibility sum rule was badly violated, while in STLS IV (Ref. 8), where the compressibility sum rule is almost satisfied, $g(0)$ becomes negative for $r_s \simeq 3$. It seems then that thus far it has not been possible to satisfy both the compressibility sum rule and the requirement that $g(0)$ be positive in the metallic range

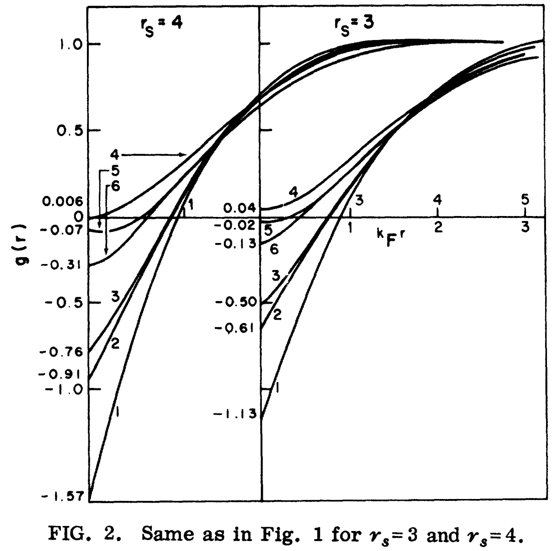

FIG. 2. Same as in Fig. 1 for $r_s = 3$ and $r_s = 4$.

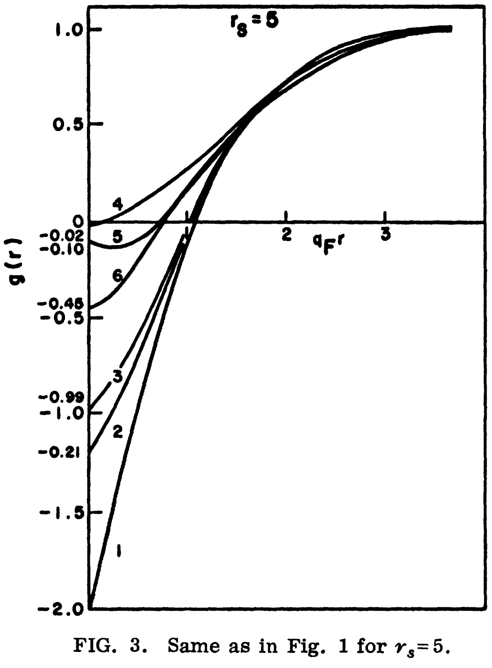

FIG. 3. Same as in Fig. 1 for $r_s = 5$.

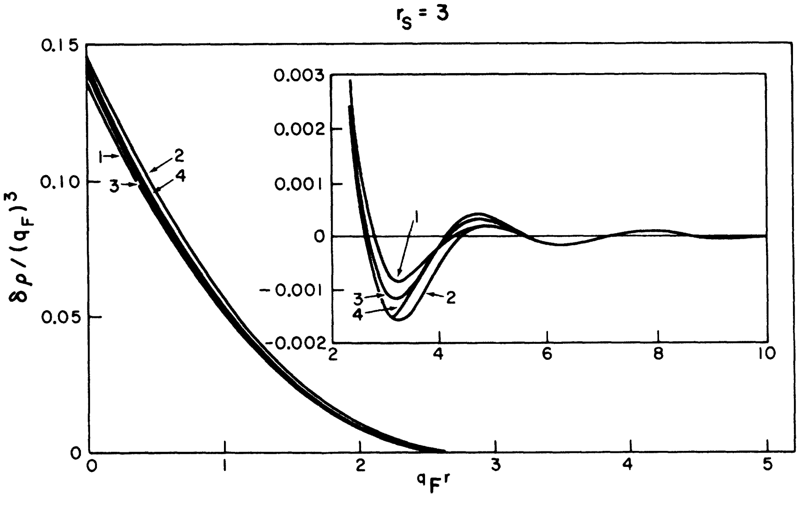

FIG. 4. Screening density $\delta\rho(r)/k_F^3$ vs $k_F r$ at $r_s=3$. Curves 1, 2, 3, and 4 are, respectively, Hubbard, STLS I, STLS IV, and present theory.

$2<r_s<6$. In our form of the theory this shortcoming has two possible origins. The first and more obvious is that in calculating the frequency moment of the higher-order Green's function we have retained only the term corresponding to the kinetic part of the Hamiltonian, thus neglecting possible correlations of higher order in the Coulomb potential. The second is the fact that in $S(\vec{k},\omega)$ we need the full ω dependence of $G(\vec{k},\omega)$, while we have used $G(\vec{k},0)$ in the definition of $\epsilon(\vec{k},\omega)$. We are now investigating both these possibilities.

B. Screening of a Fixed Impurity Charge

In linear response theory the number density fluctuation induced in the electron liquid by a unit fixed impurity charge is

$$\langle\rho(\vec{k},0)\rangle = 1-[1/\epsilon(\vec{k},0)] , \tag{2.7}$$

where $\epsilon(\vec{k},0)$ is the static dielectric function. Equation (2.7) implies for the screening density at a distance r from the impurity

$$\delta\rho(r)=\frac{k_F^3}{2\pi^2 r}\int_0^\infty k\sin(kr)\left(1-\frac{1}{\epsilon(k,0)}\right)dk , \tag{2.8}$$

where r is in units of k_F^{-1} and k in units of k_F. In Figs. 4 and 5 we compare our results with those obtained by some other authors at $r_s=3$ and $r_s=6$.

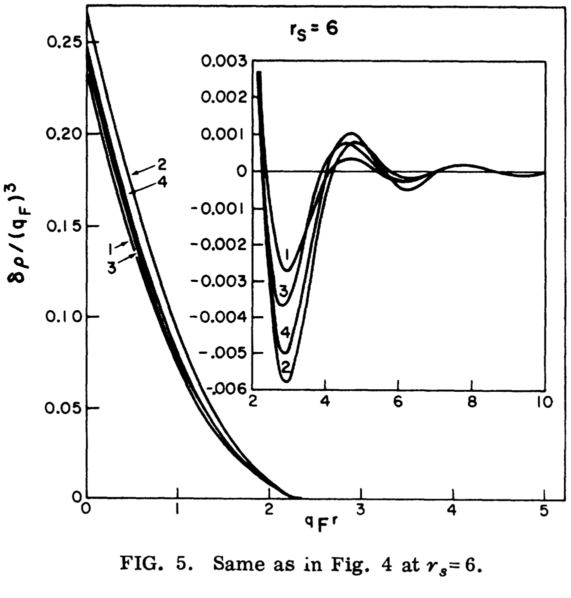

FIG. 5. Same as in Fig. 4 at $r_s=6$.

C. Correlation Energy

Hubbard's[2] formula connecting the correlation energy per electron with the dielectric function can be transformed into

$$E_{\text{corr}}=\frac{3}{2\pi\alpha r_s}-\frac{4}{\pi\alpha r_s^2}\int_0^{r_s}\gamma(r_s)\,dr_s \quad \text{(Ry)} \tag{2.9}$$

with

$$\gamma(r_s)=-\tfrac{1}{2}\int_0^\infty [S(k)-1]\,dk , \tag{2.10}$$

where k is in units of k_F as usual, and $\alpha=(4/9\pi)^{1/3}$. We notice that Eq. (2.9) may be written as

$$E_{\text{corr}}=(1/r_s^2)\int_0^{r_s} V_{\text{corr}}(r_s)\,dr_s , \tag{2.11}$$

with $V_{\text{corr}}(r_s)=(4/\pi\alpha)[\frac{3}{8}-\gamma(r_s)]$. With our values of $\gamma(r_s)$ (Table I) it is easily seen that V_{corr} satisfies Ferrell's[10,11] condition

TABLE I. Values of $\gamma(r_s)$.

r_s	1	2	3	4	5
$\gamma(r_s)$	0.455 98	0.494 09	0.521 64	0.543 72	0.562 27

TABLE II. Correlation energy (Ry/electron).

r_s	1	2	3	4	5
Present theory	−0.134	−0.095	−0.079	−0.068	−0.061
STLS I	−0.124	−0.092	−0.075	−0.064	−0.056
STLS IV	−0.125	−0.097	−0.080	−0.070	−0.063
Hubbard	−0.131	−0.102	−0.086	−0.076	−0.069
Nozières and Pines	−0.115	−0.094	−0.081	−0.072	−0.065
RPA	−0.157	−0.124	−0.105	−0.094	−0.085

$$\frac{dV_{\mathrm{corr}}(x)}{dx} \leqslant 0 \ . \qquad (2.12)$$

The values of the correlation energy obtained from ϵ_{I} are compared in Table II with those obtained by other authors.

Putting our values of the correlation energy in the expression for the cohesive energy of alkali metals obtained in the approximations discussed by Pines and Nozières,[4] the values reported in Table III are obtained.

D. Plasmon Dispersion Relation

From expression (1.1) for the dielectric function it follows that in the small-k limit one has

$$\epsilon(\vec{\mathrm{k}}, \omega) \underset{k \to 0}{=} 1 - \frac{\omega_p^2(0)}{\omega^2} \left(1 + \tfrac{9}{5} k^2 \frac{4\alpha r_s}{\pi} - \gamma k^2\right) + O(k^2) \ , \qquad (2.13)$$

where $\omega_p(0) = (4\pi n e^2/m)^{1/2}$ is the plasmon frequency at $k = 0$, k is in units of k_F, and

$$\gamma = \lim_{k \to 0} \frac{G(k)}{k^2}$$

is $\frac{1}{4}$ in the present theory.

Equation (2.13) implies for the plasmon dispersion relation

$$\omega_p(k) = \omega_p(0) + \beta \hbar k^2/m \qquad (2.14)$$

TABLE III. Cohesive energy of alkali metals (kcal/mole).

	Li	Na	K	Rb	Cs
Present theory	−38.4	−24.9	−21.5	−20.6	−20.1
STLS I	−36.0	−23.9	−19.9	−17.8	−17.6
STLS IV and Nozières and Pines	−38.1	−26.4	−22.6	−20.6	−20.4
Experimental	−38.4	−25.9	−21.5	−19.5	−18.7

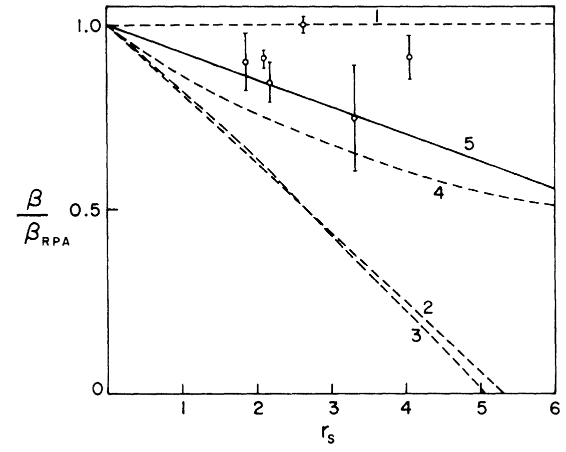

FIG. 6. Coefficients of the leading term in the plasmon dispersion (in units of its RPA value) vs r_s. Curves 1, 2, 3, and 4 are, respectively, the results of RPA, Hubbard, STLS (Ref. 6), and STLS (Ref. 7). Curve 5 gives the results of this paper. The experimental values (for Be, Al, Sb, Mg, Li, and Na in order of increasing r_s) are taken from Ref. 12.

and

$$\beta/\beta_{\mathrm{RPA}} = 1 - \tfrac{5}{9}[(4\alpha r_s/\pi)]\gamma \ . \qquad (2.15)$$

In Fig. 6, the values of $\beta/\beta_{\mathrm{RPA}}$ obtained using $\gamma = \frac{1}{4}$ are compared with some previous theoretical results and some experimental points.[12] Though the comparison with the experimental points may not be very significant due to the absence of knowledge of the influence of the ion lattice, it is nonetheless interesting to observe that the underestimate of the dispersion in the Hubbard and STLS I approximations is removed. This correction of the underestimate can be attributed to the fact that the present dielectric function satisfies quite well the compressibility sum rule and then seems to be good at small wavelengths.

III. CORRECTION TO RPA IN THE LARGE-k LIMIT

In this section we make a connection with the paper by Geldart and Taylor[5] in which the correction to the RPA polarization in the large-k limit, due to Hartree-Fock exchange and self-energy, is calculated.

First of all, we notice that the function $F_{AB}(k) = F_A(k) + F_B(k)$ defined in Ref. 5, in the notation established in I, reads

$$F_{AB}(\vec{\mathrm{k}}) = \frac{\pi^2 k^2}{\alpha r_s} \frac{Q_0(\vec{\mathrm{k}}, 0)}{1 - P_0(\vec{\mathrm{k}}, 0)} \ , \qquad (3.1)$$

where

$$P_0(k,0) = -\frac{3\alpha r_s}{4\pi^3}\int d\vec{q}_1\, d\vec{q}_2 \left[1 - \frac{2\vec{q}_2\cdot\vec{k}+k^2}{2\vec{q}_1\cdot\vec{k}+k^2}\right]\frac{1}{|\vec{q}_1-\vec{q}_2|^2}$$

$$-\left[1+\frac{2\vec{q}_2\cdot\vec{k}+k^2}{2\vec{q}_1\cdot\vec{k}+k^2}\right]\frac{1}{|\vec{q}_1+\vec{q}_2+\vec{k}|^2}\;\theta_<(\vec{q}_1)\,\theta_<(\vec{q}_2)\,\theta_>(\vec{q}_1+\vec{k})\,\theta_>(\vec{q}_2+\vec{k})\;, \qquad (3.2)$$

as defined in Eq. (4.5) of I.

In the large-k limit we can write

$$\frac{1}{2\vec{q}_1\cdot\vec{k}+k^2} \underset{k\to\infty}{=} \frac{1}{k^2}\left(1-\frac{2\vec{q}_1\cdot\vec{k}}{k^2}+\frac{(2\vec{q}_1\cdot\vec{k})^2}{k^4}-\ldots\right), \qquad (3.3)$$

so that the leading term in $P_0(\vec{k},0)$ is

$$P_0(k,0) \underset{k\to\infty}{=} \frac{3\alpha r_s}{16\pi^3}\,\frac{1}{k^2}\left[8\int\frac{d\vec{q}_1 d\vec{q}_2}{k^2}+\frac{16}{k^4}\int d\vec{q}_1 d\vec{q}_2\,\frac{(\vec{k}\cdot\vec{q}_1)^2}{|\vec{q}_1-\vec{q}_2|^2}-\frac{16}{k^4}\int d\vec{q}_1 d\vec{q}_2\,\frac{(\vec{k}\cdot\vec{q}_1)(\vec{k}\cdot\vec{q}_2)}{|\vec{q}_1-\vec{q}_2|^2}\right]. \qquad (3.4)$$

We notice that, apart from a constant, this expression is exactly the one obtained by summing Eqs. (2) and (4) of Ref. 5.

The evaluation of the integrals is rather tedious but can be performed analytically; it gives

$$P_0(k,0) \underset{k\to\infty}{=} \frac{40\alpha r_s}{9\pi}\,\frac{1}{k^4}\,. \qquad (3.5)$$

If we observe that

$$Q_0(k,0) \underset{k\to\infty}{=} \frac{16}{3}\,\frac{\alpha r_s}{9\pi}\,\frac{1}{k^4}\,,$$

the correction to the RPA polarization may be written as

$$F_{AB}(k) \underset{k\to\infty}{=} \frac{\pi^2 k^2}{\alpha r_s}\,Q_0 P_0 = \frac{5}{3}\left(\frac{4\pi}{3}\right)^2\frac{8\alpha r_s}{\pi^2 k^6}\,. \qquad (3.6)$$

Equation (3.6) is the same as Eq. (6) of Ref. 5 apart from a constant. This difference can be seen to be due to an error contained in the calculation in Ref. 5 of the integrals in Eq. (3.4). It appears from Eq. (3.6) and the compressibility result (which gives the Hartree-Fock value[11]) that the present treatment is equivalent to the Hartree-Fock time-dependent approximation for both large- and small-k values.

IV. CONCLUSION AND SUMMARY

In this note a number of properties of the electron liquid have been considered; for each property calculations based on the dielectric response function calculated in I have been performed, and the results are compared with the results of such calculations based on different forms of the response function and also, where possible, with data derived from experiments. The reader will notice that ϵ_I leads in each case to results which agree with experiment and satisfy general requirements, such as sum rules, at least as well as any other available response function. For some properties ϵ_I leads to results which satisfy all known requirements better than any other available form of ϵ.

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†Permanent address: Istituto di Fisica dell'Università, Padova, Italy.

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