TABLE I. Comparison of energies (in Ry) for states of high symmetry (with respect to $\Gamma_1 = 0$), calculated by different authors. $\langle\vec{k}|W|\vec{k}\rangle_{\Gamma_1} = -1.059$ Ry $= -(E_F + \phi)$, $\phi = 0.31$ Ry.

	Heine (Ref. 1)	Segal (Ref. 6)	Harrison (Refs. 3–5)	Snow (Ref. 7)	Connolly (Ref. 8)	Present paper	Free electron
Γ_1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
X_4'	0.592	0.622	0.585	0.597		0.590	0.677
X_1	0.717	0.698	0.693	0.679		0.700	0.677
X_3					1.20	1.199	
X_5'					1.16	1.259	
L_1		0.512		0.483		0.544	0.501
L_2'		0.483		0.467		0.447	0.501
K_1	0.742	0.723	0.713	0.705		0.699	0.761
K_3	0.699	0.699	0.679	0.673		0.654	0.761
Fermi level			0.84	0.81			0.86

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Screening of a Fixed Charge in the Electron Liquid

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The static dielectric function given by Kleinman and Langreth has been used to calculate the screening charge density around a fixed foreign charge in an electron liquid for values of r_s which correspond to metallic densities. The results are compared with the earlier results based on the Hubbard approximation, and with those of Singwi and Tosi obtained by a self-consistent procedure.

Since Hubbard[1] proposed approximate methods based on the diagrammatic technique to include the effect of exchange interactions in the RPA expression[2] for the dielectric function in metals, several improvements over his procedure have appeared in the literature.[3–5] The main difficulty with the Hubbard approximation is that it does not account for short-range correlations due to Coulomb repulsion in the electron liquid. Singwi *et al.*[3] used an ansatz to take account of these short-range correlatio~s in an approximate way through a simple physically meaningful function called the pair-distribution function. This ansatz relates the two-particle distribution function $f(1,1')$ to the one-particle distribution function $f(1)$ and $f(1')$ by

$$f(1,1') = f(1) f(1') g(\vec{x} - \vec{x}') , \tag{1}$$

where $g(\vec{x} - \vec{x}')$ is the pair-distribution function. Here, 1 and $1'$ stand for $\vec{x}$, $\vec{p}$, t and $\vec{x}'$, $\vec{p}'$, t, respectively — the usual position, momentum, and time variables for the two particles. Using Eq. (1) for $f(1,1')$ in the equation of motion of the one-particle distribution function $f(1)$ in the presence of an external perturbation, Singwi *et al.*[3] obtained an expression for the dielectric function which requires a self-consistent procedure for numerical evaluation of quantities such as the screening density.

On the other hand, Kleinman has modified Hubbard's results by self-consistent field considerations,[4] and later by a diagrammatic technique,[6] to get the expressions for dielectric function and vertex function in closed form, and which also include short-range correlations. More recently, Langreth[5] has given a variational approach for the same problem. In this variational technique, he has taken account of Hermitian properties of various types of interactions, which Kleinman did not. However, the interesting point to note is that he confirms Kleinman's results for the static case ($\omega = 0$). The purpose of the present communication is to put forth the numerical results obtained for the screening density due to a static charged impurity, using Langreth's expression for the static dielectric function, and to make a comparison with the earlier calculations.

For the external perturbation caused by a static impurity of unit charge, situated at the origin, the induced number-density fluctuation in the linear-response regime is given by[7]

$$\langle \rho(\vec{q}, 0)\rangle = 1 - 1/\epsilon(\vec{q}, 0), \tag{2}$$

where $\epsilon(\vec{q}, 0)$ is the static dielectric function. The screening density at a distance r is then given by

$$\delta\rho(r) = \frac{1}{2\pi^2 r}\int_0^\infty dq\, q \sin(qr)\left(1 - \frac{1}{\epsilon(q, 0)}\right). \tag{3}$$

Now the static dielectric function, according to Kleinman[4] and Langreth,[5] is given by

$$\epsilon(q, 0) = 1 + F(q)/[1 - f(q)F(q)], \tag{4}$$

where

TABLE I. Values of $\delta\rho(r)/q_F^3$ for various values of r_s.

rq_F	$r_s = 2$	$r_s = 3$	$r_s = 4$	$r_s = 5$	$r_s = 6$
0.0	0.1001	0.1400	0.1775	0.2135	0.2486
0.1	0.093 67	0.1304	0.1647	0.1975	0.2294
0.4	0.073 70	0.1007	0.1253	0.1485	0.1707
0.7	0.055 74	0.074 37	0.090 81	0.1059	0.1200
1.0	0.040 30	0.052 15	0.062 11	0.070 84	0.078 75
1.3	0.027 63	0.034 33	0.039 49	0.043 68	0.047 21
1.6	0.017 76	0.020 79	0.022 71	0.023 93	0.024 69
1.9	0.010 50	0.011 18	0.011 12	0.010 65	0.009 899
2.2	0.005 525	0.004 878	0.003 838	0.002 608	0.001 271
2.5	0.002 412	0.001 202	−0.000 138 8	−0.001 499	−0.002 844
2.8	0.000 702 0	−0.000 568 5	−0.001 793	−0.002 929	−0.003 979
3.1	−0.000 045 5	−0.001 097	−0.002 003	−0.002 769	−0.003 415
3.4	−0.000 214 6	−0.000 938 0	−0.001 479	−0.001 872	−0.002 148
3.7	−0.000 105 5	−0.000 508 1	−0.000 734 4	−0.000 833 3	−0.000 839 2
4.0	0.000 075 2	−0.000 078 8	−0.000 087 5	−0.000 003 0	0.000 143 3
4.3	0.000 210 0	0.000 209 1	0.000 313 8	0.000 475 7	0.000 669 3
4.6	0.000 254 1	0.000 318 2	0.000 450 0	0.000 609 0	0.000 776 3
4.9	0.000 213 8	0.000 278 8	0.000 381 8	0.000 491 3	0.000 594 8
5.2	0.000 122 7	0.000 154 4	0.000 204 4	0.000 249 6	0.000 282 8
5.5	0.000 021 3	0.000 011 9	0.000 010 2	0.000 000 2	−0.000 021 7
5.8	−0.000 057 8	−0.000 097 6	−0.000 134 1	−0.000 177 5	−0.000 229 1
6.1	−0.000 097 0	−0.000 148 4	−0.000 197 2	−0.000 249 5	−0.000 305 6
6.4	−0.000 095 1	−0.000 140 0	−0.000 181 4	−0.000 223 2	−0.000 265 0
6.7	−0.000 063 5	−0.000 089 6	−0.000 112 1	−0.000 132 8	−0.000 151 3
7.0	−0.000 019 3	−0.000 023 2	−0.000 024 0	−0.000 022 4	−0.000 018 1
7.3	0.000 020 6	0.000 034 8	0.000 051 0	0.000 068 8	0.000 088 7
7.6	0.000 044 7	0.000 068 4	0.000 092 6	0.000 117 2	0.000 142 7
7.9	0.000 048 9	0.000 072 5	0.000 095 3	0.000 117 4	0.000 139 1
8.2	0.000 036 2	0.000 052 2	0.000 066 6	0.000 079 8	0.000 091 8
8.5	0.000 014 1	0.000 018 9	0.000 022 2	0.000 024 2	0.000 024 8
8.8	−0.000 008 4	−0.000 014 0	−0.000 020 6	−0.000 028 2	−0.000 036 8
9.1	−0.000 024 1	−0.000 036 2	−0.000 048 7	−0.000 061 5	−0.000 074 7
9.4	−0.000 029 1	−0.000 042 6	−0.000 055 8	−0.000 068 7	−0.000 081 5
9.7	−0.000 023 7	−0.000 034 0	−0.000 043 6	−0.000 052 4	−0.000 060 8
10.0	−0.000 011 6	−0.000 015 8	−0.000 019 2	−0.000 022 0	−0.000 024 1
10.3	0.000 002 4	0.000 004 5	0.000 007 2	0.000 010 5	0.000 014 2

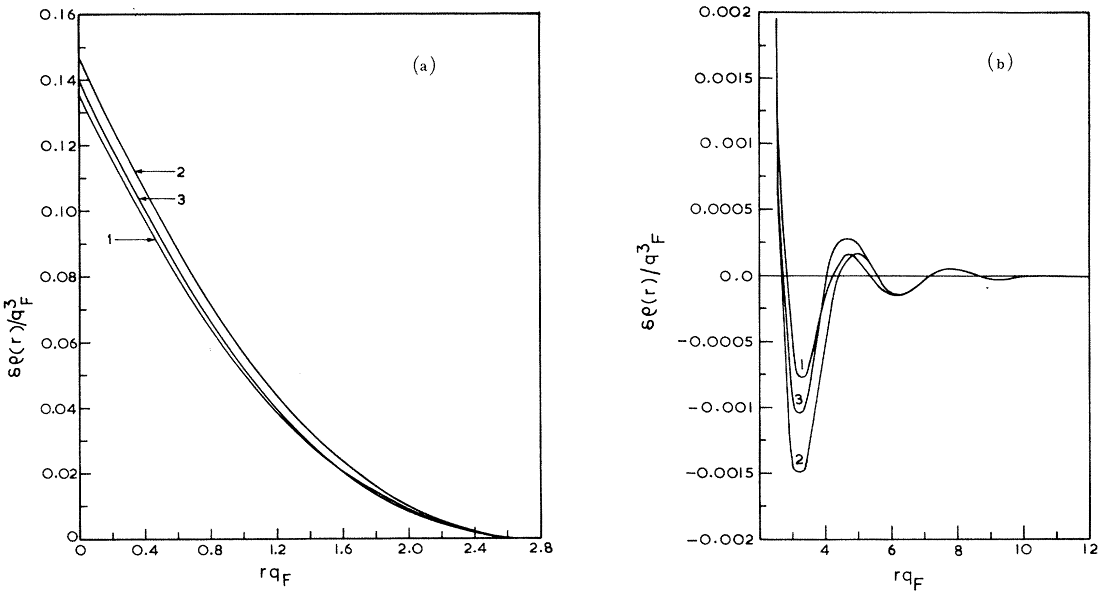

FIG. 1. Screening density $\delta\rho(r)/q_F^3$ versus rq_F for $r_s=3$(a) for small values of rq_F and (b) for large values of rq_F]; curve 1, Hubbard (Ref. 2); curve 2, Singwi and Tosi (Ref. 8); curve 3, present results.

$$F(q)=\frac{q_{FT}^2}{q^2}\left[\frac{1}{2}+\frac{q_F}{2q}\left(1-\frac{q^2}{4q_F^2}\right)\ln\left|\frac{q+2q_F}{q-2q_F}\right|\right] \qquad (5a)$$

and

$$f(q)=\frac{1}{4}\left(\frac{q^2}{q^2+q_F^2+Q_S^2}+\frac{q^2}{q_F^2+Q_S^2}\right). \qquad (5b)$$

In these expressions, q_F is the radius of the Fermi sphere, q_{FT} is the inverse Fermi-Thomas length, and Q_s is a screening parameter given by the Nozieres-Pines interpolation formula[5]

$$q_F^2/(q_F^2+Q_S^2)=\tfrac{1}{2}[1+0.158(q_{FT}/2q_F)^2], \qquad (6)$$

which has been used to reproduce the compressibility limit properly. Substituting $\epsilon(q,0)$ from Eq. (4) in Eq. (3), we get

$$\frac{\delta\rho(r)}{q_F^3}=\frac{1}{2\pi^2}\int_0^\infty dq\,\frac{q\sin(qrq_F)}{rq_F}\,\frac{F(q)}{1+F(q)[1-f(q)]}, \qquad (7)$$

where q has been expressed in the units of q_F.

The integration in Eq. (7) has been done numerically, using Simpson's rule. Very good convergence was obtained with the interval 0.01 to upper limit 200. The calculated values of $\delta\rho(r)/q_F^3$ for values of r_s varying from 2 to 6 have been tabulated in Table I. We have compared the results with those based on the Hubbard approximation as calculated by Langer and Vosko,[2] and with those of Singwi and Tosi,[8] in Figs. 1 and 2.

It should be noted here, that in Hubbard's original approximation as used by Langer and Vosko,[2] $f(q)$ of Eq. (5b) was taken to be

$$f(q)=\tfrac{1}{2}q^2/(q^2+q_F^2). \qquad (8)$$

The screening parameter was added later by Hubbard himself in private communications to several authors,[9–11] so that $f(q)$ was written as

$$f(q)=\tfrac{1}{2}q^2/(q^2+q_F^2+Q_s^2). \qquad (9)$$

But the values of $\delta\rho(r)/q_F^3$ obtained by using Eq. (9) for $f(q)$ and Eq. (6) for Q_s are extremely close to those obtained by Langer and Vosko, and can not be distinguished in the graphs of Figs. 1 and 2.

Clearly the results differ significantly from those of Hubbard. In particular, the first minimum is about 35% deeper than in Hubbard's case for $r_s=3$, and about 60% deeper for $r_s=6$. Also, near the origin, our computed charge density is greater than that obtained in the Hubbard approximation by about 4% for $r_s=3$, and by about 6% for $r_s=6$. However, the values of the charge density near the origin, as well as the depth of first minimum, are smaller than those given by Singwi and Tosi.[8] We also note that the next maximum, which corresponds to the second shell of ions around the impurity, is slightly greater than the

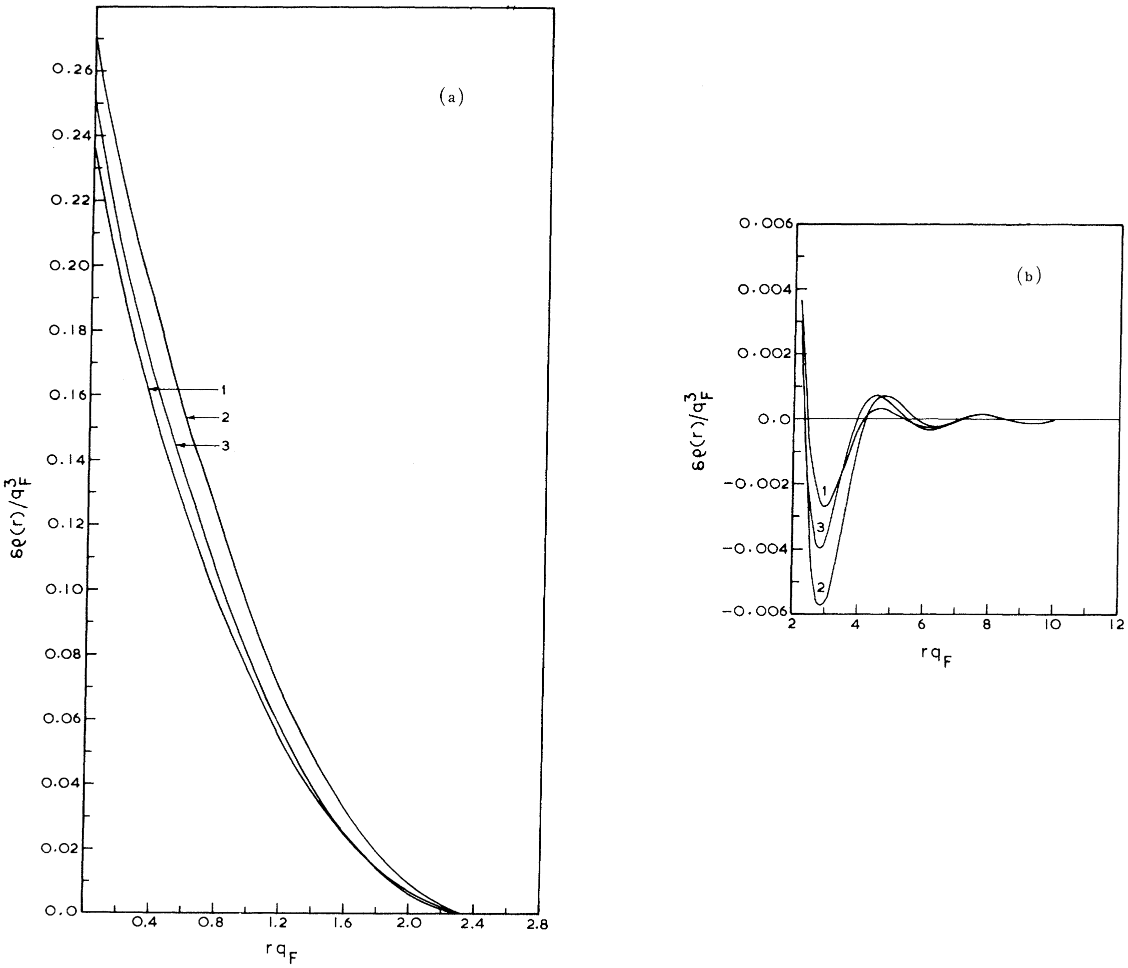

FIG. 2. Screening density $\delta\rho(r)q_F^3$ versus rq_F for $r_s=6$ (a) for small values of rq_F, (b) for large values of rq_F; curve 1, Hubbard (Ref. 2); curve 2, Singwi and Tosi (Ref. 8); curve 3, present results.

corresponding maximum in Singwi's curve. This difference becomes more clear in Fig. 1(b) for $r_s=3$, where the scale has been enlarged compared to Fig. 2(b) for $r_s=6$. Of course, there is negligible difference between results for $rq_F>6$. Thus, we see that both the self-consistent field considerations of Kleinman and the variational technique of Langreth yield results for screening density around a static impurity which lie in between the results based on Hubbard's approximation (which neglects the short-range interaction due to Coulomb repulsion) and the results of Singwi and Tosi (obtained by a self-consistent procedure).

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