# Linear Response of a Metal to an External Charge Distribution\*

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The linear response of a metal to an external-charge distribution is computed in the random-phase approximation (RPA}. The surface is assumed to be perfectly reflecting and the boundary-value problem is solved by a symmetric continuation of the metal. The linear response of the metal to an external point charge is found to be described by a function  $\nu$  which depends only on the properties of the surface and the metal. From  $\nu$ , we compute a surface function S which fully describes the electrical properties outside the metal. Graphs of S as a function of the parallel momentum  $K$  are given for the quantum-mechanical RPA and for the quasiclassical BPA which is obtained by neglecting interference effects. The potential and normal fields outside the metal are well approximated by the analytic expressions which are obtained when  $S(K)$  is replaced by  $e^{-\lambda K}$ , where  $\lambda$  has the physical meaning of a screening length.

### I. INTRODUCTION

In an earlier paper,<sup>1</sup> we treated the linear response of a semi-infinite electron gas to an embedded impurity near the surface. The response was calculated using the random-phase approximation (RPA) and assuming a perfectly reflecting boundary. This treatment leads to a one-dimensional integral equation for the symmetrized charge' density, which was solved numerically. The linear response of a metal to an external charge can be treated in the same way and is, in fact, a much simpler problem. In this paper we present the results of such a treatment.

The response of a metal to a charge a short distance from the surface is important for a number of physical processes,  $2,3$  and many authors<sup>2-6</sup> have dealt with this problem. Most of the earlier treatments are confined to the Thomas-Fermi approximation for the response<sup>3, 4</sup>; others employ the RPA, but either are purely formal<sup>5</sup> or neglect important interference effects. $6$  After the completion of our calculations, we became aware of the recent work of Newns,<sup>2</sup> which is basically equivalent to ours although different in several ways. Our general mathematical results are in agreement with his, and we have noted the relations which can be directly compared.

Newns presents numerical results only for onedimensional charge distributions while we have obtained the Green's function which may be used to calculate the response for any charge distribution. In particular, the response of the metal to an ion or an atom is easy to compute from our results. Our derivation is also distinct from that given by Newns; we treat a semi-infinite gas and symmetrize the potential to obtain an integral equation whose solution describes the dielectric response, he

treats a finite slab and obtains the response by matrix inversion. The results are the same in the limit where the thickness of the slab is allowed to become infinite.

In Sec. II a description of the formulation' of the problem is presented, and the formulas for the potential and the normal component of the field are given in terms of the dielectric response of the system and the position of the external charge. The linear response of the metal to any externalcharge distribution is found to be simply described in terms of the potential at the surface due to the external charge and of a function which depends only on the properties of the surface and the metal.<sup>7</sup>

In Sec. HI the quantum-mechanical RPA developed in I is described and numerical results are presented. Section III contains most of the relevant new results of this paper.

In Sec. IV the results for the quasiclassieal RPA described in I are presented. This approximation is obtained by neglecting the interference term in the quantum-mechanical RPA so that the symmetrized charge density and potential are simply related by the ordinary RPA linear-response function, as they are for an infinite medium. $<sup>8</sup>$  This</sup> quasiclassical calculation allows for loss of coherence at the surface and may provide a better description of a real metal surface than the quantum-mechanical calculation. It is known to provide an adequate description of the response of the surface in the high-frequency limit,<sup>9</sup> and can actually be given rigorous justification in that limit. However in this paper we deal in detail with the static case only.

#### II, FORMULATION

We consider an electron gas which fills the halfspace  $z < 0$  and a fixed external charge Z. Within

 $\overline{a}$ 

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the linear-response theory the charge density  $\rho$ is related to the total potential  $V$  by

$$
\rho(\mathbf{\bar{r}},\,t) = \int d\mathbf{\bar{r}}'\,dt'\,\chi(\mathbf{\bar{r}},\,t;\,\mathbf{\bar{r}}',\,t')\,V(\mathbf{\bar{r}}',\,t'),\tag{1}
$$

where  $\chi$  is the linear-response function and is independent of the external disturbance. For the semi-infinite gas considered here,

$$
\chi(\overline{\mathbf{r}}, t; \overline{\mathbf{r}}', t') = \chi(\overline{|\mathbf{R}} - \overline{\mathbf{R}}', t - t'; z, z') ,
$$

where  $\overline{R}$  is the tangential component of  $\overline{r}$  and z is the perpendicular component. Fourier transforming with respect to  $\tilde{K}$  the tangential component of  $\tilde{k}$  and  $\omega$  the energy variable, (1) becomes

$$
\rho(K, z; \omega) = \int_{-\infty}^{\infty} dz' \chi(K, \omega; z, z') V(K, z'; \omega) . (2)
$$

We shall only present numerical results for the static case,  $\omega = 0$ , and in the following, the  $\omega$  dependence will be suppressed, although it is a simple matter to include it in our treatment.

The potential in a charged system is also related to the charge density by Poisson's equation, which can be written

$$
V(K, z) = (2\pi/K) \left[ Ze^{-K|z-a|} + \int_{-\infty}^{0} dz' e^{-K|z-z'|} \rho(K, z') \right], \quad (3)
$$

where  $a$  denotes the distance of the external point charge  $Z$  from the surface. The boundary-value problem is conveniently treated in terms of the symmetric potential and charge density,

$$
V_s(K, k_z) = 2 \int_{-\infty}^0 dz \cos k_z z \ V(K, z)
$$
 (4)

and

$$
\rho_s(K, k_\mathbf{z}) = 2 \int_{-\infty}^0 dz \cos k_\mathbf{z} z \, \rho(K, z) \tag{5}
$$

We point out that  $V_s(K, z)$  coincides with  $V(K, z)$  for  $z < 0$  and that  $\partial V_s / \partial z$  is discontinuous at  $z = 0$ .

Inserting (3) into (4), we obtain

$$
V_s(\vec{k}) = (4\pi/k^2) [\sigma(K) + \rho_s(\vec{k})], \qquad (6)
$$

where

$$
\sigma(K) = Ze^{-Ka} - K \int_{-\infty}^{\infty} dk_{\pi} \rho_s(\vec{k}) / 2\pi k^2
$$
 (7)

is a fictitious surface charge which is the source of the difference between V and  $V_s$  and satisfies the relation

$$
4\pi\sigma = 2\frac{\partial V}{\partial z}\bigg|_{z=0} \qquad (8)
$$

Inserting (3) into (2), we obtain an integral equation for  $\rho$  or, introducing the symmetric transform of  $\chi$ 

$$
\chi_s(K; k_\alpha, k'_\alpha) = 4 \int_{-\infty}^0 dz \int_{-\infty}^0 dz' \cos k_\alpha z \cos k'_\alpha z' \chi(K; z, z');
$$
 (9)

from (2) and (6), we obtain an integral equation for  $\rho_{s}(\vec{k})$ . Examining (6), we see that the integral equation for  $\rho_s$  will be coupled to the equation for  $\sigma$ [Eq. (7)]. However, if we set

$$
\chi(\tilde{\mathbf{r}},t;\tilde{\mathbf{r}}',t')=\chi(|\vec{\mathbf{R}}-\vec{\mathbf{R}}'|,t-t';z,z')\quad ,\qquad \qquad \rho_s(\vec{\mathbf{k}})=\sigma(K)\left[\nu(\vec{\mathbf{k}})-1\right],\qquad (10)
$$

then  $\sigma(K)$  cancels and  $\nu(\vec{k})$  satisfies the integral equation

$$
\nu(K, k_s) = 1 + 2 \int dk'_s \frac{\chi_s(K; k_s, k'_s) \nu(K, k'_s)}{(K^2 + k'_s)^2} \ . \tag{11}
$$

Inserting (10) in (7), we find

$$
\sigma(K) = Ze^{-Ka} \left( \frac{1}{2} + K \int dk_{\alpha} \frac{\nu(\vec{k})}{2\pi k^2} \right) \quad . \tag{12}
$$

The dielectric response of the metal to the external charge can be determined from  $\nu$  and  $\sigma$ . The potential inside the medium is, from (6) and (10),

$$
V(\vec{\mathbf{r}}) = 4\pi \int d\vec{k} \; \frac{e^{i\vec{k} \cdot \vec{\mathbf{r}}}\sigma(K) \nu(\vec{k})}{(2\pi)^3 k^2}, \quad z < 0 \tag{13}
$$

and outside the metal  $V(\tilde{r})$  is the solution of Poisson's equation with  $-\sigma$  and the charge and its image as sources,

$$
V(\vec{r}) = Z \left\{ \left[ (z-a)^2 + R^2 \right]^{-1/2} + \left[ (z+a)^2 + R^2 \right]^{-1/2} \right\}
$$

$$
- \int d\vec{k} \, \sigma(K) \, e^{i\vec{k} \cdot \vec{R} - Kz} / 2\pi K \,, \quad z > 0 \,. \tag{14}
$$

The electric field normal to the surface is given by '

$$
E_{\mathbf{z}}(R,0) = -\frac{\partial V}{\partial z}\bigg|_{z=0} = -\int d\vec{\mathbf{K}} \frac{\sigma(K) e^{i\vec{\mathbf{K}} \cdot \vec{\mathbf{K}}}}{2\pi} \quad . \quad (15)
$$

The linear-response function  $\chi$  does not depend on the location or size of the external charge and, consequently, the function  $\nu$ [Eq. (11)] is independent of these quantities<sup>7</sup>; i.e.,  $\nu$  depends only on the metal and surface properties. This property of  $\nu$  depends on being able to define a surface so that  $\rho(\vec{K}, z) = 0$  for  $z > 0$ , and on the external charge being located outside of the metal. For an embedded charge,<sup>1</sup> the solution is much more difficulted definition. since the function  $\nu$  depends on the location of the charge.

The surface charge density  $[Eq. (12)]$  can be written in the form

$$
\sigma(K) = Ze^{-Ka}\left[1 + S(K)\right],\tag{16}
$$

where  $S(K)$  is independent of the size and location of the external charge. For an embedded charge'

 $\sigma$  has a more complicated dependence on  $a$  and does not simply scale as  $e^{-Ka}$ . It is also convenient to rewrite the potential and the normal field outside of the surface in terms of  $S<sub>10</sub>$ 

$$
\Delta V(R, z) = V(R, z) - Z [(z - a)^{2} + R^{2}]^{-1/2}
$$
  
=  $- Z \int d\vec{k} S(K) e^{i\vec{k} \cdot \vec{k} - K(\vec{k} + \vec{a})} / 2\pi K, \quad z > 0$  Here (17)

and

$$
\Delta E_z(R, z) = E_z(R, z) - Z(z - a) [(z - a)^2 + R^2]^{-3/2}
$$
  
=  $- Z \int d\vec{k} S(K) e^{i\vec{k} \cdot \vec{R} - K(x + a)}/2\pi$ ,  $z > 0$ . (18)

These are just the potential and field less the potential and field of the external charge.

The average value of the normal field over the surface can be computed from  $(15)$  as

$$
\int d\vec{R} E_{\bf{z}}(R,0) = -2\pi\sigma(K=0) ,
$$

and if

$$
\lim_{K \to 0} K \int dk_{z} \nu(k) k^{-2} = 0 , \qquad (19)
$$

then

$$
\int d\vec{R} E_{\alpha}(R, 0) = -4\pi Z . \qquad (20)
$$

This relation must be true for a metal and is indeed satisfied for the two RPA approximations, quantum-mechanical and quasiclassical, which we developed in I and for which numerical results are presented in Secs. III and IV.

# III. QUANTUM-MECHANICAL RPA

In I we considered the time-independent RPA response of a semi-infinite electron gas to a fixed embedded charge impurity. The linear-response function obtained there can be used in the formulas of Sec. II to calculate the dielectric properties of the system. The RPA response function is most simply obtained<sup>11</sup> by considering the single-particle Hamiltonian  $H_0 + e V(r)$ , where  $H_0$  is the Hamiltonian of a free electron and  $V(r)$  is the self-consistent potential, then expanding the density matrix as potential, then expanding the density matrix as  $\rho^{(0)} + \rho^{(1)}$ , where  $\rho^{(0)}$  is the unperturbed density matrix, and retaining only first-order terms in  $\rho^{(1)}$  and V in the Liouville equation for the system. Using the complete set of states for the half-space which vanish at the boundary and correspond to specular reflection from the surface,

$$
\psi_{\mathbf{z}}(\mathbf{\bar{r}}) = \langle \mathbf{\bar{r}} | \mathbf{\bar{k}} \rangle = (2/\Omega)^{1/2} \sin k_{\mathbf{z}} z e^{i\mathbf{\bar{K}} \cdot \mathbf{\bar{r}}}, \quad k_{\mathbf{z}} > 0 \tag{21}
$$

where  $\Omega$  is the volume, the static RPA response of the system,  $(2)$ , is given by<sup>1</sup>

$$
\rho_s(\vec{k}) = L(k)V_s(\vec{k}) - \Omega^{-1/3} \sum_{k'_g} L(K; k_g, k'_g) V_s(K, 2k'_g).
$$
\n(22)

$$
L(K; k_z, k'_z) = \frac{2e^2}{\Omega^{2/3}} \sum_{\vec{\mathbf{k}}'} \frac{f(\vec{\mathbf{k}}' + \frac{1}{2}\vec{\mathbf{k}}) - f(\vec{\mathbf{k}}' - \frac{1}{2}\vec{\mathbf{k}})}{E_{\vec{\mathbf{k}}'} \cdot (1/2)\vec{\mathbf{k}} - E_{\vec{\mathbf{k}}'} \cdot (1/2)\vec{\mathbf{k}}},
$$
\n(23)

and we have used

$$
H^0\big|\vec{\mathbf{k}}\,\rangle = E_{\vec{\mathbf{k}}}\big|\vec{\mathbf{k}}\,\rangle = (k^2/2m)\,\big|\vec{\mathbf{k}}\,\rangle
$$

and

$$
\rho^{(0)}\big|\vec{\mathbf{k}}\rangle = f(k)\big|\vec{\mathbf{k}}\rangle,
$$

where  $f(k)$  is the zero-temperature Fermi distribution function which vanishes for  $k > k<sub>F</sub>$ , the Fermi momentum. Performing the indicated integrations,<sup>12</sup>

$$
L(K; k_z, k_z') = -\frac{me^2}{\pi K^2} f(|k_z' + \frac{1}{2}k_z|) (K^2 - 2k_z k_z')
$$

$$
\times \left[1 - \text{Re}\left(1 - \frac{4K^2[k_p^2 - (k_z' + \frac{1}{2}k_z)^2]}{[K^2 - 2k_z k_z']^2}\right)^{1/2}\right],
$$
(24)

and a further integration gives

$$
L(k) = \Omega^{-1/3} \sum_{k'_g} L(K; k_g, k'_g)
$$
  
= 
$$
-\frac{\alpha^2}{8\pi} \left( 1 + \frac{1 - \kappa^2}{2\kappa} \ln \left| \frac{1 + \kappa}{1 - \kappa} \right| \right) ,
$$
 (25)

where  $\kappa = k/2k_F$ . The Thomas-Fermi wave number  $\alpha$  is given by

$$
(\alpha/2k_F)^2 = me^2/\pi k_F = 0.166 r_s,
$$

where  $r_s$  is the Wigner-Seitz radius in units of the Bohr radius and we have taken  $\hbar = 1$ . From now on all lengths will be expressed in units of  $(2k_F)^{-1}$ .

We see that  $L(k)$  is the ordinary RPA linear-response function for an infinite medium. $<sup>8</sup>$  The second</sup> term in (22) comes from the quantum-mechanical interference between the impinging and reflected electrons and is strongly dependent on the assumed properties of the surface.

comparing (2) and (22), we see that for the full quantum-mechanical RPA  $\nu$ , as defined in (11), is given by

$$
\text{cular reflection from the surface,}
$$
\n
$$
\nu(\vec{k}) = \frac{1}{\epsilon(k)} \left( 1 - 4\pi \int \frac{dk_x'}{2\pi} \frac{L(K; k_x, k_x')}{K^2 + 4k_x'^2} \nu(K, 2k_x') \right),
$$
\n
$$
\psi_k(\vec{r}) = \left\langle \vec{r} \right| \vec{k} \rangle = (2/\Omega)^{1/2} \sin k_x z \, e^{i\vec{K} \cdot \vec{R}}, \quad k_x > 0 \tag{21}
$$
\n
$$
(26)
$$

where  $\epsilon(k)$  is the RPA dielectric function for an infinite medium

$$
\epsilon(k) = 1 - 4\pi L(k)/k^2 \quad . \tag{27}
$$

[Notice that in I  $\nu$  is called  $\nu_0$  and defined by Eq. (34).]

We have solved the integral equation (26) numerically by an iteration procedure, which is rapidly convergent. The function  $\nu$  satisfies the sum rule

$$
\int \left[ \nu(\vec{k}) - 1 \right] dk_{\mathbf{z}} = 0 \tag{28}
$$

which is easily obtained by multiplying (26) by  $\epsilon(k)$ and integrating with respect to  $k_z$  when (25) is used to evaluate the integral involving  $L(K; k<sub>s</sub>, k'<sub>s</sub>)$ . This sum rule insures that the charge density goes to zero at the surface as can be seen by Fourier transforming (10) with respect to  $k_{\rm z}$ . As stated in I,  $L(K; k_{z}, k'_{z})$  is a well-behaved continuous function of  $k'_g$  for  $k > 2k_F$  and

$$
[\nu(\vec{k}) - 1] \sim -\alpha^2 k_\mathbf{z}^2 / 3k^8, \quad \text{as } k \to \infty . \tag{29}
$$

Numerically it is found that

$$
\nu(\vec{k}) \sim c k^2, \quad \text{as } k \to 0 , \tag{30}
$$

where  $c$  is a positive constant.



FIG. 1. Plots of  $S(K)$  as a function of  $K/2k_F$ . The curves are for the quantum-mechanical calculation (solid line), the quasiclassical calculation (dot-dashed line), and the Thomas-Fermi approximation of Hef. 4 or Appendix (dashed line). The Thomas-Fermi wave number is  $\alpha$  (in units of  $2k_r$ ).

TABLE I. Screening length  $\lambda$  for the quantum-mechanical and quasiclassical approximations. For the Thomas-Fermi approximation,  $\lambda = 2/\alpha$  where  $\alpha$  is the Thomas-Fermi wave number.

$2k_F\lambda_{\rm CM}$	$2k_F\lambda_{\rm QC}$	$2k_F(\lambda_{\rm QM}-\lambda_{\rm QC})$
7.5	4.3	3.2
6.2	3.1	3.1
5.6	2.5	3.1

The solution of (26) is used to compute  $S(K)$  [Eq. (16)], which is then used in (17) and (18) to compute the field and potential at the surface. In Fig. 1,  $S(K)$  is plotted for this calculation, for the quasiclassical calculation of Sec. IV and for the Thomas-Fermi calculation<sup>4</sup> of the Appendix. The curves are given for three values of the Thomas-Fermi parameter  $\alpha$  which correspond to the values  $r_s$  $= 1.51$ , 3.40, and 6.05 for the Wigner-Seitz radius and span the range of metallic densities. Using (29), we can obtain the asymptotic value of  $S(K)$ 

$$
S(K) \sim 5\alpha^2/768K^6, \quad \text{as } K \to \infty , \tag{31}
$$

and for small values of K we find that  $S(K) \sim e^{-\lambda K}$ , where the values of  $\lambda$  are given in column two of Table I.

Approximating  $S(K)$  by the exponential, we can compute  $\Delta V$  [Eq. (17)] and  $\Delta E_{\rm g}$ [Eq. (18)] analytically,

$$
\Delta V(R, z) = - Z[(z + a + \lambda)^2 + R^2]^{-1/2}, \quad z > 0 \quad (32)
$$

and

$$
\Delta E_z(R, z) = -Z(z + a + \lambda) \left[ (z + a + \lambda)^2 + R^2 \right]^{-3/2}, \ z > 0.
$$
\n(33)

These are very good values for these quantities and agree within about  $1\%$  with the numerically calculated values. The Friedel oscillations<sup>13</sup> on the surface are too small to be computed within the accuracy with which we have determined  $\nu(\vec{k})$ .

#### IV. QUASICLASSICAL RPA

In I we obtained the quasiclassical approximation by neglecting the interference term in (22). Then the symmetrized charge density is given by

$$
\overline{\rho}_s(\overline{k}) = L(k) V_s(\overline{k}) . \qquad (34)
$$

Strictly speaking, this equation is valid only for long wavelengths and  $L(k)$  should be the limit of (25) for  $\vec{k}$  + 0.<sup>1</sup> However, we have considered (34) to be valid for all values of  $k$  and solved the problem in this case. By comparing the solution with the quantum-mechanical case, we can determine the effect of neglecting the interference term.

Substituting (34) into (7) gives

 $\overline{\rho}_{\rm s}(\overline{\mathbf{k}}) = 4\pi L(k) \sigma(K)/k^2 \epsilon(k)$  . (35)

Comparing this with (10) or directly from (26), we have

$$
\overline{\nu}(k) = 1/\epsilon(k) \tag{36}
$$

and, using (27) and (25), the limiting behavior is

$$
\overline{\nu}(k) - 1 \sim -\alpha^2/3k^4, \quad \text{as } k \to \infty \tag{37}
$$

and

$$
\overline{\nu}(k) \sim k^2/\alpha^2, \quad \text{as } k \to 0 \ . \tag{38}
$$

The function  $S(K)$  for this approximation is plotted in Fig. 1 and its asymptotic value is

$$
S(K) \sim \alpha^2/16K^4, \quad \text{as } k \to \infty \tag{39}
$$

For small values of K we can approximate  $S(K)$  by  $e^{-\lambda K}$  where the values of  $\lambda$  are given in the third column of Table I. Using this approximation for  $S(K)$ , we again obtain the analytical forms  $(32)$  and (33) for  $\Delta V$  and  $\Delta E_{\rm g}$ . The agreement with the nu-. merical calculated values is not as good as in the quantum-mechanical case, but still within 5%. The Friedel oscillations<sup>13</sup> are appreciable but small in this case.

In I we compared the quantum-mechanical and quasiclassical results and argued that the quasiclassical results describe a system where the true surface is some distance above the plane  $z = 0$ . Comparing the results of this section with those of Sec. III, we find that this interpretation is still valid. In particular, from the fourth column of Table I, we see that the surface should be displaced a distance of  $\sim 3.1/2k_{F}$ .

#### V. SUMMARY

The linear response of a metal to an external charge distribution can be computed from the function  $\nu(\vec{k})$  which only depends on the properties of the metal and the surface. We have solved the integral equation for  $\nu(\vec{k})$  in the quantum-mechanical RPA described in Sec. III which imposes the condition of specular reflection at the surface. In Sec. IV we obtain an analytic expression for  $\nu(\mathbf{k})$ in the quasiclassical RPA which cannot be fully justified in terms of a model for the surface. In Fig. 1 the function  $S(K)$ , which is obtained by integrating  $\nu(\vec{k})/k^2$  over  $k_{\vec{k}}$  is plotted for these two RPA calculations and the Thomas- Fermi approximation described in the Appendix. All of these approximations are seen to satisfy

$$
\lim_{K \to 0} S(K) = 1.
$$

It is easily seen from  $(12)$ ,  $(16)$ , and  $(19)$  that this

is equivalent to the property (20), which is a consequence of the perfect screening of long-wavelength disturbances in a metal.

The function  $S(K)$  fully describes all of the electrical properties of the surface due to external charges and in particular for an arbitrary distribution of external charge  $\rho_{\text{ext}}(\vec{r}')$ , the potential outside the metal is obtained from  $(17)$  by a simple integration,

$$
\Delta V(\vec{\mathbf{R}}, z) = -\int_0^\infty dz' \int \frac{d\vec{\mathbf{K}}}{2\pi K} S(K) \rho_{\text{ext}}(\vec{\mathbf{K}}, z')
$$

$$
\times e^{i\vec{\mathbf{K}} \cdot \vec{\mathbf{R}} - K(z + z')}, \quad z > 0.
$$
(40)

The approximation

$$
S(K) = e^{-K\lambda} \tag{41}
$$

is found to give analytic expressions  $(32)$  and  $(33)$ in good agreement with the numerically computed potential and normal field outside the metal. When this approximation for  $S(K)$  is used the computation of electrical properties is trivial: As can be seen from  $(32)$  and  $(33)$ , the classical image theorem holds, except that the "image" charge is now located at  $z = -(a+\lambda)$ . For the quantum-mechanical RPA, this remarkable property can be used to obtain results which are accurate for all values of  $a$ .

The screening length  $\lambda$  is given in Table I for the various approximations of this paper. A full plot of  $\lambda$  as a function of  $r_s$  for the quantum-mechanical RPA and Thomas-Fermi approximation is given by Newns<sup>14</sup> in Fig. 6 of his paper. Newns only computes the screening length for a one-dimensional potential, but the quantity he defines is, in our notation,

$$
d(r_s) = -\lim_{K \to 0} \frac{V(K, z)}{E_z(K, z)} \bigg|_{z=0} = -\frac{1}{2} \left. \frac{dS}{dK} \right|_{K=0}, \tag{42}
$$

and is equal to  $\frac{1}{2}\lambda$  when S is represented by (41). Newns<sup>2</sup> has discussed the comparison with experiment and finds that the experimental data are consistent with a screening length larger than the Thomas-Fermi value  $\lambda = 2/\alpha$ .

The discontinuity of the linear-response function at twice the Fermi momentum results in an oscillatory behavior of the potential and field at the surface as a function of the radial coordinate on the surface. These Friedel oscillations are not reproduced by the approximation (41) for  $S(K)$ . However, their amplitudes are very small and they are unimportant for most electrical properties.

The full quantum-mechanical RPA response is completely described by the function  $\nu(\vec{k})$ . Since only one integral equation must be solved, there is little numerical advantage in making the quasiclassical approximation where  $\nu(\vec{k})$  can be obtained analytically. When the charge is inside the metal an integral equation must be solved for each value of the distance of the embedded charge from the surface to obtain the quantum-mechanical RPA  $r_{\text{exponse}}$ , and the quasiclassical approximation greatly reduces the numerical work required. The comparison between the two solutions is easier to make for the external charge and supports our interpretation of the embedded charge results.

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### APPENDIX

Here we quote some of Newns<sup>4</sup> results for the

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 $6J.$  W. Gadzuk, Solid State Commun.  $5$ , 743 (1967); NASA Technical Report No. R-283, 1968 (unpublished); R. W. Davies, Surface Sci. 11, 419 (1968); E. Gerlach, in Molecular Processes on Solid Surfaces, edited by E. Drauglis, R. D. Gretz, and R. I. Jaffe (McGraw-Hill, New York, 1969), p. 181.

This result is expressed by Eq.  $(66)$  of Ref. 2, since

Thomas-Fermi approximation and relate them to our calculations by expressing the approximation in our notation. If the RPA dielectric function (27) is expanded for small values of  $k$  the result is the Thomas-Fermi dielectric function  $\epsilon(k) = 1 + \alpha^2/k^2$ . Using this function,  $S(K)$  is given by

$$
S(K)=(t-K)^2/\alpha^2
$$

where  $t=(K^2+\alpha^2)^{1/2}$  and is plotted in Fig. 1. The limiting values of S are easily found to be

$$
S(K) \sim 1 - 2K/\alpha + \frac{3}{2}K^2/\alpha^2, \quad \text{as } K \to 0
$$

and

$$
S(K) \sim \alpha^2/4K^2 \ , \text{ as } K \to \infty.
$$

Computing  $\Delta V$  (see Fig. 1 of Ref. 4) and  $\Delta E_z$  numerically, one finds that when  $(z+a) > 2/\alpha$  these functions are well approximated by the analytic solutions (32) and (33) obtained with  $S(K) \sim e^{-2K/\alpha}$ [i.e.,  $\lambda = 2/\alpha$  in Eq. (40)]. This expression for  $S(K)$  leads to Gomer and Swanson's<sup>3, 4</sup> approximations for the potential energy of a charged particle near a metal surface.

 $10$ It is clear that the function S and the "dielectric function"  $\epsilon_K$ [Eq. (60), Ref. 2] defined by Newns must be related. The correspondence is  $S(K) = (\epsilon_K - 1)/(\epsilon_K + 1)$  or in terms of  $\nu(\vec{k})$ ,  $\epsilon_{\vec{k}}^{-1} = 2K \int dk_{\vec{k}} \nu(\vec{k}) / 2\pi k^2$ .

<sup>11</sup>H. Ehrenreich and M. H. Cohen, Phys. Rev.  $115$ , 786 (1959). '

 $12$  This expression is equivalent to the expression for  $A(0)$  [Eq. (35), Ref. 2] defined by Newns, but  $-\infty < k'_z$  $<\infty$ , so that  $-A_{\mathbf{K}, k_{\mathbf{g}}}, 2k_{\mathbf{g}}(0)$  is proportional to  $L(K; k_{\mathbf{g}}, k_{\mathbf{g}})$ + $L(K; k_g, -k'_g)$ , where  $k'_g > 0$ .

 $^{13}$ J. Friedel, Advan. Phys.  $3, 446$  (1954); Nuovo Cimento Suppl. 7, 287 (1958).

 $^{14}$  In the revised version of Ref. 2, Fig. 7 contains a curve labeled "truncated electron gas", which is equivalent to our quasiclassical RPA.

 $\epsilon_K$  is independent of the external charge.

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 ${}^{9}E$ . A. Stern and R. A. Ferrell, Phys. Rev. 120, 130 (1960); P. J. Feibelman, Phys. Rev. 176, <sup>551</sup> (1968).