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Dynamic response approach to dynamic image potential

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Abstract. A dielectric response approach to the dynamic image potential of a charged particle approaching a planar metal surface is formulated. A self-consistent scheme for calculating the instantaneous speed of the particle, and its image potential is also derived. It is shown that the scheme does not rely on the actual approximations made while describing the response of the metal with surface. Various approximations are discussed and the corresponding numerical results compared. The effect of self-consistency and inclusion of dispersion in metal is noticeable.

Keywords. Image potential; response function; surface dielectric function.

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1. Introduction

When a charged particle approaches a planar metal surface from vacuum, it excites elementary excitations of the metal, setting up electromagnetic fields. The interaction of the electromagnetic fields with the incoming charged particle then gives rise to the dynamical image potential (Mahan 1974). The causal nature of the response of the metal to the charged particle, makes the dynamic image potential dependent on the velocity of the incoming charge, and it is this aspect which is of considerable importance in the experimental studies involving scattering of charged particles from metal surfaces. Broadly, there are two theoretical approaches: one, where the incoming charge is treated classically, and the other, where the particle is treated quantum-mechanically. The latter is essential for the case of an electron approaching a metal, and the theoretical formulation here has been *via* the model Hamiltonian approach (Lucas 1971; Mahan 1972; Ritchie 1972; Sunjic *et al* 1972; Ray and Mahan 1972; Gumhalter 1977; Shah and Mukhopadhyay 1983). On the other hand in the former case, the theory can be developed in terms of the linear dielectric response of the metal and therefore, the details of the excitations of the metal can be incorporated in the formulation in a straightforward manner—an advantage over the latter method.

In the dielectric response approach to dynamic image potential problem, earlier work (Newns 1970; Feibelman 1971; Heinrichs 1973; Harris and Jones 1973; Ekardt 1983; Puri and Schaiach 1983) assumed a constant speed of the incoming charged particle, although self-consistent methods *via* the model Hamiltonian approach have incorporated modifications in the speed of the charged particle due to its interaction with the metal. In this paper, we develop the dielectric response approach with similar self-consistency in the modification of speed as was done in the model Hamiltonian approach (Ray and Mahan 1972; Shah *et al* 1981, Shah and Mukhopadhyay 1983) and present numerical calculations for a simplified form (plasmon pole approximations, Sunjic *et al* 1972) for the dielectric function of the metal with a planar surface. A preliminary version of this work was presented elsewhere (Shah *et al* 1981).

2. Theory

The dynamic image potential of a particle of charge q and mass m, which can be treated classically, is given by the electrostatic self-interaction energy,

$$W(\mathbf{x}(t)) = \frac{1}{2} q V_i(\mathbf{x}(t)), \tag{1}$$

at the location $\mathbf{x}$ of the external incoming particle at instant t. Here V_i is the Coulomb potential due to the induced electronic charge density ρ_i of the metal induced by the external charge q, *i.e.*,

$$V_i(\mathbf{x}(t)) = \int \mathrm{d}\mathbf{x}' v(\mathbf{x}(t), \mathbf{x}')\rho_i(\mathbf{x}', t), \tag{2}$$

where

$$v(\mathbf{x}, \mathbf{x}') = e^2/|\mathbf{x} - \mathbf{x}'|.$$

Within linear response theory, ρ_i is given by (retardation effect due to finite speed of Coulomb interaction is ignored throughout),

$$\rho_i(\mathbf{x}', t) = \int \mathrm{d}\mathbf{x}'' \int_{-\infty}^{\infty} \mathrm{d}t' \chi(\mathbf{x}', \mathbf{x}'', t - t') V_{\text{ext}}(\mathbf{x}'', t'), \tag{3}$$

where χ is the retarded density-density response function for the metal (*i.e.* interacting electron system) with $\chi = 0$ for $t < t'$. Here, the external potential is

$$V_{\text{ext}}(\mathbf{x}'', t') = q/|\mathbf{x}'' - \mathbf{x}(t')|.$$

Thus the entire problem is determined by the specification of the retarded density-density response function χ of the metal-vacuum system.

In order to proceed further, we now assume that the metal is represented by a semi-infinite jellium with its positive background extended in the $z > 0$ region and the vacuum-metal interface parallel to the xy plane. We also assume for simplicity that the external charge approaches the metal from $z \to -\infty$ at $t \to -\infty$ with an initial speed v_0 in the direction normal to the metal surface, *i.e.*, along the z-axis. We shall also be concerned with the situations where the external particle is located outside the metal. With the preceeding approximate description, the metallic system is translationally invariant in the xy plane, so that

$$\chi(\mathbf{x}, \mathbf{x}', t) \equiv \chi(\mathbf{r} - \mathbf{r}', z, z', t), \tag{4}$$

where $\mathbf{r} \equiv (x, y, 0)$, etc. This property can be exploited to simplify the expressions above, by introducing Fourier transforms (FT) in the x-y plane. In fact, it is convenient to introduce FT in space as well as time variables such that,

$$\chi(k, z, z', \omega) = \int_{-\infty}^{\infty} \mathrm{d}t \exp(i\omega t) \int \mathrm{d}\mathbf{r} \exp(i\mathbf{k} \cdot \mathbf{r}) \chi(\mathbf{r}, z, z', t). \tag{5}$$

Then, after straightforward algebraic manipulations, we have from (1)–(5),

$$W(z(t)) = \frac{q^2}{4\pi}\int_0^\infty dk \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} d\omega \exp[-i\omega(t-t')]\mathscr{F}(k, z(t), z(t'), \omega), \tag{6}$$

where

$$\mathscr{F} \equiv \frac{2\pi e^2}{k}\int_{-\infty}^{\infty} dz' \int_{-\infty}^{\infty} dz'' \exp[-k|z'-z(t)|]\chi(k, z', z'', \omega) \times \exp[-k|z''-z(t')|]. \tag{7}$$

The essential problem now is to determine the function $\mathscr{F}$ from χ. However, for the situation we are concerned with, further simplification is possible. We note that $\chi(k, z', z'', \omega)$ vanishes for z' or z'' outside the metal. Also, the retarded nature of χ ensures that contributions to t'-integral above comes for $t' < t$ provided we maintain the order of integration in (6). Thus for the charge particle outside the metal, we have $z'-z(t) > 0$, $z''-z(t') > 0$ and $z(t)$, $z(t') < 0$, so that

$$\mathscr{F} \equiv F(k, \omega)\exp[k(z(t)+z(t'))], \tag{8}$$

where

$$F(k, \omega) = \frac{2\pi e^2}{k}\int_{-\infty}^{\infty} dz' \int_{-\infty}^{\infty} dz'' \exp[-k(z'+z'')]\chi(k, z', z'', \omega). \tag{9}$$

Thus the dynamic image potential at $z(t)$ outside the metal is given by,

$$W(z(t)) = \frac{q^2}{4\pi}\int_0^\infty dk \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} d\omega \times \exp\{-i\omega(t-t') + k[z(t)+z(t')]\}\, F(k, \omega), \tag{10}$$

where the order of integration should be maintained.

There are two aspects of the problem at hand now. The first is to determine the form factor $F(k, \omega)$, characteristic of the metal vacuum system and the second is to express z as a function of t or t', so that the t' integral can be carried out.

The form factor $F(k, \omega)$ requires determination of χ, which by itself presents a very difficult task even though we have simplified the description of the metal in terms of a semi-infinite jellium. To elucidate the point, we use a short-hand notation (*i.e.* a matrix notation where sum or integrals over intermediate variables are understood), and write

$$\rho_i = \chi V_{\text{ext}} = \chi_0 V_{\text{eff}} = \chi_0(V_{\text{ext}} + V_i),$$
$$= \chi_0(V_{\text{ext}} + v\rho_i) = \chi_0(V_{\text{ext}} + v\chi V_{\text{ext}}),$$

so that $\chi = \chi_0 + \chi_0 v\chi$, *i.e.*,

$$\chi(k, z, z', \omega) = \chi_0(k, z, z', \omega) + \iint dz_1 dz_2 \chi_0(k, z, z_1, \omega) \times \frac{2\pi e^2}{k}\exp(-k|z_1 - z_2|)\chi(k, z_2, z', \omega), \tag{11}$$

where, in the so-called time-dependent Hartree (or random phase) approximation, χ_0 is the retarded density-density response function of the non-interacting electron system of semi-infinite jellium. The function χ_0 can be constructed from one electron wave functions. However, for realistic (*e.g.*, self-consistent local density functional approach) description of the semi-infinite jellium, the wave functions can be obtained only in numerical form so that finding χ itself requires considerable computational efforts (Feibelman 1974). On the other hand, at the expense of quantitative accuracy (but not physics), with additional approximation for χ_0, it is possible to handle things analytically. One such approximation is the so-called semi-classical infinite barrier model (SCIB) with which we shall be concerned hereafter. This model has been described at length elsewhere (Mukhopadhyay and Lundqvist 1978; Mukhopadhyay 1978), and it corresponds to a model where the ground state electron density profile coincides with the positive background of the semi-infinite jellium. It is also an alternative description of the so-called specular reflection model. Following the method of construction given in reference (Mukhopadhyay and Lundqvist 1978), we have for SCIB model

$$\chi_0(k, z, z', \omega) = \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} \chi_{B0}(q, \omega)[\exp(ip(z - z')) + \exp(ip(z + z'))], \tag{12}$$

for $z, z' > 0$; χ_0 is identically zero for $z, z' < 0$. Here $q^2 = k^2 + p^2$, and $\chi_{B0}(q, \omega)$ refers to the frequency and wavevector-dependent response function for infinite homogeneous non-interacting electron system (jellium). With this form of χ_0 in (11), one may attempt to solve for χ. However, we are interested in $F(k, \omega)$ and it is more convenient to rewrite (11) as,

$$\alpha(z, z') = \alpha_0(z, z') + \int \mathrm{d}z_1 \alpha_0(z, z_1)\alpha(z_1, z'), \tag{13}$$

where

$$\alpha(z, z') = \frac{2\pi e^2}{k} \int \mathrm{d}z_1 \chi(k, z, z_1, \omega) \exp(-k|z_1 - z'|), \tag{14}$$

and a similar expression for α_0 in terms of χ_0. Then for the SCIB model,

$$F(k, \omega) = \int_0^{\infty} \mathrm{d}z \alpha(z, 0) \exp(-kz), \tag{15}$$

where α is to be determined from (13). From (12) we have

$$\begin{aligned} \alpha_0(z, z') &= \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} Q_0(q, \omega) \cos pz \exp(kz'), \text{ for } z' < 0 \\ &= -\int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} Q_0(q, \omega) \cos pz [2 \cos pz' - \exp(-kz')], \quad \text{for } z' > 0, \end{aligned} \tag{16}$$

where

$$Q_0(q, \omega) = -4\pi e^2 \chi_{B0}(q, \omega)/q^2,$$

the Lindhard polarizability. From (13) and (16), after careful and lengthy algebraic manipulation, we obtain

$$\begin{aligned} F(k, \omega) &= \int_0^{\infty} \mathrm{d}z \exp(-kz) \frac{2\varepsilon_s}{1 + \varepsilon_s} \left[\int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi\varepsilon_B} \cos pz - \delta(z) \right] \\ &= \frac{1 - \varepsilon_s(k, \omega)}{1 + \varepsilon_s(k, \omega)}, \end{aligned} \tag{17}$$

where

$$\varepsilon_s^{-1}(k,\omega) = \frac{k}{\pi}\int_{-\infty}^{\infty}\frac{\mathrm{d}p}{k^2+p^2}\frac{1}{\varepsilon_B(q,\omega)}, \tag{18}$$

with $q^2 = k^2+p^2$ and $\varepsilon_B(q,\omega) = 1+Q_0(q,\omega)$, the RPA dielectric function for the infinite homogeneous electron system (jellium) with bulk metallic density. This form for $F(k,\omega)$ was first derived by Heinrichs (1973) using boundary conditions which is avoided in our derivation. We note that ε_s corresponds to surface dielectric function and it contains all the excitations in the metal with surface. For example, $\varepsilon_s(k,\omega)+1 = 0$ corresponds to the dispersion relation for the surface plasmons (Ritchie and Marusak 1966) which gives the most dominant contribution to $F(k,\omega)$, although numerically the dispersion relation does not very well agree with realistic situation (Feibelman 1974).

We now turn to the second problem of expressing z as function of t. Usually, here one makes the constant speed approximation and writes $z(t) = v_0 t$, so that the particle approaches from $z \to -\infty$ at $t \to -\infty$. However, it is not necessary to have an explicit form for $z(t)$, if we note, in anticipation, that the speed $v(t)$ at instant t is not modified substantially from v_0, and its modification arises essentially from the polarization effects during immediate past. This means that for $z(t')$ we can use a Taylor's expansion about $z(t)$ and write,

$$z(t') \simeq z(t) - (t-t')v(t). \tag{19}$$

With this approximation, the t' integration in (10) can be done after performing the ω-integration for a specific form of $F(k,\omega)$ as given by (14). However, (9) shows that χ and hence $F(k,\omega)$ admits the usual dispersion relation for retarded function, so that,

$$F(k,\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{\omega'-(\omega+i\delta)}\,\mathrm{Im}\,F(k,\omega'). \tag{20}$$

This relation can be utilized to interchange the t' and ω integration in (10), and the t' integration can be performed first to obtain,

$$\int_{-\infty}^{\infty}\mathrm{d}t'\int_{-\infty}^{\infty}\mathrm{d}\omega\exp\{i\omega(t-t')+k[z(t)+z(t')]\}F(k,\omega)$$
$$\simeq 2\pi\exp(2kz(t))F(k,ikv(t)). \tag{21}$$

This result is then independent of the approximation made in evaluating $F(k,\omega)$. We also note that the instantaneous location $z(t)$ and speed $v(t)$ appear in the formula requiring self-consistency. The image potential is then given by,

$$W(z) = \frac{q^2}{2}\int_0^{\infty}\mathrm{d}k\exp(2kz)F(k,ikv), \tag{22}$$

where $z \equiv z(t)$, $v \equiv v(t)$, and for F, the approximate form of (17) can be used.

To find $v(t)$, we now employ the energy conservation principle (Ray and Mahan 1972; Shah and Mukhopadhyay 1983), *i.e.*

$$\frac{1}{2}mv_0^2 = \frac{1}{2}mv^2(t)+W[z(t)], \tag{23}$$

and determine $v(t)$ and $W[z(t)]$ self-consistently from (22) and (23), with F given by (17).

The numerical work for the self-consistent scheme described above remains rather a formidable task, despite several approximations, mainly because of the complicated structure of $\varepsilon_B(q, \omega)$, the RPA dielectric function, and thereby of $\varepsilon_s(k, \omega)$. We reduce the numerical effort by choosing a simple approximate form for $\varepsilon_s(k, \omega)$, the so-called surface dielectric function, suggested first by Sunjic *et al* (1972), *i.e.*,

$$\varepsilon_s(k, \omega) = 1 + \left(\frac{k^2}{\kappa^2} + \frac{k}{\kappa} - \frac{\omega^2}{\omega_p{}^2}\right)^{-1}, \tag{24}$$

where $\kappa(\kappa = 3\alpha/\sqrt{r_s}$ in atomic units, $\alpha = (4/9\pi)^{1/3}$ and r_s is the usual electron gas parameter) is the Thomas-Fermi wavevector corresponding to the electron-density in the bulk of the metal and ω_p is the plasma frequency. This form for ε_s represents the static and dynamic limits of the surface dielectric function for both large and small limits of k (Sunjic *et al* 1972). We now have from (22),

$$\begin{aligned} W(z) &= -\frac{q^2}{4}\int_0^\infty \mathrm{d}k \exp(2kz)\left(\frac{k^2}{\kappa^2} + \frac{k}{\kappa} + \frac{k^2 v^2}{\omega_p{}^2} + \frac{1}{2}\right)^{-1} \\ &= -\frac{q^2}{2}\frac{\kappa}{(1 + v^2\kappa^2/\omega_s{}^2)^{1/2}} \operatorname{Im} \int_0^\infty \frac{\mathrm{d}\xi e^{-\xi}}{\xi + \xi_0 - i\mu}, \end{aligned} \tag{25}$$

where,

$$\xi_0 = \kappa|z|/(1 + v^2\kappa^2/\omega_p{}^2) > 0,\ \mu = \xi_0(1 + v^2\kappa^2/\omega_s{}^2)^{1/2} > 0,$$

$\omega_s = \omega_p/\sqrt{2}$ the surface plasmon frequency, and we have set $\xi = 2k|z|$.

Using the definition for exponential integral function of complex argument $c = a + ib$, (Gautschi and Cahill 1970),

$$E_1(c) = \int_c^\infty (e^{-t}/t)\,\mathrm{d}t,\ (|\arg c| < \pi)$$

or alternatively, using

$$e^c E_1(c) = \int_0^\infty e^{-\mu}/(\mu + c)\,\mathrm{d}\mu,$$

we rewrite (25) as

$$W(z) = -\frac{q^2}{2}\frac{\kappa}{(1 + v^2\kappa^2/\omega_s{}^2)^{1/2}} \operatorname{Im}\left[\exp(\xi_0 - i\mu)E_1(\xi_0 - i\mu)\right], \tag{26}$$

where the standard formulae (Gautschi and Cahill 1970) can be used to compute E_1. When $\kappa \to \infty$, *i.e.*, the Thomas Fermi screening wavelength vanishes, we obtain the classical result (where $\varepsilon_B(q, \omega)$ is dispersionless, *i.e.*, $\varepsilon_B = 1 - \omega_p{}^2/\omega^2$, in which case $\varepsilon_s = \varepsilon_B$):

$$W_{cl}(z) = -\frac{q^2\omega_s}{2v} f(2\omega_s|z|/v), \tag{27}$$

where $f(x)$ is a standard tabulated integral function (Gautschi and Cahill 1970) defined as,

$$f(x) = \int_0^\infty \frac{\mathrm{d}t\, e^{-xt}}{1 + t^2}. \tag{28}$$

The classical result (27) has been derived before by several authors within constant speed approximation (*i.e.* v_0 in place of v above), (Lucas 1971) as well as within the self-consistent scheme described above (Ray and Mahan 1972; Shah and Mukhopadhyay 1983).

The case of dispersion *via* $\varepsilon_B(q, \omega)$ has been considered before, but within constant speed approximation (Sunjic *et al* 1972; Heinrichs 1973). Our working formula (26), coupled with the self-consistency requirement (23), differs in that our method is self-consistent. The details of our numerical work are presented below.

3. Calculation and results

We have calculated the image potential values numerically for different incident energy $\varepsilon_0 = mv_0^2/2$ of an incoming electron (*i.e.* $q = e$) and for different electron densities of the metal, characterized by the well-known electron gas parameter r_s (in the range $2 \leqslant r_s \leqslant 5$). Some of the results are presented in figures 1–3. The potential is plotted against z, the distance of the electron from the metal surface, and the incident energy expressed in terms of the classical plasmon energy $\hbar\omega_p$. Figure 1 corresponds to $r_s = 2$ and $\varepsilon_0 = 0{\cdot}125\hbar\omega_p = 2{\cdot}08$ eV, whereas figures 2 and 3 correspond to $r_s = 4$, $\varepsilon_0 = \hbar\omega_p = 5{\cdot}89$ eV and $0{\cdot}125\hbar\omega_p = 0{\cdot}74$ eV respectively. In all figures, curve 1 corresponds to the classical dispersionless case with constant speed approximation (*i.e.*, based on (27)) considered earlier (see Mahan 1974 and references therein); curves 2 and 3 correspond

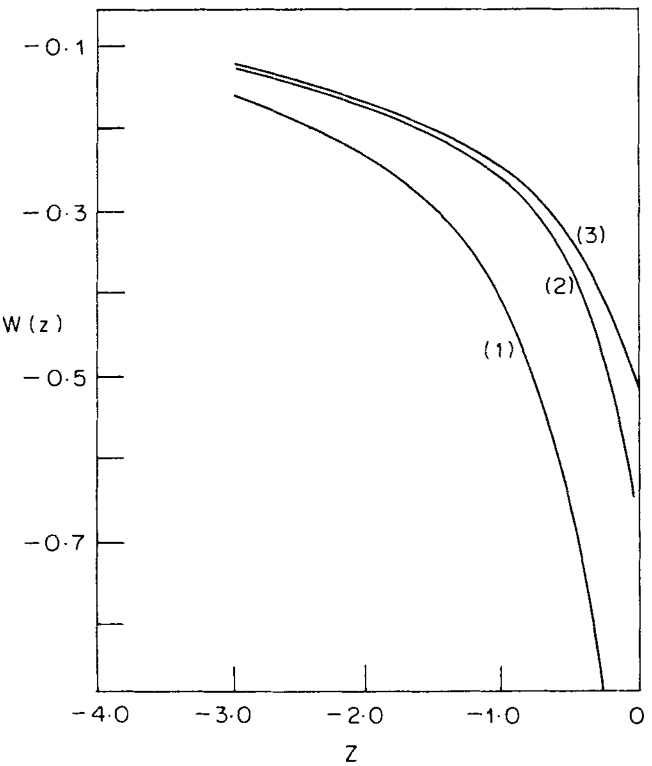

Figure 1. The dynamic image potential $W(z)$ vs z, for $r_s = 2$ and $\varepsilon_0 = 0{\cdot}125\hbar\omega_p$.

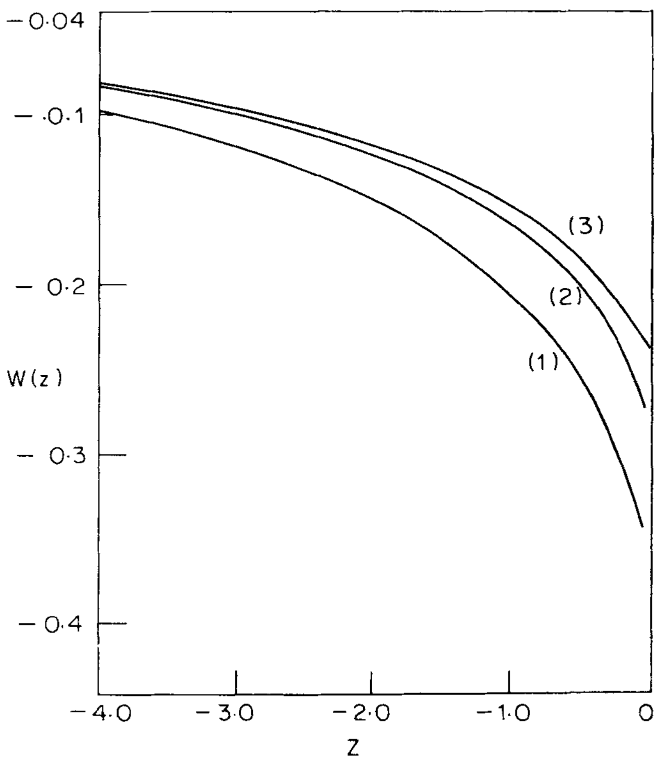

Figure 2. $W(z)$ vs z, for $r_s = 4$ and $\varepsilon_0 = \hbar\omega_p$.

respectively to our approximate formula (26), with constant speed approximation (Sunjic *et al* 1972) and with self-consistency respectively. We have also calculated results for the classical case but with self-consistency (Ray and Mahan 1972) and the corresponding curves (not shown in figure) lie between curves 1 and 2, closer to curve 2.

From the figures, we find considerable effect on the dynamic image potential due to dispersion in ε_s as well as due to the self-consistency requirement. Also, the modifications increase as the incident energy and the metallic electron density decrease (*i.e.*, for smaller ε_0 and larger r_s). This trend has been noticed in earlier work too.

A study of the image potential results shows that the maximum potential depth W_m is obtained at the metal surface (*i.e.*, for the present model, at $z = 0$), for a particle initially at rest. To obtain W_m, we set $\varepsilon_0 = 0$ in the energy conservation relation (23), and find v for W_m. For the classical case it gives (Mahan 1974; Shah and Mukhopadhyay 1983),

$$W_{m0} = -(3\pi^2/8)^{1/3} r_s^{-1} \, Ryd. \tag{29}$$

In the present case (*i.e.*, with dispersive ε_s and self-consistent scheme) we have from (23) and (26),

$$W_m = uW_{m0}, \tag{30}$$

where u satisfies the equation

$$u^3 + 3\beta u^2 - 1 = 0, \tag{31}$$

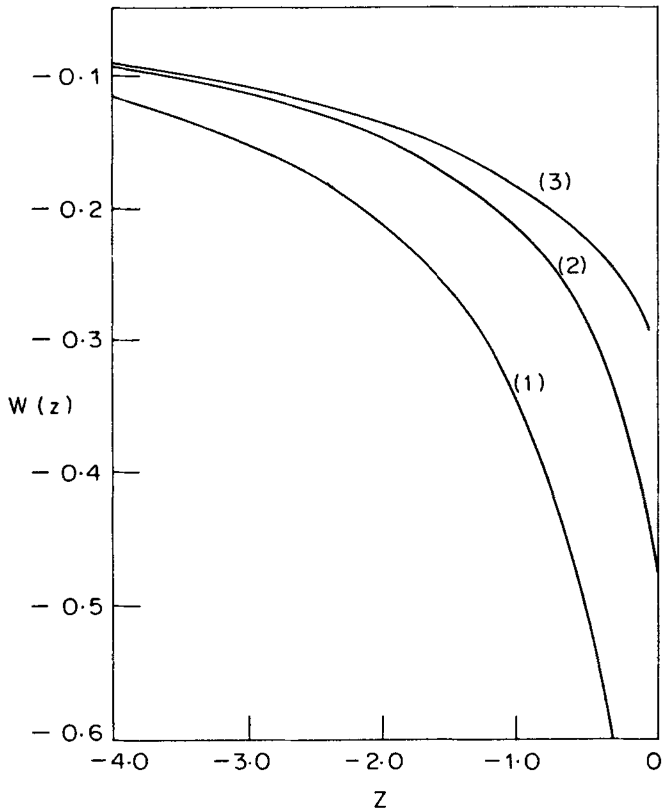

Figure 3. $W(z)$ vs z, for $r_s = 4$ and $\varepsilon_0 = 0{\cdot}125\hbar\omega_p$; Curve 1—classical with constant speed, Curve 2—present model with constant speed, Curve 3—present model with self-consistency.

Table 1. Maximum average number of excitations for classical (Q_{m0}) and present (Q_m) cases, and maximum potential depth (in Rydbergs) for classical (W_{m0}) and present (W_m) cases. Also included are the values for $u(= W_m/W_{m0})$ for different r_s values.

r_s	u	W_{m0} (Ryd)	W_m (Ryd)	Q_{m0}	Q_m
2	0·938	−0·773	−0·725	1·786	1·675
3	0·958	−0·516	−0·444	2·188	2·096
4	0·968	−0·387	−0·375	2·526	2·445
5	0·974	−0·309	−0·301	2·824	2·751

with $\beta = (6\ 2^{1/3} r_s)^{-1}$, having the solution,

$$u = [\tfrac{1}{2} - \beta^3 + (\tfrac{1}{4} - \beta^3)^{1/2}]^{1/3} + [\tfrac{1}{2} - \beta^3 - (\tfrac{1}{4} - \beta^3)^{1/2}]^{1/3} - \beta. \qquad (32)$$

The numerical value of u for different r_s is given in table 1.

Another quantity which can be calculated, is Q, the average number of excitations, excited at the metal surface by an electron making a round trip (Mahan 1974):

$$Q = -2W(0, v)/\hbar\omega_s.$$

It is obvious that an improvement in the estimate of the image potential provides an identical improvement in the estimate of Q. Our analysis then shows, that inclusion of dispersion effects reduces the average number of surface modes created. This in turn reduces significantly the possibility of inelastic scattering, thus providing knowledge of the potential essential for studying elastic scattering experiments. We can also estimate the maximum Q value, $Q_m = -2W_m/\hbar\omega_s$. The probability that the incoming electron does not cause any excitation is $\exp(-Q_m)$. This being a quantity which can be measured in low energy electron scattering experiments, the estimation of Q_m is useful. Table 1 lists values of W_m and Q_m, along with the corresponding values W_{m0} and Q_{m0} for the case of dispersionless ε_s.

4. Conclusion

We have shown, from the response function approach, how a self-consistent scheme for the calculation of the image potential can be arrived at. To our knowledge, we have for the first time, shown that formula (22) is independent of the approximation made in describing the response of the metal. We have also included, though in an approximate manner, the effect of the dispersion in the surface dielectric function, in the self-consistent scheme, and found modifications in the image potential calculations over earlier work (Sunjic *et al* 1972; Ray and Mahan 1972). Finally, we would like to point out that further improvements over the present calculations, lie essentially in the description of the form factor $F(k, \omega)$, *via* more accurate description of the metallic response function χ. Also, the effect of surface irregularities can be incorporated here in an approximate manner. We have taken up studies along these lines now, and will present the results in a later publication.

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