

NONLOCAL DYNAMICAL POTENTIALS NEAR CURVED SURFACES

LEONARDO MARUŠIĆ AND MARIJAN ŠUNJIĆ

Department of Physics, University of Zagreb, POB 162, 10000 Zagreb, Croatia

Received 10 July 1998; Accepted 16 November 1998

We present a self-consistent quantum-mechanical formulation of the nonlocal dynamical potential near the surface of a solid describable in a coordinate system in which Laplace equation is separable. We apply the formulation to calculate image potential on surfaces with uniform curvature, i.e. planar, spherical and cylindrical surfaces. We also calculate the dielectric function $\epsilon(\omega)$ and dispersion relations of surface modes in these systems.

PACS numbers: 73.20.Mf, 77.90.+k

UDC 538.971, 538.956

Keywords: surface of a solid, nonlocal dynamical potential, self-consistent quantum-mechanical formulation, image potential, planar, spherical and cylindrical surfaces, dielectric function, dispersion relations of surface modes

1. Introduction

Knowledge of the self-consistent dynamical response of solids of various shapes to an external charged particle is important in understanding many physical phenomena, e.g. potential energies of charged particles near surfaces, bound or resonant states of such particles and optical transitions between them, energy losses of electrons in EELS experiments, electron tunneling in metal-insulator-metal systems, semiconductor heterojunctions and systems like STM, BEEM, etc. These problems have been extensively studied mostly within the long-wavelength limit, i.e. by neglecting the dispersion in solids. First calculations have been performed in the local limit, i.e. by treating a charged particle as a classical static charge at a point \vec{r} interacting with surface excitations (phonons, plasmons), and that

was done for a number of different geometries [1–3]. In the nonlocal case, the induced potential between the two charges at points \vec{r} and \vec{r}' near a solid surface, due to their interaction with surface excitations, has been calculated using several different formalisms, for planar and spherical surfaces [4–8]. Most accurate calculations of image potential were done for planar jellium surface. They were first performed within the framework of DFT and LDA [9], but recently they use diagrammatic methods to correct LDA results [10–12]. More detailed *ab initio* calculations, which would take into account the band structure of the metal, still do not exist.

We use the method of Newns [4] and generalize it to any coordinate system in which the Laplace equation is separable. In this paper we specifically treat the solids invariant to transformations (translations and/or rotations) in two coordinates, i.e. with planar, spherical and cylindrical boundary surfaces. The definition of our model, and the two-dimensional Fourier transforms of all quantities involved is given in Sect. 2. In Sect. 3, we calculate the self-consistent nonlocal potential W , surface dielectric function $\epsilon_Q(\omega)$ and the dispersion relations of surface modes, and finally, in Sect. 5, we apply our general results to discuss explicitly the three special cases. The systems with lower symmetry, i.e. invariant to transformation in only one coordinate, are discussed in Sect. 4, and we show that symmetry of these systems is insufficient to complete all the calculations analytically.

2. Formulation of the problem

We describe the solid by its response function $R(\vec{r}, \vec{r}', \omega)$. Coordinates are chosen so that the surface (and therefore boundary conditions) is defined in one of them, which we call *broken* or, in analogy with the spherical solid, *radial* coordinate, and the other two we call *angular* coordinates. In the *radial* direction, the solid is finite in all systems considered, and in the *angular* direction the solid is finite for spherical coordinates, and infinite in other cases. We assume that electron cannot penetrate into the solid, which means that it will interact only with surface excitations, because within the longwave limit, bulk excitations do not produce any field outside the solid, i.e. they are fully screened by the surface excitations.

Dynamically screened potential W between the points \vec{r} and \vec{r}' is given by:

$$W(\vec{r}, \vec{r}', \omega) = V(\vec{r}, \vec{r}') + W^{ind}(\vec{r}, \vec{r}', \omega), \quad (1)$$

where

$$W^{ind}(\vec{r}, \vec{r}', \omega) = \int_{\tau} d^3 r_1 d^3 r_2 V(\vec{r}, \vec{r}_1) R(\vec{r}_1, \vec{r}_2, \omega) W(\vec{r}_2, \vec{r}', \omega). \quad (2)$$

Here τ is the volume of the solid, V the direct Coulomb interaction, R the response function [13] describing the charge fluctuations in the solid, and W^{ind} the induced part of the nonlocal potential W .

Due to the symmetry of the system, we expand all these quantities using the solutions $g_Q(\Omega)$ of the *angular* part of the Laplace equation

$$[\Delta_{\Omega} + \lambda_Q(r)]g_Q(\Omega) = 0 \quad (3)$$

in the appropriate geometry. The functions $g_Q(\Omega)$ form a complete and orthonormal set

$$\sum_Q g_Q^*(\Omega)g_Q(\Omega') = \delta(\Omega - \Omega'), \quad (4)$$

$$\int g_Q^*(\Omega)g_{Q'}(\Omega)\rho(\Omega)d\Omega = \delta_{QQ'}. \quad (5)$$

The index Q denotes the conserved quantum numbers, Ω are the associated coordinates, or degrees of freedom, and $\rho(\Omega)d\Omega$ is the *angular* part of the volume differential d^3r . In particular, we can expand V , W and R as:

$$V(\vec{r}, \vec{r}') = \sum_Q g_Q^*(\Omega)g_Q(\Omega')V_Q(r, r'), \quad (6)$$

$$W(\vec{r}, \vec{r}') = \sum_Q g_Q^*(\Omega)g_Q(\Omega')W_Q(r, r'), \quad (7)$$

$$R(\vec{r}, \vec{r}') = \sum_Q g_Q^*(\Omega)g_Q(\Omega')R_Q(r, r'). \quad (8)$$

Inserting (2), (6), (7) and (8) into (1), we get:

$$W_Q(r, r', \omega) = V_Q(r, r') + \int f(r_1)dr_1 f(r_2)dr_2 \quad (9)$$

$$V_Q(r, r_1)R_Q(r_1, r_2, \omega)W_Q(r_2, r', \omega),$$

where $f(r)dr$ is *radial* part of the volume differential in a particular geometry.

This procedure is valid only for planar, cylindrical and spherical geometries. Other geometries require a slightly different derivation, and will be treated separately.

The Poisson equation for the Fourier components of the Coulomb potential now becomes:

$$[\Delta_r - \lambda_Q(r)]V_Q(r, r') = \frac{4\pi e^2}{f(r)}\delta(r - r'), \quad (10)$$

and the solution is:

$$V_Q(r, r') = v_Q[\phi_Q^>(r)\phi_Q^<(r')\theta(r - r') + \phi_Q^<(r)\phi_Q^>(r')\theta(r' - r)], \quad (11)$$

where $\phi_Q^<$ and $\phi_Q^>$ are the two solutions of *radial* part of the Laplace equation:

$$[\Delta_r - \lambda_Q(r)]\phi_Q^< = 0, \quad (12)$$

chosen so that $\phi_Q^<$ converges for $r \rightarrow 0$, and $\phi_Q^>$ for $r \rightarrow \infty$. $V(\vec{r}, \vec{r}')$ is direct Coulomb interaction $e^2/|\vec{r} - \vec{r}'|$ which can be expanded in terms of the solutions of the Laplace

equation [14]:

$$\frac{e^2}{|\vec{r} - \vec{r}'|} = -4\pi e^2 \frac{h'_1}{h'_2 h'_3} \sum_Q g_Q^*(\Omega') g_Q(\Omega) \frac{\rho(\Omega')}{W} [\phi_Q^>(r) \phi_Q^<(r') \theta(r - r') + \phi_Q^<(r) \phi_Q^>(r') \theta(r' - r)], \quad (13)$$

where W is the Wronskian. Comparing that with (6) and (11), we get

$$v_Q = -4\pi e^2 \frac{h'_1}{h'_2 h'_3} \frac{\rho(\Omega')}{W}. \quad (14)$$

Table 1 contains all the quantities mentioned above for planar, spherical and cylindrical geometries.

TABLE 1. Coordinates, boundary surfaces, quantum numbers and other quantities needed for the calculation of the nonlocal potential in planar, spherical and cylindrical systems.

Coordinate system	Planar	Spherical	Cylindrical
Angular coordinates (Ω)	x, y	ϑ, φ	z, φ
Quantum numbers (Q)	k_x, k_y	ℓ, m	k, m
$g_Q(\Omega)$	$e^{i\vec{k}\vec{\rho}} / (2\pi)$	$Y_{\ell m}(\Omega)$	$e^{ikz} e^{im\varphi} / (2\pi)$
Radial coordinate (r)	z	r	ρ
Boundary surface	$z = 0$	$r = a$	$\rho = a$
$\lambda_Q(r)$	$k^2 = k_x^2 + k_y^2$	$\ell(\ell + 1)/r^2$	$k^2 + m^2/\rho^2$
Density function $\rho(\Omega)$	1	$\sin \vartheta$	1
Wronskian	$-2k$	$-(2\ell + 1)/r^2$	$-1/\rho$
$h_1/(h_2 h_3)$	1	$1/(r^2 \sin \vartheta)$	$1/\rho$
v_Q	$2\pi e^2/k$	$4\pi e^2/(2\ell + 1)$	$4\pi e^2$
$f(r)dr$	dz	$r^2 dr$	$\rho d\rho$
$\phi_Q^<(r)$	e^{kz}	r^ℓ	$I_m(k\rho)$
$\phi_Q^>(r)$	e^{-kz}	$r^{-\ell-1}$	$K_m(k\rho)$
λ_q	$-k^2 - n^2\pi^2/a^2$	$-x_{\ell n}^2/a^2^{(1)}$	$-k^2 - x_{mn}^2/a^2^{(2)}$
$h_q(r)$	$\cos(n\pi z/a)$	$j_\ell(x_{\ell n} r/a)$	$J_m(x_{mn} \rho/a)$

(1) $x_{\ell n}$ are zeroes of derivatives of spherical Bessel functions.

(2) x_{mn} are zeroes of derivatives of cylindrical Bessel functions.

3. Derivation of the non-local electrostatic potential

Now, we introduce a complete orthonormal set of functions $h_{Qq}(r)$, which are the solutions of the equation:

$$[\Delta_r - \lambda_Q(r)]h_{Qq}(r) = \lambda_q h_{Qq}(r), \quad (15)$$

with the boundary condition:

$$\left. \frac{\partial h_{Qq}(r)}{\partial r} \right|_{r=a} = 0. \tag{16}$$

This condition is much more convenient to use (compared to $h_{Qq}(r = a) = 0$), because the functions h_{Qq} are going to be used for Fourier transformation of the quantities, such as W and R , which do not vanish on the surface.

Functions h_{Qq} for various systems are listed in Table 1.

Acting on (9) from the left with $f(r)h_{Qq}(r)[\Delta_r - \lambda_Q(r)]$, integrating inside the solid, and using the fact that the potential V satisfies the Poisson equation (10), we find:

$$\begin{aligned} & \int f(r)dr h_{Qq}(r)[\Delta_r - \lambda_Q(r)] W_Q(r, r', \omega) = \\ & = -4\pi e^2 \int f(r)dr h_{Qq}(r) \int f(r_1)dr_1 R_Q(r, r_1, \omega) W_Q(r_1, r', \omega). \end{aligned} \tag{17}$$

The first term on the r.h.s. of (9) vanished because r' is outside the solid.

We introduce single and double Fourier transforms in terms of the functions h_{Qq} :

$$W_{Qq}(r', \omega) = \int f(r)dr h_{Qq}(r) W_Q(r, r', \omega), \tag{18}$$

$$R_{Qqq'}(\omega) = \int f(r)dr f(r')dr' h_{Qq}(r) h_{Qq'}(r) R_Q(r, r', \omega). \tag{19}$$

The r.h.s. of (17) can be Fourier transformed into:

$$-4\pi e^2 \sum_q R_{Qqq'}(\omega) W_{Qq'}(r', \omega), \tag{20}$$

and the l.h.s. can be rewritten as [4,7]:

$$\begin{aligned} & \int W_Q(r, r', \omega)[\Delta_r - \lambda_Q(r)] h_{Qq}(r) f(r)dr + \\ & \int \nabla_r [(\nabla_r W_Q(r, r', \omega)) h_{Qq}(r)] f(r)dr - \\ & \int \nabla_r [(\nabla_r h_{Qq}(r)) W_Q(r, r', \omega)] f(r)dr. \end{aligned} \tag{21}$$

The first term in (21), according to (15) and (18), is equal to $\lambda_q W_{Qq}(r', \omega)$. The second term is:

$$f(a)[\nabla_r W_Q(r, r', \omega) h_{Qq}(r)]_{r=a} = f(a)h_{Qq}(a)W'_Q(a, r', \omega),$$

where the prime denotes the differentiation with respect to r .

And finally, the last term in (21) vanishes because of (16), so that (17) becomes

$$\sum_{q'} E_{Qqq'}(\omega) W_{Qq'}(r', \omega) = -f(a) h_{Qq}(a) W'_Q(a, r', \omega), \quad (22)$$

where we have introduced the matrix:

$$E_{Qqq'}(\omega) = 4\pi e^2 R_{Qqq'}(\omega) + \lambda_q \delta_{qq'}. \quad (23)$$

Multiplying (22) by the inverse matrix E we get:

$$W_{Qq}(r', \omega) = -f(a) \sum_{q'} E_{Qqq'}^{-1}(\omega) W'_Q(a, r', \omega) h_{Qq'}(a), \quad (24)$$

or

$$W_Q(r, r', \omega) = -f(a) \sum_{qq'} E_{Qqq'}^{-1}(\omega) W'_Q(a, r', \omega) h_{Qq'}(a) h_{Qq}(r). \quad (25)$$

We still have to calculate $W'_Q(a, r', \omega)$ from the solution $W_Q(r, r', \omega)$ outside the solid, where V_Q is given by (11), and the induced potential W_Q^{ind} satisfies the equation:

$$[\Delta_r - \lambda_Q(r)] W_Q^{ind}(r, r', \omega) = 0. \quad (26)$$

The solution for $r, r' \geq a$ (i.e. outside the solid) is:

$$W_Q^{ind}(r, r', \omega) = \frac{\phi_Q^>(r)}{\phi_Q^>(a)} W_Q^{ind}(a, r', \omega). \quad (27)$$

Therefore, differentiating the equation:

$$W_Q(r, r', \omega) = V_Q(r, r') + W_Q^{ind}(r, r', \omega) \quad (28)$$

in the region $a < r < r'$, and using (11) and (27) we find:

$$W'_Q(a, r', \omega) = \frac{\phi_Q^<(a)}{\phi_Q^<(a)} V_Q(a, r') + \frac{\phi_Q^>(a)}{\phi_Q^>(a)} W_Q^{ind}(a, r', \omega), \quad (29)$$

which may be written as:

$$W'_Q(a, r', \omega) = \alpha_Q^> W_Q(a, r', \omega) + (\alpha_Q^< - \alpha_Q^>) V_Q(a, r'), \quad (30)$$

where

$$\alpha_Q^>< = \left. \frac{d}{dr} \ln \phi_Q^>< \right|_{r=a}. \quad (31)$$

Inserting (30) into (25) for $r = a$ (i.e. at the boundary surface), and solving for W we get:

$$W_Q(a, r', \omega) = \frac{1 - \alpha_Q}{\varepsilon_Q(\omega) - \alpha_Q} V_Q(a, r'), \quad (32)$$

where

$$\alpha_Q = \frac{\alpha_Q^>}{\alpha_Q^<} = \frac{\phi_Q^< \phi_Q^>'}{\phi_Q^> \phi_Q^<'}, \quad (33)$$

and we have introduced the dielectric function $\varepsilon_Q(\omega)$, defined by:

$$\varepsilon_Q^{-1}(\omega) = -\alpha_Q^< f(a) \sum_{qq'} E_{Qqq'}^{-1}(\omega) h_{Qq}(a) h_{Qq'}(a). \quad (34)$$

From this expression and (23), we see that the inverse dielectric function for all three systems could be expressed in terms of the response function $R_{Qqq'}(\omega)$ in the same manner as for the planar system [4]. This allows the calculation $\varepsilon_Q^{-1}(\omega)$ by making an appropriate approximation (e.g. the random phase approximation [7], or including the local exchange and correlation [15]) for the response function. Also, it becomes straightforward to calculate $\varepsilon_Q^{-1}(\omega)$ from (34) in a semiclassical limit by neglecting non-diagonal terms of $E_{Qqq'}(\omega)$, as, e.g., in the semi-classical infinite barrier model (SCIBM) [4,16].

From (27), (28) and (32), we now obtain:

$$W_Q^{ind}(r, r', \omega) = -\frac{\varepsilon_Q(\omega) - 1}{\varepsilon_Q(\omega) - \alpha_Q} \frac{\phi_Q^>(r)}{\phi_Q^>(a)} V_Q(a, r'), \quad (35)$$

or, using (11),

$$W_Q^{ind}(a, r', \omega) = -v_Q \frac{\phi_Q^<(a)}{\phi_Q^>(a)} \phi_Q^>(r) \phi_Q^>(r') \frac{\varepsilon_Q(\omega) - 1}{\varepsilon_Q(\omega) - \alpha_Q}. \quad (36)$$

This expression is the central result of this paper, representing the nonlocal electrostatic potential near a solid surface in a simple form. From the denominator of that expression, we see that dispersion relations for SP modes are given by:

$$\varepsilon_Q(\omega) = \alpha_Q. \quad (37)$$

4. Surfaces with nonuniform curvature

As we mentioned before, procedure described in Sect. 2 is valid only for surfaces with uniform curvature, i.e. for planar, spherical and cylindrical surfaces, because in these cases the system is translationally invariant in direction parallel to the surface. Therefore, we can use expansions (6)–(8). In all other cases, only the expansion (6) is correct (because direct

Coulomb potential $V(\vec{r}, \vec{r}')$ depends only on points \vec{r} and \vec{r}' , and has nothing to do with the surface and its shape). But for W and R the expansions are:

$$W(\vec{r}, \vec{r}', \omega) = \sum_{QQ'} g_Q^*(\Omega) g_{Q'}(\Omega') W_{QQ'}(r, r', \omega), \quad (38)$$

$$R(\vec{r}, \vec{r}', \omega) = \sum_{QQ'} g_Q^*(\Omega) g_{Q'}(\Omega') R_{Q'}(r, r', \omega). \quad (39)$$

Using that instead of (9), we get:

$$\begin{aligned} W_{QQ'}(r, r', \omega) = & V_Q(r, r') \delta_{QQ'} + \int f(r_1) dr_1 f(r_2) dr_2 \\ & \sum_{Q_1} V_Q(r, r_1) R_{QQ_1}(r_1, r_2, \omega) W_{Q_1 Q'}(r_2, r', \omega), \end{aligned} \quad (40)$$

or, in matrix notation:

$$\begin{aligned} \widehat{W}(r, r', \omega) = & \widehat{V}(r, r') + \int f(r_1) dr_1 f(r_2) dr_2 \\ & \widehat{V}(r, r_1) \widehat{R}(r_1, r_2, \omega) \widehat{W}(r_2, r', \omega), \end{aligned} \quad (41)$$

where matrix \widehat{V} is diagonal, which means that in the product $\widehat{V} \widehat{R} \widehat{W}$, only multiplication $\widehat{R} \widehat{W}$ is matrix multiplication, but multiplication of \widehat{V} with any other matrix is just ordinary multiplication. Trouble is that our procedure is based on the assumption that differential d^3r could be factorized in *radial* and *angular* parts i.e.:

$$d^3r = f(r) dr \rho(\Omega) d\Omega, \quad (42)$$

where $\rho(\Omega)$ is the density function for normalization of functions $g(\Omega)$ (as we can see from (5)), which allows to eliminate $\rho(\Omega)$ from (1), and get equation (9) dependent only on *radial* coordinate. Unfortunately, the assumption (42) is valid only in planar, spherical and cylindrical coordinates. As a consequence, v_Q can not be evaluated analytically and written in a simple form such as (11).

However, the formal procedure described in Sect. 3 is completely general, and using it, we can find a solution analogous to (35):

$$\widehat{W}^{ind}(a, r', \omega) = - \frac{\phi_Q^>(r)}{\phi_Q^>(a)} \widehat{V}(a, r') [\widehat{\epsilon}(\omega) - 1] [\widehat{\epsilon}(\omega) - \widehat{\alpha}]^{-1}. \quad (43)$$

This expression is valid for all systems in which the Laplace equation is separable, but $V_Q(a, r')$ has to be calculated numerically, except, of course, for systems with uniform curvature, where symmetry of the system allows to calculate it analytically.

5. Discussion and conclusion

General solution (36) could become quite complicated when applied to some special system because, if functions ϕ_Q are Bessel or Legendre functions, α_Q will be a combination of these functions and their derivatives. The exceptions are planar and spherical systems where ϕ_Q 's, and, therefore α_Q 's, are very simple. In particular, for a planar system $\alpha_Q = -1$, and for a spherical system $\alpha_Q = -\frac{\ell+1}{\ell}$, but for a cylindrical system

$$\alpha_{km} = \frac{I_m(ka)K'_m(ka)}{I'_m(ka)K_m(ka)}. \quad (44)$$

Using quantities from Table 1, we can evaluate the inverse dielectric function for a **planar** system:

$$\varepsilon_k^{-1}(\omega) = \frac{k}{a} \sum_{nn'} \left[4\pi e^2 R_{knn'}(\omega) - \left(k^2 + \frac{n^2 \pi^2}{a^2} \right) \delta_{nn'} \right]^{-1} (nn')^{\frac{1}{2}}, \quad (45)$$

for a **spherical** system:

$$\varepsilon_\ell^{-1}(\omega) = \frac{2\ell}{a^2} \sum_{nn'} \left[4\pi e^2 R_{knn'}(\omega) - \frac{x_{\ell n}^2}{a^2} \delta_{nn'} \right] \left(1 - \frac{\ell(\ell+1)}{x_{\ell n}^2} \right)^{-\frac{1}{2}} \left(1 - \frac{\ell(\ell+1)}{x_{\ell n'}^2} \right)^{-\frac{1}{2}}, \quad (46)$$

and for a **cylindrical** system:

$$\varepsilon_{km}^{-1}(\omega) = \frac{2}{a^2} \frac{I'_m(ka)}{I_m(ka)} \sum_{nn'} \left[4\pi e^2 R_{mkn'}(\omega) - \left(k^2 + \frac{x_{mn}^2}{a^2} \right) \delta_{nn'} \right]^{-1} \left(1 - \frac{m^2}{x_{mn}^2} \right)^{-\frac{1}{2}} \left(1 - \frac{m^2}{x_{mn'}^2} \right)^{-\frac{1}{2}}, \quad (47)$$

where $I'_m(x) = \frac{d}{dx} I_m(x)$.

From (36), we can calculate the potential energy of an electron in the vicinity of a surface:

$$V(\vec{r}, \omega) = \frac{1}{2} W^{ind}(\vec{r}, \vec{r}, \omega), \quad (48)$$

$$V(\vec{r}, \omega) = -\frac{1}{2} \sum_Q \left\{ v_Q \frac{\phi_Q^<(a)}{\phi_Q^>(a)} [\phi_Q^>(r)]^2 \frac{\varepsilon_Q(\omega) - 1}{\varepsilon_Q(\omega) - \alpha_Q} \right\} |g_Q(\Omega)|^2. \quad (49)$$

For a planar system, α_Q does not depend on Q . If we neglect dispersion, assuming that $\varepsilon_Q(\omega)$ does not depend on Q , the series in (49) is analytically summable, leading to the well known classical result [17]:

$$V(z, \omega) = -\frac{\varepsilon(\omega) - 1}{\varepsilon(\omega) + 1} \frac{e^2}{4z}. \quad (50)$$

In a spherical system, for an electron on the z -axis, we get [8,18]:

$$V(r, \omega) = -\frac{e^2}{2a} \sum_{\ell} \left(\frac{a}{r}\right)^{2\ell+1} \frac{\varepsilon_{\ell}(\omega) - 1}{\varepsilon_{\ell}(\omega) + 1 + \frac{1}{\ell}}. \quad (51)$$

The ℓ -summation cannot be carried out analytically except for a metal surface where $\varepsilon(\omega) \rightarrow \infty$, which leads to the classical image potential [17].

For a cylindrical system, for an electron on the x -axis ($\varphi = 0$), we have:

$$V(\rho, \omega) = -\frac{e^2}{2\pi a} \sum_{km} \frac{I'_m(ka)}{K_m(ka)} K_m^2(k\rho) \frac{\varepsilon_{km}(\omega) - 1}{\varepsilon_{km}(\omega) - \alpha_{km}}, \quad (52)$$

with α_{km} given by (44).

As an illustration, Fig. 1 shows the image potentials for an electron near planar and spherical metal ($\varepsilon \rightarrow \infty$) surface. Units on the x -axis are scaled with respect to the radius of the sphere (i.e. $a = 1$), and the origin for the planar potential is shifted to $z = a$. It is obvious that very close to the surface, there is practically no difference between the planar and spherical surfaces because, if the electron is so close, the spherical surface appears planar. Far away from the surface, the difference between those two potentials increases and at a distance $a/2$ from the surface, potential for the spherical surface is already 20% larger.

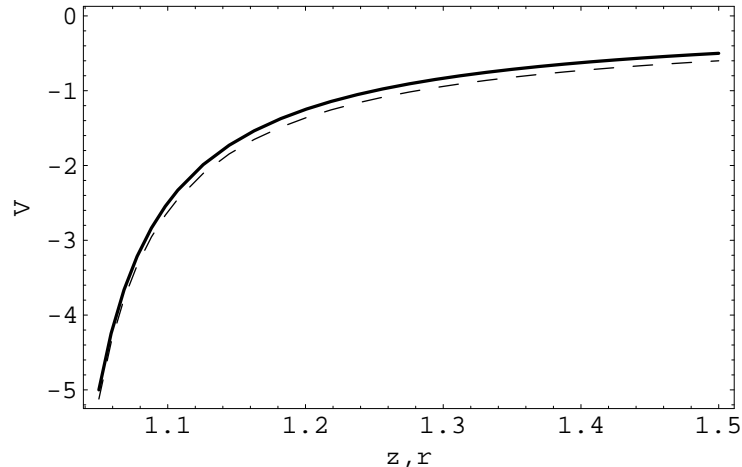


Fig. 1. Image potential for planar and spherical surfaces. Solid line: planar surface, dashed line: spherical surface.

Note that the functions ϕ_Q always appear in ratios, so they do not have to be normalized, while the functions g_Q and h_{Qq} are used for Fourier transformations and have to be normalized.

In conclusion, we have formulated a self-consistent nonlocal dynamical potential near a solid surface describable in separable coordinates, assuming a uniform curvature. From that general result, we have evaluated the potential energy of an electron in the vicinity of a curved surface, generally and in three special cases, and also the surface mode dispersion relations. We have shown how the inverse dielectric function of the solid with a curved surface could be expressed in terms of the response function. We also showed that a similar procedure could be performed for systems with nonuniform curvature, but only up to certain point because of a reduced symmetry of the systems, so that the analytic method has to be continued numerically. Our results are not very helpful for practical calculations, because it is probably easier to treat each case by the method appropriate for that particular geometry instead of the general treatment we presented here (and also because the two most important cases, planar and spherical, were already solved). But they are interesting from the formal point of view because of their generality.

References

- 1) R. Rupin and R. Engelman, Rep. Prog. Phys. **33** (1970) 144;
- 2) R. Brako, J. Hrnčević and M. Šunjić, Z. Physik **B 21** (1975) 193;
- 3) A. Ronveaux, A. Moussiaux and A. A. Lucas, Can. J. Phys. **56** (1977) 1423;
- 4) D. M. Newns, Phys. Rev. **B 1** (1970) 3304;
- 5) F. Hache, D. Richard and C. Girard, Phys. Rev. **B 38** (1988) 7990;
- 6) Z. Penzar and M. Šunjić, Physica Scripta **30** (1984) 431;
- 7) Z. Penzar, J. Petravić and M. Šunjić, Fizika **16** (1984) 119;
- 8) A. C. Sharma, Phys. Rev. **B 36** (1987) 4413;
- 9) N. D. Lang and W. Kohn, Phys. Rev. **B 3** (1971) 1215;
- 10) A. G. Eguiluz and W. Hanke, Phys. Rev. **B 39** (1989) 10433;
- 11) A. G. Eguiluz, M. Heinrichmeier, A. Fletzar and W. Hanke, Phys. Rev. Lett. **68** (1992) 1359;
- 12) J. J. Deisz, A. G. Eguiluz and W. Hanke, Phys. Rev. Lett. **71** (1993) 2793;
- 13) D. Pines and P. Nozieres, *The Theory of Quantum Liquids*, W.A.Benjamin, Inc. (1966);
- 14) M. Abramowitz and I. A. Stegun (eds.), *Handbook of Mathematical Functions*, Dover Publishing (1965);
- 15) see e.g. N. H. March and S. Lundqvist (eds.), *Theory of Inhomogenous Electron Gas*, Plenum, New York (1983);
- 16) R. M. Ritchie and A. L. Marusak, Surf. Sci. **4** (1966) 294;
- 17) J. D. Jackson, *Classical Electrodynamics*, Wiley (1975);
- 18) W. R. Smythe, *Static and Dynamic Electricity*, 3rd ed., McGraw-Hill (1968), as quoted in P. A. Antoniewicz, G. T. Bennett and J. C. Thompson, J. Chem. Phys. **77**(9) (1982) 4573.

NELOKALNI DINAMIČKI POTENCIJALI UZ ZAKRIVLJENE POVRŠINE

Razmatra se samosuglasna kvantno-mehanička formulacija nelokalnog dinamičkog potencijala uz površinu čvrstine koja se može opisati u koordinatnom sustavu u kojemu je Laplaceova jednačina separabilna. Ta se formulacija primjenjuje za proračun zrcalnog potencijala uz površine jednolike zakrivljenosti, tj. uz planarne, sferne i cilindrične površine. Izračunali smo također dielektričnu funkciju $\epsilon(\omega)$ i disperzijske relacije za površinske modove u tim sustavima.

æ