Effect of a macroscopic field near a crystal boundary on the slow-electron reflection coefficient

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The energy dependence of the reflection coefficient of slow electrons is obtained in the threshold approximation. It is shown that the rate at which the macroscopic potential approaches the vacuum value affects most strongly the energy dependence of the reflection coefficient.

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1. INTRODUCTION

The reflection and transmission coefficients of electrons through the potential barrier at the interface of a solid with vacuum (or some other medium) at energies $\lesssim 1$ eV in vacuum has repeatedly attracted the attention of the theoreticians. One reason is that these coefficients are capable of describing many processes that take place on the interface, such as photoemission, thermionic emission, reflection of slow electrons from surfaces, and others. Another reason is that the experimental methods of research into this field are still far from perfect. The exact solution of problems of this kind is exceedingly complicated because they require knowledge of the details of the potential near the surface, and these data are lacking in most cases. It is therefore not surprising that under these circumstances certain importance is attached to attempts at determining the so-called threshold singularities of the energy dependence so the the transmission coefficient (see Ref. 1 and the citations therein, even if it is necessary to resort for this purpose to substantial simplifying assumption.

The purpose of the present paper is further development of the indicated ideas under assumptions that are less stringent than usual. In particular, an attempt will be made to separate the influences of the long- and short-range forces on the coefficient of the transmission of an electron through the potential barrier at the interface with vacuum.

2. EFFECT OF THE IMAGE-FORCE POTENTIAL ON THE COEFFICIENT OF TRANSMISSION OF AN ELECTRON THROUGH A POTENTIAL BARRIER ON A CRYSTAL–VACUUM INTERFACE

We consider first, by way of example, the normal incidence of slow electrons from a vacuum (or a medium with dielectric constant ε) on a metal boundary. The transmission coefficient obtained in this manner coincides, as is well known, with the coefficient of transimission from a solid to a vacuum in the threshold approximation.

At distances a_0 from the boundary on the order of the interatomic distances at which the micropotential becomes constant and beyond, the behavior of the electron is described by the one-dimensional Schrödinger equation with a long-range image-force potential:

$$\left(\frac{\partial^2}{\partial z^2}+k^2+\frac{2m\alpha}{\hbar^2|z|}\right)\varphi(z)=0, \quad \alpha=\frac{e^2}{4\varepsilon}. \tag{1}$$

The z axis is directed into the interior of the crystal. The wave function φ in the region $z<0$, however, is influenced not only by this macroscopic potential and even not only by the micropotential in the region $|z| \sim a_0$, where it varies most strongly, but also by the micropotential in the interior of the crystal.[2-3] The influence of the last two factors is taken into account, for example, in the theory of LEED (low-energy electron diffraction). We, however, are interested in the low-energy region ($\lesssim 1$ eV), when there are still no diffraction processes.

In its formulation, our problem is closest to that of finding the threshold singularities in the cross section for particle scattering near the threshold of some process, and more specifically to the resonant scattering of charged particles,[4] which is described by using a Schrödinger equation with a long-range potential, while the short-range potential is accounted for via the boundary condition. It is precisely these properties which determine the constant $\varkappa$, to which the logarithmic derivative of the solution at zero is equated. The reason why this derivative is constant is that a low energy real or virtual level is present in the spectrum of the micropotential, and this is why the scattering is called resonant. Thus, the separation of the threshold singularies imposes in this case rather stringent requirements on the micropotential.

We shall attempt to divide the problem into two stages and consider separately the effect of the long-range forces, as is done in the theory of scattering of charged particles, describing in this case the micropotential by a certain reflection coefficient that must be found by solving an analogous problem, but now without the macroscopic potential. We choose a distance $|z_1| \sim a_0$ at which the three-dimensional character of the potential and of the wave function can be neglected. Since the micropotential becomes one-dimensional precisely at lengths $\sim a_0$, this can always be done. We now divide the macropotential into two smooth parts, V_1+V_2, such that one of them differs negligibly little at $|z| \geqslant |z_1|$ from the image-force potential, and at $|z|<|z_1|$ it becomes constant at distances much smaller than a_0 from z_1; we then solve the problem with the new macropotential V_1, and relegate V_2 to the micropotential. Since the potential energy of the

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electron is perfectly finite at $z=z_1$, namely $\sim\alpha/a_0$, this subdivision can always be so effected that the wave functions of the threshold electrons are hardly changed.

The described artifice allows us, first, to match the wave functions in the one-dimensionality region and, second, describe this matching with the aid of one parameter. In fact, since the wave function is one-dimensional at $z\sim z_1$, it should take the form

$$\varphi\approx u_1+Ru_2, \tag{2}$$

where u_1 and u_2 are the incident and reflected waves, normalized to unity flux, for the problem with $V_1=0$, and R is the reflection coefficient. By virtue of the formulation of the problem, there is no second linearly independent solution, since it corresponds to a wave indident on the surface from the inside. The proposed breakdown is convenient because in the notation (2) the logarithmic derivative, which is needed for the matching of the wave functions at $z=z_1$, is simple in form and is described by a single parameter R, that depends now only on the new micropotential and is, generally speaking a function of the energy (and not a constant).

The boundary condition can thus be represented in the form

$$\frac{\varphi'}{\varphi}\Big|_{z=z_1}=ik_1\frac{1-R}{1+R},\quad \frac{\hbar^2k_1^2}{2m}=\frac{\hbar^2k^2}{2m}+\frac{\alpha}{|z_1|}, \tag{3}$$

where k is the wave vector of the electron in vacuum.

The problem has now been reduced to a solution of Eq. (1) with the boundary condition (3). The procedure here is fully analogous to that described in the book by Landau and Lifshitz,[4] We therefore note here only that since the matching of (3) is carried out here at $z\neq 0$, and the behavior at zero is of no importance at all, we need a general solution of (1), which includes also the one with the singularity at zero. Further, the solution in Ref. 4 was obtained for the case

$$ka_0\ll 1, \tag{4}$$

$$a_0/a_c\ll 1,\quad a_c=\hbar^2/m\alpha \tag{4'}$$

for a repulsion-force potential. In analogy with Ref. 4, we can obtain for the case of attraction forces the following equation for the reflection coefficient $|r|^2$ (r is the amplitude of the reflection coefficient)

$$\begin{aligned} &i\frac{1-r}{1+r}=\frac{1}{\pi}\left(1-\exp\left[\frac{-2\pi}{ka_c}\right]\right)\left[h(ka_c)+\frac{\varkappa a_c}{2}\right],\\ &\varkappa=-ik_1\frac{R-1}{R+1}+\frac{2\ln(2|z_1|/a_c)+4\gamma}{a_c},\\ &h(k)=\frac{1}{k^2}\sum_{n=1}^{\infty}\frac{1}{n(n^2+k^{-2})}-\gamma+\ln k,\\ &h(k)\approx k^2/12,\quad k\ll 1;\quad h(k)\approx-\gamma+\ln k+1.2/k^2,\quad k\gg 1, \end{aligned} \tag{5}$$

$\gamma=0.577\ldots$ is the Euler constant.

The transition to the case $\alpha=0$, when there is no image-force potential, leads naturally to a solution $r=R(k)$ that does not contain the characteristics of the macropotential. A similar expression for r is obtained also in the case of large k:

$$ka_c\gg 1,\quad k\gg(2\alpha m/\hbar^2|z_1|)^{1/2}=k_0. \tag{6}$$

It should also be noted that, in contrast to the theory of particle scattering, r in (5) depends significantly on the difference $1-|R|$. In particular, if $\varkappa$ is real, as in Ref. 4, then $|r|=1$ and there is no energy dependence. It is easy to show that for $\varkappa$ to be complex it is necessary and sufficient to satisfy the inequality $|R|\neq 1$. The transmission coefficient is then $\sim 1-|R|$ and can be small if $|R|$ is close to 1. We note that this is a perfectly realistic case[5] and can be observed in semiconductors, where the electron effective mass differs strongly from the mass of the free electron.

In the opposite limiting case, $ka_c\ll 1$, there is no explicit dependence on k in (5), and if $R(k)$ is constant in the threshold region, then r is independent of energy, although it can be quite small. Finally, in the intermediate case, if realized at all,

$$k_0\gg k\gg 1/a_c, \tag{7}$$

it can be shown that $1-|r|^2\sim k/k_1$ if $1-|R|$ is not too small.

Next, in contrast to Ref. 4, the inequality (4′), which greatly simplifies the calculations and is valid at $\varepsilon\gg 1$, may not hold at $\varepsilon=1$, i.e., for emission into vacuum. In this case the calculations become much more complicated and (5) assumes in the threshold approximation (i.e., at $ka_c\ll 1$, $|z_1|\sim a_c$) the form

$$\begin{aligned} &ik_1a_c\frac{1-R}{1+R}=\frac{\Phi'}{\Phi},\quad \Phi\cong\frac{2\pi\rho_0J_1(2(2\rho_0)^{1/2})}{(2\rho_0)^{1/2}}i\frac{1-r}{1+r}\\ &\qquad-(2\rho_0)^{1/2}\pi Y_1(2(2\rho_0)^{1/2}),\quad \rho_0=|z_1|/a_c, \end{aligned} \tag{8}$$

where J_1 and Y_1 are Bessel functions of the first and second kind.[6] The dependence of r on ρ_0 thus becomes more substantial.

3. CASE OF ZERO MACROPOTENTIAL

The formal artifice employed above, of breaking up the macropotential into two parts, cannot be used if the macroscopic part of the potential does not exist at all. This can occur when the crystal is in contact with a sufficiently well conducting medium, say an electrolyte. In this situation the wave functions will be matched in the region $z\sim a_0$, where the three-dimensional character of the potential cannot be neglected, and this makes the calculations much more difficult. For a qualitative description of the energy dependence of the transition coefficient we can nevertheless use the general assumption that the reflection-coefficient amplitude is analytic in the energy, in analogy with the assumption usually made in the theory of scattering near the threshold of a reaction.[4] It is then convenient to consider the incidence of an electron on a surface from the interior of the crystal. We consider the structure of the wave function that describes reflection of an electron from the surface at near-threshold energies. Near the threshold, where the potential is still large enough to be able to neglect in the Schrödinger equation (in the threshold approximation) the dependence of the function on the energy (reckoned from the vacuum level), the sought wave function can be represented in the form

$$\varphi=\alpha_1\varphi_1+\alpha_2\varphi_2, \tag{9}$$

where φ_1 and φ_2 are two aribtrary linearly independent solutions (in accord with the formulation of the problem) that have no singularities whatever at $k=0$. On the other hand the coefficients α_1 and α_2 have a strong dependence on k near the threshold. At large distances from the surface the wave function should have the form of an incident (u_1) and reflected (ru_2) wave near the crystal and of a transmitted (or damped) wave (u_3). At distances $|z| \sim a_0$ from the surface these functions should match the function (9) on certain, generally speaking nonplanar surfaces (since the potential is three-dimensional).

The values of the function (9) or of its derivatives are thus the boundary conditions for the corresponding Dirichlet boundary-value problems of the Helmholtz equation, to which the Schrödinger equation in vacuum is equivalent[7]: the envelopes of the wave functions inside the crystal can be similarly treated. The asymptotic expressions for the solutions of the indicated boundary-value problems, as is well known, depend linearly on α_1 and α_2. It is this circumstance which makes it possible to express α_1, α_2, and r in terms of the logarithmic derivative of the asymptotics, in analogy with the procedure in particle-scattering theory[4]:

$$\frac{\alpha_1 a_1' + \alpha_2 a_2'}{\alpha_1 a_1 + \alpha_2 a_2} = \frac{(u_1 + r u_2)'}{u_1 + r u_2}\Big|_{z=z_2}, \qquad \frac{\alpha_1 b_1' + \alpha_2 b_2'}{\alpha_1 b_1 + \alpha_2 b_2} = \frac{u_3'}{u_3}\Big|_{z=z_2} = \lambda, \tag{10}$$

where u_1 and u_2 are the envelopes of the wave functions corresponding to the incident and reflected wave; a_1, a_1', b_1, b_1', . . . are quantities calculated from the functions φ_1 and φ_2 (functionals of φ_1 and φ_2), while z_1 and z_2 should be located in the one-dimensionality regions. The choice of z_2 depends on the change, of no importance here, of the phase of r.

It must be noted, however, that the matching surface and hence the values of the wave functions and of their wave derivatives on it may generally speaking depend on the wave vector. To separate the threshold singularities we must therefore make one more assumption, that this dependence is not critical in the threshold approximation at least for a certain range of sufficiently small but finite k, and it is for these that the sought formula will be obtained.

We have thus two equations for the two unknowns α_1/α_2 and r, and among the coefficients in (10) only one quantity depends in practice on k, namely the logarithmic derivative of the transmitted wave u_3, which is designated λ in (10). Since we should have $|r|^2 = 1$ below the threshold, it is clear that the form of $r(\lambda)$ should be ($\lambda = -|k|$ is real below the threshold)

$$r(\lambda) = \frac{1+\beta\lambda}{1+\beta^*\lambda} e^{i\eta}, \tag{11}$$

where η is a real constant and ρ a complex one. We easily find from (11) that above the threshold, when $\lambda = ik$, the transmission coefficient is

$$D = \text{const} \cdot k. \tag{12}$$

The expression (12) is arrived at for a rather large class of one-dimensional potentials that tend rapidly enough (faster than $|z|^{-2}$) to the vacuum value, including potentials with abrupt breaks, such as steps.[4] Equation (12) should also be realized in numerical calculations within the framework of the jellium model or in the egg-shaped-potential approximation, usually employed in LEED studies, when it is usually specified that the potential is one-dimensional or a nearly one-dimensional near the boundary and tends rapidly enough to a maximum value. The description of the numerical-calculation methods is the subject of an extensive literature (see, e.g., Refs. 2 and 3) and we shall not dwell here on this question. We note only that expressions of type (12) [but not (5)] will appear also in those cases when a macropotential is present but tends to a constant value rapidly enough (faster than $|z|^{-2}$), for example as a result of screening effects. This can be demonstrated by reasoning and derivations similar to those used in the derivation of Eq. (5).

Investigation of oblique incidence of the electrons on a crystal surface in the threshold approximation reduces to the following. It must only be borne in mind that k now means the normal component of the momentum and not the total momentum, and that R depends not only on k but also on the parallel component.

4. CONCLUSION

Thus, the energy dependence of the transmission coefficient D of an electron through a potential barrier on the crystal boundary near the threshold is very strongly influenced by the rate at which the macroscopic part of the potential in the vacuum (or in some medium) tends to a constant value. If this potential varies rapidly enough, D tends to zero [see Eq. (12)] near the threshold, and in the case of the image-force potential, which decreases slowly, the coefficient tends to a constant. Intermediate cases are of course also possible.

The foregoing analysis holds for attracting and uniform potentials. If these conditions are not satisfied (particularly the latter), the investigation becomes much more complicated (see Ref. 8).

It is known that a change of $D(k)$ brings about a change of the corresponding equations that describe processes connected with emission of electrons from a crystal, for example formulas, for the thermionic or photoemission.[1] In particular, a change from (5) to (12) corresponds to violation of the known Fowler's law for the dependence of the photocurrent on the emission frequency near the threshold.

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