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Comparison of image-potential theories

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We study a simple model which contains the basic physics of the image-potential problem but which allows a nearly exact solution. The predictions of this numerical solution are compared to those of various approximate theories that have been recently proposed. We find no support for the suggested anomalies; conventional image-potential theory appears to be adequate.

I. INTRODUCTION

In the last few years reports of several experiments have appeared[1–3] which probe the close-range interaction between an electron and a metal surface and whose interpretation seems to challenge the conventional view. Instead of supporting an attractive-image-potential energy of $V_I = -e^2/4x$ where x is the distance from the metal and V_I is to saturate at the inner potential, one claims evidence for an early saturation of V_I,[1] or an oscillation in time of V_I as an electron leaves,[4] or a suppression of V_I if the exiting electron is tunneling.[2] Although the main motivation for the suggestion of these anomalies is the desire to fit experimental data, there is also some theoretical support in each case. However, since the suggestions are rather diverse and not clearly consistent with each other, the theoretical situation is similarly confusing.[5]

In this paper we examine within the context of a single model the implications of various theoretical approaches. Our model has been purposely idealized and simplified so that its content is tractable and transparent. Although it is consequently too crude to allow direct comparisons with experiments, it does contain the key physics thought to be relevant. By extracting its predictions according to various theoretical prescriptions, we can learn which approximation schemes are valid for it and hopefully also for more realistic systems.

In Sec. II we describe the model and the calculations we have done. We find no support for any theoretical anomalies.[2,4] In Sec. III we discuss to what extent our conclusions may carry over to more complex systems.

II. MODEL CALCULATIONS

The basic problem we analyze is the transmission of an electron past a barrier that presents both static and dynamic potential energies. The latter aspect is due to the transient polarization of the other electrons in a metal by an exiting electron. It is often idealized to a coupling between the one electron and the metal's surface and bulk plasmon fields. We further simplify the situation by working in one dimension and by allowing only one polarizable mode to be present.

The many-body Hamiltonian which we study is

$$H = \frac{p^2}{2m} + V(x) + \hbar\omega(a^\dagger a) + \lambda(x)(a + a^\dagger) , \tag{1}$$

where p and m are the electron's momentum and mass, ω is the frequency of the polarizable mode, and $a^\dagger(a)$ is the creation (annihilation) operator for this harmonic mode. The static potential energy felt by the electron is $V(x)$ and is presumed to be nonzero only close to $x=0$. The coupling, $\lambda(x)$, of the electron to the polarizable mode is also localized near $x=0$.

If the electron were held stationary, the effective potential energy would be given by the adiabatic dependence

$$V_a(x) = V(x) - \lambda^2(x)/\hbar\omega , \tag{2}$$

which is found by completing the square for the part of H that involves the polarizable mode. Thus the analog of the conventional image potential for our model is $-\lambda^2(x)/\hbar\omega$. The recent theoretical suggestions all concern possible modifications to this result. The concept of an effective potential energy, however, is not unambiguous since the electron's quantum-mechanical motion is only properly described via a nonlocal self-energy. We hence do not compare various theories in terms solely of what "image potential" they predict, but in addition calculate the transmission coefficient T for an electron to pass through the barrier region. For simplicity, the incident electron energy E is kept less than $\hbar\omega$ and the mode is initially in its unperturbed ground state so that only virtual excitations of the mode are possible and $T(E)$ is the elastic transmission coefficient of the electron.

A general solution of Schrödinger's equation for the Hamiltonian of (1) may be expanded as

$$\langle x \mid \Psi \rangle = \sum_n \phi_n(x) \mid n \rangle , \tag{3}$$

where the $\mid n \rangle$ are normalized eigenstates of $a^\dagger a$. The ϕ_n's are determined by the set of coupled equations:

$$\left[\frac{p^2}{2m} + V - E\right]\phi_0 + \lambda\phi_1 = 0 , \tag{4a}$$

$$\lambda\phi_0 + \left[\frac{p^2}{2m} + V + \hbar\omega - E\right]\phi_1 + \sqrt{2}\lambda\phi_2 = 0 , \tag{4b}$$

$$\sqrt{2}\lambda\phi_1 + \left[\frac{p^2}{2m} + V + 2\hbar\omega - E\right]\phi_2 + \sqrt{3}\lambda\phi_3 = 0 , \tag{4c}$$

and so on. We shall work in a weak coupling limit, which bounds the extent of virtual excitation of the polarization mode. Specifically we truncate the set (4) by requiring

$$\phi_n(x) \equiv 0 \quad \text{for } n \geq m . \tag{5}$$

We have studied the cases $m=2,3$ and comment below on their difference and on the justification of (5).

Finally, in order to find a simple, exact solution of the truncated set (4), we assume that both $V(x)$ and $\lambda(x)$ are piecewise constant. Then in each region of constant V and λ, the functions $\phi_n(x)$ can all be expanded in terms of plane waves, $e^{\pm ikx}$, where the numbers of distinct k's is m. For example, when $m=2$, one has

$$\langle x \mid \Psi \rangle = \sum_k \sum_{n=0}^{1} \alpha_n^k e^{ikx} \mid n \rangle \;, \tag{6}$$

with $k=\pm k_1, \pm k_2$ determined by

$$\left[\frac{\hbar^2 k^2}{2m}+V-E\right]\left[\frac{\hbar^2 k^2}{2m}+V+\hbar\omega-E\right]-\lambda^2=0 \;, \tag{7}$$

and four of the eight α_n^k's obtained from

$$\left[\frac{\hbar^2 k^2}{2m}+V-E\right]\alpha_0^k+\lambda\alpha_1^k=0 \;. \tag{8}$$

Solutions of the form (6) are matched at each discontinuity of V and λ by requiring continuity of value and slope separately for the coefficients of $\mid 0 \rangle$ and $\mid 1 \rangle$. Outside the interaction zone, i.e., when $V=0=\lambda$, only outgoing waves are retained except for the incident wave

$$\exp[i(2mE)^{1/2}x/\hbar] \mid 0 \rangle$$

coming from $x=-\infty$. Of course T is the absolute square of the amplitude of this same wave as $x \to +\infty$.

A. Single-bump case

As a first example we show in Fig. 1 results for $T(E)$ when the barrier is a single rectangular bump. Both V and λ are finite only for $0 \le x \le L_1$. We have chosen $L_1=4$ Å, $V_1=10$ eV, $\lambda_1=7$ eV, and $\hbar\omega=20$ eV. In addition to the weak coupling solutions outlined above, we have plotted the predictions of more approximate treatments. All of these use an effective Hamiltonian that no longer contains the polarizable mode:

$$H_{\text{eff}}=\frac{p^2}{2m}+V(x)+V_I(x) \;. \tag{9}$$

The new term $V_I(x)$, which is the analog of the image potential, is supposed to represent in an averaged sense the effect of the dynamic coupling in (1). The three possibilities illustrated either ignore $V_I(x)$, or use the adiabatic form $-\lambda^2(x)/\hbar\omega$ or self-consistently require

$$V_I(x)=[-\lambda^2(x)/\hbar\omega]T(E) \;.$$

This last form was proposed by the IBM group.[2]

The close similarity of the weak coupling solutions for $m=2,3$ to each other suggest that $\lambda/\hbar\omega$ is sufficiently small to justify the truncation of (4). We have found that differences between them scale roughly as $(\lambda/\hbar\omega)^2$ and do not become major until $\lambda > \hbar\omega/2$. Hence the weak coupling predictions for the parameter choices of Fig. 1 should be close to the exact solution of (1).

Next, note that these results agree quite well with those obtained from (9) using the conventional adiabatic image potential for V_I: $-\lambda^2(x)/\hbar\omega$. The two alternate choices of V_I give noticeably different results for T. In particular,

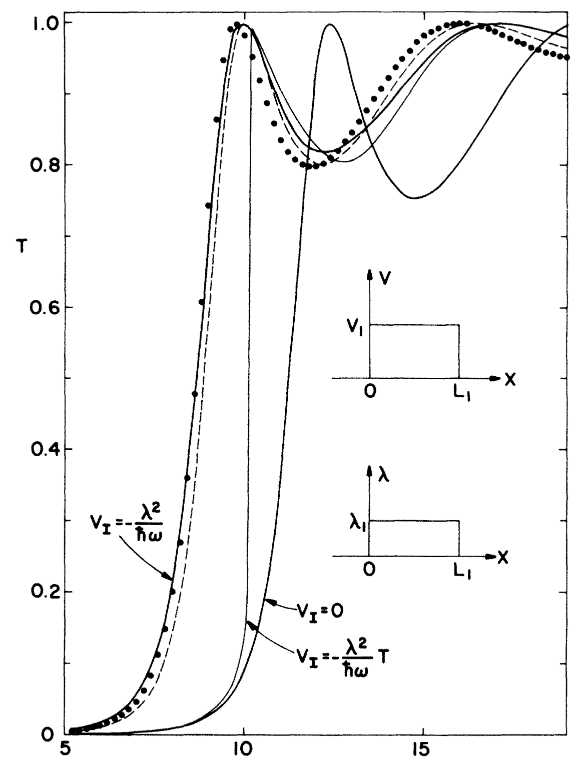

FIG. 1. Transmission coefficient T vs incident electron energy E. The shape of the barrier parameters are shown in the insets. See text for numerical values of the parameters. The approximate image potentials used for three of the curves are noted. The remaining two results were found using the weak coupling solutions of the full Hamiltonian with $m=2$ (dashed curve) or $m=3$ (dots).

it is precisely where the choice of the IBM group differs from the conventional one; i.e., where the electron is tunneling and $T \ll 1$, that their predictions disagree significantly with the nearly-exact weak coupling solutions. This defect in their theory was pointed out earlier by Johnson,[6] who studied a more general model via Green's-function techniques, and our numerical results substantiate his conclusions. Indeed, applying his methods to our model does yield $V_I=-\lambda^2/\hbar\omega$ except close to the discontinuities of V and λ.

It is difficult to give a precise reason why the choice of V_I proposed by the IBM group is wrong. The explicit formula results from approximating a nonlocal interaction, which itself is obtained from a variational estimate of a bound-state energy.[7] Too many uncontrolled approximations are involved in their theory to make an *a priori* assessment. We can only point to Fig. 1 to show that the prescription cannot be correct in general.

B. Double-bump case

We now change the barrier shape into two rectangular bumps in an effort to allow the dynamics of the polarizable mode to become (possibly) visible in T. The argument we are trying to test was first proposed in the context of photostimulated field emission[4,8] in order to explain the experimental observations of rapid oscillations in electron yield with applied, static field. Roughly speaking, it says that the sudden departure of an electron through a metal surface leaves the surface plasmons not in a state of adiabatic polarization, but instead in a state of oscillation. This should lead in turn to an oscillatory image potential and oscillations in T vs E.

To exhibit these implications one uses an image-potential theory based on the trajectory approximation.[9–12] The electron is treated as a point charge following a prescribed path and the resulting time-dependent perturbation on the polarizable modes of the system leads to an induced potential energy. For instance, following the prescription of Echenique *et al.*,[12] we obtain for our model with a single bump (Fig. 1),

$$V_I(x) = -\frac{\lambda_1^2}{\hbar\omega}\left[1-\cos\frac{\omega x}{v}\right], \tag{10}$$

when $0<x<L_1$. Here we have assumed that the electron has moved at a fixed speed v from $-\infty$ to x. Note that this image potential starts from zero at $x=0$ and never settles down to the adiabatic value $-\lambda_1^2/\hbar\omega$. Still, from the viewpoint of classical mechanics an electron subject to (9) with (10) for V_I would have $T=1$ for $E>V_1$ and $T=0$ for $E\le V_1$. However, if we force the electron to encounter a second, higher static barrier V_2 at $x=L_1$, as shown in Fig. 2, then its transmission coefficient might show an oscillatory variation determined by $\cos(\omega L_1/v)$. This rough argument, which can be refined to some extent,[4,13] thus leads one to expect oscillations in T vs E

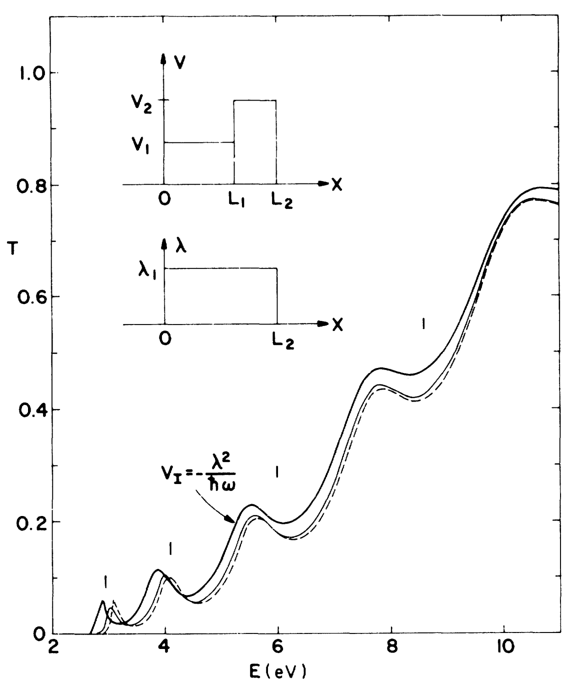

FIG. 2. Transmission coefficient T vs incident electron energy E. The shape of the barrier parameters are shown in the insets; the electron is incident from the left. See text for numerical values of the parameters. The solid curve was computed from (9) using the conventional image potential. The other two curves were found from the weak coupling solution of (1) with $m=2$ and $\lambda^2/\hbar\omega$ held fixed. They differ in the choice of λ and ω: $\hbar\omega=20$ eV, dashed curve, and $\hbar\omega=30$ eV, thin line.

whose period will depend on ω, the frequency of the polarization mode.

In Fig. 2 we show $T(E)$ for a double-step model of $V(x)$. Only the weak coupling solution for $m=2$ is shown. The parameters used are $L_1=10$ Å, $L_2=12$ Å, $V_1=5$ eV, $V_2=10$ eV, $\lambda_1^2/\hbar\omega=2.45$ eV, and $\hbar\omega=20$ or 30 eV. There are definitely oscillations in T over the range of E shown. However, their period depends negligibly on ω and the weak coupling curves seem to again mimic the result found from the conventional image potential. We interpret the oscillations as due to standing waves of the electron momentarily trapped by the potential in the region $0<x<L_1$. Indeed the ticks in Fig. 2 show where L_1 is an integer multiple of one-half the wavelength of an electron with kinetic energy $E-V_1+\lambda_1^2/\hbar\omega$. A similar interpretation may be applied to the oscillations in Fig. 1.

Thus the rough argument sketched above[4] is apparently wrong, although a specific *a priori* reason for this is not obvious. Some work has been done on refining its details[8,13] but this has not changed its basic prediction about the ω dependence of the oscillations in T. We feel that a crucial assumption is the classical localization of an electron to a fixed trajectory, even if the latter may be self-consistently determined.[13] Within a quantum-mechanical description, the electron cannot be precisely located while it is in the barrier region. Hence for the two-step model of Fig. 2, there is no clear relevance of the comparison of the polarization mode's period with classical transit times across L_1. Another worrisome point is the neglect of recoil implicit in the trajectory approximation. This defect is unfortunately most important as $v\to 0$, which is just where the new argument's predictions are most striking.

III. DISCUSSION

So far we have criticized the modified theories of the image potential only within the context of our idealized model. We have suggested reasons why they are deficient but the strongest argument against them has been their explicit disagreement with the weak coupling solutions. When we now turn to more realistic models we lose this argument since we no longer have nearly exact results with which to compare. Thus it is more difficult to draw firm conclusions.

One way to lessen this problem is to use Green's-function techniques to make a better treatment appear to be essentially the same as our simple model. For instance we can recast the set (4) truncated at $m=2$ as

$$\phi_0(x)=\phi_0^0(x)+\int dx' G_0(x,x')\lambda(x')\phi_1(x'), \tag{11a}$$

$$\phi_1(x')=\int dx'' G_1(x',x'')\lambda(x'')\phi_0(x''), \tag{11b}$$

where

$$G_n(x,x')=\left\langle x\left|\left[E-\frac{p^2}{2m}-V-n\hbar\omega+i0^+\right]^{-1}\right|x'\right\rangle \tag{12}$$

are single-particle Green's functions and

$$\phi_0^0(x)=\exp[i(2mE)^{1/2}x/\hbar]$$

is the appropriate choice for a transmission problem. Alternatively one can introduce a self-energy via

$$\phi_0(x)=\phi_0^0(x)+\int dx'\int dx''G_0(x,x')\Sigma(x',x'')\phi_0(x'') , \tag{13}$$

where

$$\Sigma(x,x')=\lambda(x)G_1(x,x')\lambda(x') . \tag{14}$$

Now consider a three-dimensional model wherein the static potential V has translational invariance parallel to the surface and the polarization coupling is to a continuum of surface plasmons, labeled by the two-dimensional wave vectors $\underline{Q}$. If an electron whose wave vector parallel to the surface is $\underline{K}$ is incident on such a barrier its (approximate) elastic wave function may be written as

$$\Phi_0(\vec{x})=\phi_0(x,\underline{K})e^{i\underline{K}\cdot\underline{X}} , \tag{15}$$

where the three-dimensional vector $\vec{x}=(x,\underline{X})$, with x ($\underline{X}$) normal (parallel) to the surface. The equation for $\phi_0(x,\underline{K})$ is

$$\phi_0(x,\underline{K})=\phi_0^0(x,\underline{K})+\int dx\int dx'G_0(x,x';\underline{K})\times\Sigma(x',x'';\underline{K})\phi_0(x'',\underline{K}) , \tag{16}$$

where $\phi_0^0(x,\underline{K})=\exp[i(2mE-\hbar^2K^2)^{1/2}x/\hbar]$ and

$$\Sigma(x,x';\underline{K})=\sum_{\underline{Q}}\lambda(x,-\underline{Q})G_1(x,x';\underline{K}+\underline{Q})\lambda(x',\underline{Q}) , \tag{17}$$

with

$$G_n(x,x';\underline{K})=\left\langle x\left|\left[E-\frac{p^2}{2m}-\frac{\hbar^2K^2}{2m}-V-n\hbar\omega+i0^+\right]^{-1}\right|x'\right\rangle . \tag{18}$$

The function ϕ_0 determines the elastic scattering amplitude and we have used a weak coupling form for Σ, allowing only one surface plasmon to be (virtually) excited at a time by the coupling $\lambda(x,\underline{Q})$, which is proportional to $e^{-Q|x|}$.

We do not wish to push the analysis of these equations further since they are essentially the set studied by Jonson.[6] Instead we emphasize the similarity between (13), (14), and (12) on the one hand and (16), (17), and (18) on the other. Our numerical results and conclusions apply to the former set, while a fairly realistic model description is possible with the latter. The two sets are quite similar in structure and give us confidence that the qualitative aspects of our one-dimensional results would again be found in a three-dimensional calculation.

One should note, however, that we have not described a completely realistic model[14]: V depends only on x, both bulk plasmon and electron-hole pair coupling are ignored, only weak coupling solutions are considered, etc. Yet we have made contact with the models that were used in the recent theories that suggest anomalies in the image potential.[2,4] Perhaps the reason for the discrepancies[1-3] between experiment and conventional theory, which our calculations support, lies in these further omissions.

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