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Dynamical effects in electron tunneling: Self-consistent semiclassical image potentials

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The problem of dynamical screening and local potentials for electrons tunneling in the metal-insulator-metal system is treated in the self-consistent GW approximation. The self-energy is evaluated for electron coupling to the long-wavelength charge-density oscillations. The analytic results for dynamical image potentials, obtained in the semiclassical (local) limit, contain explicitly the competing influences of screening dynamics, tunneling electron energy, and recoil. The role of dynamical image potentials on the tunneling rates for thin barriers is discussed.

INTRODUCTION

Recent experimental advances in the measurement of tunneling through well-characterized barriers, and the observation[1] of possible dynamical effects for tunneling times comparable to the plasmon, i.e., screening times have again emphasized the need for a theoretical description of effective barriers seen by the tunneling electrons, that would take into account the dynamics of the charge fluctuations and their coupling to the tunneling electrons.

Very early, indications of deviations from the classical image potential were observed experimentally, and several attempts were made to find semiempirical corrections.[2] More recently it was realized that the origin of image potential is in the electron interaction with polarization modes in the solid, in particular, surface (or interface) plasmons[3,4] which also led to the semiclassical formulation of the dynamical image potential for uniformly moving particles.[5-8] Application of this surface-plasmon model to electron tunneling was attempted by several authors,[9-15] for various experimental situations and trying to explain different physical phenomena. Two papers[9,15] are especially relevant for the present work; Jonson[9] formulated the image potential in terms of a nonlocal self-energy which he approximately calculated for dispersionless surface plasmons (SP) in a barrier outside the semiinfinite metal. Persson and Baratoff[15] calculated the tunneling rates directly, without discussing the image potentials and barrier shapes. Though this is probably justified, because the role of fluctuating potentials in tunneling cannot be fully represented by their (static) averages, we feel that it should be very useful to calculate and discuss the shapes of the tunneling barriers for different dynamical parameters. Moreover, this is the correct extension of the "dynamical image potential" concept[5-8] developed for uniformly moving free particles to the tunneling electrons.

FORMULATION OF THE PROBLEM

Following the formulation of Jonson,[9] we define the image potential for tunneling electrons in terms of the nonlocal energy-dependent self-energy, in the self-consistent GW approximation,[16] i.e., neglecting vertex corrections in the electron coupling to the charge fluctuations in the metal-insulator-metal system.

In the long-wavelength limit, applicable in this situation several Å away from the boundaries of the external static barrier $V_0(z)$, this reduces to the interaction with two interface plasmons.[3,4]

For planar barriers $V_0 \equiv V_0(z)$, using the parallel ($\boldsymbol{\rho}$) translational invariance, the wave function is

$$\psi(r) \simeq e^{i\mathbf{k}\cdot\rho}\phi_{\mathbf{k}}(z) , \tag{1}$$

where $\mathbf{k}$ is the parallel electron momentum. The electronic wave functions $\phi_{\mathbf{k}}$ are solutions of the self-consistent equation

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}+V_0(z)+\frac{\hbar^2k^2}{2m^*}-E\right]\phi_{\mathbf{k}}(z) + \int dz'\Sigma_{\mathbf{k}}(z,z';E)\phi_{\mathbf{k}}(z')=0 \tag{2}$$

with the self-energy arising from the electron-SP interaction in the GW approximation.

$$\Sigma_{\mathbf{k}}(z,z';E)=\int d\mathbf{Q}\int d\omega G_{\mathbf{k}-\mathbf{Q}}(z,z';E-\hbar\omega)W_{\mathbf{Q}}(z,z';\omega) . \tag{3}$$

As the problem is essentially nonlocal, it is convenient to introduce an effective induced local potential

$$V_{\mathbf{k}}(z,E)=\int dz'\Sigma_{\mathbf{k}}(z,z';E)\phi_{\mathbf{k}}(z')/\phi_{\mathbf{k}}(z) \tag{4}$$

which has to be evaluated self-consistently from the equation

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}+V_{\text{eff}}(\mathbf{k},z,E)-\left[E-\frac{\hbar^2k^2}{2m^*}\right]\right]\phi_{\mathbf{k}}(z)=0 . \tag{5}$$

The total effective potential

$$V_{\text{eff}}(\mathbf{k},z;E)=V_0(z)+V_{\mathbf{k}}(z,E) \tag{6}$$

contains the external static potential barrier $V_0(z)$ and the self-consistent induced potential $V_{\mathbf{k}}$.

In the surface-plasmon-pole approximation for W the self-energy (3) becomes

$$\Sigma_{\mathbf{k}}(z,z';E)=\sum_p \int d\mathbf{Q}\,\Gamma_i^*(z)G_{\mathbf{k}-\mathbf{Q}}(z,z';E-\hbar\omega_i)\Gamma_i(z')\ , \tag{7}$$

where $p=\pm$ denotes the parity, $i\equiv(p,Q)$, ω_i are the surface mode frequencies for wave vectors Q

$$\omega_i\equiv\omega_{pQ}=\frac{\omega_p}{\sqrt{2}}(1+pe^{-2aQ})^{1/2}\ , \tag{8}$$

and Γ's are the coupling matrix elements, which, inside the planar barrier of width $2a$, have the form[18,4,8]

$$\Gamma_i(z)=\left[\frac{e^2\hbar\omega_p^2}{4\pi Q\omega_i}\right]^{1/2} g_i(z)\ ,$$
$$g_i(z)=e^{-Qa}\frac{1}{2}(e^{Qz}+pe^{-Qz})\ . \tag{9}$$

In (8) and (9) ω_p is the frequency of bulk charge-density oscillations in the metal electrodes, which, in principle, need not be simple plasmons. For simplicity we have neglected the high-frequency screening and taken $\varepsilon_\infty=1$ everywhere.

We shall here notice that the attenuation constant corresponding to the Green's function in the self-energy (7),

$$q(z)=\left[\frac{2m^*}{h^2}[V_{\mathrm{eff}}(\mathbf{k},z;E)-E+\hbar\omega_i+\Delta E_{\mathbf{k}}(Q)]\right]^{1/2}\ , \tag{10}$$

where

$$\Delta E_{\mathbf{k}}(\mathbf{Q})=\hbar^2(Q^2+2\mathbf{k}\cdot\mathbf{Q})/2m^*\equiv\hbar\mathbf{v}_\parallel\cdot\mathbf{Q}+\frac{h^2Q^2}{2m^*} \tag{11}$$

is large, and therefore make a semiclassical (local) approximation

$$\lim_{q\to\infty} G(z,z';\hbar^2q^2/2m^*)=-\frac{2m^*}{h^2q^2}\delta(z-z')\ . \tag{12}$$

This amounts to averaging (3) over z' on a scale $1/q$. In this way, by contracting $z'=z$ in the self-energy (7), we have reduced our result to the semiclassical approximation, earlier used in the formulation of the dynamical image potential for free particles.

Inserting these expressions and (9) into (7) and (4) leads to the result for the energy-dependent-induced (exchange-correlation) potential in the region $-a\le z\le a$:

$$V_{\mathbf{k}}(z,E)=-\frac{e^2}{2}\hbar\omega_p^2\sum_p\int dQ\int\frac{d\phi}{2\pi}\frac{1}{2\omega_i}\frac{|g_i(z)|^2}{\hbar\omega_i+\varepsilon_{\mathbf{k}}(z,E)+\Delta E_{\mathbf{k}}(Q)}\ , \tag{13}$$

where ε is

$$\varepsilon_{\mathbf{k}}(z,E)=V_{\mathrm{eff}}(\mathbf{k},z,E)-E\ . \tag{14}$$

DISCUSSION

Equation (13) is the semiclassical or local expression for the dynamical image potential for tunneling electrons. It can be generalized to any tunneling geometry and potential $V_0(z)$ by changing the coupling functions Γ_i and SP frequencies ω_i.

The character of the dynamical corrections is shown explicitly in the denominator of (13). The first term defines the dynamics of the screening mechanism. The second term can be written in terms of the local energy-dependent attenuation parameter $k(z)$, given by

$$\kappa(z)=\left[\frac{2m^*}{h^2}\varepsilon_{\mathbf{k}}(z,E)\right]^{1/2} \tag{15}$$

and is thus related to the local electron attenuation. The third term $\Delta E_{\mathbf{k}}(\mathbf{Q})$ contains the influence of parallel electron motion. ($\mathbf{v}_\parallel$) and the recoil term.[5–8] It is obvious that κ here does not enter as the "tunneling velocity" but plays a role of the spatial attenuation parameter. (In terms of the path integral formulation this means that the motion of a tunneling particle is not obtained from the real particle motion by going to an imaginary trajectory but to imaginary time.)

We can remember that in the case of an electron moving freely with the normal velocity $v_\perp$ the corresponding term was

$$\mathbf{v}_\parallel\cdot\mathbf{Q}+iQv_\perp\ , \tag{16}$$

i.e., the normal velocity was also coupled to the SP momentum. Instead, κ in (13) should be considered as a spatial attenuation parameter, leading to the time-decay constant $\tau_d=h/\varepsilon(z)$. In this way the dynamics in (13) enters via the ratio $\eta=\tau_s/\tau_d$ of the two characteristic times, τ_s and τ_d, where τ_d depends on the local decay of the tunneling electron. We notice that this η differs from the ratio τ_s/τ_t, sometimes used[1,9,15] to discuss the dynamical corrections to the image potential in tunneling.[17]

In the following we shall study the $\mathbf{k}=0$ case, which is simpler, but contains all essential physics. In this case the potential (13) depends on two ratios: $\eta(z)=\varepsilon(z)/h\omega_s$ and $\xi=E_a/h\omega_s$, and scales with $e^2/4a$. Here

$$E_a=\frac{\hbar^2}{2m^*(2a)^2} \tag{17}$$

is a characteristic energy of electrons in a barrier of width $2a$.

In Fig. 1 we show a series of potentials for different barriers, SP frequencies, and energies evaluated self-

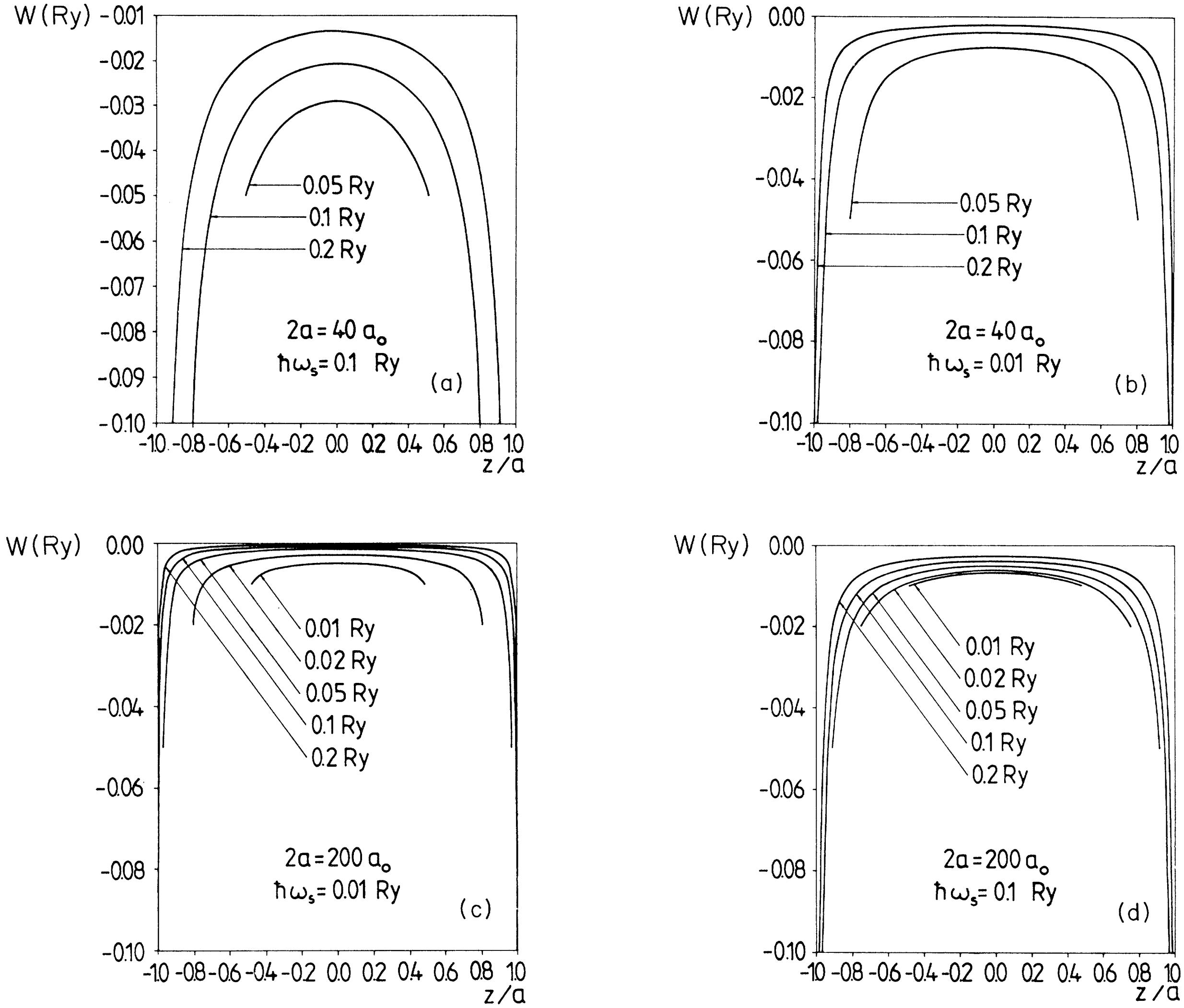

FIG. 1. Self-consistently calculated dynamical image potentials in the barriers of widths $2a=40a_0$ and $200a_0$, in the first iteration. The SP energies are $\hbar\omega_s=0.1$ and 0.01 Ry, $m^*=0.07m$. The electron energies are 0.01, 0.02, 0.05, 0.1, and 0.2 Ry.

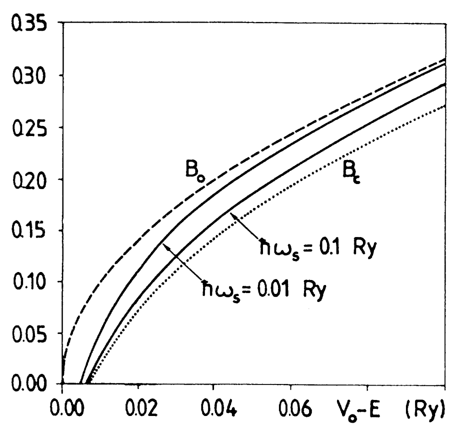

FIG. 2. Tunneling rates for the barrier with $2a=200a_0$, $m^*=0.07m$, calculated with no image potential (B_0), classical image potential (B_c), and the dynamical image potential (B) for two SP frequencies: $\hbar\omega_s=0.1$ and 0.01 Ry. The rates are given in units of $(2a/a_0)(m^*/m)^{1/2}$.

consistently. Self-consistent results are always lower than the first iteration, though appreciable differences occur only near the interfaces.

TUNNELING RATES

The shape of the potential barrier—its width and height—determines the conductance of the barrier, and we shall illustrate how the dynamical screening modifies conductance. The tunneling rate in WKB is

$$T(E)=e^{-2B(E)} \tag{18}$$

with

$$B(E)=\int_{-z_0}^{z_0}\kappa(z)dz\ , \tag{19}$$

where κ is given by (15), and $\pm z_0$ are the turning points. In the absence of the screening the exponent in (18) would have the form

$$B_0(E)=2a\kappa_0\ , \tag{20}$$

where $\kappa_0=[2m^*(V_0-E)/\hbar^2]^{1/2}$. Both $B(E)$, where the potential V_k in $\kappa(z)$ was evaluated self-consistently, and $B_0(E)$ are shown in Fig. 2 for the barrier width $2a=200$ Å, and for two SP frequencies.

At this point we have to emphasize that the WKB theory applies to the tunneling through a static or time-averaged barrier, and it would be easy to find arguments against this treatment for the case of a fluctuating potential. However, the use of this barrier provides a good and simple estimate of the dynamical effects in electron tunneling, though for more refined work one probably has to adopt a more sophisticated path integral/instanton approach, as in Ref. 15. On the other hand, in the latter approach one cannot study explicit forms of the image potentials in the barrier, as presented in this paper.

CONCLUSION

In conclusion, in this work we have calculated analytic expressions for the dynamical image potentials for tunneling electrons in the semiclassical approximation, taking into account SP dispersion and coupling in a particular metal-insulator-metal geometry. We have shown how finite SP frequencies, when comparable to other characteristic energies, prevent formation of a full (static) image potential, and thus modify the barrier conductance.

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