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DYNAMICAL EFFECTS IN FINITE FIELD ELECTRON TUNNELING

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Dedicated to Professor Boran Leontić on the occasion of his 70$^{\text{th}}$ birthday

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The problem of dynamical screening for electrons tunneling in the metal-insulator-metal system, based on a generalization of the Jonson's nonlocal theory of exchange-correlation potential, is reviewed. The self-energy is evaluated within the GW approximation for electrons coupled to the long-wavelength charge-density oscillations. Effective potential barriers are obtained by selfconsistent non-local numerical calculation, and then used to get transmission coefficient exactly and within the WKB approximation. The method is also extended to the case with an external potential applied on metal electrodes, and transmission coefficient is plotted as a function of electron energy and external potential.

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1. Introduction

The problem of dynamical effects in electron tunneling, and their formulation in terms of the interaction with surface plasmons (SP), was first given by Jonson [1], and later extended to metal-insulator-metal (M-I-M) systems, using nonlocal dynamical image potential [2], or its local limit [3]. In our previous papers [4, 5], we solved that problem numerically in order to get selfconsistent results even in the nonlocal case and also when an external electric field is applied. Using that approach we calculated effective potentials and analyzed them.

In this paper we use those methods and results in order to calculate the transmission probabilities exactly and to compare them with the WKB approximation. We also analyze the influence of the external voltage applied on the electrodes.

2. Formulation of the problem

As in Refs. [4] and [5], we consider electron tunneling in the M-I-M system, where the insulator is represented by a static barrier $V_0(z)$ of height V_0 and width $2a$. In the presence of an external voltage V, the static barrier is

$$V_0(z) = V_0 - eV\frac{z+a}{2a}\,. \tag{1}$$

We can calculate the local dynamical image potential

$$W_{\mathbf{k}}(z,E) = \int \mathrm{d}z' \Sigma_{\mathbf{k}}(z,z',E)\frac{\phi_{\mathbf{k}}(z')}{\phi_{\mathbf{k}}(z)} \tag{2}$$

using wave functions $\phi_{\mathbf{k}}$ obtained from the equation

$$\left[-\frac{\hbar^2}{2m^*}\frac{\mathrm{d}^2}{\mathrm{d}z^2} + \tilde{V}_{\mathbf{k}}(z,E) + E_\perp\right]\phi_{\mathbf{k}}(z) = 0\,, \tag{3}$$

where $\tilde{V}_{\mathbf{k}}$ is the total effective potential given by

$$\tilde{V}_{\mathbf{k}}(z,E) = V_0(z) + W_{\mathbf{k}}(z,E) \tag{4}$$

and $E_\perp$ is the "perpendicular" energy that can be evaluated from total energy using

$$E = \frac{\hbar^2 k^2}{2m^*} + E_\perp\,. \tag{5}$$

Self energy $\Sigma_{\mathbf{k}}$ is calculated in a self-consistent GW approximation [6]

$$\Sigma_{\mathbf{k}}(z,z',E) = \int \mathrm{d}\mathbf{q}\mathrm{d}\omega \mathcal{G}_{\mathbf{k}-\mathbf{q}}(z,z',E-\hbar\omega_i)W_{\mathbf{q}}(z,z',\hbar\omega). \tag{6}$$

If we evaluate the nonlocal potential $W_{\mathbf{q}}$ in the surface-plasmon-pole approximation and integrate with respect to ω, the self energy (6) becomes

$$\Sigma_{\mathbf{k}}(z,z',E) = \sum_p \int \mathrm{d}\mathbf{q}\Gamma_i^*(q,z)\mathcal{G}_{\mathbf{k}-\mathbf{q}}(z,z',E-\hbar\omega_i)\Gamma_i(q,z') \tag{7}$$

where $p=\pm$ denotes the SP mode parity, $i\equiv(p,q)$, ω_i are the SP mode frequencies for wave vector $\mathbf{q}$

$$\omega_i = \omega_{p\mathbf{q}} = \frac{\omega_p}{\sqrt{2}}\left(1+pe^{-2qa}\right)^{\frac{1}{2}} \tag{8}$$

(ω_p is bulk plasma frequency), and the Γ's are the matrix elements of the SP coupling [7].

The propagator $\mathcal{G}_{\mathbf{k}-\mathbf{q}}$ is the solution of the equation

$$\left[-\frac{\hbar^2}{2m^*}\frac{\mathrm{d}^2}{\mathrm{d}z^2}+\tilde{V}_{\mathbf{k}}(z,E)+E'_\perp\right]\mathcal{G}_{\mathbf{k}}(z)=-\delta(z-z'), \tag{9}$$

where the perpendicular energy $E'_\perp$ in the intermediate state should be evaluated from

$$E=\hbar\omega_i+\frac{\hbar^2(\mathbf{k}-\mathbf{q})^2}{2m^*}+E'_\perp \tag{10}$$

instead of (5). It can be shown that solution of Eq. (9) is given by

$$\mathcal{G}_{\mathbf{k}-\mathbf{q}}(z,z',E-\hbar\omega_i)=-\frac{2m^*}{\hbar}\frac{\phi^L_{\mathbf{k}-\mathbf{q}}(z^>)\phi^R_{\mathbf{k}-\mathbf{q}}(z^<)}{W(E)}\,, \tag{11}$$

where $\phi^{L,R}$ are solutions of equation (3) (with $E'_\perp$ instead of $E_\perp$) propagating from left and right, respectively, and W is their Wronskian.

3. *Tunneling rates*

It is interesting to analyze the influence of the dynamically modified potentials (4) on the tunneling rates. We can calculate them within the WKB approximation, as in Refs. [2] and [3], but since we solve our problem numerically, we can also calculate them exactly. After we get self-consistent result for the effective potential, we can once again solve the equation (3), obtain exact wave functions, and use them to calculate tunneling rate as the ratio between the transmitted and the incoming wave.

In the WKB approximation we define the transmission coefficient as

$$T_{WKB}=e^{-2B_{WKB}(E)}. \tag{12}$$

Here $B(E)$ is the attenuation rate [2, 3]

$$B_{WKB}(E)=\int\limits_{z_1}^{z_2}\kappa(z)\mathrm{d}z\,, \tag{13}$$

where z_1 and z_2 are turning points, and κ is

$$\kappa(z)=\sqrt{\widetilde{V}_{\mathbf{k}}(z,E)-E}\,. \tag{14}$$

In order to compare exact numerical results with the WKB approximation, we shall define the exact attenuation rate as

$$B(E)=-\frac{1}{2}\ln T(E)\,, \tag{15}$$

where $T(E)$ is the exactly calculated transmission coefficient.

4. *Results and discussion*

Figure 1 shows the exact attenuation rates for $\mathbf{k} = 0$, and for two different SP frequencies $\hbar\omega_s = 0.01$ and 0.1 Ry, as functions of electron energy, compared with WKB results. In our previous paper [4], this WKB result was compared with

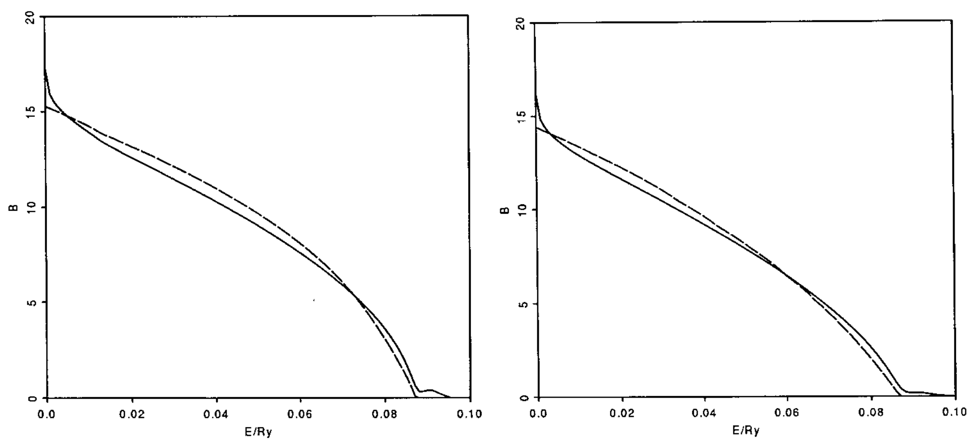

Fig. 1. Attenuation rates for barrier width $2a = 200a_0$, potential step $V_0 = 0.1$ Ry, external voltage $eV = 0.2V_0$ and effective mass $m^* = 0.07m$ as functions of electron energy. Solid lines: exact numerical results; dashed lines: WKB results. SP frequencies are: a) $\hbar\omega_s = 0.01$ Ry, b) (right) $\hbar\omega_s = 0.1$ Ry.

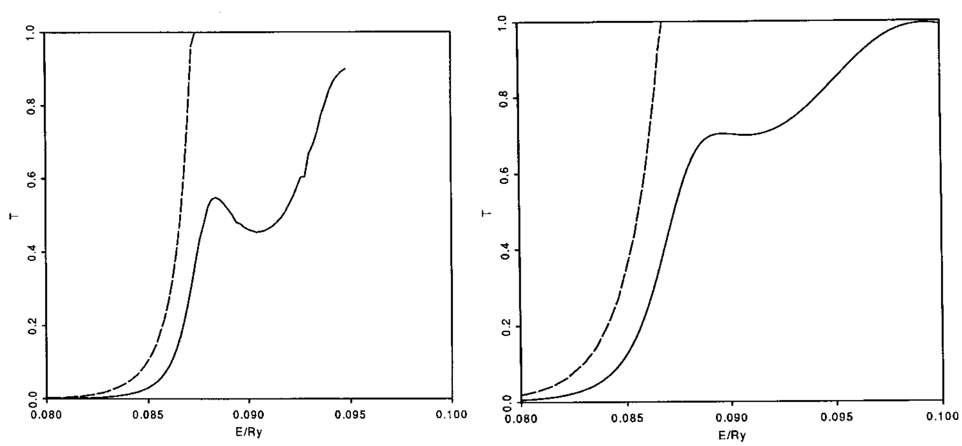

Fig. 2. Transmission coefficients for the same parameters as in Fig. 1.

the attenuation rates through the static and classical barrier, so here we omit the curves corresponding to these two limiting cases in order to concentrate on the comparison of the exact and WKB results for the dynamical potential. The chosen parameters (barrier width, $2a$, and height, V_0, external voltage, eV, and effective mass, m^*) are typical for the GaAs-AlGaAs system which is an example of a semiconductor heterojunction having a band structure equivalent to the M-I-M system. SP frequencies in such a system vary from 0.01 Ry to 0.1 Ry, depending on the doping. We can see that the WKB result behaves reasonably well, except of course for very low energies, and above the top of the effective barrier, where it fails for the well known reasons. Above the barrier the exact result oscillates, which can be better observed from Fig. 2 which shows the transmission coefficient for electron energies between $0.8\,V_0$ and $1\,V_0$. Irregularities of the curve for $\hbar\omega_s = 0.01$ Ry are due to numerical difficulties that arise from the concept of effective potential as we discussed in Ref. [5], and for the same reason we could not continue the calculation up to $E = V_0$.

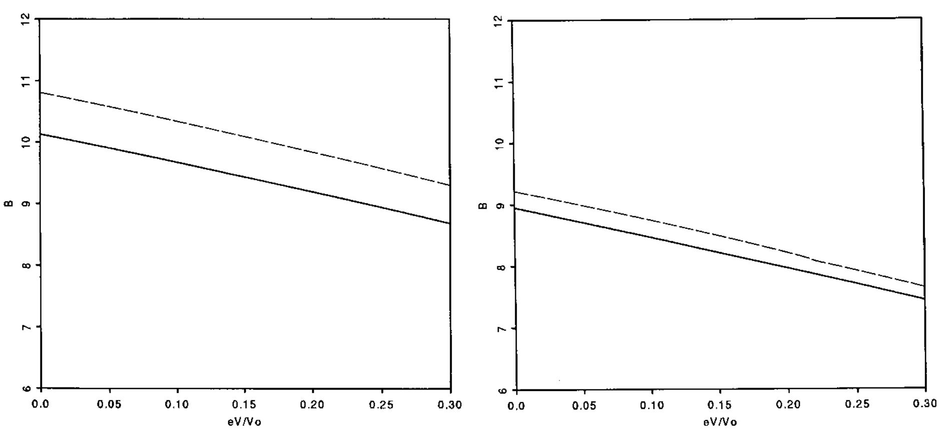

Fig. 3. Attenuation rates for barrier width $2a = 200a_0$, *potential step* $V_0 = 0.1$ Ry, *electron energy* $E = 0.5V_0 = 0.05$ Ry *and effective mass* $m^* = 0.07m$ *as functions of external voltage. Solid lines: exact numerical results; dashed lines: WKB results. SP frequencies are: a)* $\hbar\omega_s = 0.01$ Ry, *b) (right)* $\hbar\omega_s = 0.1$ Ry.

In Figs. 1 and 2 attenuation rates and transmission coefficients are shown for an external voltage $eV = 0.2\,V_0$. The results would be very similar for any other reasonable voltage (even for $V = 0$). In Figs. 3 and 4 we show B and T versus applied voltage for fixed electron energy $E = 0.5\ V_0 = 0.05$ Ry. We can see that in that region WKB provides a very good qualitative description of the phenomena, but quantitatively WKB transmission coefficients are several times larger than the exact ones. That means that for calculations of currents, we do need exact trans-

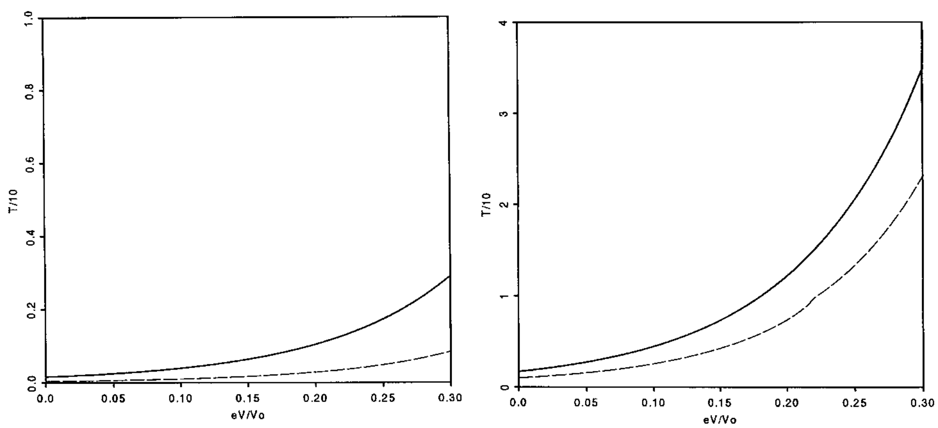

Fig. 4. Transmission coefficients for the same parameters as in Fig. 3.

mission coefficients, which, even without selfconsistency, could be evaluated only by means of numerical calculations.

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DINAMIČKI EFEKTI U TUNELIRANJU ELEKTRONA S KONAČNIM POLJEM

Razmatramo problem dinamičkog zasjenjenja za elektrone koji tuneliraju sistemom metal-izolator-metal, na osnovi poopćenja Jonsonove nelokalne teorije potencijala zamjene i korelacije. Izračunali smo svojstvenu energiju u GW aproksimaciji za elektrone vezane s oscilacijama nabojne gustoće velike valne duljine. Dobili smo efektivne potencijalne bedeme samosuglasnim numeričkim računom i njih smo primijenili za dobivanje točnih i približnih (dobivenih WKB metodom) vrijednosti propusnih koeficijenata. Metodu smo proširili i na slučaj s vanjskim poljem na metalnim elektrodama, a koeficijenti propusnosti se prikazuju kao funkcije energije elektrona i vanjskog potencijala.