Dynamic image potentials and field emission

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(Received 20 May 1983)

A numerical calculation is presented of a quantum-mechanical model of an electron leaving a metal under the pull of an electric field. The calculation includes possible interference phenomena from the electron virtual emission of a surface plasmon. The emitted current is calculated as a function of electric field.

INTRODUCTION

There have been a number of theoretical calculations of the effective image potential acting upon an electron as it leaves a metal surface.[1-7] These discussions have been given impetus by the report of Lee and Reifenberger[8] of oscillations in the photoassisted field emission current when plotted versus the applied electric field. Recent models[5-7] have focused upon the possible role of the dynamic formation of the image charge, and whether its transients could provide the oscillations in the current. Recent experiments by Reifenberger's group[9] have confirmed the experimental observation. However, most recent theoretical papers have been unable to provide an explanation.[4,6,7]

Our calculations also do not provide an explanation of the observed oscillations. Here we report an accurate computer solution to the quantum-mechanical equations which describe the possible interference phenomena caused by the dynamic formation of the image charge. No oscillations are found.

The first theoretical predictions of oscillations were by Mahan.[1] He calculated the transient potential acting upon a classical particle which moves through the interface at a constant velocity. The dynamic image potential was found to oscillate as the particle left the surface, due to the transients associated with the formation of the image potential. Other theorists have confirmed this classical prediction.[2,3] However, a quantum-mechanical calculation by Jonson did not find such oscillations.[4] Subsequent quantum calculations on low-energy electrons have confirmed Jonson's result.[6,7] Of course, the quantum-mechanical models are correct, and the classical model provides an incorrect picture for low-energy electrons.

Here we present a fully quantum-mechanical solution for the potential shown in Fig. 1. There is a metal in the region $z<0$, and a vacuum with an electric field F in the region $z>0$. The surface plasmons are included as a set of boson oscillators. The Hamiltonian is[10]

$$\begin{aligned} H &= \frac{p^2}{2m} + V_0(z) + \omega_s \sum_k a_k^\dagger a_k \\ &\quad + \sum_k \left(\frac{\pi e^2 \omega_s}{kA}\right)^{1/2} e^{-k|z|}(a_k + a_k^\dagger) \ , \\ V_0 &= \Theta(z)(V_{00} - eFz) \ . \end{aligned} \tag{1}$$

The surface plasmons form the image potential which acts upon the electron while it is near the surface. Their influence is strong and long range: The asymptotic image potential is $-e^2/4|z|$. Recent theoretical work[4,7] has shown that the best one-electron approximation to the dynamic image potential is just the static one. This leads us to formulate the problem as

$$\begin{aligned} H &= H_0 + V' \ , \\ H_0 &= \frac{p^2}{2m} + V_0(z) + U(z) + \omega_s \sum a_k^\dagger a_k \ , \\ V' &= -U(z) + \sum_k \left(\frac{\pi e^2 \omega_s}{kA}\right)^{1/2} e^{-k|z|}(a_k + a_k^\dagger) \ , \\ U(z) &= \frac{-e^2}{4(z^2+a^2)^{1/2}} \ . \end{aligned} \tag{2}$$

The static image potential U is built into the initial Hamiltonian H_0, where the parameter a prevents the divergence at the origin. With this choice, the effects of V' should be small. In the one-plasmon approximation, the equation for the wave function of an electron of energy E is

$$\psi_E(z) = \phi_E(z) + \int dz'\, G_E(z,z') \left[-U(z')\psi_E(z') + \frac{e^2\omega_s}{2} \int dz' \frac{G_{E-\omega_s}(z',z'')}{|z|+|z'|} \psi_E(z'') \right] , \tag{3}$$

where $\phi_E(z)$ is the wave function which is an eigenstate of H_0, while $\psi_E(z)$ is the eigenstate of H. In V', the effects of $-U$ enter in first-order perturbation theory, while the effects of the surface plasmons enter in second order.

Equation (3) was also obtained by Young. The question is whether the terms in V' will interfere with the unperturbed wave function ϕ_E, and hence explain the oscillations of Lee and Reifenberger. Young evaluated this expression in an approximate way, which was equivalent to the earlier model of Jonson, and found no oscillations. We have evaluated this expression on the computer without making these drastic approximations. We also do not find oscillations.

Lest this conclusion seem obvious, our initial expectation was that we would find oscillations. The reason is that there is a possible interference phenomena as the electron

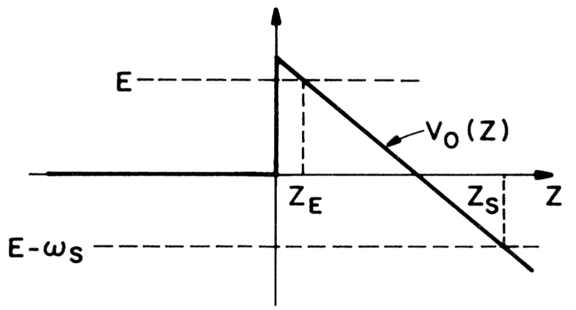

FIG. 1. Dark solid line is the electron potential energy near the metal surface in photoassisted field emission. Electrons leaving the metal have energy E, but may change to $E-\omega_s$ after emitting a surface plasmon.

traverses the region $z_E < z < z_s$ in Fig. 1. If the electron emits a surface plasmon, its energy in the final state is $E-\omega_s$. This wave function oscillates in space for $z > z_s$, and is evanescent for $z < z_s$. In a semiclassical view of this process, the electron of energy E cannot emit a surface plasmon until it is in the region $z \gtrsim z_s$. For the electron of energy E, the region $z_E < z < z_s$ is lossless, while the region $z > z_s$ is lossy. Thus it is possible to get interference if the electron reflects from the lossy region. Although approximate analytical evaluations of Eq. (3) showed that such oscillatory terms could exist, our numerical solutions do not show them. Hence the effect must be very small. Furthermore, the analytical estimates show that the current would oscillate with a period given by the inverse power of the electric field F. This prediction does not agree with Lee and Reifenberger, who found $F^{-1/2}$ rather than F^{-1}.

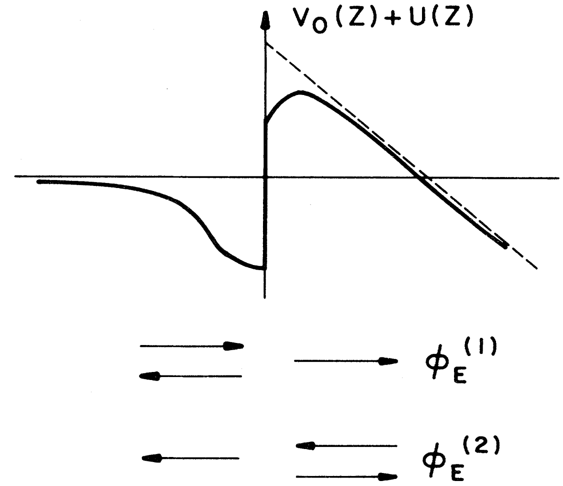

FIG. 2. Schematic illustration on the construction of the Green's function in Eq. (4).

CALCULATIONS AND RESULTS

The Green's functions in Eq. (3) are

$$G_E(z,z') = \frac{\phi_E^{(1)}(z^>)\phi_E^{(2)}(z^<)}{W(E)} , \quad z^> = \max(z,z'), \quad z^< = \min(z,z') . \tag{4}$$

As shown in Fig. 2, $\phi_E^{(1)}$ is a wave going to the right, while $\phi_E^{(2)}$ is a wave going to the left. $W(E)$ is their Wronskian. Since we are interested in how the current is affected, we only need the wave function in the limit as $z \to \infty$:

$$\lim_{z\to\infty} \psi_E(z) = \phi_E^{(1)}(E)[1+Q(E,F)],$$
$$Q(E,F) = \frac{1}{W(E)} \int_{-\infty}^{\infty} dz' \, \phi_E^{(2)}(z') \left[-U(z')\psi_E^{(1)}(E') + \frac{e^2\omega_s}{2} \int_{-\infty}^{\infty} dz'' \frac{G_{E-\omega_s}(z',z'')}{|z'|+|z''|} \psi_E^{(1)}(z'') \right] . \tag{5}$$

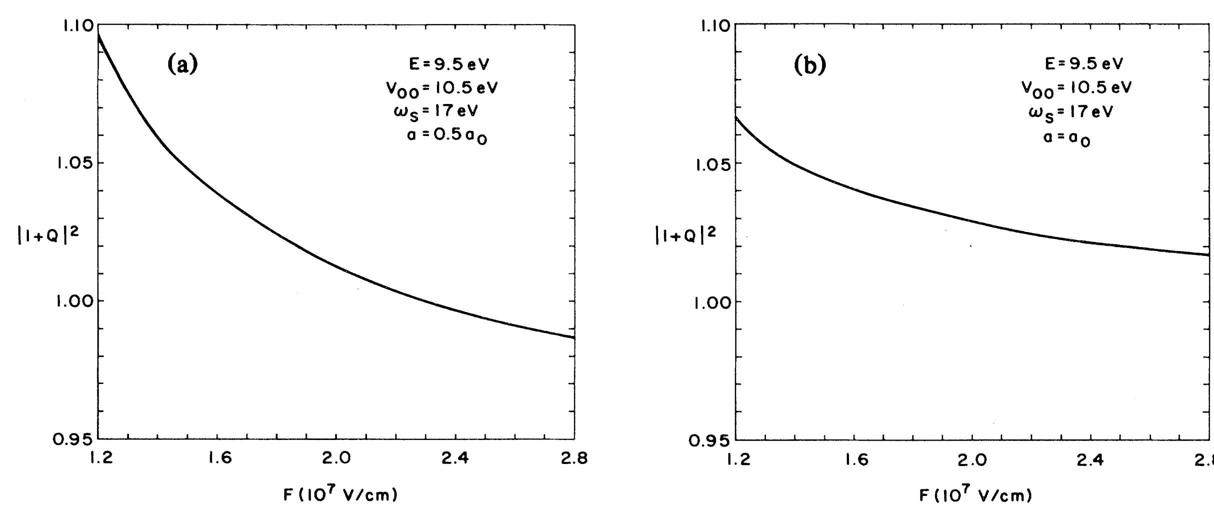

FIG. 3. Interference factor $|1+Q|^2$ vs the electric field in the region of experimental interests (Ref. 5). Numerical calculations were carried out for different values of the parameter a, for $a = 0.5a_0$ in (a) and $a = a_0$ in (b), where $a_0 = 0.529$ Å is the Bohr radius.

We calculate the quantity $Q(E,F)$ and see whether it interferes with the "1" term as a function of F. We assume that the effects of V' are small so that we can replace $\psi_E^{(1)}$ by $\phi_E^{(1)}$ on the right in Eq. (5). Our numerical solution shows that $|1+Q|^2$ is close to 1, so that the effects are indeed small, and our assumption is confirmed.

The first step in the calculation was to numerically calculate the four functions $\phi_E^{(1)}(z)$, $\phi_E^{(2)}(z)$, $\phi_{E-\omega_s}^{(1)}(z)$, and $\phi_{E-\omega_s}^{(2)}(z)$. They are one-particle eigenstates of the potential $V_0(z)-e^2/4(z^2+a^2)^{1/2}$. Asymptotic expressions were generated at large z, and then Numerov's method[11] was used to step inward through the origin. After these functions are found, the numerical integrations in Eq. (5) are straightforward. Parameters are chosen to model tungsten, with $V_{00}=10.5$ eV, $\hbar\omega_s=17$ eV, and values of E were selected near the top of the barrier to model the experimental conditions of photoassisted field emission.

Figure 3 shows two graphs of the quantity $|1+Q|^2$ for $E=9.5$ eV, and for values of the electric field between 1.2–2.8×10^7 V/cm. The experimental oscillations were observed in this range of field. No oscillations are evident in our result. Instead, the values are near unity, which shows that Q is monotonic. The effects of V' are small, in agreement with other calculations done on step barriers.

ACKNOWLEDGMENTS

We thank R. Reifenberger and W. L. Schaich for igniting our interests in this problem. Discussions with W. Hänsch, M. Jonson, and A. Puri have also been helpful. This research was supported by the National Science Foundation through Grant No. DMR-80-16883.

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