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LETTER TO THE EDITOR

Image force for a particle moving near a solid surface

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Abstract. Effects of surface plasmon dispersion and single-particle effects on the image force are studied for parallel incident particles. The inclusion of such effects avoids the unphysical logarithmic divergence of the parallel force at the surface. The probability of surface plasmon excitation is reduced with respect to the undispersed model.

It is well known that the image force acting on a charged particle moving outside a solid surface plays an important role in a set of problems related to particle–surface interactions.

Recently Muscat and Newns (1977), following earlier work by Takimoto (1966), calculated the force, both along and perpendicular to the direction of motion, acting upon a fast particle moving parallel to a solid surface. These authors use an undispersed surface dielectric function to represent the response of the surface. Within this model the transverse force acting on an electron moving parallel to a solid surface was shown to be finite everywhere, including at the surface itself, while the longitudinal force presents a logarithmic singularity at the surface. This force, dissipative in character, is important in RHEED experiments (Masud and Pendry 1976). This unphysical singularity is a consequence of neglecting surface plasmon dispersion and single-particle effects in the response of the medium. In this paper we propose a simplified method to estimate the importance of such effects. We study specifically the effect that the inclusion of surface plasmon dispersion and single-particle excitations will have on the image force and consequently on the probability of causing real surface excitations.

The model we take is that of a solid on the right-hand side ($Z > 0$), characterised by a bulk dielectric constant $\epsilon(\boldsymbol{k}, \omega)$, and a vacuum on the left-hand side ($Z < 0$).

The force acting on a charge Z_1 moving parallel to the surface in a fixed trajectory with uniform velocity v and at a distance Z_0 from the surface is given by $\boldsymbol{F} = -\nabla\phi(\boldsymbol{r}, t)$ where

$$\phi(\boldsymbol{r}, t) = (-Z_1^2/2\eta)\int_{-\infty}^{\infty} \exp(-\mathrm{i}\omega t)\,\mathrm{d}\omega \int \mathrm{d}^2Q \exp(-\mathrm{i}\boldsymbol{Q}\,.\,\boldsymbol{b}) \times \{[1-\epsilon(Q,\omega)]/[1+\epsilon(Q,\omega)]\}\exp(-Q|Z+Z_0|)\delta(\omega - \boldsymbol{Q}\,.\,\boldsymbol{v}) \qquad (1)$$

where $k = (Q, k_\perp)$ (Q and $k_\perp$ indicate the components of the wavevector $\boldsymbol{k}$ parallel and normal to the surface respectively and $\epsilon(Q, \omega)$ is the surface dielectric constant (Ritchie and Marusak 1966, Newns 1970) given by

$$\epsilon(Q, \omega) = (Q/\eta)\int_{-\infty}^{\infty} \mathrm{d}k_\perp[(k_\perp^2 + Q^2)\epsilon(k, \omega)]^{-1}. \qquad (2)$$

From now on we shall take $Z_1 = 1$ and we shall use atomic units throughout.

We could now take any of the well-known dielectric functions for the bulk and use it in equation (1) via equation (2). Instead, and in the spirit of Lundqvist's plasmon pole approximation to the bulk dielectric constant (Lundqvist 1967), we define a surface plasmon pole approximation to $\epsilon(Q, \omega)$ given by

$$\epsilon(Q, \omega) = 1 + \{\omega_p^2/[\omega(\omega + i\gamma) - \omega_p^2 - \alpha Q - \tfrac{1}{4}Q^4]\} \tag{3}$$

where ω_p is the bulk plasmon frequency, γ is a positive infinitesimal constant and α is given by

$$\alpha = \sqrt{\tfrac{3}{5}}v_F\omega_S. \tag{4}$$

The surface plasmon dispersion is then given by

$$\omega_{SQ}^2 = \omega_S^2 + \alpha Q + \tfrac{1}{4}Q^4. \tag{5}$$

This dielectric constant has been derived by looking at the behaviour of equation (2) for small and large Q with $\epsilon(k, \omega)$ given by the Lindhard dielectric function. It reproduces the surface plasmon dispersion relation described by Ritchie and Marusak (1966) and Inkson (1971) for small Q and takes into account in an approximate manner the individual character of the response throughout the Q^4 term.

The force acting on the particle $F = -\nabla\phi$ will have two components. The perpendicular component is given by

$$F_\perp(Z_0) = \omega_S^2 \int_0^\infty [Q \exp(-2Q|Z_0|)\theta(\omega_{SQ} - Qv)/\omega_{SQ}(\omega_{SQ}^2 - Q^2v^2)^{1/2}]\,dQ \tag{6}$$

where θ is the step function. For the parallel force we find

$$F_\parallel(Z_0) = (\omega_S^2/v) \int_0^\infty [\exp(-2Q|Z_0|)\,\theta(Qv - \omega_{SQ})/(Q^2v^2 - \omega_{SQ}^2)^{1/2}]\,dQ. \tag{7}$$

In figure 1 we show the results of calculation of the longitudinal force for an electron moving with velocity $v = 6$ au parallel to an aluminium surface in our approximation

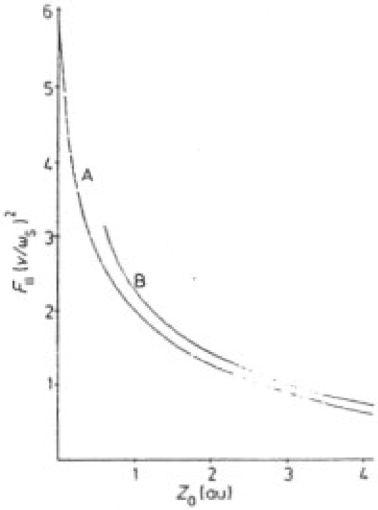

Figure 1. Longitudinal force $F_\parallel$ acting on an electron moving parallel to an aluminium surface. Dispersed model for $\epsilon(Q, \omega)$ (curve A); undispersed model (curve B).

and in the undispersed model. Inclusion of dispersion and single-particle effects avoids the unphysical logarithmic divergence predicted by the undispersed model.

Muscat and Newns (1977) studied the influence of the image force on the trajectory of an electron in grazing-incidence reflection inelastic electron spectroscopy. By using conservation of energy (neglecting the dissipative part) at the point at which the particle strikes the surface, they obtained a relationship between the contact angle β' at which the particle strikes the surface and the angle β made by the linear trajectory when the particle is far away from the surface. They found

$$\beta'^2 = \beta^2 + (2/v^2)|V_R(0)| \tag{8}$$

where $V_R(0)$ is the image potential at the surface. An estimate of the effect of the bending of the trajectory on the surface plasmon excitation probability can be obtained by calculating the total probability of surface plasmon excitation for a linear trajectory making a small angle β with the surface, which is given by

$$P(\beta) = (\omega_S^2/v \tan\beta) \int_0^\infty \theta(Qv - \omega_{SQ})\, dQ/Q\omega_{SQ}(Q^2v^2 - \omega_{SQ}^2)^{1/2} \tag{9}$$

and then substituting β' from equation (8) for β in equation (9). This is equivalent to assuming a linear trajectory of constant angle β', that is, we underestimate the value of $P(\beta(Z))$. Figure 2 shows the limiting maximum probability for excitation of surface

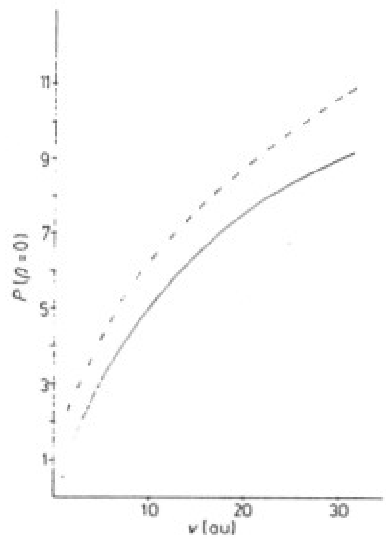

Figure 2. Maximum probability of surface excitations $P(\beta = 0)$ as a function of the particle velocity, $r_s = 2{\cdot}07$. Undispersed model, broken curve; dispersed model, full curve.

plasmons $P(\beta = 0)$ as a function of particle velocity both in our approximation and in the undispersed model for an electron moving parallel to an aluminium surface. Figure 3 shows $P(\beta)$ for an electron with $v = 31$ au moving near an aluminium surface for both our model and the undispersed model. We also show the results of a calculation in which the bending of the trajectory caused by the transverse force is neglected. The total

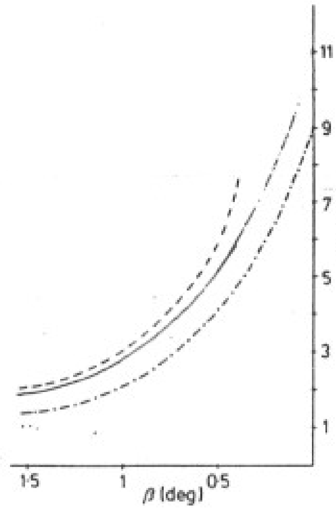

Figure 3. Probability of surface mode excitations as a function of the angle of incidence for an electron incident with velocity $v = 31$ au at an aluminium surface. $r_s = 2{\cdot}07$. Undispersed model, full curve; dispersed model, chain curve; undispersed model neglecting the bending of the trajectory (as given by equation (8)), broken curve.

probability of surface mode excitation in grazing-incidence reflection inelastic electron spectroscopy is reduced with respect to the undispersed model, following the experimental trend.

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