Asymmetric behavior in the excitation of plasmons by ions entering or leaving a material in an oblique trajectory

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Abstract. In this work we analyze the production of bulk and surface plasmons by fast ions entering or leaving a material at different incidence angles. In the framework of a semi classical dielectric formulation, we study the different contributions to the induced potential, mainly in the vicinity of the surface, analyzing the differences and similarities that arise when in and out trajectories are compared. In particular, we find some novel oscillatory structures for both perpendicular and oblique trajectories.

1. Introduction
The excitation of plasmons in a material bombarded by swift ions is relevant in different techniques for the spectroscopic analysis of surfaces, thin-foils and nanostructures [1, 2]. On the theoretical ground, these collective excitations are usually studied by means of second quantization or dielectric formulations, as complementary approaches for the analysis of quantum and semiclassical aspects of the problem [3]. For instance, we have recently analyzed the excitation of plasmons by a swift ion traversing a metal-vacuum planar interface in a normal trajectory and studied the differences and similarities that arise between incoming and outgoing trajectories [4]. The aim of the present communication is to extend this analysis to oblique trajectories. This seemingly simple objective is not without pitfalls. For instance, the standard method of cutting off the plasma response function only along the direction parallel to the interface, which has been customarily employed since its introduction by G. D. Mahan [5] four decades ago, is sound for perpendicular trajectories, but fails at other incidence angles. The reason for this failure is that it introduces a spurious spatial asymmetry that might lead to incorrect results, as for instance an unrealistic dependence of the energy loss on the angle at asymptotic distances from the surface. In the present article we avoid this approximation on the cutoff, a generalization that differentiates the present results from previous analyses.

In the following two sections we evaluate the induced potential and the energy dissipation rates due to bulk plasmon excitations. Finally, in section 4, we analyze the dependence of the in-out asymmetry with respect to the incidence angle $\theta$. 

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2. Induced Potential

In order to analyze the in-out asymmetry of plasmon production by swift ions in oblique trajectories, we avoid any complication of the problem and consider the simplest possible scenario. For instance, we use a Drude-type approximation of the dielectric function \( \epsilon(k, \omega) \), namely \( \epsilon(\omega) = 1 - \omega_p^2 / (\omega + i\gamma) \) [6]. Here, \( \omega_p \) and \( \gamma \) are the plasma frequency and damping rate of the metal, respectively (in particular, we use aluminum constants, with \( \omega_p = 15.8 \) eV). Let us point out that for swift projectiles, the discussion in this article still applies when allowance is made for spatial dispersion, provided that their velocity is large compared with the minimum phase-velocity of the plasmons in the medium [7].

We describe the metal-vacuum interface by means of the specular reflection and extended pseudo-medium models [8, 9, 10, 11]. Furthermore, we assume that the ion’s trajectory is undisturbed by the plasmon excitation events, an approximation which holds for sufficiently large kinetic energies, namely \( mv^2/2 \gg \hbar \omega_p \), where \( m \) and \( v \) are the mass and velocity of the projectile, respectively. With these provisions, and following the analysis in our previous articles [3, 4], the surface \((S)\) and bulk \((B)\) contributions to the potential induced by an ion of charge \( Z \) and velocity \( v \) should be given by (atomic units are used throughout this article),

\[
\phi(\mathbf{r}, t) = \phi_S(\mathbf{r}, t) + \phi_B(\mathbf{r}, t),
\]

where

\[
\phi_S(\mathbf{r}, t) = Z \omega_S \int_{-\infty}^{t} dt' e^{-\gamma(t-t')/2} \sin[\omega_S(t-t')] \\
\times \int_{0}^{k_c} dq J_0 \left(q|\vec{\rho} - \vec{v}_||t'|\right) e^{-q(|z|+|v_\perp t'|)}
\]

\[
\phi_B(\mathbf{r}, t) = Z \omega_P \Theta(-z) \int_{-\infty}^{t} dt' e^{-\gamma(t-t')/2} \sin[\omega_P(t-t')] \Theta(-v_\perp t') \\
\times \int_{0}^{k_c} dq J_0 \left(q|\vec{\rho} - \vec{v}_||t'|\right) \left(e^{-q(|z|+v_\perp t'|) - e^{-q(|z|+v_\perp t'|)}\right).
\]

Here \( \vec{v}_||(t) \) and \( v_\perp(t) \) are the components of the projectile’s velocity parallel and perpendicular to the surface, respectively. Similarly, \( \vec{\rho} \) and \( z \) are the projections of the position \( \mathbf{r} \) in directions perpendicular and parallel to \( \hat{z} \). The interface is located on the plane \( z = 0 \), with the metal occupying the semi-space \( z < 0 \). We have also defined the usual cutoff in the plasma response function,

\[
k_c = \omega_P \sqrt{\frac{1}{v_F^2} - \frac{1}{v^2}},
\]

where \( v_F = (3\sqrt{\pi} \omega_P/2)^{2/3} \) is the Fermi velocity. Both cases, of a particle leaving \( v_\perp > 0 \) or entering \( v_\perp < 0 \) the solid are considered.

However, as it was stated in the previous section, these results were obtained on the assumption that the cutoff \( k_c \) could be kept only in the components parallel to the surface, while the integration over the perpendicular component could be extended to infinity. This approximation might lead to spurious dependencies on the incidence angle, as it can be seen, for instance, in Fig. 7a of ref. [3]. To avoid this effect, we had to trace back the calculations leading to (1) and (2). For instance, the bulk contribution to the induced potential can now be written as

\[
\phi_B(\mathbf{r}, t) = \Theta(-z) \left[ \tilde{\phi}(\mathbf{r}, t) - \tilde{\phi}(\mathbf{r} - 2z\hat{z}, t) \right],
\]

where \( \Theta(x) \) is the Heaviside function and

\[
\tilde{\phi}(\mathbf{r}, t) = \frac{Z \omega_P}{2\pi^2} \Theta(-z) \int_{-\infty}^{t} dt' \int_{k<k_c} d\mathbf{k} e^{-\gamma(t-t')/2} \sin[\omega_P(t-t')] \Theta(-v_\perp t') \frac{e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{v} t')}}{k^2}.
\]
Note that the integral in \( k \) can be performed analytically in terms of Sine integral functions.

3. Results and Conclusions

Let us first investigate the particular case of a particle heading towards the interface from inside the material (i.e., \( v_\perp > 0 \) and \( t < 0 \)). In this case, since \( \tilde{\phi}(r, t) \) decreases exponentially in front of the projectile (i.e. \( z > 0 \)), its reflection \( \tilde{\phi}(r - 2z\hat{z}, t) \), which is moving towards the interface from outside the metal, would be negligible inside it. Thus, if the projectile is still far away from the surface, it would be possible to neglect the reflected contribution and approximate the induced potential \( \phi_B(r, t) \) by its direct term alone. However, once the particle has crossed the surface (i.e. \( t > 0 \)), the potential will start to decrease (due to the reduction of the integration range on \( t' \)), but its reflection will start to be relatively important. It would seem as if the wake that has been accompanying the projectile inside the solid almost without any distortion, is reflecting at the surface while begins to fade away (see figure 1, left and central panels).

For the opposite situation of a particle moving towards the surface from outside the solid (i.e., \( v_\perp < 0 \) and \( t < 0 \)), the Heaviside function vanishes and so does the induced potential \( \phi_B(r, t) \). Only when the particle has crossed the surface (i.e. \( t > 0 \)), the range of integration on \( t' \) becomes different from zero (namely, \( 0 < t' < t \)), and the induced potential starts to build up. In this case, the projectile will be moving across the waves of its own reflected wake (see figure 1, right panel).

![Figure 1. Bulk induced potential in aluminum due to an external ion, normalized to the ion atomic number \( Z \), with \( v = 4 \) a.u. and incidence angle \( \theta = 45 \) deg. Left and central panel: outgoing trajectory, particle inside and outside the material, respectively. Right panel: incoming trajectory, particle inside the material (in this case, the bulk induced potential is zero before the particle enters the material).](image)

These differences between the incoming and outgoing trajectories have their effect on the energy lost by the ion per time unit which is evaluated as

\[
\frac{dW}{dt} = -Z \left. \frac{\partial \phi(r, t)}{\partial t} \right|_{r=vt},
\]

In figure 2 we show the corresponding bulk contribution

\[
\left. \frac{dW}{dt} \right|_B = -Z \Theta(-v_\perp t) \left[ \left. \frac{\partial \tilde{\phi}(r, t)}{\partial t} \right|_{r=(v_\parallel + v_\perp)t} - \left. \frac{\partial \tilde{\phi}(r, t)}{\partial t} \right|_{r=(v_\parallel - v_\perp)t} \right],
\]

as a function of the distance to the surface \( z = v_\perp t \) of the incoming \( (v_\perp < 0) \) or outgoing \( (v_\perp > 0) \) ion. Firstly we note that the direct contribution to the energy lost by an outgoing
projectile is constant (and equal to that within an infinite medium) up to the crossing of the surface, and becomes zero beyond it. The reflected contribution is practically zero also inside the material, except in the vicinity of the surface. This begrenzung effect is due to the interaction of the projectile with the reflection of the front part of the wave accompanying it.

On the other hand, we see in figure 2 that the energy lost by an incoming projectile is very different to the outgoing case. We still see the same direct and reflected terms, but now they show oscillations that were not present for outgoing trajectories. These terms cancel partially, but a remanent oscillation persists that is still clearly visible in the total energy loss. This effect was already studied in a previous article [4] for normal incidence, but it was erroneously attributed to an interference between the direct and reflected contributions to the induced potential acting on the ion. Here we see that the oscillations are already present in both terms and occur as result of the transient construction of the direct wake upon penetration and the surfing of the reflected wake by the projectile. Furthermore, we see that they persist with oblique trajectories, even though their amplitude decrease with increasing angles.

![Figure 2. Energy lost per time unit for oblique incoming and outgoing trajectories of the charged particle (black lines), compared with the perpendicular case (red lines). Dashed: direct term; dash-dotted: reflected term; continuous: total energy loss rate. Velocity and incidence angle are the same as in previous figures.](image)

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