WAKE POTENTIAL IN THE VICINITIES OF A SURFACE

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ABSTRACT

An expression for the potential set up by a swift ion when it crosses a solid-vacuum interface is presented. The evaluation of this expression is carried out by using the plasmon-pole approximation for the dielectric function.

The wake phenomena associated to the motion of a swift charged point particle in an electron gas has been extensively studied in the past [1]. Many authors have studied the dynamical corrections to the image potential [2-4]. The surface potential when the particle moves parallel to the surface and with constant velocity has also been considered [2,6]. It has also been shown that the image potential is mainly due to the interaction with surface plasmons [7,8]. The self-energy of a moving charge near a surface has also been studied in detail [3].

The problem we want to deal with consists in deriving expressions for the potential induced by the moving charge, i.e., finding the response of the semi-infinite medium. We shall adopt the specular reflection model (SRM), first introduced by Ritchie and Marusak [9] to study the dispersion relation for surface plasma modes. In this model each semi-infinite medium is treated as if it was infinite under a symmetrisation of the charges being inside it, and adding a charge distribution on the surface which is eliminated after imposing the matching conditions for the potential. Some authors have applied this model to similar physical problems [4,5]. In order to have a good knowledge of the induced potential near the surface it is necessary to study the effect of the surface on electron production induced by swift

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ions, as is the case in convoy electrons and in particular the wake-riding electrons, which has been the subject of intense experimental [10] and theoretical work [11].

Let us consider a swift charged point particle which is travelling in the vicinities of a flat solid-vacuum interface with velocity $\vec{v}$, and let Z_1 be the charge of the particle. We shall use the notation $\vec{r} = (\vec{R},z)$, $\vec{k} = (\vec{Q},k_z)$, $\vec{v} = (\vec{v}_\parallel,\nu_z)$, where $\vec{R}$, $\vec{Q}$ and $\vec{v}_\parallel$ are the components parallel to the surface, and the z-axis is chosen in the perpendicular direction. The trajectory of the particle, whose recoil is negligible, is described by the equation $\vec{r} = \vec{v}t$, so that it reaches the surface, located at $z = 0$, when $t = 0$. The bulk solid $(z < 0)$ is taken to be described by its dielectric function $\varepsilon(k,\omega)$.

Let us concentrate on the outgoing particle case $(\nu_z > 0)$. The charge stays in the metal side $(z < 0)$ while t is negative. Thus, the symmetrised charge density [4] for the extended metal should read

$$\rho^{metal}(\vec{r},t) = Z_1 \left[\left\{\delta(\vec{r}-\vec{v}t) + \delta(\vec{r}-\vec{v}'t)\right\} \theta(-t) + \rho^S(\vec{R},t)\delta(z)\right], \tag{1}$$

with $\vec{v}' = (\vec{v}_\parallel,-\nu_z)$ the specular reflection of $\vec{v}$, and $\theta(x)$ the Heaviside step function. The ingredients of this charge density are the real charge and its specular image, (which are only present for negative times, i.e., while the real charge is in the metal side), and a surface-charge distribution, that is used to match the potential at the surface. After inserting this charge density into Poisson's equation and expressing the potential in terms of its Fourier transform

$$\phi(\vec{r},t) = \frac{1}{(2\pi)^4} \int d\vec{k} \int d\omega\, e^{i(\vec{k}\vec{v}-\omega t)}\, \tilde{\phi}(\vec{k},\omega), \tag{2}$$

we obtain

$$\tilde{\phi}^{metal}(k,\omega) = \frac{4\pi Z_1}{k^2\varepsilon(k,\omega)} \left\{ \int_{-\infty}^{0} \left[e^{i(\omega-\vec{k}\vec{v})t} + e^{i(\omega-\vec{k}\vec{v}')t}\right] dt + \int d\vec{R} \int_{-\infty}^{\infty} dt\, e^{i(\omega t-\vec{Q}\vec{R})}\, \rho(\vec{R},t)\right\}.$$

After undoing the Fourier transform in the variable z, it becomes

$$\tilde{\phi}^{metal}(\vec{Q},\omega,z) = 4\pi Z_1 \left[U_0(z) + \rho^S(\vec{Q},\omega)\, I_0(z)\right], \quad (z < 0) \tag{3}$$

where $\varepsilon(k,\omega)$ is assumed to depend on k_z only through $k^2 = Q^2 + k_z^2$,

$$U_0(z) = \frac{1}{\pi}\int_{-\infty}^{\infty} dk_z \int_{-\infty}^{0} dt\; e^{i(\omega-\vec{Q}\vec{V}_{\parallel}-k_z\nu_z)t} \left(\frac{\cos(k_z z)}{k^2\varepsilon(k,\omega)}\right), \tag{4}$$

and

$$I_0(z) = \int_{-\infty}^{\infty} dk_z \;\frac{\cos(k_z z)}{k^2\varepsilon(k,\omega)}. \tag{5}$$

We proceed in the same way with the vacuum side ($z > 0$), where now

$$\rho^{\mathrm{vacuum}}(\vec{r},t) = Z_1 \left[\left\{\delta(\vec{r}-\vec{v}t) + \delta(\vec{r}-\vec{v}'t)\right\}\theta(t) - \rho^{s}(\vec{R},t)\,\delta(z)\right]. \tag{6}$$

The complete charge scheme is depicted in fig.1. The term proportional to $-\rho^{s}(\vec{R},t)$ provides the continuity of the perpendicular component to the surface of the electric displacement. Solving again Poisson's equation it is easily found that

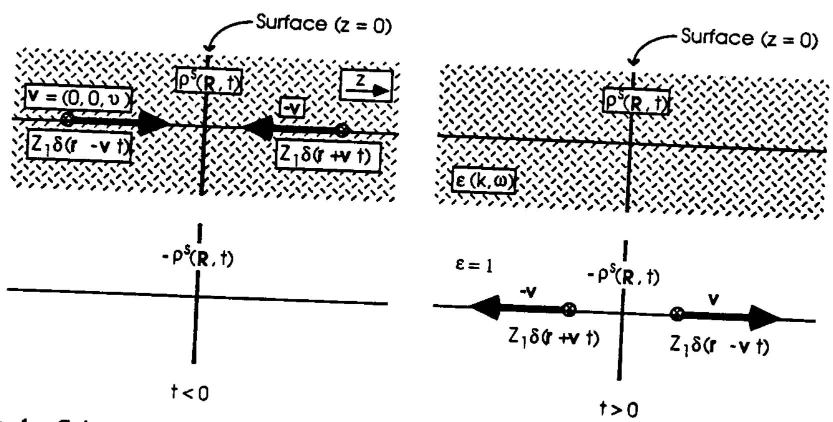


Figure 1. Schematic representation of the charges used in the specular reflection model to calculate the induced potential created by a charged point particle which crosses a solid-vacuum interface from the solid side. Z_1 is the charge of the particle. For the sake of simplicity we plot the case of perpendicular motion, i.e., the velocity of the particle is given by $\vec{v} = (0,0,\nu)$. The particle leaves the solid at $t = 0$. The two drawings at the left hand side show the charge situation when $t < 0$ and the ones at the right are used when $t > 0$. The upper drawings stand for $z < 0$, that is, inside the solid, $\varepsilon(k,\omega)$ being its bulk dielectric function, while the lower ones represent the vacuum, $z > 0$, where $\varepsilon(k,\omega) = 1$. The surface is placed at $z = 0$.

$$\tilde{\phi}^{vacuum}(\vec{Q},\omega,z) = 4\pi Z_1\left[U_1(z) - \rho^S(\vec{Q},\omega)\,\frac{\pi}{Q}\,e^{-Qz}\right], \quad (z > 0) \tag{7}$$

where $U_1(z) = \frac{1}{\pi}\int_{-\infty}^{\infty} dk_z \int_0^{\infty} dt\; e^{i(\omega-\vec{Q}\vec{V}_\parallel-k_z\nu_z)t}\left(\frac{\cos(k_z z)}{k^2}\right) =$

$$= \frac{e^{i\tilde{\omega}|z|/\nu_z}}{\nu_z\,\tilde{K}^2} + \frac{i\tilde{\omega}\,e^{-Q|z|}}{\nu_z^2\,\tilde{K}^2\,Q}, \quad \text{with } \tilde{\omega} = \omega - \vec{Q}\vec{V}_\parallel\,, \quad \text{and } \tilde{K}^2 = Q^2 + \frac{\tilde{\omega}^2}{\nu_z^2}.$$

The continuity of the potential at the surface $(z = 0)$ fixes the value of $\rho^S(\vec{Q},\omega) = Q(U_1^+ - U_0^-)/(\pi + QI_0^-)$, where the upper signs + and - stand for the limits when z approaches 0 while remaining positive or negative respectively (both limits are equal because U_0, U_1 and I_0 depend only on $|z|$).

The analysis of the incoming particle case follows the same calculations but taking

$$\rho^{metal}(\vec{r},t) = Z_1\left[\left\{\delta(\vec{r}-\vec{v}t) + \delta(\vec{r}-\vec{v}'t)\right\}\theta(t) + \rho^S(\vec{R},t)\,\delta(z)\right]$$

$$\rho^{vacuum}(\vec{r},t) = Z_1\left[\left\{\delta(\vec{r}-\vec{v}t) + \delta(\vec{r}-\vec{v}'t)\right\}\theta(-t) - \rho^S(\vec{R},t)\,\delta(z)\right],$$

instead of eqs.(1) and (6). This assumes the particle is traveling from positive to negative z's. The important point is to realize the difference in the signs of the step functions.

A first evaluation of the wake potential may be carried out by using the classical frequency-dependent dielectric function $\varepsilon(\omega)$. We find the same results for the surface wake than those in ref.[12], while for the image potential in the vacuum our results reproduce those of ref.[3] for a non-dispersive medium.

Let us now consider the solid to be described by the plasmon-pole dielectric function, which has been previously used to calculate the bulk wake [1],

$$\varepsilon(k,\omega) = 1 + \frac{\omega_p^2}{\frac{k^4}{4} + \beta^2 k^2 - \omega(\omega + i\eta)},$$

with $\beta = \sqrt{3/5}\;v_F$, (v_F is the Fermi velocity) and $\omega_p = \sqrt{3/r_s^3}$ the plasmon frequency. η is a positive constant that represents the damping of the plasma modes. For the sake of simplicity we consider an outgoing particle in a perpendicular trajectory, $\vec{v} = (0,0,\nu)$. Similar expressions are found when $\vec{v}_{\parallel}$ is not set to 0. Then $I_0(z)$ is obtained from eq.(5) and the result is [3]

$$I_0(z) = \frac{\pi}{Q} \frac{\omega(\omega + i\eta)}{\Omega} e^{-Q|z|} + \frac{\pi\omega_p^2}{\Lambda_+ - \Lambda_-} \left\{ \frac{\exp\left[-|z| \sqrt{Q^2 + 2\Lambda_-}\right]}{\Lambda_- \sqrt{Q^2 + 2\Lambda_-}} - \frac{\exp\left[-|z| \sqrt{Q^2 + 2\Lambda_+}\right]}{\Lambda_+ \sqrt{Q^2 + 2\Lambda_+}} \right\},$$

where $\Omega = \omega(\omega + i\eta) - \omega_p^2$ and $\Lambda_\pm = \beta^2 \pm [\beta^4 + \Omega]^{1/2}$. From this we may calculate $U_0(z)$, defined in eq.(4), after realizing that (for $\vec{v}_{\parallel} = 0$)

$$U_0(z) = \frac{1}{2\pi} \int_{-\infty}^{0} dt\, e^{i\omega t} \left\{ I_0(z - \nu t) + I_0(z + \nu t) \right\},$$

and we find

$$U_0(z) = \frac{\exp(-i\omega|z|/\nu)}{\nu k^2\, \varepsilon(k,\omega)} - \frac{\omega(\omega + i\eta)}{\Omega} \frac{i\,\omega}{\nu^2 k^2 Q} e^{-Q|z|}$$
$$+ \frac{i\,\omega\,\omega_p^2}{\Lambda_+ - \Lambda_-} \left\{ \frac{\exp\left[-|z| \sqrt{Q^2 + 2\Lambda_+}\right]}{\Lambda_+ \sqrt{Q^2 + 2\Lambda_+}\left[\nu^2(Q^2 + 2\Lambda_+) + \omega^2\right]} - \frac{\exp\left[-|z| \sqrt{Q^2 + 2\Lambda_-}\right]}{\Lambda_- \sqrt{Q^2 + 2\Lambda_-}\left[\nu^2(Q^2 + 2\Lambda_-) + \omega^2\right]} \right\}.$$

The final expression for the potential comes from eqs.(2), (3) and (7)

$$\phi(\vec{r},t) = \frac{1}{2\pi^2} \int_0^\infty dQ\, Q\, J_0(RQ) \int_0^\infty d\omega\, \mathrm{Re} \left\{ e^{-i\omega t}\, \tilde{\phi}(\vec{Q},\omega,z) \right\},$$

where ($\vec{v}_{\parallel} = 0$ and $\nu_z = \nu$),

$$\tilde{\phi}(Q,\omega,z) = \tilde{\phi}^{\mathrm{metal}}(Q,\omega,z)\, \theta(-z) + \tilde{\phi}^{\mathrm{vacuum}}(Q,\omega,z)\, \theta(z).$$

We have evaluated ϕ^{ind}, the wake potential minus the bare Coulomb potential, for $\vec{r} = \vec{v}t$, $\nu = 4$ a.u. and $Z_1 = 1$. We have done this for an incoming ion as well. The results are plotted in fig.2. In both cases (incoming and outgoing ion) the induced potential at the origin presents

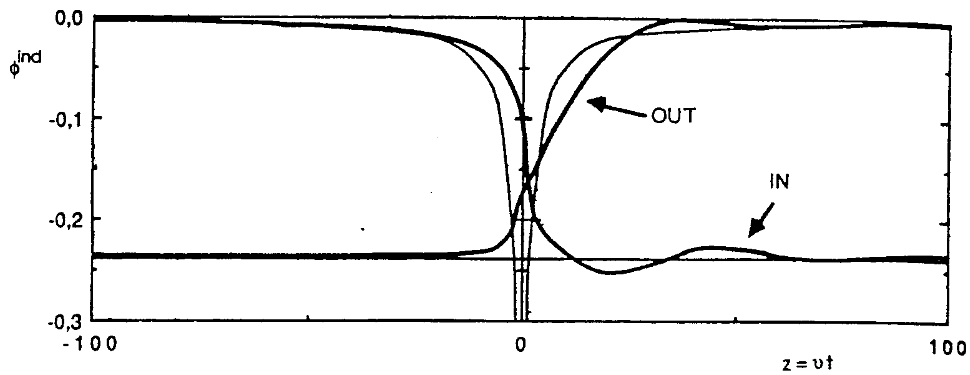


Figure 2. Induced potential at the position of the charge set up by a charged particle which is crossing a solid-vacuum interface in a direction perpendicular to the surface. IN is the situation where the particle is coming from the vacuum and penetrates into the solid, and OUT represents the particle coming from the solid. In both cases the particle is moving from left to right with a velocity ν = 4 a.u. The equation of motion is $z = \nu t$, and this is the quantity that appears in the horizontal axis. The bulk medium is described by the plasmon-pole dielectric function with $r_s = 2$ and a damping η = 0.015 a.u. (aluminum). The potential presents oscillations after the particle has crossed the surface in both cases. The period of these oscillations is approximately given by $2\pi\nu/\omega_s$. The classical induced potential and the bulk induced potential at the position of the particle are also plotted.

oscillations once the particle has crossed the surface. The period of these oscillations is approximately given by $2\pi\nu/\omega_s$, where $\omega_s = \omega_p/\sqrt{2}$ is the surface plasma frequency [3].

Fig.3 shows the wake formation and destruction process for an incoming and outgoing proton respectively along the points of the trajectory. The potential remains almost unchanged until the particle crosses the surface (t = 0). In fig.4 we plot the wake destruction process for ν = 6 a.u. and for points not only in the trajectory.

To summarize, we have found expressions for the induced potential created by an ion when it crosses a solid-vacuum surface. A numerical evaluation has been carried out for a perpendicular trajectory and with the plasmon-pole dielectric function to describe the bulk metal. We find that in the case of an outgoing trajectory the potential remains nearly unchanged until the projectile crosses the surface. The induced potential at the position of the ion presents oscillations, due to the surface plasmon excitations, once the projectile has crossed the surface in both the outgoing and the incoming trajectories.

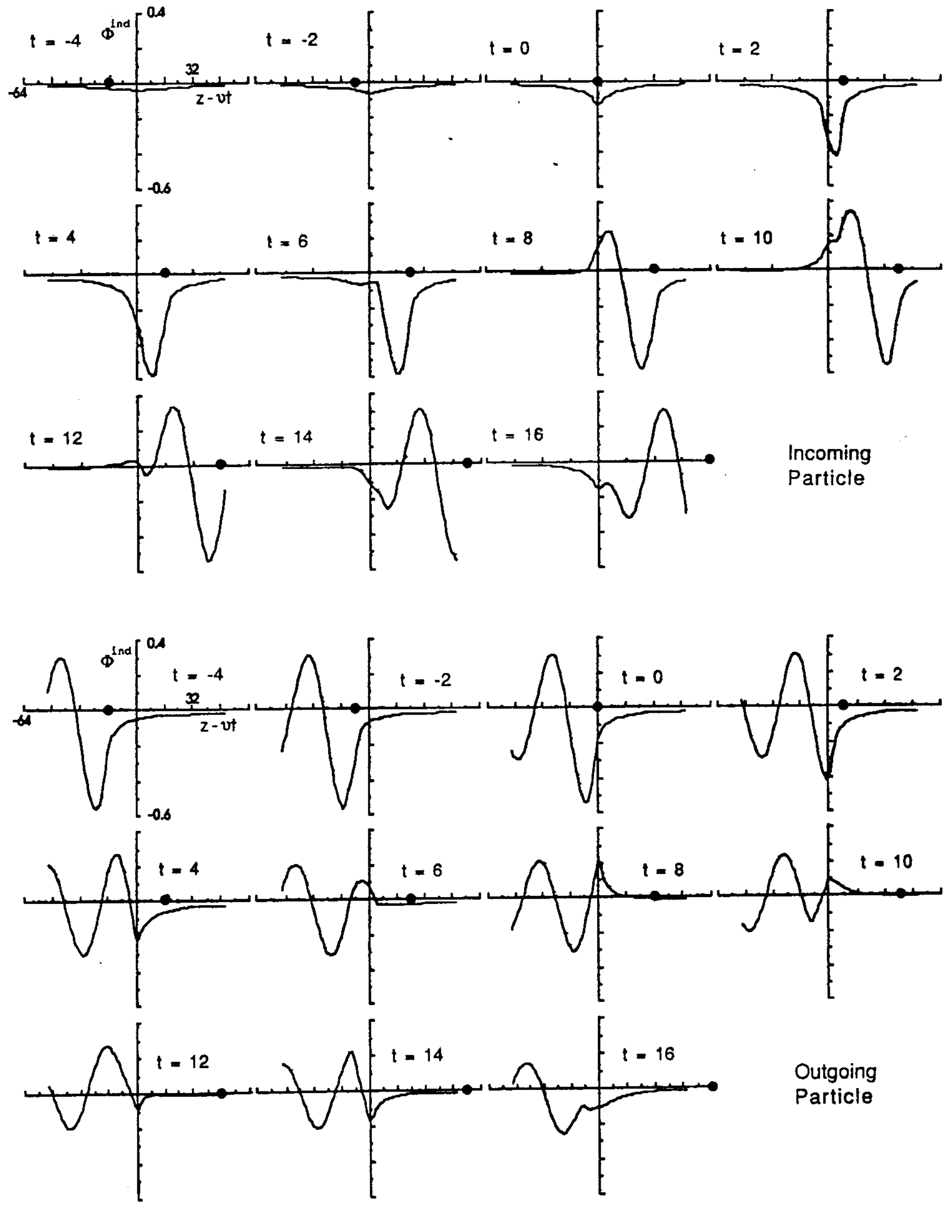


Figure 3. Wake destruction and formation process for a proton crossing an Al-vacuum interface under the same conditions as in fig.2. Here we plot the induced potential for points along the trajectory and t = -4, -2, 0, ..., 16 a.u. when the particle is incoming and outgoing. The proton is shown as a black circle.

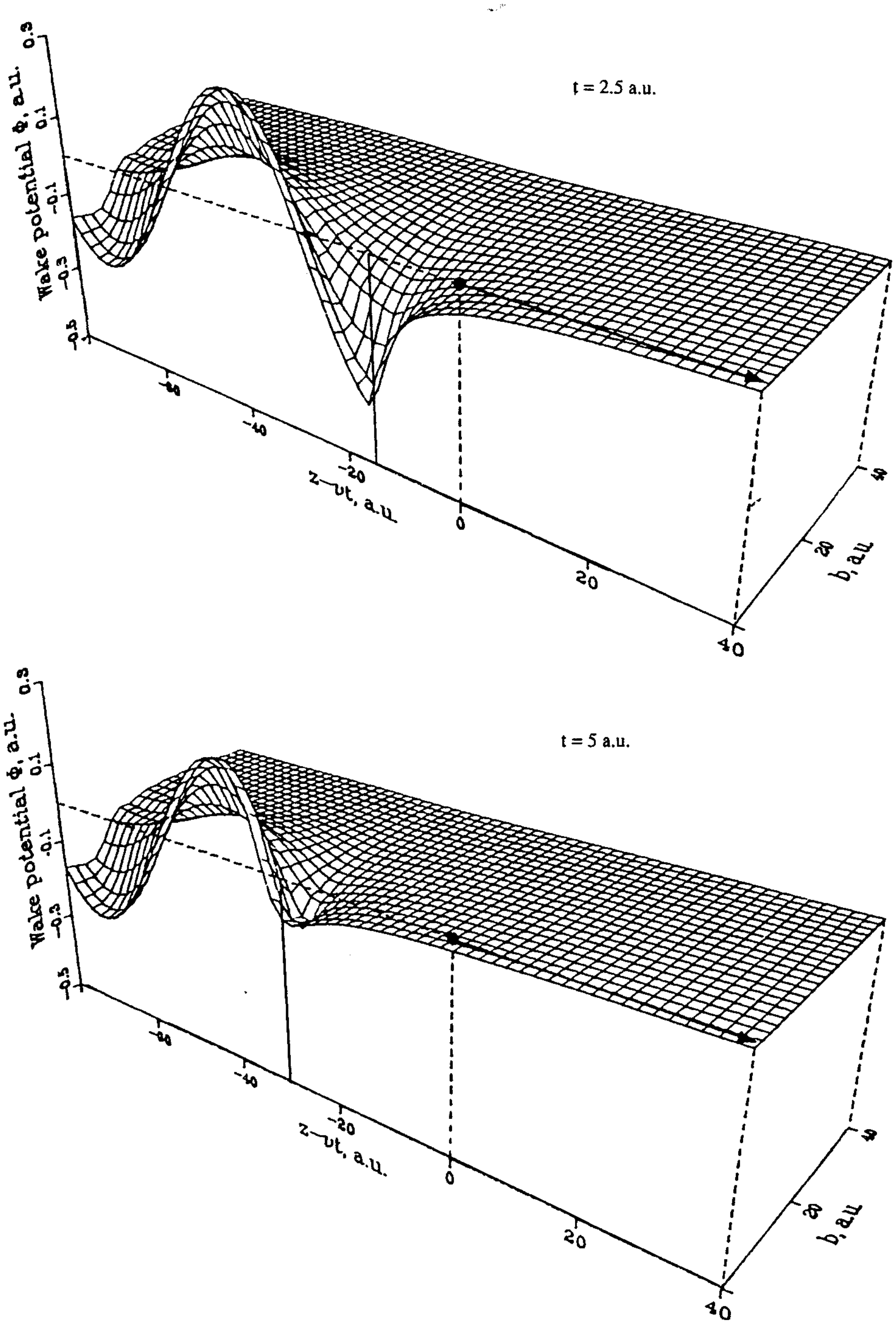
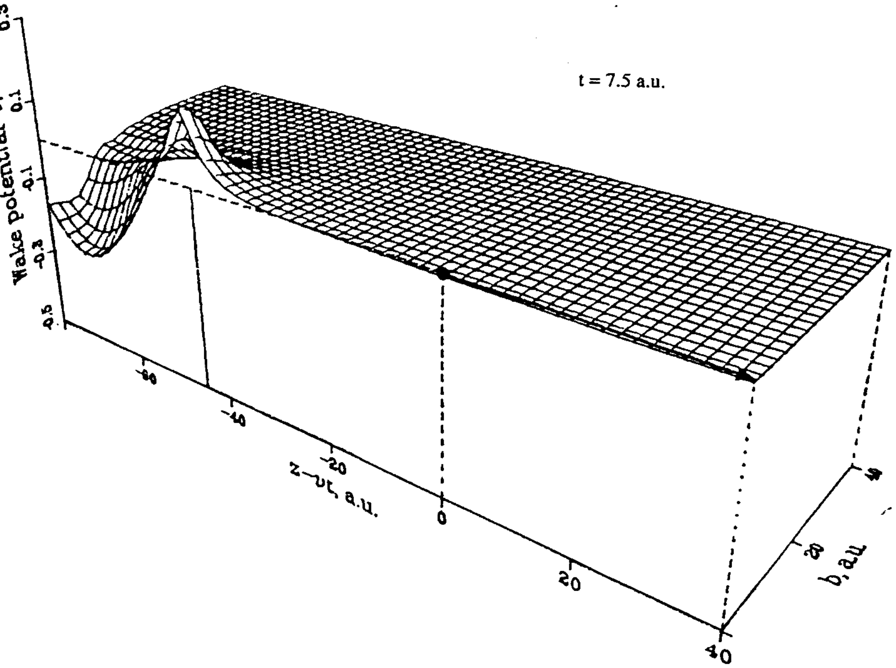


Figure 4. Induced wake potential created by an outgoing proton under the same conditions as in fig.2 except that the velocity is now ν = 6 a.u. The wake is plotted on a grid in z - νt and b (the direction perpendicular to the trajectory) for t = 2.5, 5, 7.5 and 10 a.u. The surface is represented by a vertical solid line. It comes out clearly how the wake begins to vanish only once the proton has crossed the surface.



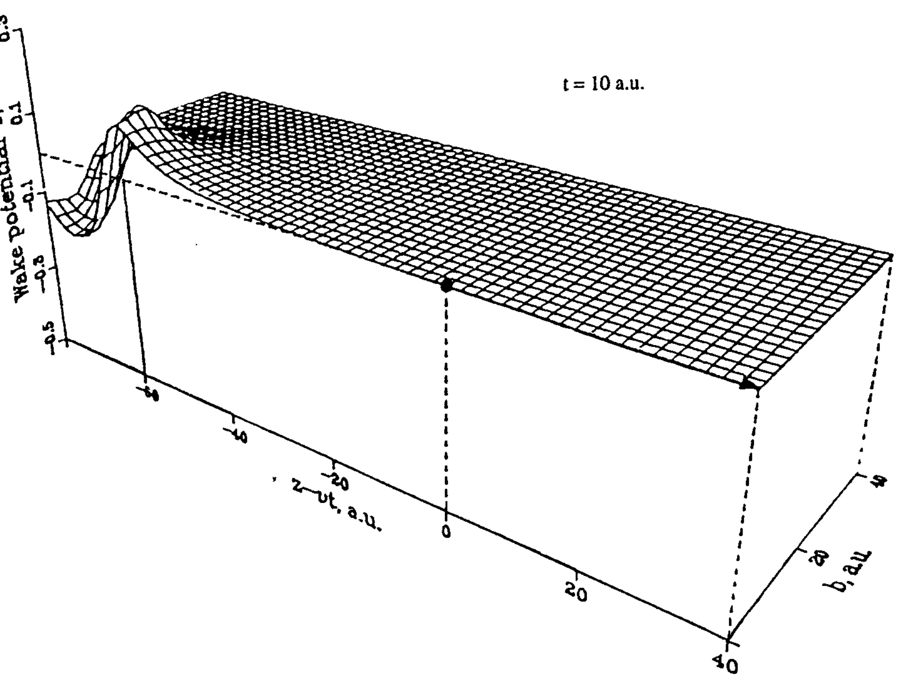


Figure 4. part 2

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REFERENCES

1. J Neufeld and R.H. Ritchie, Phys. Rev. *98* (1955) 1632; *99* (1955) 1125; V.N. Neelavathi, R.H. Ritchie and W. Brandt, Phys, Rev. Lett *33* (1974) 302, *34* (1975) 650(E); P.M. Echenique, F. Flores and R.H. Ritchie, *Dynamic Screening of Ions in Condensed Matter,* Solid State Physics Series. Vol. *43*, p.229, Erhenreich and Turnbull, eds, Academic (1990); P.M. Echenique, R.H. Ritchie and W. Brandt, Phys. Rev. *B20* (1979) 2567.
2. D. Chan and P. Richmond, J. Phys. *C9* (1976) 163; N. Takimoto, Phys. Rev. *146* (1965) 366; J. Heinrichs, Phys. Rev. *B8* (1973) 1346; Yu.A. Romanov and V.Ya Aleshkin, Sov. Phys. Solid State *23* (1981) 147; B.N. Libenson and V.V. Rumyantsev, Sov. Phys. JEPT *59* (1984) 999; M.L.Glasser and G. Gumbs, Phys. Rev. *B35* (1987) 7490; N.J.M. Horing, H.C. Tso and G. Gumbs, Phys. Rev. *B36* (1987) 1588; K. Suzuki, M. Kitagawa and Y.H. Otsuki, Phys. Status Solidi *B82* (1977) 643; J.P. Muscat and D.M. Newns, Surface Sci. *64* (1977) 641.
3. F. Flores and F. Garcia-Moliner, J. Phys. *C12* (1979) 907; P.M. Echenique, R.H. Ritchie, N. Barberán and J.C. Inkson, Phys. Rev. *B23* (1981) 6486.
4. F. García-Moliner and F. Flores, *Introduction to the Theory of Solid Surfaces,* Cambridge University Press, (1979).
5. R. Núñez, P.M. Echenique and R.H. Ritchie, J. Phys. *C13* (1980) 4299.
6. Y.H. Ohtsuki, *Charged Beam Interaction with Solids*, London, Taylor & Francis Ltd., (1983).
7. R.H. Ritchie, Phys. Lett. *A38* (1972) 189.
8. A.A. Lucas, Phys. Rev. *B4* (1971) 2939.
9. R.H. Ritchie and A.L. Marusak, Surf. Sci. *4* (1966) 234.
10. Y. Yamazaki, Proc. 10th W. Brandt Workshop, Alicante, Spain (1987).
11. J. Burgdörfer, Nucle. Inst. and Meth. *B24/25* (1987) 139.
12. P.M. Echenique, Ph.D. Thesis, Universidad Autónoma de Barcelona (1977) (unpublished).

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