## Wake potential of a swift ion near a metal surface

## Godfrey Gumbs

Department of Physics, University of Lethbridge, Lethbridge, Alberta, Canada T1K 3M4

## M. L. Glasser

Department of Mathematics and Computer Science, Clarkson University, Potsdam, New York 13676 (Received 27 January 1987)

The scalar electric potential due to a point charge having constant velocity parallel to a solid surface is calculated explicitly. The calculation is based on the random-phase-approximation theory of the dynamic electronic-response properties of a semi-infinite solid-state plasma. The classical infinite-barrier model is used to represent the surface.

Although several important advances have been made in the theory of the scalar electric potential in a homogeneous, isotropic medium due to a swift charge having constant velocity, there has been no work reported so far on the scalar potential of an ion moving near a solid surface. The work reported in the present paper is concerned with the scalar electric potential due to a swift charge Ze moving with uniform velocity v parallel to the surface of a semi-infinite solid-state plasma. The first explicit calculation for the oscillatory wake potential which is produced by an ion moving in an electron gas was given by Neufeld and Ritchie<sup>1</sup> 30 years ago. The most recent analysis for the interaction of fast ions with an electron gas has been carried out by Ashley and Echenique,<sup>2</sup> who calculated the influence of damping on wake binding energies. (For a list of references, see Refs. 2 - 9.

The quantum plasma fills the half-space z > 0 and the charged particle moves with uniform velocity v = vi parallel to the xy plane at a distance  $|z_0|$  from the pla-

nar surface at z=0. The impressed Coulomb potential  $U(\mathbf{r},t)=Ze \mid \mathbf{r}-vt\mathbf{i}-z_0\hat{\mathbf{z}}\mid^{-1}$  at the space-time point  $(\mathbf{r},t)$  is dynamically screened, resulting in the *induced* electrostatic potential ( $\hat{\mathbf{z}}$  is a unit vector perpendicular to the planar surface)

$$V(\mathbf{r},t) = \int d\mathbf{r}' \int dt' [\epsilon^{-1}(\mathbf{r}t,\mathbf{r}'t') - \delta(\mathbf{r}-\mathbf{r}')\delta(t-t')] \times U(\mathbf{r}',t'), \qquad (1)$$

where  $\epsilon^{-1}$  is the inverse of the longitudinal dielectric function. Since the system is translationally invariant in the  $\mathbf{r}_{\parallel} = (x, y)$  plane and time, we may Fourier transform with respect to space  $\mathbf{r}_{\parallel} - \mathbf{r}'_{\parallel} \rightarrow \overline{\mathbf{q}}$  and time  $t - t' \rightarrow \omega$ .

We take the response properties of the semi-infinite solid-state plasma to be given by the classical infinite-barrier model with bulk properties characterized by the random-phase approximation (RPA). In this approximation, which neglects the off-diagonal density-response matrix elements,  $\epsilon^{-1}(z,z';\overline{q},\omega)$  is given in the semi-infinite limit of plasma thickness by  $^{10}$ 

$$\begin{split} \epsilon^{-1}(z,z';\overline{q},\omega) &= \eta_{+}(-z) \left[ \delta(z-z') - \frac{e^{\frac{\overline{q}z}{D}}}{D\left(\overline{q},\omega\right)} \left[ \delta(z') - 2\eta_{+}(z')\kappa_{\infty}(z';\overline{q},\omega) \right] \right] \\ &+ \eta_{+}(z) \left[ v_{\infty}(z;\overline{q},\omega) \frac{\overline{q}}{D\left(\overline{q},\omega\right)} \left[ \delta(z') - 2\kappa_{\infty}(z';\overline{q},\omega)\eta_{+}(z') \right] + \left[ \kappa_{\infty}(z+z';\overline{q},\omega) + \kappa_{\infty}(z-z';\overline{q},\omega) \right] \eta_{+}(z') \right] \,. \end{split}$$

Here  $\eta_+(x)$  is the Heaviside unit step function, and the surface dispersion formula  $D(\overline{q},\omega)$  is given in terms of the bulk dielectric function  $\epsilon_B(\overline{q},q_z;\omega)$ , where  $q_z$  is the component of the wave vector perpendicular to the surface:

$$D(\overline{q},\omega) \equiv 1 + \frac{2\overline{q}}{\pi} \int_0^\infty dq_z \frac{1}{(q_z^2 + \overline{q}^2)\epsilon_R(\overline{q},q_z;\omega)} . \quad (3)$$

Also, we have

$$\kappa_{\infty}(z;\overline{q}\omega) \equiv \frac{1}{\pi} \int_{0}^{\infty} dq_{z} \frac{\cos(q_{z}z)}{\epsilon_{B}(\overline{q},q_{z};\omega)} , \qquad (4a)$$

$$v_{\infty}(z;\bar{q}\omega) \equiv \frac{1}{\pi} \int_0^{\infty} dq_z \frac{\cos(q_z z)}{(q_z^2 + q^2)\epsilon_R(\bar{q},q_z;\omega)} . \tag{4b}$$

The step functions  $\eta_{+}(z)$  and  $\eta_{+}(-z)$  in Eq. (2) separate the contributions to the scalar potential when the field point  $(\mathbf{r}_{\parallel}, z)$  is inside or outside the quantum plasma.

Assuming that the charged particle moves parallel to the surface at a distance  $z_0$  outside the plasma, we substitute Eq. (2) into Eq. (1) and obtain

$$V(\mathbf{r},t) = \frac{Ze}{[R^2 + (z_0 + |z|)^2]^{1/2}} - Ze \int d^2\bar{\mathbf{q}} \frac{1}{\pi \bar{q}} e^{-\bar{q}(z_0 + |z|)} \operatorname{Re} \left[ \frac{e^{i\bar{\mathbf{q}} \cdot \mathbf{R}}}{D(\bar{q}, q_z v)} \right]$$
(5a)

for the *outside* case (z < 0) and

$$V(\mathbf{r},t) = Ze \int d^2 \overline{\mathbf{q}} \frac{e^{-\overline{q}z_0}}{\pi} \operatorname{Re} \left[ e^{i\overline{\mathbf{q}} \cdot \mathbf{R}} v_{\infty}(z; \overline{q}, q_z v) \left[ \frac{1}{2} + \frac{1}{D(\overline{q}, q_z v)} \right] \right] - \frac{Ze}{\left[ R^2 + (z_0 + z)^2 \right]^{1/2}}$$
 (5b)

for the inside case (z > 0). Here Re(x) stands for the real part of x and R = (x - vt, y).

In the high-speed regime, we use the local approximation  $\epsilon_B(q,\omega) \approx (\omega^2 - \omega_p^2)/\omega^2$  in Eqs. (3) and (4) and then substitute the results into Eqs. (5);  $\omega_p$  is the bulk plasmon frequency in the long-wavelength limit. For z < 0, we obtain

$$V(\mathbf{r},t) \approx -Ze^{\frac{\omega_p^2}{2\pi}} \int_{-\infty}^{\infty} dq_z \int_{-\infty}^{\infty} dq_y \frac{1}{(q_x^2 + q_y^2)^{1/2}} e^{i(q_x\bar{x} + q_yy)} \exp[-(q_x^2 + q_y^2)^{1/2}(z_0 + |z|)] \frac{1}{\omega_p^2 - 2q_x^2 v^2 + i0^+},$$
 (6)

where  $\bar{x} = x - vt$ . Doing the  $q_y$  integral first, we obtain (see p. 17, No. 27 of Ref. 11)

$$V(\mathbf{r},t) = 4\frac{Ze}{2\pi}\omega_p^2 \int_0^\infty dq_x \cos(q_x \bar{x}) \frac{K_0(q_x [y^2 + (z_0 + |z|)^2]^{1/2})}{2q_x^2 v^2 - \omega_p^2} , \qquad (7)$$

where  $K_0(x)$  is a modified Bessel function and the integral in Eq. (7) is a Cauchy principal value. Using Parseval's trick to perform the integral in Eq. (7), we obtain the electrostatic potential outside the plasma for a charge moving at high speed outside as

$$V(\mathbf{r},t) = \frac{Ze\omega_{p}\pi}{2\sqrt{2}v}\cos\left[\frac{\omega_{p}\bar{x}}{v\sqrt{2}}\right] \left[\mathbf{L}_{0}\left[\frac{\omega_{p}}{v\sqrt{2}}[y^{2}+(z_{0}+|z|)^{2}]^{1/2}\right] - I_{0}\left[\frac{\omega_{p}}{v\sqrt{2}}[y^{2}+(z_{0}+|z|)^{2}]^{1/2}\right] + \frac{Ze\omega_{p}\sqrt{2}}{2v}\Phi_{1}\left[\frac{\omega_{p}|\bar{x}|}{v\sqrt{2}}, \frac{1}{|\bar{x}|}[y^{2}+(z_{0}+|z|)^{2}]^{1/2}\right],$$
(8)

where  $L_0(x)$  is a modified Struve function,  $I_0(x)$  is a Bessel function of imaginary argument, and

 $\Phi_1(\alpha,\beta) \equiv \int_0^1 du \frac{\sin[\alpha(u-1)]}{(u^2 + \beta^2)^{1/2}} . \tag{9}$ 

The first term in Eq. (8) exhibits oscillations of wave-

length  $2\sqrt{2\pi v/\omega_p}$  associated with the surface-plasmon frequency for small wave number,  $\omega_p/\sqrt{2}$ .

To obtain the induced electrostatic potential inside the plasma due to a very fast particle, we substitute the long-wavelength approximation for  $\epsilon_B(q,\omega)$  into Eq. (5b) and obtain

$$V(\mathbf{r},t) = \pi Z e \int \frac{d^2 \bar{\mathbf{q}}}{(2\pi)^2} e^{i\bar{\mathbf{q}} \cdot \mathbf{R} - \bar{q}z_0} \left[ 2 + \frac{\omega_p^2}{q_x^2 v^2 - \omega_p^2} + \frac{\omega_p^2}{2q_x^2 v^2 - \omega_p^2} \right] - \frac{Z e}{\bar{x}^2 + (z_0 + z)^2]^{1/2}} . \tag{10}$$

After performing the integrals in Eq. (10) (see Ref. 11, p. 16, No. 26), we obtain the electrostatic potential inside a semi-infinite plasma due to a fast charged particle. The result is

$$V(\mathbf{r},t) = \mathbf{Z}e\,\pi \left[ \Phi_0 \left[ \frac{\omega_p}{v} \right] + \Phi_0 \left[ \frac{\omega_p}{v\sqrt{2}} \right] \right] , \tag{11}$$

where the function and  $\Phi_0(x)$  is

$$\Phi_0(x) \equiv x^2 \int_{-\infty}^{\infty} dq_x \int_{-\infty}^{\infty} dq_y e^{i(q_x \bar{x} + q_y y)} \frac{\exp[-(q_x^2 + q_y^2)^{1/2}(z_0 + z)]}{(q_x^2 - x^2)(q_x^2 + q_y^2)^{1/2}} . \tag{12}$$

The wake potential induced by a swift charge in a homogeneous electron gas has been studied by several authors.<sup>12</sup> However, to interpret the various terms contributing to Eqs. (8) and (11) we evaluate the induced electric potential in the local approximation. We obtain

$$V_{B}(r_{\parallel},z;t) = \frac{2Ze}{\pi v} \omega_{p}^{2} \int_{0}^{\infty} d\bar{q} \, \bar{q} J_{0}(\bar{q}(y^{2}+z^{2})^{1/2}) \int_{0}^{\infty} d\omega \cos\left[\frac{\omega \bar{x}}{v}\right] \frac{1}{(\bar{q}^{2}+\omega^{2}/v^{2})(\omega^{2}-\omega_{p}^{2})} . \tag{13}$$

With the use of tables, we evaluate the  $\omega$  integral and obtain

$$V_B(r_{\parallel},z;t) = -Zev\omega_p^2 \int_0^{\infty} d\bar{q} \, \bar{q} J_0(\bar{q}(y^2+z^2)^{1/2}) \frac{1}{\omega_p^2 + v^2 \bar{q}^2} \left[ \frac{1}{\omega_p} \sin \left[ \frac{\omega_p \mid \bar{x} \mid}{v} \right] + \frac{1}{v\bar{q}} e^{-\bar{q}\bar{x}} \right]. \tag{14}$$

Calculation shows that

$$V_{B}(\mathbf{r},t) = \frac{Ze\omega_{p}}{2v} \sin\left[\frac{\omega_{p} \mid \overline{x} \mid}{v}\right] K_{0} \left[\frac{\omega_{p}}{v} r_{\perp}\right] - \frac{Ze\omega_{p}}{v} \left\{\pi/2\cos(\omega_{p} \mid \overline{x} \mid v) [I_{0}(\omega_{p}r_{\perp}/v) - \mathbf{L}_{0}(\omega_{p}r_{\perp}/v)] - \Phi_{1}(\omega_{p} \mid \overline{x} \mid /v r_{\perp}/\mid \overline{x}\mid)\right\},$$
(15)

where  $r_1 \equiv (y^2 + z^2)^{1/2}$ . These calculations show that the electric potential inside the electron-gas plasma consists of the direct unscreened Coulomb potential between the moving charge and an electron inside the plasma as well as a dipole term which has no counterpart in the bulk case. The long-wavelength electron-density fluctuations screen the Coulomb potential giving rise to the oscillations which are exhibited in the electric potential. The potential in Eq. (15) for the homogeneous electron gas exhibits oscillations of wavelength  $2\pi v/\omega_p$  associated with the long-wavelength bulk-plasmon frequency.

Referring to Eqs. (8) and (11), the electric potential for a semi-infinite electron gas has an oscillatory behavior of wavelength  $2\sqrt{2\pi v/\omega_p}$  associated with the low-wavenumber surface-plasmon frequency  $\omega_p/\sqrt{2}$ .

Figure 1 shows the wake potential  $V(z,R)/Zeq_F$  for y=0 in the R,z plane, as derived from Eq. (5b). One sees the distinct oscillations parallel to the R (i.e.,  $\bar{x}$ ) axis. The total potential is shown with contributions due to particle-hole excitations as well as surface-plasmon modes. The parameters used in computing Fig. 1 are given in the caption.

$$\rho(\mathbf{r},t) = -\frac{1}{4\pi e} \int_{-\infty}^{\infty} dz' \int \frac{d^2 \overline{q}}{(2\pi)^2} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{i(\overline{\mathbf{q}}\cdot\mathbf{r}_{\parallel}-\omega t)} \left[ \frac{\partial^2}{\partial z^2} - \overline{q}^2 \right] \left[ \epsilon^{-1}(z,z';\overline{q},\omega) - \delta(z-z') \right] U(z';\overline{q},\omega) . \tag{16}$$

This results in a force exerted on the moving charge by the quantum plasma given by

$$\mathbf{F} = e \int d\mathbf{r} \, \rho(\mathbf{r}, t) \nabla [V(\mathbf{r}, t) + U(\mathbf{r}, t)] \,, \tag{17}$$

where  $V(\mathbf{r},t)$  and  $\rho(\mathbf{r},t)$  are obtained from Eqs. (5) and (16), respectively. In a straightforward way, we obtain the components of the force parallel (||) and perpendicular (1) to the surface. These are

$$\mathbf{F}_{\parallel} = -2\pi \mathbf{Z}^{2} e^{2} \int_{-\infty}^{\infty} dz \int \frac{d^{2}\overline{q}}{(2\pi)^{2}} i \overline{\mathbf{q}} e^{-\overline{q} | z + z_{0}|} \epsilon^{-1} (-z_{0}, z; \overline{\mathbf{q}}, q_{x} v) , \qquad (18)$$

$$\mathbf{F}_{\perp} = -\pi \mathbf{Z}^{2} e^{2} \widehat{\mathbf{z}} \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz' \int_{-\infty}^{\infty} dz'' \int \frac{d^{2}\overline{q}}{(2\pi)^{2}} \exp[-\overline{q}(|z' + z_{0}| + |z'' + z_{0}|)]$$

$$\times \left[ \left[ \frac{\partial^{2}}{\partial z^{2}} - \overline{q}^{2} \right] \epsilon^{-1} (z, z'; \overline{q}, q_{x} v) + 2\overline{q} \delta(z - z') \delta(z' + z_{0}) \right]$$

$$\times \frac{\partial}{\partial z} \epsilon^{-1} (z, z''; -\overline{q}, -q_{x} v) . \qquad (19)$$

A detailed study of the force may be carried out with the use of Eq. (2) for the inverse dielectric function.

Substituting Eq. (2) into Eq. (18), calculation shows that

$$\mathbf{F}_{\parallel} = -\frac{Z^2 e^2}{\pi} \int d^2 \mathbf{\bar{q}} (\mathbf{\bar{q}}/\mathbf{\bar{q}}) e^{-2\mathbf{\bar{q}}z_0} \operatorname{Im} \left[ \frac{1}{D(\mathbf{\bar{q}}, q_x v)} \right] , \quad (20)$$

where Im(x) stands for the imaginary part of x. The different factors in Eq. (20) are intuitively understandable. Im(1/D) takes into account the process in which

energy is transferred to electrons by a probe coupled to the density fluctuations. The factor  $\exp(-2\bar{q}z_0)$  characterizes the decay of the force  $\mathbf{F}_{\parallel}$  as the distance  $z_0$  of the charge Ze from the surface in the region outside the metal increases. The friction parameter obtained by Ferrell  $et\ al.^{13}$  for the specular reflection model of a bounded electron gas may be immediately obtained from Eq. (20) since the fractional momentum loss of the particle per unit time is  $\mathbf{F}_{\parallel} \cdot \mathbf{v}$ .

Mahanty and Summerside, <sup>14</sup> as well as Muscat and Newns, <sup>15</sup> have calculated the force on a charged particle

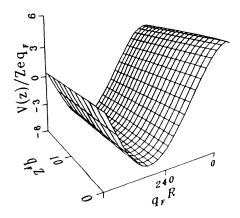


FIG. 1. Scalar electric potential inside a semi-infinite quantum plasma. A charged particle travels with velocity  $v = 0.5v_F = 0.4 \times 10^8$  cm sec<sup>-1</sup> outside the plasma in the positive x direction at a distance  $z_0 = 3q_F^{-1}$  from the planar surface located at z = 0. The interparticle spacing in units of the Bohr radius is  $r_s = 6$  and the effective mass of the electron is set equal to the bare mass  $m_e$ . The potential values were computed from Eq. (5b) with the use of the RPA longitudinal dielectric function of a bulk plasma at zero temperature.

moving with constant velocity parallel to a planar metal surface. The purpose of their calculation was to examine the effect of spatial dispersion on this force. The hydrodynamic model was employed in their calculations. In our treatment of spatial dispersion within the quantum plasma, both particle-hole excitations as well as surface and bulk-plasmon modes contribute at arbitrary velocity of the charged particle. Expressing the surface dispersion formula  $D(\bar{q},\omega)$  in terms of its real and imaginary parts,  $D=D_R+iD_I$ , the surface-plasmon contribution corresponds to  $\text{Im}(1/D)=-\pi\delta(D_R)$  and the contribution of the electron-hole spectrum corresponds to regions of frequency-wave-vector space where  $D_1$  is finite.

Harris and Jones<sup>16</sup> have discussed the interaction potential for a classical charged particle *impinging* on a metal surface which is simulated by a classical infinite barrier bounding a semi-infinite electron gas. There is no need to underscore the completeness of the work in Ref. 16. In the present paper we restricted our attention to fast-particle motion parallel to a planar surface. This may also be of interest to experimentalists. The closed-form expressions which we obtained illustrate that the general formulation of the problem may be applied to any model for which the inverse dielectric function can be derived in a tractable form. We hope that this preliminary investigation will stimulate the interest of experimentalists. More-detailed numerical results and applications will be presented elsewhere.

This work was supported by the Natural Sciences and Engineering Research Council of Canada, as well as the Alexander von Humboldt-Stiftung (G.G.) and by the National Science Foundation (M.L.G.).

<sup>&</sup>lt;sup>1</sup>J. Neufeld and R. H. Ritchie, Phys. Rev. **98**, 1632 (1955); **99**, 1125 (1955).

<sup>&</sup>lt;sup>2</sup>J. C. Ashley and P. M. Echenique, Phys. Rev. B **31**, 4655 (1985).

<sup>&</sup>lt;sup>3</sup>R. A. McCorkle and G. J. Iafrate, Phys. Rev. Lett. **39**, 1263 (1977)

<sup>&</sup>lt;sup>4</sup>P. M. Echenique, R. H. Ritchie, and W. Brandt, Phys. Rev. B 20, 2567 (1979).

<sup>&</sup>lt;sup>5</sup>J. C. Ashley and R. H. Ritchie, Phys. Status Solidi B 83, K159 (1977).

<sup>&</sup>lt;sup>6</sup>R. H. Ritchie, W. Brandt, and P. M. Echenique, Phys. Rev. B 14, 4808 (1976).

<sup>&</sup>lt;sup>7</sup>M. H. Day, Phys. Rev. B 12, 514 (1975).

<sup>&</sup>lt;sup>8</sup>V. N. Neelavathi, R. H. Ritchie, and W. Brandt, Phys. Rev. Lett. 33, 302 (1974).

<sup>&</sup>lt;sup>9</sup>D. S. Gemmell, J. Remillieux, J. C. Poizat, M. J. Gaillard, R. E. Holland, and Z. Vager, Phys. Rev. Lett. 34, 1420 (1975).

<sup>&</sup>lt;sup>10</sup>N. J. M. Horing, E. Kamen, and H.-L. Cui, Phys. Rev. B 32, 2184 (1985).

<sup>11</sup> Table of Integrals, Series and Products, edited by I. S. Gradshteyn and I. M. Ryzhik (Academic, New York, 1965).

<sup>&</sup>lt;sup>12</sup>A. L. Fetter and J. D. Walecka, Quantum Theory of Many-Particle Systems (McGraw-Hill, New York, 1971), pp. 158-162.

<sup>&</sup>lt;sup>13</sup>T. L. Ferrell, P. M. Echenique, and R. H. Ritchie, Solid State Commun. 32, 419 (1979).

<sup>&</sup>lt;sup>14</sup>J. Mahanty and P. Summerside, J. Phys. F 10, 1013 (1980).

<sup>&</sup>lt;sup>15</sup>Muscat and Newns, Surf. Sci. **64**, 649 (1977).

<sup>&</sup>lt;sup>16</sup>J. Harris and R. O. Jones, J. Phys. C 6, 3585 (1973).