

WAKE POTENTIAL AND WAKE BINDING ENERGY FOR PROTONS AND ANTIPROTONS

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We investigate the wake binding energies of electrons trapped in the first potential well caused by a swift proton and an antiproton in two different solids. Binding is possible in aluminium for both protons and antiprotons in a large range of velocities. In carbon the binding is drastically reduced when one takes into account realistic values of the damping.

A fast ion moving in condensed matter causes an oscillatory wake of the electron density fluctuations. The space–time distribution of such perturbations was first studied by Neufeld and Ritchie [1] and Ritchie [2]. Since then many authors have evaluated the wake potential using more sophisticated dielectric functions [3–9]. A brief discussion of the wake phenomena and related topics is given by Ritchie and Echenique [10,11].

Neelavathi, Ritchie and Brandt [3] considered the existence of wake-bound electrons trapped in the first well of the wake potential. When the ion is travelling along a target, these electrons emerge from the solid with the ion, and it has been speculated that they could give rise to one of the contributions to the convoy-electron distribution, that is, the distribution of accompanying free electrons travelling with nearly the same velocity as the ion when it leaves the target. Electron capture probabilities into wake-riding states are much larger in the case of negatively charged trailing ions than when positive ions are used, for the bound electron is located approximately three times closer to the ion in the former [12]. Capture and loss cross sections have been evaluated for the case of swift protons [13]. Several calculations of the wake binding energies have been carried out [3–9] and experimental data are consistent with the existence of such states [14] for negatively charged ions, while for positive ones no conclusion can be drawn [15]. Very recently a Monte Carlo simulation has been carried out to explore the possibility that wake-bound electrons can contribute to the cusps appearing in the forward electron emission using antiprotons as probes [12].

The wake potential (i.e., the scalar electric potential) in a homogeneous, isotropic medium due to a moving point charge Z_1 having a constant velocity v is given by

$$\Phi_w(b, z) = \frac{Z_1}{\pi v} \int_0^\infty Q J_0(Qb) dQ \int_{-\infty}^\infty \frac{e^{i\omega z/v}}{k^2 \epsilon_{k, \omega}} d\omega \quad (1)$$

(when relativistic effects are neglected), where b and z are cylindrical coordinates which refer to the direction of motion and are defined by $b = (x^2 + y^2)^{1/2}$ and $\tilde{z} = z - vt$ relative to the position $(x, y, z) = (0, 0, vt)$ of the charge. The wave number $k = (Q^2 + \omega^2/v^2)^{1/2}$ has a component Q in the b -direction.

We compute the binding energy in the first potential well for an electron which is located at $\tilde{z} \approx -3\pi v/2\omega_p$ for positive ions and $\tilde{z} \approx \pi v/2\omega_p$ for negative ones. The potential can be fitted by an expression of the form

$$V(b, \tilde{z}) = -\Phi_w = -V_0 + \frac{1}{2}\alpha^2 b^2 + \frac{1}{2}\alpha_0^2 (\tilde{z} - \tilde{z}_0)^2 \quad (2)$$

in the neighborhood of its minimum and hence the electron binding energies will be the usual ones for the harmonic-oscillator potential. The ground-state wave function in this approximation is of a Gaussian type:

$$\psi_0(b, \tilde{z}) = \left[\frac{\alpha^2 \alpha_0}{\pi^3} \right]^{1/4} e^{-\alpha b^2/2} e^{-\alpha_0 (\tilde{z} - \tilde{z}_0)^2/2}. \quad (3)$$

More accurate results can be obtained by using a variational method and taking as trial wave function the previous one and then minimizing the binding energy given by the expression

$$E_w = \langle \Psi_0 | (-\frac{1}{2}\nabla^2) | \Psi_0 \rangle + \langle \Psi_0 | -\Phi_w | \Psi_0 \rangle. \quad (4)$$

In our calculations we have used the plasmon-pole dielectric function for carbon ($r_s = 1.6$, r_s being defined by $n = 1/(3\pi/4r_s^3)$, where n is the density of the valence electrons) and aluminium ($r_s = 2$) and the extrapolated dielectric function proposed by Ritchie and Howie [16] which was obtained by fitting a sum of Drude-type functions to optical data and then extrapolating this result for $k \neq 0$. The latter is applied only to

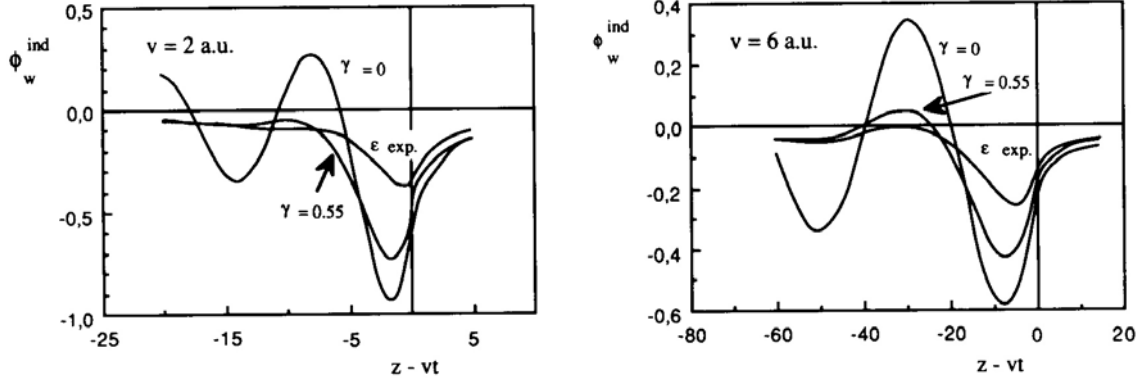


Fig. 1. The induced scalar potential created by a proton, $\phi_w^{\text{ind}} = \phi_w - 1/r$, is plotted here along the trajectory ($b = 0$) for two velocities ($v = 2$ a.u. and $v = 6$ a.u.). Three different dielectric functions have been used for each velocity to represent the response of the carbon medium; the plasmon-pole function with $r_s = 1.6$ and zero damping; the same function but making use of a realistic damping ($\gamma = 15$ eV); and finally the extrapolated dielectric function proposed by Howie and Ritchie [16].

carbon. The expression for it reads as follows:

$$\frac{1}{\epsilon_{k,\omega}} = 1 - \sum_{j=1}^n A_j \frac{\Omega_j^2(k) - \omega^2 + i\Gamma_j(k)\omega}{(\Omega_j^2(k) - \omega^2)^2 + \Gamma_j^2(k)\omega^2}, \quad (5)$$

where the damping and central frequency extrapolations to $k \neq 0$ are taken to be

$$\Gamma_j(k) = (\Gamma_j^2 + k^2/4)^{1/2}$$

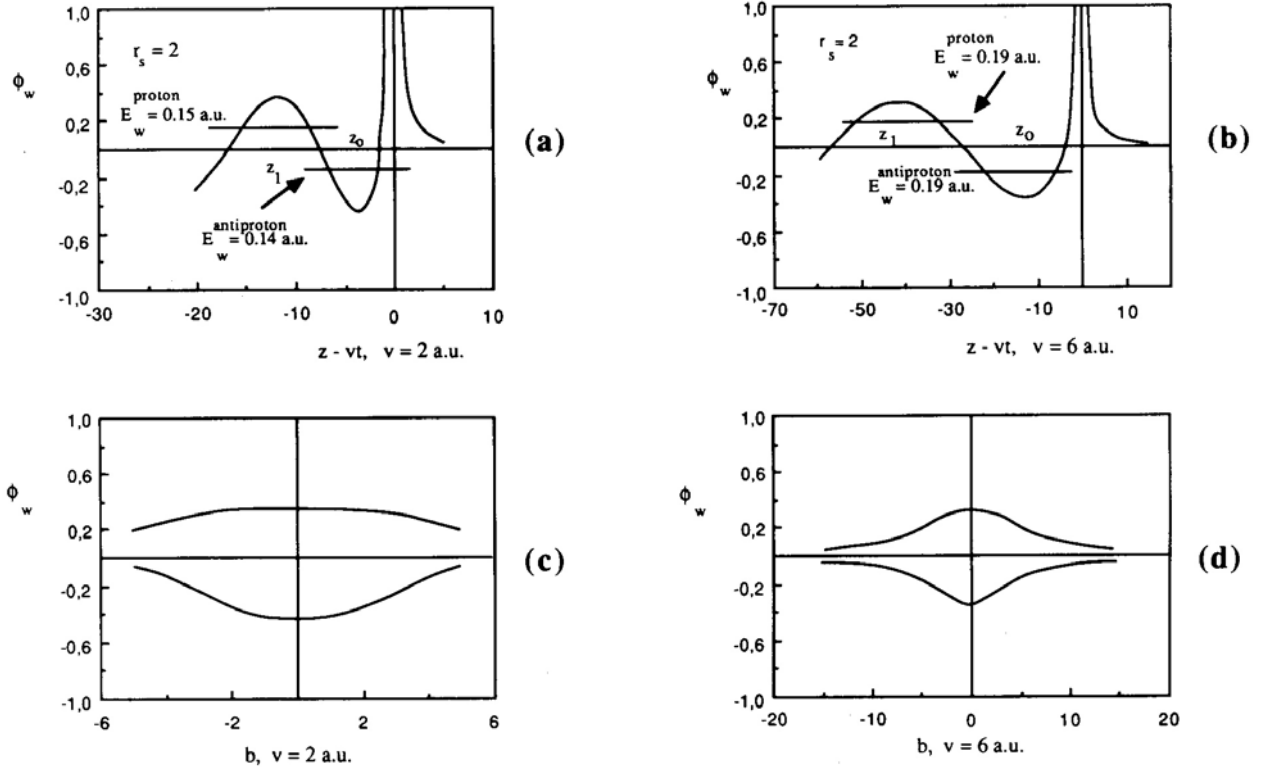


Fig. 2. Scalar potential created by a proton travelling in aluminium at $b = 0$. The medium is described by the plasmon-pole dielectric function with $r_s = 2$. Two different velocities have been plotted: $v = 2$ a.u. and $v = 6$ a.u. (c) and (d) represent perpendicular cuts of the potential at the position of its minimum and its maximum. For $v = 2$ these values are $\bar{z}_0 = -3.69$ a.u. and $\bar{z}_1 = -11.90$ a.u. respectively, while for $v = 6$ we get $\bar{z}_0 = -12.62$ a.u. and $\bar{z}_1 = -41.32$ a.u. The wake binding energy levels are also shown as horizontal bars, the binding being the distance from the bar to the $z-vt$ axis. The potential is given in a.u.

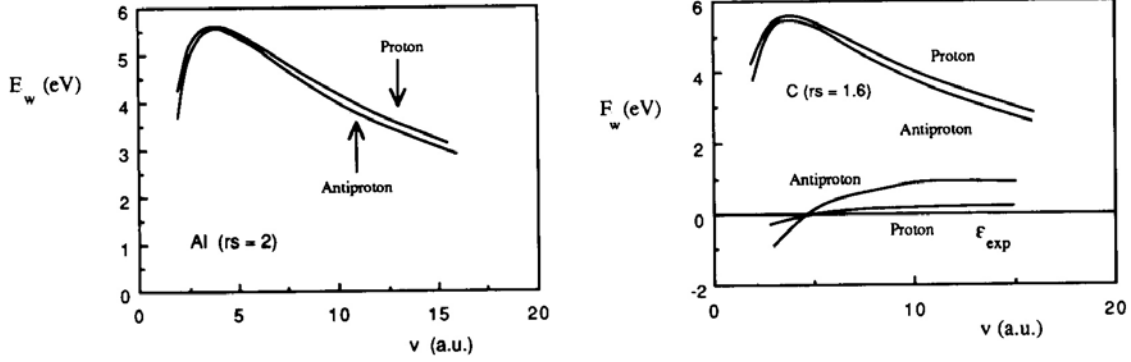


Fig. 3. Wake binding energies for an electron trapped in the first minimum of the potential created by a proton and an antiproton travelling in aluminium which is described by the plasmon-pole dielectric function with $r_s = 2$ and by the extrapolated fitted dielectric function for carbon. The wake binding is drastically reduced in carbon.

and

$$\Omega_j(k) = \left(\Omega_j^2 + (k^2/2)^p \right)^{1/p}$$

with $p = 2/3$. Γ_j and Ω_j are experimentally fitted constants [16].

In fig. 1 curves are plotted that show the induced scalar potential, that is, the wake scalar potential once the bare Coulomb potential is subtracted, calculated according to eq. (1) for a proton moving with a speed $v = 2$ a.u. and $v = 6$ a.u. and located at $\bar{z} = 0$. Damping effects seem to increase with the distance to the ion [3,8] and hence the binding energy of an electron trapped in the wake of a proton is strongly dependent upon the damping. This effect is smaller in the case of negatively charged leading ions. The extrapolated dielectric function deviates from this behaviour for it has a damping with dispersion. The medium is supposed to be carbon and is described by a plasmon-pole dielectric function with and without damping and also by the experimental dielectric function. The plasmon-pole dielectric function and the RPA one give nearly equivalent results in the range of the velocities used here [7]. The results obtained from the extrapolated dielectric function are

rather different: a deviation occurs from the plasmon pole behaviour but it coincides with the damping case at large distances. This can be explained because this function was fitted to optical data for $k = 0$, and a dispersive damping was assumed.

Fig. 2 shows the wake binding energies related to the wake potential for protons and antiprotons travelling in aluminium. The perpendicular cuts of the potential are shown at the position of the first minimum and maximum. The binding energy obtained for leading protons justifies the harmonic-well approximation, because at this energy level the potential is practically harmonic. For antiprotons a certain asymmetry can be observed with respect to the minimum of the potential.

The results for the wake binding energies are plotted in fig. 3. These values are obtained by minimizing eq. (4), using eq. (3) as wave function. Quite similar results can be obtained from the harmonic-well approximation expressed by eq. (2). Binding energies are computed for carbon and aluminium, described by the plasmon-pole dielectric function ($r_s = 1.6$ and $r_s = 2$ respectively) and for the extrapolated dielectric function given by eq. (5). Binding is drastically reduced in the latter, while the

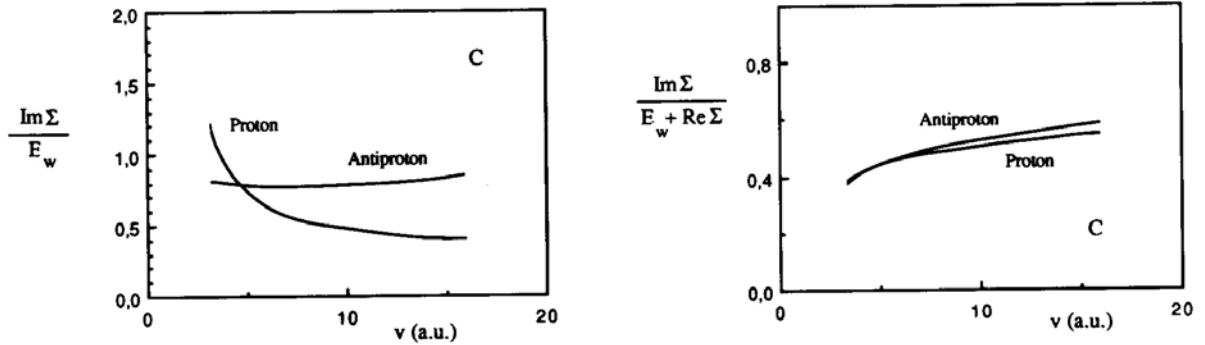


Fig. 4. Imaginary part of the self-energy (for $n' \neq n$; see the text) divided by E_w and $E_w + \text{Re } \Sigma$ for bound electrons trailing protons and antiprotons moving in carbon described by the plasmon-pole dielectric function.

plasmon-pole description allows it. This reduction of the binding energies when considering the extrapolated dielectric function is mainly due to its dispersive damping. Damping effects on the binding energies have already been studied by Ashley and Echenique [8].

In order to include nonlocal correlation effects we can obtain the dewaking, i.e., the rate of electron loss from the wake-riding state to the continuum. This is directly related to the imaginary part of the self-energy, while the real part of this quantity is simply added to the already computed binding energy. The expression that accounts for the self-energy of the bound electron-ion composite computed in the pair approximation reads as follows (see for instance refs. [9–11]):

$$\Sigma_{kn, E_{kn}} = \sum_{n'} \int \frac{d^3q}{(2\pi)^3} |\rho_{n'n}(\mathbf{q}) - Z_1 \delta_{n'n}|^2 \times v_q \left(\epsilon_{\mathbf{q}, \mathbf{v} \cdot \mathbf{q} + \omega_n - \omega_{n'}}^{-1} - 1 \right) \quad (6)$$

where \mathbf{k} is the momentum of the electron-ion composite and n labels the internal state. ω_n stands for the energy of the internal motion and $\rho_{n'n}(\mathbf{q}) = \langle n' | \exp(-i\mathbf{q} \cdot \mathbf{r}) | n \rangle$. ω_0 is the wake binding energy already computed ($\omega_0 \equiv E_w$). We take arbitrarily $n = 0$ to be the wake-riding bound state and $n > 0$ represents the states of the continuum. The term $n' = 0$ does not suppose a change in the internal state and hence can be interpreted as a contribution to the stopping power of the pair.

The results for the self-energy Σ , in the approximation used in ref. [5], are plotted in fig. 4. The imaginary part of the self-energy (for $n' \neq n$) is of the same order of magnitude as the binding energy. In the case of carbon, and using the plasmon-pole dielectric function, for protons and antiprotons (the results are quite similar indeed for both types of projectiles) the value of $\text{Im } \Sigma / (E_w + \text{Re } \Sigma)$, which gives the relative width of the wake-bound state, varies between 0.3 and 0.5 in the velocity range of interest ($v \sim 2\text{--}10$ a.u.).

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