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Self-consistent wake binding energies

P. M. Echenique
Cavendish Laboratory, University of Cambridge, Cambridge, CB3 0HE, England

W. Brandt*
Department of Physics, New York University, New York, New York 10003

R. H. Ritchie†
Health and Safety Research Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831

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We consider an electron that is trailing a swift ion in condensed matter and is trapped in the wake of the ion. The many-body theory of such a wake-bound state is developed, including polaronlike nonlocal self-trapping effects. The binding energy is computed self-consistently for several cases.

Since the early work of Neufeld and Ritchie[1] and Ritchie,[2] a great deal of experimental and theoretical work has been concerned with the distribution in space and time of perturbations of electron motion in solids caused by the passage of swift charged particles. Neelavathi, Ritchie, and Brandt[3] (NRB) pointed out that the oscillatory wake of electron density fluctuations trailing a fast ion may (a) influence the motion of nearby ions traveling with nearly the same velocity, and (b) give rise to wake-bound electron states. Subsequently, Brandt, Ratkowski, and Ritchie[4] showed experimentally and theoretically that the energy loss of proton clusters in solids is influenced by the presence of such wakes. They bombarded thin foils with swift $H_2{}^+$ and $H_3{}^+$ ions and found that the energy lost by an ion cluster in a foil was larger than that which would have occurred if the constituent ions were isolated from one another. The augmented energy loss is mainly due to the retarding effect of the wake of a leading ion on a trailing one. Gemmell *et al.*[5] found that it was necessary to include in their calculations the wake potential generated by the leading ion in order to explain the experimental distributions in energy and angle of protons emerging from crystals bombarded with $(\mathrm{HeH})^+$ beams under planar channeling conditions. The force acting on the trailing ion, arising because there is an excess of polarized electrons behind the leading ion, tends to move it towards the track when it is in the region

$$(-\pi v/\omega_p) < \tilde{z} < 0 .$$

Here $\mathbf{v}$ is the velocity, ω_p the plasma frequency, and $\tilde{z}$ is the coordinate along the direction of motion in a reference frame moving with the cluster with origin at the leading ion.

Recent experiments with swift channeled ions that have atomic numbers ranging from 5 to 9 and carry a single electron in a K-orbital state show resonant excitation of the electron due to coherent periodic perturbation by atoms in the bounding crystal rows.[6] A pronounced splitting in the resonant dips of the surviving fraction of these ions as a function of ion speed may be attributed in substantial portion to the wake of the ion.[7] Hybridization of excited hydrogenic levels on the ion (wake energy splitting) is a measure of the mean retarding force on the ion and has its origin in the wake.[7,8] Bell and co-workers[9] have measured the shift in the x-ray energy corresponding to the transition between the $^1P_1$ and $^1S_0$ multiplets in heliumlike sulfur projectiles. This decrease in binding energy may be attributed to the wake of the ion.[8]

When swift ions penetrate gaseous or solid targets, they emerge with accompanying free electrons traveling with nearly the same velocity as the ion. These are the so-called convoy electrons.[10] For gaseous targets this phenomenon was first observed by Crooks and Rudd[11] and explained by Macek[12] in terms of charge-transfer—to—continuum states associated with the Coulomb potential of ions moving in vacuum. Some investigators[13,14] have observed two components in the measured velocity distribution. It has been suggested[15] that some of the convoy electrons from solids might originate from wake-bound electrons trailing the swift ion in the solid. Part of the binding energy of such an electron must originate from polarization induced by the electron itself. Besides its intrinsic interest, a self-consistent calculation of the wake-bound electron state could lead to a better understanding of the spectrum of convoy electrons emerging from a solid. Little quantitative attention has been given to capture and loss processes involving weak-bound states.[16]

In the calculation of the wake potential by Neufeld and Ritchie,[1] a local dielectric function was used to represent the response of the medium. They also studied the shock-wave aspects of the wake by employing a spatially dispersive dielectric function. The local form was also used in the first papers of NRB (Ref. 3) and Gemmell *et al.*[5] Day[17] considered the effect of including plasmon dispersion on the binding energy of wake-bound electrons in an electron gas described by Lindhard's classical dielectric function.[18] More realistic calculations[19-21] using a quantal dielectric function differ appreciably from Day's.

These authors[19-21] presented a detailed study of the wake potential and of the density fluctuations within the plasmon-pole approximation and estimate the binding energy of wake-riding states. The concluded that although the binding energies are smaller than the ones calculated by NRB binding existed over the whole range of experimental velocities (2—20 a.u.). These results are in agreement with those found by Day and Ebel[22] who used a semiclassical dielectric function to represent the response of the medium and a variational procedure in which an exponential trial function was employed. The validity of the plasmon-pole approximation for this problem was confirmed by Mazarro *et al.*[23] who presented a detailed study of the wake using the full random-phase approximation dielectric function to describe the response of the electron gas. The binding energies calculated in the random-phase approximation[23,24] are in general agreement with the ones obtained within the plasmon-pole approximation for the medium response.

Although most of the theoretical work related to these problems is couched in the language of the electron gas, the results are of much wider applicability. They apply to semiconductors and insulators, where collective excitations centered at some resonance frequency ω_0 are known to exist.[25] Ritchie *et al.*[19] pointed out that the form of the wake may be influenced by the damping of the collective excitations in such media to a greater extent than in metals. Recently Ashley and Echenique[26] have evaluated the effect of damping using the Mermin[27] dielectric function to describe the response of the electron gas.

Most published theoretical work on the wake has used classical electrodynamics to describe the response of the medium via a causal dielectric function. Ritchie and Echenique[28] have presented a completely quantal treatment of the wake potential.

None of the calculations of the binding energies quoted above include the effect of the self-wake of the trapped electron on its binding energy in the trough of the leading ion. In fact, once the electron is trapped, polaronlike nonlocal effects in the wake will tend to increase the binding further. We present in this paper the results of a calculation including such effect. The response of the medium is taken to be the full random-phase-approximation (RPA) function.

SELF-ENERGY APPROACH

The quantum-mechanical interaction of an ion-bound electron with an interacting electron gas has been studied by Ritchie and Echenique.[28] The energy of a electron-ion complex can be described in terms of the destruction and creation operators $C_{\mathbf{K}n}, C^{\dagger}_{\mathbf{K}n}$. The electron-ion system has center-of-mass momentum $\mathbf{K}$ and internal state specified by the quantum index n. We have then, the free Hamiltonian H_0,

$$H_0=\sum_{\mathbf{K}}\sum_{n} E_{\mathbf{K}n}C^{\dagger}_{\mathbf{K}n}C_{\mathbf{K}n}\ , \tag{1}$$

where

$$E_{\mathbf{K}n}=\frac{K^2}{2(M+1)}+\omega_n\ . \tag{2}$$

Here ω_n is the energy of internal motion and M the ion mass. We use atomic units throughout ($e=\hbar=m=1$). The Hamiltonian of an interacting electron gas H_{eg} is

$$H_{\mathrm{eg}}=\sum_{\mathbf{p}} E_p A^{\dagger}_{\mathbf{p}}A_{\mathbf{p}}+\frac{1}{2\Omega}\sideset{}{'}\sum_{\mathbf{q}}\sum_{\mathbf{p}}\sum_{\mathbf{p}'} v_q A^{\dagger}_{\mathbf{p}-\mathbf{q}}A_{\mathbf{p}}A^{\dagger}_{\mathbf{p}'+\mathbf{q}}A_{\mathbf{p}'}\ , \tag{3}$$

where $A_{\mathbf{p}}$ is a destructive operator for an electron with momentum $\mathbf{p}$ and $E_p=p^2/2$. The normalization volume is Ω, $v_q=4\pi/q^2$ is the momentum representation of the Coulomb interaction energy, and the prime in the sum over q means that the term $\mathbf{q}=0$ is to be omitted to account for the presence of the uniform positive background charge. The energy of interaction between the ion-electron system and the electron gas may be written as

$$H_I=\frac{1}{\Omega}\sum_{\boldsymbol{\kappa}}\sum_{\mathbf{p}}\sum_{\mathbf{q}} v_q[\rho_{n'n}(\mathbf{q})-Z\delta_{n,n'}]C^{\dagger}_{\boldsymbol{\kappa}-\mathbf{q},n'}C_{\boldsymbol{\kappa},n}A^{\dagger}_{\mathbf{p}+\mathbf{q}}A_{\mathbf{p}}\ ,$$

where $\rho_{nn'}(\mathbf{q})=\langle n\,|\,e^{i\mathbf{q}\cdot\mathbf{r}}\,|\,n'\rangle$, is the matrix element of the density operator with respect to the static vectors of the internal motion, and Z is the ion charge. The Dyson equation for $G_{\kappa n,\omega}$, the exact Green's function of the interaction system, may be solved formally as

$$G_{\kappa n,\omega}=(\omega-E_{\kappa n}+\Sigma_{\kappa n,\omega})^{-1}\ , \tag{4}$$

where $\Sigma_{\kappa n,\omega}$ is the irreducible self-energy of the ion-electron pair due to the interaction with the medium. It may be represented by an infinite sum of diagrams in which interactions with the medium occur in all possible ways except that no diagrams are to be included that can be separated into two unconnected parts by cutting only a single line representing the propagator of the electron-ion pair. The analysis is similar to that for the interaction of a single particle with the medium. We work in the pair approximation.[29] Then we have

$$\Sigma_{\kappa n,\omega}=i\sum_{n'}\int\frac{d^3q}{(2\pi)^3}v_q M_q^2 \times\int\frac{d\omega'}{2\pi}G_{\boldsymbol{\kappa}-\mathbf{q},n',\omega-\omega'}(\epsilon^{-1}_{\mathbf{q},\omega'}-1)\ , \tag{5}$$

where $M_q=\rho_{nn'}(q)-Z\delta_{nn'}$.

A first order perturbative solution of this equation is found by replacing G by G^0 the free ion-electron Green's function in the right hand side of Eq. (5). G^0 is obtained from Eq. (4) by neglecting Σ. Then we have

$$\Sigma_{\kappa n,\omega}=i\sum_{n'}\int\frac{d^3q}{(2\pi)^3}v_q\,|\,M_q\,|^2\int\frac{d\omega'}{2\pi}(\epsilon^{-1}_{\mathbf{q},\omega'}-1)D\ , \tag{6}$$

where

$$D=[\omega-\omega'-E_{\boldsymbol{\kappa}-\mathbf{q},n'}+i\delta\,\mathrm{sgn}(E_{\boldsymbol{\kappa}-\mathbf{q},n'}-\mu)]^{-1}$$

and μ is the chemical potential. The ω' integral may be evaluated by rotating the contour so it lies along the imaginary axis of the ω' plane. If we are interested in the quasiparticle properties of the ion-electron gas we look at $\omega=E_{\kappa n}$ and then we get in the nonrecoil approximation, justified because $M\gg 1$,

$$\Sigma_{\kappa n,E_{\kappa n}}=\sum_{n'}\int\frac{d^3q}{(2\pi)^3}\,|\,\rho_{n'n}(q)-z\delta_{nn'}\,|^2 \times v_q(\epsilon^{-1}_{q,\mathbf{v}\cdot\mathbf{q}+\omega_n-\omega_{n'}}-1)\ , \tag{7}$$

where **v** is the velocity of the center of mass that we take to be the ion pair velocity since it has been assumed that $M \gg 1$.

From the structure of Eq. (7) it may be seen that distinct contributions to Σ originate from (a) transitions of the projectile in which its internal state remains unaltered and (b) transitions in which the internal state changes. Consider the four terms of Eq. (7) that appear when the absolute square bracket is multiplied out. The term proportional to Z^2 arises from the reaction of the ion on itself through polarization induced in the medium. This is of no interest here and will not be considered further. The two terms proportional to Z may be considered to originate (a) in the action of the ion on the electron and (b) in the action of the electron on the ion. The second of these may also be disregarded for present purposes. The remaining portion Σ_n^e of the self-energy is written as

$$\Sigma_n^e = \sum_{n'} \int \frac{d^3q}{(2\pi)^3} v_q \int d^3r\, u_{n'}^*(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} u_n(\mathbf{r}) \times [\rho_{nn'}^*(q) - Z\delta_{nn'}] \times (\epsilon_{q,\mathbf{v}\cdot\mathbf{q}+\omega_n-\omega_{n'}}^{-1} - 1) , \tag{8}$$

where $u_n(\mathbf{r}) \equiv \langle \mathbf{r} \mid n \rangle$ and $\delta_{nn'}$ is the Kronecker delta.

An expression for the self-energy as it depends on the coordinate **r** may be found directly by the argument that Σ_n^e in Eq. (8) may be considered to be the expectation value of the space-dependent self-energy $\Sigma_n^e(\mathbf{r})$ with respect to the wave function of relative motion in the nth state, i.e.,

$$\Sigma_n^e = \int d^3r\, u_n^*(\mathbf{r}) \Sigma_n^e(\mathbf{r}) u_n(\mathbf{r}) . \tag{9}$$

Equating the integrands of Eqs. (8) and (9), it follows that

$$\Sigma_n^e(\mathbf{r}) = \sum_{n'} \int \frac{d^3q}{(2\pi)^3} v_q \frac{u_{n'}^*(\mathbf{r})}{u_n^*(\mathbf{r})} e^{i\mathbf{q}\cdot\mathbf{r}} \times (\rho_{n'n}^* - Z\delta_{nn'})(\epsilon_{q,\mathbf{v}\cdot\mathbf{q}+\omega_n-\omega_{n'}}^{-1} - 1) . \tag{10}$$

The term in Eq. (10) that is proportional to Z_1,

$$\Sigma_{Z_1 w}(\mathbf{r}) = -Z_1 \int \frac{d^3q}{(2\pi)^3} v_q e^{i\mathbf{q}\cdot\mathbf{r}} (\epsilon_{q,\mathbf{v}\cdot\mathbf{q}}^{-1} - 1) , \tag{11}$$

may be seen to be essentially the same as the semiclassical wake potential,[1,2,19] i.e., the real part of Σ_{Zw} is the standard wake potential expressed in atomic units and multiplied by the electron charge (-1).

The part of Eq. (10) containing the factor $\rho_{nn'}^*(q)$ arises from the action of the electron's wake on the electron itself. The set of single-particle eigenfunctions $\{\langle \mathbf{r} \mid n \rangle\}$ that determines the matrix elements $\rho_{n'n}$ should be solved self-consistently, given that the self-energy enters the Schrödinger equation for $\{\langle \mathbf{r} \mid n \rangle\}$. An exact solution cannot be obtained. Useful approximations valid for eigenvalue spectra closely space compared with ω_0 may be obtained by invoking closure to evaluate the sum over n' in Eq. (10). If the spacing between eigenvalues is large compared with ω_0 it may be a good approximation to neglect all terms except for $n' = n$.[28]

Here we will consider the term $\rho_{n'n}(k)\rho_{n'n}^*(k)$ for $n' = n$, and will focus on the influence on the bound electron of the wake set up by the bound electron itself. Thus we get

$$\Sigma_{\kappa n, E_{\kappa n}} = \int \frac{d^3q}{(2\pi)^3} \mid \rho_{nn}(q) \mid^2 (\epsilon_{q,\mathbf{v}\cdot\mathbf{q}}^{-1} - 1) . \tag{12}$$

WAKE BINDING ENERGY

We want to calculate the ground-state energy of an electron trapped in the first trough of potential energy of the wake set up by a fast-moving leading ion, but taking into account the interaction of the trapped electron, now moving at a speed v relative to the medium, with the medium itself.

The scalar electric potential $\Phi^w(\mathbf{r},t)$ in an homogeneous isotropic medium due to a swift point charge Z_1 having constant velocity **v** is given in the reference frame of the moving ion by

$$\Phi_{Z_1}^w(\mathbf{r},t) = \frac{Z_1}{(2\pi)^2} \int \frac{d^3k}{k^2} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\epsilon_{k,\mathbf{k}\cdot\mathbf{v}}} , \tag{13}$$

or in a cylindrical coordinate system,

$$\Phi_{Z_1}^w(\mathbf{r},t) = \frac{Z_1}{\pi v} \int_0^\infty Q J_0(Qb) dQ \int_{-\infty}^{\infty} \frac{e^{i\omega\tilde{z}/v}}{k^2 \epsilon_{k,\omega}} d\omega . \tag{14}$$

The cylindrical coordinates b and $\tilde{z}$ refer to the direction of motion and are defined as $b = (x^2+y^2)^{1/2}$ and $\tilde{z} = z - vt$ relative to the positive $(x,y,z) = (0,0,vt)$ of the moving charge Z_1. The wave number $k = (Q^2+\omega^2/v^2)^{1/2}$ has component **Q** in the b direction.

An electron trapped in a bound state having a wave function $\Psi_0(\mathbf{r})$, will set up a wake potential given by

$$\phi^w(\mathbf{r},t) = -\int \rho_0(\mathbf{r}') \Phi_{Z_1=1}^w(\mathbf{r}-\mathbf{r}') d^3r' , \tag{15}$$

where $\rho_0(r)$ is the probability density of an electron in the state $\Psi_0(\mathbf{r})$: thus

$$\rho_0(\mathbf{r}) = \mid \Psi_0(\mathbf{r}) \mid^2 . \tag{16}$$

Thus the ground-state energy E_0 of an electron in a state described by a wave function will then be

$$E_0 = \langle \Psi_0 \mid (-\tfrac{1}{2}\nabla^2) \mid \Psi_0 \rangle + \langle \Psi_0 \mid (-\Phi_{Z_1}^w) \mid \Psi_0 \rangle + \tfrac{1}{2} \langle \Psi_0 \mid (-\Phi^w) \mid \Psi_0 \rangle , \tag{17}$$

where $-\frac{1}{2}\nabla^2$ is the kinetic-energy operator and we have included a factor of $\frac{1}{2}$ in the last term to account for the fact that it represents the self-energy of the electron due to the polarization of the medium that the electron itself has created. E_0 can be written more explicitly as

$$E_0 = \langle \Psi_0 \mid (-\nabla^2) \mid \Psi_0 \rangle + \frac{-Z_1}{2\pi^2} \int \frac{d^3k}{k^2} \frac{1}{\epsilon_{k,\mathbf{k}\cdot\mathbf{v}}} \int d^3r \rho(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{(-1)}{4\pi^2} \int \frac{d^3k}{k^2} \frac{\rho_0(\mathbf{r})}{\epsilon_{k,\mathbf{k}\cdot\mathbf{v}}} \times \int d^3r \int d^3r' \rho_0(\mathbf{r}) \rho_0(\mathbf{r}') e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} , \tag{18}$$

or

$$E_0=\langle\Psi_0|(-\tfrac{1}{2}\nabla^2)|\Psi_0\rangle+\left[-\frac{Z_1}{2\pi^2}\right]\int\frac{d^3k}{k^2}\frac{\rho_0(\mathbf{k})}{\epsilon_{k,\mathbf{k}\cdot\mathbf{v}}}+\left[\frac{-1}{4\pi^2}\right]\int\frac{d^3k}{k^2}\frac{|\rho_0(\mathbf{k})|^2}{\epsilon_{k,\mathbf{k}\cdot\mathbf{v}}}\,, \tag{19}$$

where $\rho_0(\mathbf{k})$ is the Fourier transform of the probability density $\rho_0(\mathbf{r})$ given by

$$\rho_0(\mathbf{k})=\int d^3r\, e^{i\mathbf{k}\cdot\mathbf{r}}\rho_0(\mathbf{r})\,. \tag{20}$$

We could try to solve for the minimum of binding energy E_0 by a variational procedure by using Eq. (19). Alternatively, an explicit expression for the position dependent wake may be derived and then Eq. (17) may be evaluated by performing the integrals in real space.

A calculation of this type using the full RPA result to represent the medium response will clearly be a formidable task. Fortunately in the region of the first trough of the potential energy curve the potential of the leading ion is well described by fitting it to a harmonic oscillator well,[3,17,21,23] both along and transverse to the direction of motion. We are interested in estimating the order of magnitude of the effect and therefore we shall approximate the potential created by the leading ion in the neighborhood of the first potential energy trough for an electron at $(\tilde{z}-\tilde{z}_1)$ by an expression of the form

$$-\Phi^{w}_{Z_1}(b,\tilde{z})=-V_0+\tfrac{1}{2}\alpha_1^2b^2+\tfrac{1}{2}\alpha_{01}^2(\tilde{z}-\tilde{z}_1)^2\,. \tag{21}$$

For the electronic bound state, we use a trial wave function of a Gaussian type

$$\Psi_0(\mathbf{r})=\left[\frac{\alpha^2\alpha_0}{\pi^3}\right]^{1/4}e^{-\alpha b^2/2}e^{-\alpha_0(\tilde{z}-\tilde{z}_1)^2/2}\,. \tag{22}$$

The potential set up by the localized electron is calculated by approximating the point-electron wake to be used in Eq. (15) by either a harmonic well or a Gaussian.

(i) *Harmonic well approximation.* We approximate the potential set up by a point electron in the neighborhood of $\tilde{z}_0$, by an expression of the form

$$\Phi^{w}_{1}(b,\tilde{z})=-\phi_0+\tfrac{1}{2}\beta^2b^2+\tfrac{1}{2}\beta_0^2(\tilde{z}-\tilde{z}_0)^2\,, \tag{23}$$

and obtain for the expectation value, $E(\alpha,\alpha_0)$, of the Hamiltonian of Eq. (18) using the trial wave function of Eq. (22)

$$E(\alpha,\alpha_0)=\frac{\alpha}{2}+\frac{\alpha_0}{4}+Z_1\left[-V_0+\frac{\alpha_1^2}{2\alpha}+\frac{\alpha_{01}^2}{4\alpha_0}\right]+\frac{1}{2}\left[-\phi_0+\frac{1}{2}\beta_0^2\tilde{z}_0^2\right]+\frac{\beta^2}{2\alpha}+\frac{\beta^2}{4\alpha_0}\,, \tag{24}$$

leading to a ground-state energy of

$$E_0=-Z_1V_0-\phi_0/2+\tfrac{1}{4}\beta_0^2\tilde{z}_0^2+\alpha_f+\tfrac{1}{2}\alpha_{0f}\,, \tag{25}$$

where

$$\alpha_f^2=\beta^2+Z_1\alpha_1^2\,, \tag{26}$$

$$\alpha_{0f}^2=\beta_0^2+Z_1\alpha_{01}^2\,. \tag{27}$$

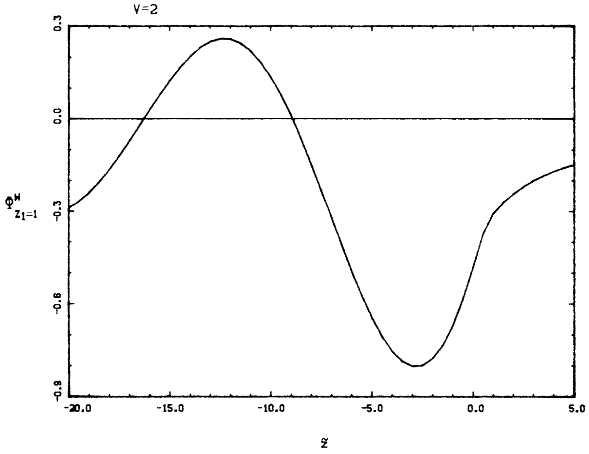

FIG. 1. Plot of the scalar electric potential generated in a metallic medium due to the presence of a swift proton with velocity $v=2$ a.u. The medium density corresponds to a one-electron radius of $r_s=2$ and the potential was computed using the RPA dielectric function. The potential of the bare ion has been subtracted out and the result is shown as a function of position along the track with $\tilde{z}=0$ corresponding to the location of the proton. All quantities are given in atomic units ($e=\hbar=m=1$). The value of $\pi v/\omega_p$ appropriate to this case is 10.3 a.u.

For very large charges this effect of the self-wake is given by the energy shift

$$\Delta=-\tfrac{1}{2}\phi_0+\tfrac{1}{4}\beta_0^2\tilde{z}_0^2+\frac{1}{Z_1}\left[\frac{\beta}{2\alpha_1}+\frac{\beta}{2\alpha_{01}}\right], \tag{28}$$

which increases slightly with increasing Z_1; the relative effect, of course, decreases with increasing Z_1.

(ii) *Gaussian approximation.* If the potential set up by the incident ion, is described by a Gaussian centered in the neighborhood of $\tilde{z}_0$, i.e.,

$$\Phi^{w}_{1}(b,\tilde{z})=-\phi_0e^{-\beta b^2}e^{-\beta_0(\tilde{z}-\tilde{z}_0)^2}\,, \tag{29}$$

then the potential created by the bound state charge distribution can be easily evaluated and is given by

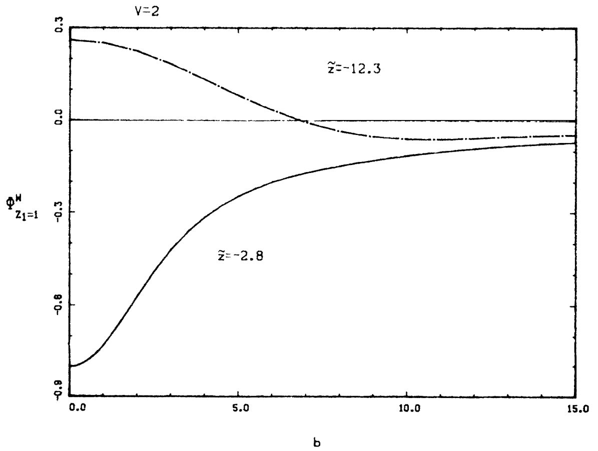

FIG. 2. Plot of the scalar electric potential calculated under the same assumptions as those of Fig. 1. The wake potential is given as a function of lateral distance b from the track for two different values of $\tilde{z}$. All quantities are given in atomic units. The value of $\pi v/\omega_p$ appropriate to this case is 10.3 a.u.

TABLE I. Binding energy of an electron trapped in the first trough of potential energy for a proton moving with velocity v in a medium with density corresponding to that in aluminum ($r_s = 2$). The medium response is described in the RPA. E_0 is the binding energy in eV without inclusion of the self-wake effect. Δ_{HW} and Δ_G are the extrabinding produced by the self-wake in the harmonic well (HW) and Gaussian approximations (G) to the trapped electron well described in the text.

v	E_0	Δ_{HW}	Δ_G
2	0.85	5.1	3.11
4	4.24	2.64	2.23
6	4.63	2.3	1.74

TABLE II. Additional binding energy Δ_G in electron volts due to the self-wake. The Gaussian approximation is used for the trapped electron wake for ions of charges Z_1 (1,2,5) moving at velocities v (2,4,6) in an electron gas of density corresponding to that of aluminum ($r_s = 2$). The electron gas response is described in the random-phase approximation. Numbers in parentheses are values of E_0 in eV.

	Z_1		
v	1	2	5
2	3.11 (0.85)	3.68 (7.5)	4.47 (29.5)
4	2.23 (4.24)	2.47 (10.5)	2.83 (37.0)
6	1.74 (4.63)	1.85 (12.0)	1.94 (35.5)

$$\phi^w(r,t) = -\phi_0 \left[\frac{\alpha^2 \alpha_0}{\pi^3} \right]^{1/2} \frac{\pi^{3/2}}{(\alpha+\beta)(\alpha_0+\beta_0)} \times \exp\left[\frac{-\alpha\beta}{\alpha+\beta} b^2 \right] \exp\left[-\frac{\alpha_0\beta_0}{\alpha_0+\beta_0} (\tilde{z}-\tilde{z}_0)^2 \right] . \tag{30}$$

The expectation value of the Hamiltonian is then

$$E(\alpha,\alpha_0) = \frac{\alpha}{2} + \frac{\alpha_0}{4} + Z_1 \left[-V_0 + \frac{\alpha_1^2}{2\alpha} + \frac{\alpha_{01}^2}{4\alpha_0} \right] - \frac{\phi_0}{2} \left[\frac{\alpha}{\alpha+\beta} \right] \left[\frac{\alpha}{\alpha+\gamma} \right] \left[\frac{\alpha}{\alpha_0+\beta_0} \right]^{1/2} \times \left[\frac{\alpha_0}{\alpha_0+\gamma_0} \right]^{1/2} \exp - \frac{\alpha_0\gamma_0}{\alpha_0+\gamma_0} \tilde{z}_0^2 , \tag{31}$$

where

$$\gamma = \alpha\beta/(\alpha+\beta) , \tag{32}$$

and

$$\gamma_0 = \alpha_0\beta_0/(\alpha_0+\beta_0) . \tag{33}$$

RESULTS

We have calculated the wake potential using the random phase approximation[18,23] to the dielectric function to describe the response of the medium. The results of such calculation along the incident ion trajectory are shown in Fig. 1 for an ion moving with velocity $v = 2$ in a medium with an electron density corresponding to that of aluminum ($r_s = 2$). In Fig. 2, we show for $v = 2$ the wake potential of the leading ion in the transverse direction both at the first trough of electron potential energy $\tilde{z}_1 = -12.3$ together with the wake created by a point electron at the position of the first minimum for the electron $\tilde{z}_0 = -2.8$.

In Table I, we show the binding energy of an electron trapped in the first minimum of potential energy for a proton moving with velocity v in a medium with density equivalent to that of aluminum. We show the binding energies calculated with and without inclusion of the trapped electron self-wake effects. We show the results obtained by using the two approximations described in the text: the harmonic well approximation, denoted as HW, and the Gaussian approximation. The harmonic well fitting has been chosen so as to give an overestimation of the self-wake effect while the Gaussian gives an underestimate. A reasonable description could be obtained by taking the mean of the two numbers.

In Table II, we show the increase in binding due to the self-wake of the trapped electron for different velocities and different ionic charge. The binding increasing slightly with increasing Z_1 [see Eq. (28)] the relative effect, of course, decreasing with increasing ionic charge. For $v = 2$ and $Z_1 = 5$ ($\Delta/E_0 \sim 0.1$) while at $Z_1 = 1$ there would be practically no binding without the self-generated wake effect.

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[*] Deceased.

[†] Also Department of Physics, University of Tennessee, Knoxville, TN 37996.

[1] J. Neufeld and R. H. Ritchie, Phys. Rev. **98**, 1632 (1955); **99**, 1125 (1955).

[2] R. H. Ritchie, Ph.D. thesis, University of Tennesse, 1959 (unpublished).

[3] V. N. Neelavathi, R. H. Ritchie, and W. Brandt, Phys. Rev. Lett. **33**, 302, 670(E) (1974); **34**, 560(E) (1975).

[4] W. Brandt, A. Ratkowski, and R. H. Ritchie, Phys. Rev. Lett. **33**, 1325 (1974); **35**, 130(E) (1975).

[5] D. S. Gemmell, J. Remillieux, M. J. Gaillard, and R. E. Holland, and F. Vager, Phys. Rev. Lett. **34**, 1920 (1975).

[6] S. Datz, C. D. Moak, O. H. Crawford, O. H. Krause, M. F. Dittner, P. F. del Campo, J. G. Biggerstaff, J. A. Miller, P. D. Hvelplund, P. Hvelplund, and H. Knudsen, Phys. Rev. Lett. **40**, 843 (1978).

[7] O. H. Crawford and R. H. Ritchie, Phys. Rev. A **20**, 1848 (1979).

[8] J. Tejada, P. M. Echenique, O. H. Crawford, and R. H.

Ritchie, Nucl. Instrum. Methods **170**, 249 (1980).

[9] F. Bell, H. O. Betz, H. Panke, and W. Stehling, J. Phys. B **9**, 3017 (1967); D. H. Jakubassa, J. Phys. C **10**, 4491 (1977).

[10] R. Laubert, I. A. Sellin, C. R. Vane, M. Sufer, S. B. Elston, G. D. Alton, and R. S. Thoe, Phys. Rev. Lett. **41**, 712 (1978).

[11] G. B. Crooks and M. E. Rudd, Phys. Rev. Lett. **25**, 1599 (1970).

[12] J. Macek, Phys. Rev. A **1**, 235 (1970).

[13] A. Gladieux and A. Chateau-Thierry, Phys. Rev. Lett. **47**, 786 (1981).

[14] R. Latz, G. Astner, H. J. Frischkorn, P. Koschar, J. Pfenning, J. Schrader, and K. O. Groeneveld, Nucl. Instrum. Methods **194**, 315 (1982).

[15] W. Brandt and R. H. Ritchie, Phys. Lett. **62A**, 374 (1977).

[16] See, however, Y. Yamazaki and N. Oda, Nucl. Instrum. Methods **194**, 415 (1982).

[17] M. H. Day, Phys. Rev. B **12**, 514 (1975).

[18] J. Lindhard, K. Dan. Vidensk. Selsk. Mat.-Fys. Medd. **28**, No. 8 (1954).

[19] R. H. Ritchie, W. Brandt, and P. M. Echenique, Phys. Rev. B **14**, 4808 (1976); P. M. Echenique, Ph.D. thesis, University of Barcelona, 1977 (unpublished).

[20] P. M. Echenique, R. H. Ritchie, and W. Brandt, Phys. Rev. B **20**, 2569 (1979).

[21] P. M. Echenique and R. H. Ritchie, Elhuyar **17**, 1 (1979).

[22] M. H. Day and M. Ebel, Phys. Rev. B **19**, 3434 (1979).

[23] A. Mazarro, P. M. Echenique, and R. H. Ritchie, Phys. Rev. B **27**, 4117 (1983).

[24] P. M. Echenique and R. H. Ritchie, Phys. Rev. B **21**, 5854 (1980).

[25] W. Brandt and R. H. Ritchie, in *Physical Mechanisms in Biology,* edited by R. D. Cooper and R. W. Wood (available from National Technical Information Service, U.S. Department of Commerce, Springfield, VA 22151) (Conference Proceedings No. CONF-721001), pp. 20—40 ; R. H. Ritchie and W. Brandt, in *Proceedings of the Fifth International Radiation Congress,* H. I. Adler and W. K. Sinclair (Academic, New York, 1975), pp. 315—324.

[26] J. C. Ashley and P. M. Echenique, Phys. Rev. B **31**, 4655 (1985).

[27] D. W. Mermin, Phys. Rev. B **1**, 2362 (1970).

[28] R. H. Ritchie and P. M. Echenique, Ann. Israeli Physical Society **4**, 245 (1981).

[29] See, e.g., T. D. Schultz, *Quantum Field Theory and the Many-Body Problem* (Gordon and Breach, New York, 1964), p. 93.