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Wake potential of swift ions in solids

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Valence-electron density fluctuations are expected to form wakes trailing charged particles moving through condensed matter with velocities larger than the Bohr velocity. We compute the resulting wake potential with a quantum-mechanical dielectric response function of the electron gas which includes plasmon dispersion as well as single-particle effects at the densities of metallic conduction electrons. The binding energy of electrons trapped in this potential ranges from ~5 eV behind protons to ~50 eV behind heavy ions moving with kinetic energies ~1 MeV/amu. The effects of quantum fluctuations on the binding energy and the lifetime of the wake-riding state are estimated.

INTRODUCTION

Recent research 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[1] (NRB) pointed out that the oscillatory wake of electron density fluctuations trailing a fast ion in a solid may (a) influence the motion of nearby ions traveling with nearly the same velocity, and (b) give rise to wake-bound electron states. Brandt, Ratkowski, and Ritchie[2] showed experimentally and theoretically that the energy loss of proton clusters in solids is influenced by the presence of these wakes. Arista and Ponce[3] derived an analytical approximation for the cluster stopping power. Gemmell *et al.*[4] studied the angular distribution of protons emerging from crystals bombarded with $(HeH)^+$ beams under planar channeling conditions. They found that in order to account for their measurements it is necessary to include the wake potential generated by the leading ion in their particle-transmission calculations, and used the expression for the wake potential employed by NRB.

For emphasis and simplicity, NRB presented a starkly schematized representation of the wake potential accompanying a swift ion. It was derived using a local metallic dielectric function to represent the response of valence electrons in the solid.[5] The binding energies of wake-bound electrons trailing ions as a function of ion charge and velocity were estimated variationally.[6] Brandt and Ritchie[7] have given an account of current work on wake phenomena.

Recently, Day[8] has 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.[9] The wake-binding energies in such a medium were found to be much smaller than those given by NRB. In particular, his treatment reduces binding energies behind 0.5-MeV protons from ~10 eV, calculated by NRB, to ~0.1 eV or less. This would preclude detection of wake-riding states behind protons.

We return to the question of binding energies of wake-riding states to explore the role played by quantum effects in the dielectric response function of the medium. In the range of short wavelengths, where single-particle recoil enters, quantum effects could become important in determining the potential close to the track. The quantum dielectric function of the electron gas can be expressed in analytical form in Lindhard's pair approximation.[10] It is known to describe many properties of real metals.[11] The full expression for the wake potential in this approximation becomes quite cumbersome and opaque. We have simplified, therefore, the quantum dielectric response function such that it retains the essential features of plasmon dispersion and particle-hole excitation while making the wake potential tractable. As a result we obtain more realistic estimates of wake-binding energies than those given by NRB and by Day. Our approach opens the way for the study of new aspects of the wake phenomenon. A full account of our numerical results will be published elsewhere.

WAKE POTENTIAL

Starting with the form employed by NRB, we write for the scalar electric potential $\Phi(\vec{r}, t)$ in an homogeneous isotropic medium due to a swift point charge Ze having constant velocity $\vec{v}$,

$$\Phi(\vec{r}, t) = \frac{Z}{\pi v} \int_0^\infty \kappa\, d\kappa\, J_0(\kappa\rho) \times \int_{-\infty}^{\infty} d\omega \exp\left(\frac{i\omega\bar{z}}{v}\right) k^{-2}\epsilon^{-1}(k, \omega). \tag{1}$$

We use atomic units throughout. The cylindrical

coordinates, $\rho=(x^2+y^2)^{1/2}$ and $\tilde{z}=z-vt$, are defined relative to the position of the charge, $(0,0,vt)$, at time t for the field point $\vec{r}=\vec{r}(x,y,z)$. The wave number k is related to the integration variable as $k^2\equiv\kappa^2+\omega^2/v^2$. If we use for the dielectric function of the medium, $\epsilon(k,\omega)$, the quantum expression appropriate for high densities,[10] we find that Eq. (1) must be evaluated numerically by double quadratures. For the present we employ a simpler expression

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

which should give an accurate description of the potential at points close to the ion track. In Eq. (2), $\beta^2=\frac{3}{5}v_F^2$ is a constant related to the Fermi velocity v_F in the electron gas of plasmon frequency ω_p, and σ is a small damping constant. Equation (2), through the term proportional to k^4, gives an approximate representation of the single-particle response of the medium with correct asymptotic behavior for large k. It satisfies the sum rules

$$\int_0^\infty \omega\,\mathrm{Im}[\epsilon(k,\omega)]\,d\omega=\int_0^\infty \omega\,\mathrm{Im}\left(\frac{-1}{\epsilon(k,\omega)}\right)d\omega=\tfrac{1}{2}\pi\omega_p^2, \tag{3}$$

and should be sufficiently accurate for our purposes over the whole (k,ω) plane. Indeed, there is extensive evidence that the plasmon-pole approximation, Eq. (2), to the dielectric function gives good accounts of the valence-electron contributions to the dynamic properties of solids.[12]

We substitute Eq. (2) into Eq. (1), perform the ω integration by closing the contour in the lower half-plane, and obtain an expression valid in the space behind the charged particle. Writing $\Phi=\Phi_1+\Phi_2+\Phi_{sc}$, we find in the limit $\sigma\to 0$,

$$\Phi_1(\tilde{z},\rho)=Z\sqrt{2}\,\omega_p^2\int_0^{Q_c}dQ\,QJ_0(\sqrt{2}\,\rho Q)\times\frac{\sin(\tilde{z}[2(\alpha-\xi)]^{1/2})}{\xi(\alpha-\xi)^{1/2}\,|Q^2+\alpha-\xi|} \tag{4}$$

and

$$\Phi_2(\tilde{z},\rho)=-\frac{Z}{\sqrt{2}}\,\omega_p^2\int_{Q_c}^\infty dQ\,QJ_0(\sqrt{2}\rho Q)\frac{e\sqrt{2}\delta\tilde{z}}{\gamma\delta}\times\mathrm{Re}\left(\frac{\exp(i\sqrt{2}\gamma\tilde{z})}{(\gamma-i\delta)[Q^2+(\gamma-i\delta)^2]}\right), \tag{5}$$

with the abbreviations,

$$Q_c=(1/\sqrt{2}v)(\tilde{v}^4-\omega_p^2)^{1/2},\quad \alpha=\tilde{v}^2-Q^2,$$

$$\xi=(\tilde{v}^4-2v^2Q^2-\omega_p^2)^{1/2},\quad \gamma=(1/\sqrt{2})(G+\alpha)^{1/2},$$

$$\delta=(1/\sqrt{2})(G-\alpha)^{1/2},$$

$$G=(Q^4+2\beta^2Q^2+\omega_p^2)^{1/2},\quad \tilde{v}^2=v^2-\beta^2.$$

Qualitatively, Φ_1 represents the oscillatory contribution to the wake potential due to plasmon excitations, and Φ_2 a part due to particle-hole excitations.

The potential Φ_{sc} represents the contribution to Φ from the poles in the ω plane of the factor k^{-2} in Eq. (1). This portion of the scalar potential is nonoscillatory in the variable $\tilde{z}$. It may be regarded as describing the bare potential of the charged particle, screened in a nonspherically symmetric manner by density fluctuations trailing the particle. In the notation of NRB, $\Phi_{sc}=Z\omega_p g(\vec{r})/v$, where

$$g(\vec{r})=\int_0^\infty\frac{x^2}{x^2+1}J_0\left(\frac{x\omega_p\rho}{v}\right)\exp\left(\frac{-x\omega_p|\tilde{z}|}{v}\right)dx. \tag{6}$$

The potential Φ_{ind} induced by the enhancement δn of the mean electron density n_0 near the projectile is of interest.[13] At the position of the projectile, $|\vec{r}|\to 0$, $\Phi_{ind}(\vec{r})=\Phi(\vec{r})-Z/r$ becomes $\Phi_{ind}(0)=-\pi Z\omega_p/2v+\Delta$. The first term is contributed by Φ_{sc}. The quantity Δ is small by comparison and derives from Φ_2 originating mainly from single-particle excitations. Equations (4) and (6) reveal that the contributions from Φ_1 and Φ_{sc} to the density enhancement, $\delta n=-\nabla^2\Phi/4\pi$, at $|\vec{r}|=0$ are zero. The enhancement comes mainly from single-particle processes underlying Φ_2 and diminishes as v^{-1} for $v\gg 1$. In the low-density limit $\omega_p\to 0$, δn approaches the value given by Coulomb scattering theory.[14]

WAKE-BINDING ENERGIES

We have carried out a numerical study of the wake potential in terms of Eqs. (4) and (5). In the neighborhood of the first potential trough for electrons at distances $\tilde{z}_0\simeq 3\pi v/2\omega_p$ behind the ion, Φ_2 and Φ_{sc} are both negligible compared with Φ_1. We computed the binding in the first potential trough by fitting the potential near its minimum with $-e\Phi\approx -V_0+a\rho^2+b(\tilde{z}-\tilde{z}_0)^2$, and calculating electron binding energies in this harmonic oscillator potential in the usual manner. Behind protons in the velocity range under discussion, the wave function of wake-bound electrons extends over ~1.5 a.u., and more localized behind particles of higher charge. We estimate that the fitting procedure introduces uncertainties $\lesssim 3\%$ in the binding energies.

Figures 1, 2, and 3 show wake-binding energies E_w, so computed for protons, oxygen ions, and sulphur ions (solid curves), and the corresponding energies calculated in the approximation of NRB (dashed curves). Our binding energies are somewhat smaller but of the same order of magnitude than those of NRB. It is instructive that they turn

out to be much larger than those found by Day based on a classical dielectric function. The approximation to the quantum-mechanical $\epsilon(k, \omega)$ used here, Eq. (2), should give an accurate potential close to the particle track. This domain is very important in obtaining reliable values of E_w. The results of the present treatment support the general conclusions reached by NRB about the wake states of electrons trailing swift particles in condensed matter.

CORRELATION EFFECTS

Nonlocal correlation effects decrease the electron density in the neighborhood of a wake-bound electron, resulting in an increase in the binding energy compared with the values shown in Figs. 1–3. This is the dynamical analog in an electron gas of the correlation effects which give rise to polarons in solids. The real part of the self-energy of a wake-bound electron gives the additional binding due to correlations. The imaginary part describes dewaking, i.e., the rate of loss of the electron from the wake-riding state due to quantum fluctuations of the system.

We estimate the self-energy $\Sigma(\omega, \vec{\kappa}, n)$ in the pair approximation as

$$\Sigma(\omega, \vec{\kappa}, n) = \frac{i}{\Omega} \sum_{\vec{\kappa}'} \sum_{n'} \sum_{\vec{k}} \int \frac{d\omega'}{2\pi} |W|^2 \frac{4\pi}{k^2} \left(\frac{1}{\epsilon_{k,\omega'}} - 1 \right) \times G(\omega - \omega', \vec{\kappa}', n'), \quad (7)$$

where Ω is the normalization volume of the system and $G(\omega, \vec{\kappa}, n)$ the Green function of the leading-ion and wake-riding–electron pair. The pair is considered to be in its nth state of internal excita-

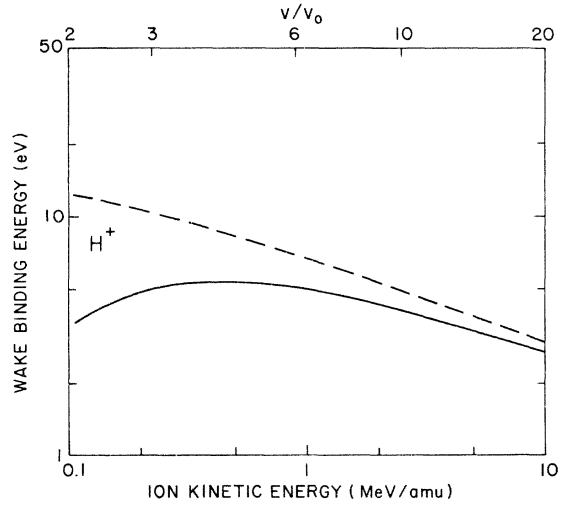

FIG. 1. Wake-binding energies of an electron in the first potential trough behind a fast proton in an electron gas at a density corresponding to the conduction band in Al metal. The lower solid curve shows the present results, while the dashed curve shows the results of NRB (Ref. 1).

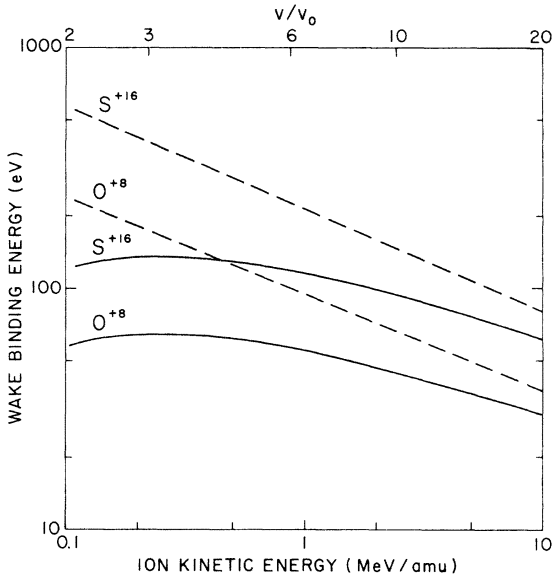

FIG. 2. Wake-binding energies of an electron in the first potential trough behind a fast bare O^{+8} ion and S^{+16} ion in an electron gas at a density corresponding to the conduction band in Al metal. The solid curves show the present results, while the dashed curves show the results of NRB (Ref. 1).

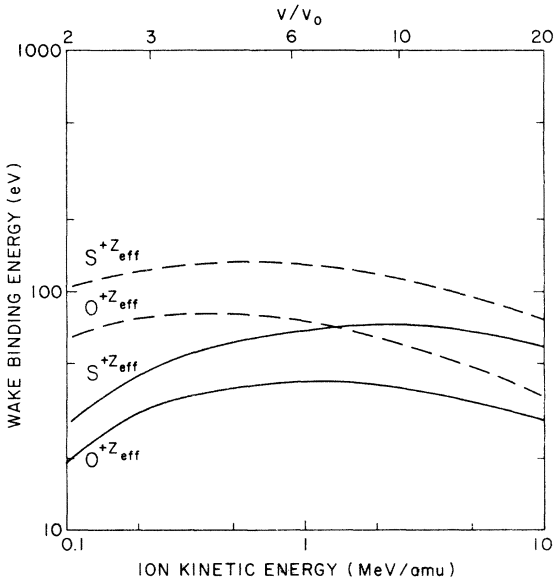

FIG. 3. Wake-binding energies of an electron in the first potential trough behind a fast $O^{+Z_{\text{eff}}}$ ion and $S^{+Z_{\text{eff}}}$ ion, where $Z_{\text{eff}}(v) = Z[1 - \exp(-v/Z^{2/3}v_0)]$, in an electron gas at a density corresponding to the conduction band in Al metal. The solid curves show the present results, while the dashed curves show the results of NRB (Ref. 1).

tion and described by a state vector $|\vec{\kappa}, n\rangle$ of eigenenergy $\omega_{\vec{\kappa},n}$, where $\vec{\kappa}$ is the center-of-mass momentum of the pair. The matrix element W of the vertex interaction between the pair and the medium can be approximated by

$$W(\vec{\kappa}', n', \vec{\kappa}, n, \vec{k}) = \langle \vec{\kappa}', n' | e^{-i\vec{k}\cdot\vec{r}} | \vec{\kappa}, n \rangle , \tag{8}$$

where $\vec{r}$ denotes the position of the wake-riding electron. The difficult task of solving Eq. (7) self-consistently by accounting for the effect of correlations on the wave function of the wake-bound electron will not be attempted here. Instead, we replace the Green function by the non-interacting form $(\omega - \omega_{\vec{\kappa},n} + i\delta)^{-1}$, employ a harmonic-oscillator wave function for the electron ground state, and approximate excited states by plane waves. We insert the total unperturbed energy of the pair $K^2/2(1+M) - E_w$, where M is the ion mass, as the trial value for ω of $\Sigma(\omega, \vec{\kappa}, n)$ and achieve limited self-consistency with respect to energy by iteration. In the present context, it suffices to use in Eq. (7) a properly acausal quantum dielectric function obtained from Eq. (2) by simply requiring that the poles of ϵ^{-1} lie on opposite sides of the real axis. Then,

$$\Sigma = -\frac{i\omega_p^2}{2^4\pi^5} \int d^3p \int \frac{d^3k}{k^2} |u_{\vec{p}}^{(0)}|^2 \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{1}{\omega'^2 - (\omega_k - i\sigma)^2} \frac{1}{\omega' - \Delta\omega - i\delta} , \tag{9}$$

where $\vec{P} = \vec{p} + \vec{k} - \vec{v}$, $\vec{p}$ being the wave vector of the electron after ionization from the wake-riding state; $u_{\vec{p}}^{(0)} = \int d^3r\, e^{i\vec{p}\cdot\vec{r}} u^{(0)}(\vec{r})$ is the Fourier transform of the ground-state wave function, $u^{(0)}(\vec{r})$ of the wake-bound electron, and $\omega_k = (\omega_p^2 + \beta^2k^2 + \frac{1}{4}k^4)^{1/2}$. The pair energy difference $\Delta\omega = \omega_{\vec{\kappa}n} - \omega_{\vec{\kappa}'n'}$ becomes

$$\Delta\omega = \vec{v}\cdot\vec{k} - [E_w + \tfrac{1}{2}(\vec{p} - \vec{v})^2] . \tag{10}$$

The function $|u_{\vec{p}}^{(0)}|^2$ is so strongly peaked about the point $\vec{P} = 0$ that we may approximate it by $(2\pi)^3$ times a δ function of its argument.

Carrying out the integrations we obtain, finally,

$$\mathrm{Re}(\Sigma) = \frac{\omega_p^2}{2\pi v} \int_0^{\infty} \frac{dk}{k\omega_k} \ln \left| \frac{\Omega_k - vk}{\Omega_k + vk} \right| , \tag{11}$$

$$\mathrm{Im}(\Sigma) = -\frac{\omega_p^2}{2v} \int_{k_1}^{k_2} \frac{dk}{k\omega_k} , \tag{12}$$

where k_1 and k_2 are the real roots of $vk = E_w + k^2/2 + \omega_k \equiv \Omega_k$. The damping due to the interaction of the wake-riding electron with the excitations in the system set up by the guiding ion is considered to be small and has been neglected.

Equation (11) leads one to estimate that in a metallic medium characterized by $r_s \simeq 2$ and in the velocity range of interest, the correlation-induced polaronlike increment of the wake-riding binding energy, $\mathrm{Re}(\Sigma) \approx 4$ eV, is comparable to the initial binding energy for $Z = 1$, and decreases slowly with increasing Z.

The relative width of the wake-bound state is given by

$$(\Delta E/E)_w \equiv \mathrm{Im}(\Sigma)/[E_w + \mathrm{Re}(\Sigma)] , \tag{13}$$

which leads to values ranging from 0.15 to 0.25 for an electron bound to a proton. Equation (12) can be approximated by setting $\omega_k \approx \omega_p$ in the integrand and by replacing k_1 and k_2 by simple forms. We find

$$\mathrm{Im}(\Sigma) \simeq \frac{\omega_p}{2v} \ln \left(1 + \frac{v^2k_c^2}{[\omega_p + E_w + \mathrm{Re}(\Sigma)]^2} \right)^{1/2} , \tag{14}$$

where $k_c \sim \omega_p/v_F$.

The mean free path Λ for dewaking due to quantum fluctuations in the electron gas becomes $\Lambda = v/2\,\mathrm{Im}(\Sigma)$. Since Eq. (14) varies only weakly with Z, Λ is approximately the same for all ions moving at the same velocity in dense media and has the value Λ (Å) $\approx r_s^{3/2}v$ where r_s, defined by $\frac{4}{3}\pi r_s^3 n_0 = 1$, and v are given in atomic units. Inasmuch as the initial and final wave functions of the ion-electron pair used in this model calculation are approximate and not mutually orthogonal, this value of Λ may constitute an underestimate of the correct value. In real metals, except under channeling conditions, additional damping is expected to occur in scattering events with ion cores.

CONCLUSIONS

The binding energy of electrons to the wakes of electron density fluctuations trailing ions moving in metallic media has been calculated in a quantum-mechanical approximation of the response function which treats the electron response accurately near the particle track, and the self-energy due to correlations has been estimated. The results apply best under conditions where interaction with ion cores is weak, such as in metals with small ionic cores, or in crystal channels. The binding energies are found to be significantly larger than those obtained by Day with a classical approximation of the response function. They are of the order of 10 eV behind protons and some 50 eV behind heavy ions. Polaronlike nonlocal effects in the wakes increase the binding energies by some 4 eV. The mean free path due to quantum fluctua-

tions for the decay of a wake-riding state is estimated to be 10–20 Å. This implies that detectable manifestations of wake-riding states in the properties of beams emerging from a solid are dictated by the last atomic layers, and may be influenced by the surface.

Although couched in the language of the electron gas, our results also apply to semiconductors and insulators, where collective excitations centered at some resonance frequency ω_0 are known to exist.[15] The form of the wake will be influenced to a greater extent than in metals by the damping of the collective excitations in such media.

Well-defined wake phenomena are expected to exist only in substances sufficiently dense that the wake can be considered continuous as subsumed in Eq. (1). Continuity requires that the mean interatomic distance in the medium be small compared to the wavelength associated with the wake, $2\pi v/\omega_0$. Under these conditions the relative density fluctuations, $\delta n/n_0$, happen to remain sufficiently small for linear-response theory to apply. Our results, therefore, should be valid for more realistic situations than implied by the simple model from which they have been derived. Wake phenomena may contribute to observable dynamic effects induced by charged particles in a wide range of materials.

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[13]The oscillatory track of electron density fluctuations trailing the charged particle may be studied by integrating the charge-density functions over all positions lateral to the particle track. The total polarization charge $Q(d)$ integrated from a distance d behind the ion to the position of the ion is thus given by

$$Q(d) = \frac{Z}{2\pi i}\int_{-\infty}^{\infty}\frac{d\omega}{\omega}\left[1-\exp\left(-i\frac{\omega}{v}d\right)\right] \times\left[\epsilon^{-1}(\omega/v,\omega)-1\right].$$

In the limit of large v one may easily show, using Eq. (2) but neglecting the term proportional to k^4 for simplicity, that $Q(\pi v/2\tilde{\omega}_p) = -Z$, where $\tilde{\omega}_p = \omega_p|1-\beta^2|^{1/2}$. In NRB, this relation was erroneously rendered as $Q(\pi v/\omega_p) = -Z$. In other words, the charge in the oscillatory wake contained under the *first quarter wave* of spatial variation is equal to the negative of the charge on the ion. We are grateful to Dr. J. C. Poizat for helpful conversations in this connection.

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