Bound Electron States in the Wake of Swift Ions in Solids*

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Fluctuations of valence-electron density are expected to occur in the wake of a fast charged particle moving through condensed matter. Electrons can be trapped into wake-riding states by the potential minima associated with domains of electron-density depletion with binding energies ranging from ~10 eV behind protons to several hundred eV behind highly charged heavy ions. Observable phenomena possibly linked to wake-riding states are discussed.

The energy loss of a fast charged particle moving in condensed matter can be described in terms of the complex dielectric function of the medium.[1] Physically the target response manifests itself as a cylindrically symmetric wake of electron-density fluctuations behind the particle.[2] Its axis defines the particle track. The wake consists of a series of domains, at distinct distances behind the projectile, in which the electron density is alternately enhanced and depleted relative to the mean density n_0 in the medium. Domains of density enhancement create regions of negative electric potential, and domains of depletion regions of positive potential. If sufficiently deep, these potential troughs can trap, respectively, positive or negative particles and sweep them along in wake-riding states trailing the projectile. Experimental verification of wake-riding states would contribute significantly to the understanding of the dynamic many-body response of condensed matter to moving charged particles. Moreover, projectile trailing by particles may contribute to several important phenomena associated with the penetration of charged particles through dense matter.

Consider a homogeneous isotropic medium characterized by the dielectric response function $\epsilon(\vec{k},\omega)$, where $\vec{k}$ and ω are the wave vector and the frequency of the perturbing field, respectively. In linear-response theory a point particle of charge Ze moving in the medium with velocity v generates a scalar potential $\Phi(\vec{r},t)$ given by[2]

$$\Phi(\vec{r},t)=\frac{2Ze}{\pi v}\int_0^\infty \kappa J_0(\kappa\rho)\,d\kappa\int_0^\infty \tilde{k}^{-2}\,\mathrm{Re}\{\epsilon^{-}(\vec{k},\omega)\exp[i(\omega/v)(z-vt)]\}\,d\omega, \tag{1}$$

where $\kappa^2=\tilde{k}^2-(\omega/v)^2$. The Cartesian coordinates of the projectile at time t are taken to be $(0,0,vt)$. The radial distance from the z axis is denoted by ρ, and J_0 is the zero-order Bessel function of the first kind. Suppose that the medium can sustain well-defined plasmons of energy $\hbar\omega_p=\hbar(4\pi n_0e^2/m_0)^{1/2}$ in the sense that the plasmon decay rate γ is so small that $\gamma/\omega_p\ll 1$. In a metal, the density of the participating electrons n_0 would correspond to the density of valence electrons. As long as $v\leq v_F\simeq v_0\equiv e^2/\hbar$, where v_F is the Fermi velocity of the electron gas, the potential set up by the moving particle is screened out over a distance $v_F/\omega_p\approx 1$ Å in typical metals. However, when $v\gg v_F$, the potential assumes the form

$$\Phi(\vec{r})=Zek[g(\vec{r})-2\sin(kz)K_0(k\rho)\exp(-\gamma kz/2\omega_p)\theta(z)], \tag{2}$$

where $k=\omega_p/v$; K_0 denotes the zero-order modified Bessel function of the second kind, and $\theta(z)$ the unit step function.[3] In Eq. (2) the coordinate system moves with the particle placed at the origin and has the positive z axis in the direction of $-\vec{v}$. The first term in Eq. (2) represents the potential in close proximity to the projectile and need not concern us here in detail. The second term represents a damped periodic potential set up by oscillatory electron density fluctuations in the wake of the projectile. The oscillatory portion of $V=-e\Phi(\vec{r})$ is shown schematically in Fig. 1.

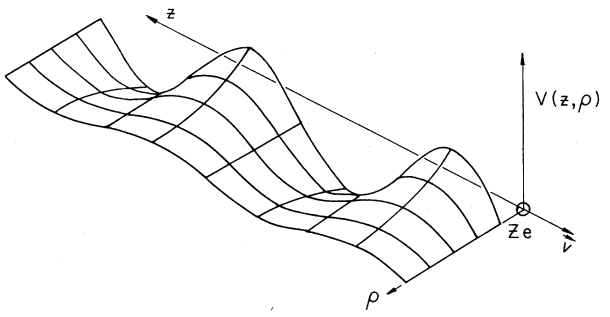

FIG. 1. Schematic representation of the oscillatory portion of the potential energy of an electron as a function of position behind a projectile of charge Ze. The charge is assumed to be moving with velocity v in the direction of the negative z axis of a coordinate system with origin placed at the projectile.

In condensed matter the potential can persist over many wavelengths behind the projectile. It is important to note that in the limit $\gamma \to 0$, the spatial integral over the electron density fluctuation from the origin to the first zero at the distance $z = \pi v/\omega_p$ is just equal to Ze, the charge of the moving ion.

In the approximation of Eqs. (1) and (2), the depth of the first trough increases linearly with Z, and is approximately $Ze\omega_p/v$. If this quantity is sufficiently large, bound quasistationary states of particles in the oscillating tail of $\Phi(r)$ may exist. In a medium with given ω_p, the number of bound states in a trough depends upon Z/v. Heavy projectiles may carry a core of tightly bound electrons extending over a distance comparable to or smaller than the Thomas-Fermi radius $a_{TF} = 0.8853 a_0 Z^{-1/3}$. Since the extension of ion cores is small compared with the wavelength $2\pi v/\omega_p$ characteristic of their wakes, which in the linear-response approximation does not depend upon Z, heavy ions can be treated in this context as point particles with a velocity-dependent effective charge number $Z_{\mathrm{eff}}(v) \leq Z$.

The nonlocal aspects of the wake phenomenon make a self-consistent solution of the wave equation of a trapped electron intractable except by numerical methods. For a first study of the bound states we make the *Ansatz* $u_0(\vec{r}) = A \exp(\alpha\zeta^2 - \beta\rho^2)$ for the ground-state wave function of a wake-riding electron. Here α and β are variational parameters, and ζ is the z coordinate measured from the center of a given positively charged potential trough. With this *Ansatz* all operations leading to a variational lower bound E_0 for the binding energy of the ground state can be carried out easily for the potential given in Eq. (2). The correlation effects between a trapped electron and the medium will tend to decrease the electron density near the trough and thus increase the binding energy further, perhaps by a fraction $1/Z$. This applies also to a positive particle wake-riding in a negatively charged potential trough, between two positively charged troughs, because here correlation tends to enhance the electron density. We neglect variations of $g(\vec{r})$ and the damping factor $\exp(-\gamma kz/2\omega_p)$ over the extension of a given trough, but evaluate them at the center of each trough. Electron-trapping, positively charged troughs appear behind the projectile at the distances z_m given by the condition $\omega_p z_m/v = \pi(4m+3)/2$, where $m = 0, 1, 2, \ldots$. Negatively charged troughs which, for example, may trap protons, appear when $\omega_p z_m/v = \pi(4m+1)/2$. In the following all energies and frequencies are expressed in units of $\mathcal{R} = e^2/2a_0 = \frac{1}{2}$ a.u. = 13.6 eV and all lengths in units of $a_0 = \hbar^2/m_0 e^2 = 1$ a.u. = 0.529 Å. The energy $E_0^{(m)}$ designates the variational ground-state energy of an electron in the mth trough.

Standard techniques lead to the result

$$E_0^{(m)} = \frac{\omega_p^2}{8v^2}\left\{W_m\left[\ln\left(\frac{W_m}{2\Gamma}\right)\right] - \left[W_m \ln\left(\frac{W_m}{2\Gamma}\right)\right]^{1/2}\right\}, \quad (3)$$

if $W_m \equiv 16Zk^{-1}\exp(-\gamma kz_m/2\omega_p)$ is much larger than unity. This condition on W_m is well satisfied in all cases we consider. Also $\ln\Gamma = 0.5772$ is Euler's constant.

Figure 2 displays the variation of the ground-state binding energy $E_0^{(0)}$ for an electron in the first potential trough ($m = 0$) behind hydrogen, oxygen, and sulfur ions as a function of their kinetic energy. The ions are assumed to move in a medium like aluminum metal for which $\hbar\omega_p = 15.4$ eV and $\gamma/\omega_p = 4.6 \times 10^{-2}$. The curves labeled O^{+8} (bare) and S^{+16} (bare) were computed assuming that the ions remain stripped during their passage through the medium. Such high-charge states may be selected in experiments with channeled ions,[4] where the low probability of small-impact-parameter collisions between a channeled ion and crystal ion cores makes electron capture from the solid unlikely compared to the situation in random media. The curves labeled $O^{+Z_{\mathrm{eff}}}$ and $S^{+Z_{\mathrm{eff}}}$ were computed assuming a velocity-dependent effective charge number of

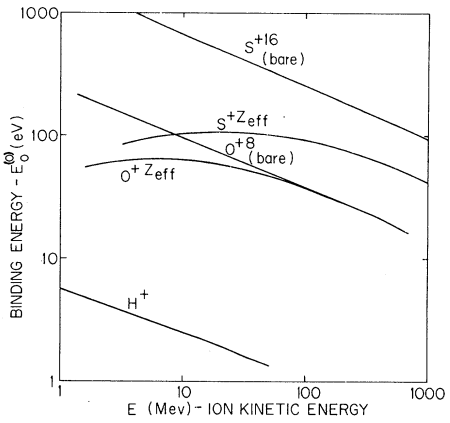

FIG. 2. Ground-state binding energies (in eV) of an electron in the first ($m=0$) trough of the polarization potential created in a medium like aluminum by ions of hydrogen, oxygen, and sulfur as a function of their kinetic energies. The curves labeled $O^{+Z_{eff}}$ and $S^{+Z_{eff}}$ were calculated for effective ion charges $Z_{eff}(v)$ as described in the text.

the form $Z_{eff}(v) = Z[1 - \exp(v/Z^{2/3}v_0)]$.[5]

Table I illustrates how the ground-state binding energy varies with the position of the trough along the wakes behind bare O^{+8} and S^{+16} ions at velocity $v = 10v_0$ in a medium like aluminum. The binding energies of wake-riding states can range from tens to hundreds of eV in situations of experimental interest. More realistic estimates, taking into account nonlinear effects in Z, should not change these values substantially and are expected to display the same trends with Z, Z_{eff}, ω_p, and v as obtained here.

Auger-type capture into these states should be efficient. Assuming that the binding energy of the states is dissipated through particle-hole pair production in the conduction band of the metal, one estimates, e.g., a mean free path of ~300 Å for capture into a wake-riding state behind a 2-MeV O^{+8} ion in Al metal. It may be possible to detect electron capture into these states by observing the associated Auger electrons, or the soft x rays generated in the capture process. The related radiative capture of electrons into inner shells of stripped swift ions in solids has been discovered recently.[6-8]

When an ion trailed by a wake-riding electron emerges from a metal into vacuum, the potential trough seen by the electron vanishes. Then in first approximation, we expect these electrons to appear outside the metal as a group of electrons with velocities centered about v, and with a spread determined by the momentum transform

TABLE I. Variational ground-state binding energies, $E_0^{(m)}$ of electrons trapped by the mth potential trough in the wakes at distances Z_m behind 2.5-MeV protons, 40-MeV O^{+8} ions and 80-MeV S^{+16} ions moving in a metal like aluminum.

m	Z_m (Å)	$E_0^{(m)}$ (eV) 2.5-MeV H^+	40-MeV O^{+8}	80-MeV S^{+16}
0	44.03	4.08	55.4	125.8
1	102.74	3.09	43.4	99.0
2	161.46	2.33	33.9	77.8
3	220.16	1.75	26.4	61.0

of the wake-riding-electron wave packet. These electrons should contribute a component to the electron distribution associated with the emergence of positive ions from metals, which so far have been explained only in terms of capture into continuum states on the positive ions *in vacuo*.[9]

We mention other possible consequences of wake-riding states in solids:

(a) The amount of charge separation in solid-state detectors of ionizing radiation may be affected by the existence of spatially coherent electron states of moving particles. Such states would be expected not only to reduce particle-hole recombination in solid-state detectors, but also to diminish the recombination of electrons with geminate ions in insulators such as organic liquids.

(b) Correlated capture and loss into wake-riding states may determine the velocity dependence of the neutral-beam fraction in experiments with charged particles emerging from solid surfaces.[10,11] The binding energy of an electron trailing an energetic proton is ~10 eV ~1 Ry in a typical metal. Thus, the interesting picture of a dynamically stabilized solid-state H atom emerges, in which the proton rides ahead, trailed by the wave packet of the electron at a distance $\sim 3\pi v/2\omega_p$. An antimorph of the entity which might exist by virtue of the wake phenomenon is the *dielectron*. Two electrons might experience strong spatial correlation due to density fluctuations. Energy lost by a dielectron in distant collisions should be altered relative to that by a single electron; its mean free path in condensed matter may be longer than that of either electron separately, enhancing the likelihood that it will produce observable effects.

(c) The experiments of Gaillard, Poizat, and Remillieux[12] on the transmission probability of

channeled H_2^+ ions through gold foils show that a significant fraction emerges from the foils as molecules. H^+H^+ pairs locked in spatial correlation may contribute significantly to this transmission probability. It would be interesting to ascertain the importance of wake-riding states of protons behind heavier ions, for example, in transmission experiments with incident fast molecules such as LiH, CH, OH, or hydrogen halides.

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Fluctuation Resistivity in One-Dimensional Metals

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The resistivity of one-dimensional metals is calculated for two models in which impurity scattering is the only mechanism for dissipating momentum. In the first model, impurity scattering is added to the Fröhlich Hamiltonian. In the fluctuation regime above an incommensurate Peierls transition it is found that the resistivity is enhanced. For a general two-body interaction Hamiltonian it is found that charge-density–wave fluctuations predominate over Cooper-pair fluctuations leading to enhanced resistivity.

There has been much speculation recently that enhanced conductivity can be obtained from fluctuation contributions in one-dimensional metals.[1-6] A general feature of one-dimensional metals is their inherent instability towards the formation of a charge-density wave with a period of twice the Fermi wave vector ($2k_F$).[7-10] In this Letter we examine two models for which impurity scattering is the only dissipative mechanism for momentum and find that the density fluctuations lead to an enhanced resistivity, not conductivity. One is the Peierls instability arising from the electron-phonon coupling. The second problem is that of a one-dimensional metal with a general two-body Hamiltonian. In this case even though attractive interactions cause a divergence in the Cooper-pair response function, the scattering time is dominated by the divergence in the electronic polarizability at $2k_F$, and the fluctuation contribution leads to a divergence in the resistivity.

We consider first the Peierls instability with a