Spatial excitation patterns induced by swift ions in condensed matter

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It is shown that a charged particle moving with velocity $\vec{v}$ in a medium of resonance frequency Ω_0 may set up two types of electron-density fluctuations. Collective fluctuations trail the particle, composing a conical pattern in a relatively extended periodic wake of wavelength $\sim 2\pi v/\Omega_0$. They constitute a mode of energy transport from the particle track leading eventually to particle-hole excitations. Single-particle interactions give rise to bow waves ahead of the particles of wavelength $2\pi\hbar/mv$. The gradient along $\vec{v}$, at the site of the ion, of the wake potential set up by density fluctuations, multiplied by the ionic charge, yields an expression for the retarding force of the medium on the projectile in exact agreement with the Bethe stopping-power formula appropriate to the medium. The wake of a dicluster causes forces between the constituent ions which account quantitatively for measurements of the breakup behavior of swift molecular ions in thin foils. The increase in the energy straggling of a test charge, when moving in the wake of a leading ion, is shown to be small compared with the straggling induced by its own wake under normal conditions.

The theory of wake phenomena in the electron-density fluctuations excited by charged particles moving in an electron gas[1] has stimulated many experiments, in particular on the stopping power of matter for ion clusters[2] and on the space-time correlation between cluster particles[3,4] after emergence from dense media.[5] Collective density waves trailing an ion with velocity $v \gtrsim v_0 = e^2/\hbar$ in a condensed medium of resonance frequency Ω_0 have wavelengths, $\lambda_w \simeq 2\pi v/\Omega_0$, of the order of 10 Å under typical experimental conditions. In addition, as shown in this paper, close collisions cause electrons to recoil and form a bow wave ahead of the ion. Clusters are created by injecting swift molecular ions, such as H_2^+ or $(HeH)^+$, into a solid target. They lose their binding valence electrons after penetrating a few atomic layers and generate a wake given by a (generally nonlinear) superposition of wakes due to the individual ions of the cluster. This gives rise to a new interaction between particles in a cluster determined by the dynamic response of the medium. The dynamically modified Coulomb repulsion between its constituents causes the cluster to explode. Transmission experiments are usually performed on thin foils such that the time of penetration is so short that particles in the exploding clusters trace out only a very small fraction of the wake dimension. Under such circumstances, the cluster-particle interaction probes, in effect, the slope of the cluster wake potential near the origin. For example, the elegant measurements by Gemmel and co-workers[3] of the angle and energy distributions of channeled protons emerging from single crystals of Si bombarded with swift $(HeH)^+$ ions only probe distances $\sim 0.05\lambda_w$. They present convincing evidence that the force set up by the wake potential of the leading ion can influence strongly the motion of the trailing ion.

In light of the sensitivity of this important type of experiment, we have derived in linear perturbation theory expressions for the total field of density fluctuations surrounding a moving ion, with special emphasis on the behavior near the origin. This enables us to calculate the enhanced electron density at the projectile nucleus and to compare it with exact results from the theory of scattering of single electrons by moving ions. This enhanced density is germane to the discussion of the effects of dynamic screening on atomic states[6] and on transient magnetic fields at recoil nuclei in magnetized foils.[7] The mean gradient along $\vec{v}$ of the wake potential at the origin, multiplied with Ze, yields an expression for the retarding force of the medium on the ion. We show it to be, at high velocities, exactly equal to the Bethe[8] stopping-power formula. The force on the particles in a cluster derived from the wake potential agrees, in its essential aspects, with the result derived from a local dielectric response function.[1,2]

I. COLLECTIVE ASPECTS OF THE WAKE

The response of the valence electrons in many media is describable to a good approximation by the diagonal part, $\epsilon(k, \omega)$, of a (longitudinal) dielectric matrix which depends on the wave number k and frequency ω in a manner such that off-diagonal components can be neglected. The scalar electric wake potential, Φ, of an ion moving in such media is given in the linear approximation by[1,9,10]

$$\Phi(\rho,\tilde{z}) = \frac{Ze}{\pi v}\int_0^\infty \kappa J_0(\rho\kappa)\, d\kappa \times \int_{-\infty}^{\infty} d\omega \exp\left(\frac{i\omega\tilde{z}}{v}\right) \Big/ k^2\epsilon(k,\omega) \quad . \tag{1}$$

The cylindrical coordinates ρ and $\tilde{z}$ refer to the direction of motion and are defined as $\rho \equiv (x^2+y^2)^{1/2}$ and $\tilde{z} \equiv z - vt$ relative to the position $(x,y,z) = (0,0,vt)$ of the moving charge, Ze, with wave number $k = (\kappa^2 + \omega^2/v^2)^{1/2}$. The wave vector $\vec{k}$ has component κ in the ρ direction. The ion velocity, $\vec{v}$, is treated as a constant. The projectile, referred to here as the ion, may be any charged point particle with mass much greater than that of the electron. The induced electron-density fluctuation, $\delta n(\rho,\tilde{z})$, in the medium is related to Φ by Poisson's equation and is described by

$$\delta n(\rho,\tilde{z}) = -\frac{Z}{4\pi^2 v}\int_0^\infty \kappa J_0(\rho\kappa)\, d\kappa \times \int_{-\infty}^{\infty} d\omega \exp\left(\frac{i\omega\tilde{z}}{v}\right)\left(\frac{1}{\epsilon(k,\omega)} - 1\right) \quad , \tag{2}$$

such that the charge-density fluctuation is given by $(-e\,\delta n)$.

A convenient and instructive first approximation to Φ and δn can be found with the aid of the local dielectric function with a k cutoff,

$$\epsilon(k,\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)}\Theta(k_c - k) \quad , \tag{3}$$

where Ω_0 is set equal to the plasmon frequency $\omega_p = (4\pi e^2 n/m)^{1/2}$ in an electron gas of density n; $\Theta(x)$ denotes the unit step function $\Theta(x) = (\frac{1}{2})(1 + x/|x|)$, and the cutoff wave vector of magnitude $k_c \approx \omega_p/v_F$ is given in terms of the Fermi velocity $v_F = (3\pi^2 n)^{1/3}\hbar/m$ of the valence electrons in the medium. Equation (3) describes the collective dielectric response of the medium, but does not describe dispersion or single-particle behavior. The empirical constant γ describes damping. With Eq. (3), the potential given by Eq. (1) becomes

$$\Phi(\rho,\tilde{z}) = Zeh_0(\rho,\tilde{z}) + \frac{2Ze\omega_p}{v}\sin\left(\frac{\omega_p\tilde{z}}{v}\right)K_0\left(\frac{\omega_p\rho}{v}, \frac{v}{v_F}\right) \times \exp\left(\frac{\gamma\tilde{z}}{2v}\right)\Theta(-\tilde{z}) \quad . \tag{4}$$

The first term gives the screened Coulomb potential of the ion, and the second describes the oscillatory potential due to the wake of electron-density fluctuations trailing the ion.[1,9] The function

$$K_0(\xi,\eta) = \int_0^\eta \frac{yJ_0(\xi y)}{1+y^2}\, dy \tag{5}$$

approaches the modified Bessel function of zero order, $K_0(\xi)$, for large ξ; it is $K_0(0,\eta) = (\frac{1}{2})\ln(1+\eta^2)$ when $\xi = 0$.

The function $h_0(\rho,\tilde{z})$ in Eq. (4) can be written in the form

$$h_0(\rho,\tilde{z}) = \frac{1}{R} - \frac{\omega_p}{v}S_0\left(\frac{\omega_p\rho}{v}, \frac{\omega_p\tilde{z}}{v}\right) \quad . \tag{6}$$

The first term is the bare Coulomb potential per unit charge of the ion, where $R \equiv (\rho^2 + \tilde{z}^2)^{1/2}$. The second term has a factor

$$S_0(\xi,\eta) = \int_0^\infty \frac{J_0(\xi t)\exp(-|\eta| t)}{1+t^2}\, dt \tag{7}$$

and accounts for steady-state screening of the ion charge by the electrons of the medium. For simplicity we have set $\gamma = 0$ in obtaining this expression for S_0. A simple form of Eq. (4) is obtained in the limit $\gamma << \omega_p$. One readily verifies that

$$\frac{\omega_p}{v}S_0\left(\frac{\omega_p\rho}{v}, \frac{\omega_p\tilde{z}}{v}\right) = \begin{cases} \dfrac{1}{R} - \left(\dfrac{v}{\omega_p}\right)^2 \dfrac{2\tilde{z}^2 - \rho^2}{R^5} + \cdots, & \dfrac{\omega_p R}{v} >> 1 , \\[2ex] \dfrac{\omega_p}{v}\left\{\dfrac{\pi}{2} - \dfrac{\omega_p}{v}\left[|\tilde{z}|\ln\left(\dfrac{1.5262\cdots}{\omega_p|\tilde{z}|/v}\right) + \rho\right] + \cdots\right., & \dfrac{\omega_p R}{v} << 1 . \end{cases} \tag{8}$$

The function h_0, Eq. (6), vanishes in the limit $\omega_p R/v >> 1$. Since $h_0(\rho,\tilde{z}) = h_0(\rho,-\tilde{z})$, its mean $\tilde{z}$ gradient around $R = 0$ vanishes, i.e., $\langle \partial h_0/\partial\tilde{z}\rangle_{R\to 0} = 0$. Thus the screening effect described by h_0 makes no contribution to the retarding force of the medium on the ion.

As pointed out earlier,[11] one obtains

$$\lim_{R\to 0}\left(\Phi - \frac{Ze}{R}\right) = -\frac{\pi Ze\omega_p}{2v} \tag{9}$$

for the potential of the polarized medium at the site

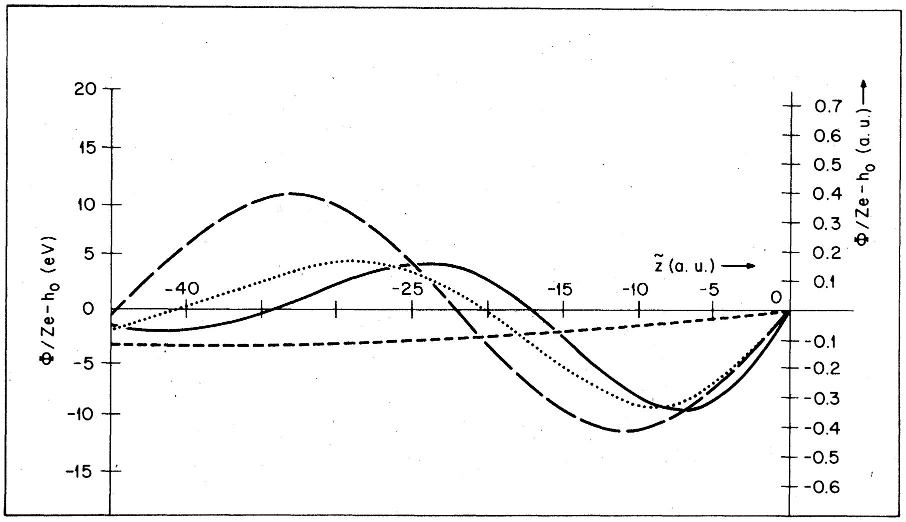

FIG. 1. Oscillatory portion of the scalar electric potential computed in the local dielectric approximation from Eq. (4). Plotted is $\Phi/Ze-h_0$ vs $\tilde{z}$ on the particle track, $\rho=0$. The plasma frequency, ω_p, and the damping rate, γ, have been chosen to represent, approximately, the response of four different solids. The solids and the corresponding values of $\hbar\omega_p$ and γ/ω_p are: Al (long-dash line) 15.4 eV, 0.616; Si (dot-dash line) 17 eV, 0.441; C (solid line) 25 eV, 0.5; Ag (short-dash line) 3.78 eV, 0.02. The ion velocity was taken to be 4 a.u.

of the ion. In this approximation, therefore, the self-energy, E_s, of a massive point charge is given by $E_s=-(Ze)^2(\pi\omega_p/4v)$. When applied to high-velocity electrons, where electron-recoil effects can be neglected, this estimate agrees, as it should, with the self-energy calculated for fast electrons in an electron gas.[12,13]

It is instructive to compare the picture of the wake as presented above with the model of a stationary charge in an electron gas. For a negative stationary charge one speaks of a correlation hole around it, and for a positive charge one speaks of a density enhancement at the charge. In either case the response of the medium can be represented as a screened Coulomb potential centered at the charge, giving rise to a negative self-energy with a null imaginary part. In comparison, a moving ion gives rise to a cylindrically symmetric potential with a part centered at the charge, even in $\tilde{z}$, plus an oscillatory part stretching behind the particle. The first part gives rise to a real part of the self-energy which is negative, and which originates from the correlation domain of dimension v/Ω_0 around the charge. Only the oscillatory portion contributes to the imaginary part of the self-energy that describes the slowing down of the charge.

Figure 1 shows plots of the oscillatory part of $\Phi/Ze-h_0$ computed from Eq. (4) as a function of $\tilde{z}$ along the trajectory, $\rho=0$, for various combinations of ω_p and γ as indicated on the figure caption.

Equation (2) with Eq. (3) yields

$$\delta n(\rho,\tilde{z})\approx-\frac{Z\omega_p^2}{2\pi v v_F\rho}J_1\left[\frac{\omega_p\rho}{v_F}\right]\times\sin\left[\frac{\omega_p\tilde{z}}{v}\right]\exp\left[\frac{\gamma\tilde{z}}{2v}\right]\Theta(-\tilde{z})\ , \tag{10}$$

where J_1 is the Bessel function of the first kind of order one. In this cutoff approximation, there is neither dispersion of the plasmon waves, nor an electron-density enhancement at $R=0$. It does not describe knock-on collisions with single electrons, but damping is included in a realistic manner.[1]

II. PLASMON DISPERSION

The polarization density retains a tractable analytical form if one goes beyond Eq. (3) and includes plasmon dispersion according to the Bloch hydrodynamic approximation by inserting into Eq. (2) the dielectric function

$$\epsilon(k,\omega)=1+\frac{\omega_p^2}{\beta^2k^2-\omega(\omega+i\gamma)}\ . \tag{11}$$

The constant $\beta=(3/5)^{1/2}v_F$ is the propagation of density disturbances in an electron gas, v_F being the Fermi velocity of the electrons in the medium.

Denoting $w\equiv(1-\beta^2/v^2)^{-1/2}$, neglecting γ as well as terms $O(\beta^4)$, Eq. (10) becomes

$$\delta n(\rho,\tilde{z}) = -\frac{Z\omega_p^2 w}{2\pi v\beta\rho}\int_{\omega_p\rho/v}^{\infty} \sin\left[\frac{\beta w\tilde{z}}{v\rho}q\right] \times J_0\left[\left(q^2-\frac{\omega_p^2\rho^2}{\beta^2}\right)^{1/2}\right] dq \qquad (12)$$

$$= \frac{Z\omega_p^2}{2\pi\beta(v^2-\beta^2)^{1/2}}\frac{\cos(\omega_p\Lambda/\beta)}{\Lambda}\Theta(\Lambda^2) \ , \qquad (13)$$

where the variable $\Lambda \equiv (\lambda^2\tilde{z}^2-\rho^2)^{1/2}$ with $\lambda^2 \equiv \beta^2/(v^2-\beta^2)$. An equation equivalent to Eq. (13) was derived by Neufeld and Ritchie,[9] and again by Fetter.[14]

A singularity in the polarization density occurs at $\Lambda = 0$, corresponding to the radial distance from the particle trajectory

$$\rho = \lambda\tilde{z} = \tilde{z}/(v^2/\beta^2-1)^{1/2} \simeq \beta\tilde{z}/v \qquad (v >> \beta) \ . \qquad (14)$$

Equation (14) defines the envelope of the collective wake, of half-angle $\sim\beta/v$. The singularity of δn at the cone is, of course, an artifact of the model dielectric function Eq. (11). When the integration in Eq. (12) is limited to $q \leq \rho k_c = \rho\omega_p/v_F$, the wake cone is marked by a maximum in δn. In fact, if the full dielectric function is employed, the maximum is replaced by a series of wavelike fluctuations as described in Sec. III.

III. SINGLE-PARTICLE WAKE CONTRIBUTIONS

We retain the salient features of the quantum expression for $\epsilon(k,\omega)$ in metals and semiconductors by setting[11,15]

$$\epsilon(k,\omega) = 1 + \frac{\omega_p^2}{\omega_g^2+\beta^2k^2+\hbar^2k^4/4m^2-\omega(\omega+i\gamma)} \ . \qquad (15)$$

As in Eq. (11), plasmon dispersion is included through the term containing β^2. Single-particle effects now are accounted for by the term equal to the square of the kinetic energy, $\hbar^2k^2/2m$, of a free electron with momentum $\hbar\vec{k}$. The small constant γ represents damping processes. The energy $\hbar\omega_g$ may be taken to account for an effective band gap in materials like semiconductors, to give a collective resonance frequency $\Omega_0 = (\omega_g^2+\omega_p^2)^{1/2}$.[16,17]

Substitution of Eq. (15) into Eq. (1) yields the potential in the form

$$\Phi(\rho,\tilde{z}) = \frac{Ze}{R} + \Phi_w(\rho,\tilde{z}) \ , \qquad (16)$$

where the wake potential, Φ_w, can be expressed as a sum of three terms,

$$\Phi_w = \phi_0 + \phi_1 + \phi_2 \ . \qquad (17)$$

The function ϕ_0 is given by

$$\phi_0 = -Ze[h(\rho,\tilde{z}) - 1/R] \ , \qquad (18)$$

where, with $k_0 \equiv \Omega_0/v$,

$$h(\rho,\tilde{z}) = \frac{\omega_p^2}{v\Omega_0}\int_0^{\infty} \frac{t^2 J_0(\rho k_0 t)\exp(-k_0|\tilde{z}|t)}{1+(\tilde{z}/|\tilde{z}|)(\gamma t/\Omega_0)+t^2}\,dt \ . \qquad (19)$$

Equation (19) reduces to $h_0(\rho,\tilde{z})$, Eq. (6), for $\gamma \rightarrow 0$ and $\omega_g \rightarrow 0$.

The term ϕ_0 accounts for nonoscillatory dynamic screening of the ion charge by electrons in the medium. Since $h \rightarrow 0$ when $Rk_0 >> 1$, the ion charge is completely screened at distances large compared with v/Ω_0. The second and third terms of Eq. (17) make oscillatory contributions that stem primarily from collective and single-particle responses of the medium, respectively.

The functions ϕ_1 and ϕ_2 are expressed as integrals with respect to the variable κ after evaluating the ω integral in Eq. (1) by the calculus of residues. The ω integrand exhibits an interesting behavior as κ increases from the long-wavelength limit, $\kappa = 0$, to large values where single-particle behavior dominates. In Fig. 2 are sketched the loci of the poles of the inverse dielectric function appearing in the integrand for a material characterized by $\Omega_0 = 0.7$, $\beta = 0.9$, and $\gamma = 0.58$, in Hartree atomic units. The poles labeled $\omega_c^{\pm}$ and $\omega_s^{\pm}$ correspond to collective and single-

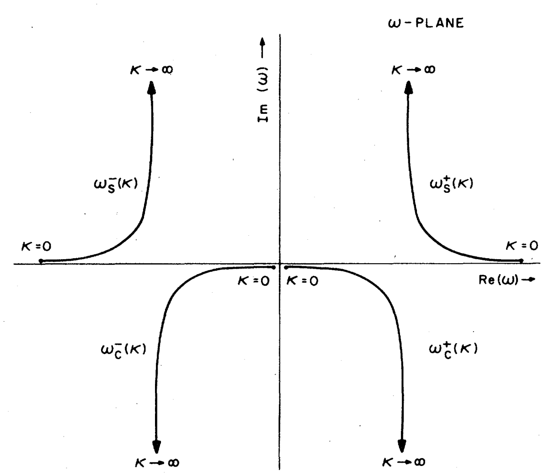

FIG. 2. Loci of poles of the inverse dielectric function $[\epsilon((\kappa^2+\omega^2/v^2)^{1/2},\omega)]^{-1}$ in the complex plane for values of the material constants of Eq. (15) given by $\Omega_0 = (\omega_p^2+\omega_g^2)^{1/2} = 0.7$ a.u., $\beta = 0.9$ a.u., and $\gamma = 0.58$ a.u. The poles at points labeled $\omega_c^{\pm}(\kappa)$ correspond to collective resonances, those labeled $\omega_s^{\pm}(\kappa)$ to single-particle excitations. The poles move, following the arrows, as the variable κ increases from zero. As $\kappa \rightarrow \infty$, $\omega_c^+ \rightarrow \omega_s^{+*}$ and $\omega_c^- \rightarrow \omega_s^{-*}$. Also, $v = 4$ a.u.

particle responses, respectively. The poles move as indicated by arrows as κ increases from zero to infinity, $\kappa \rightarrow \infty$, where $\omega_c^{\pm} = \omega_s^{\pm *}$. The fact that the two poles, ω_s^+ and ω_s^-, lie above the real ω axis is surprising at first glance, since their presence seems to signal the breakdown of causality: in effect, the single-particle excitations in the medium appear to precede the moving ion in time. In reality, the ion is treated as having been in motion long enough for the complete development of waves including knock-on electrons. There are, then, indeed precursor or bow waves of electron-density fluctuations that run ahead of the particle. Bow waves are associated primarily with electrons that have been scattered in close collisions with the ion into the forward hemisphere of directions.

The scale of spatial variations of Φ and δn due to the $\pm\omega_s$ poles is $\sim 2\pi\hbar/mv$, the de Broglie wavelength of an electron which has acquired momentum $m\vec{v}$ from the ion. In the velocity range of interest, $v > v_F$, such fluctuations are short compared to the length scale, $\sim v/\Omega_0$, associated with the poles at $\omega = \pm\omega_c$ that describe the collective fluctuations in the wake trailing the ion.

When $\gamma \rightarrow 0$, one derives closed expressions for ϕ_1 and ϕ_2 in terms of the integration variable $q = \kappa/\sqrt{2}$, viz.,

$$\phi_1(\rho, \pm\tilde{z}) = \frac{\sqrt{2}\, Zem^2\omega_p^2}{\hbar^2} \int_0^{q_c} qJ_0(\sqrt{2}\rho q) \times \frac{\sin(\sqrt{2}\tilde{z}\xi_\pm)}{\delta^2\xi_\pm(q^2+\xi_\pm^2)}\, dq \; . \tag{20}$$

The notation $\pm\tilde{z}$ in the argument of ϕ_1, Eq. (20), means that when $\tilde{z} > 0$, ξ_+ is to be used in the right-hand side of Eq. (21); similarly ξ_- is used when $\tilde{z} < 0$. Also,

$$\phi_2(\rho,\tilde{z}) = -\frac{Ze\,\omega_p^2 m^2}{\sqrt{2}\hbar^2} \int_{q_c}^{\infty} qJ_0(\sqrt{2}\rho q) \times \frac{\exp(-2^{1/2}\eta_-|\tilde{z}|)N}{\eta_+\eta_-(\eta_+^2+\eta_-^2)D}\, dq \; , \tag{21}$$

where

$$q_c = \{[m(v^2-\beta^2)/\hbar]^2 - \Omega_0^2\}^{1/2}/\sqrt{2}v \; ,$$

with

$$\xi_\pm = (\alpha^2 \pm \delta^2)^{1/2} \; , \quad \alpha^2 = m^2(v^2-\beta^2)/\hbar^2 - q^2 \; ,$$

$$\delta^2 = \{[m^2(v^2-\beta^2)/\hbar^2] - m^2(2v^2q^2+\Omega_0^2)/\hbar^2\}^{1/2}$$

In addition,

$$\eta_\pm = 2^{-1/2}\{[q^4 + 2(m\beta q/\hbar)^2 + (m\,\Omega_0/\hbar)^2]^{1/2} \pm [m^2(v^2-\beta^2)/\hbar^2 - q^2)]\}^{1/2}$$

and

$$N = (\eta_+C + \eta_-S)(q^2+\eta_+^2-\eta_-^2) + 2\eta_+\eta_-(\eta_+S - \eta_-C) \; ,$$

where

$$C = \cos(\sqrt{2}\eta_-\tilde{z}) \; , \quad S = \sin(\sqrt{2}\eta_-|\tilde{z}|)$$

and

$$D = (q^2+\eta_+^2-\eta_-^2)^2 + 4\eta_+^2\eta_-^2 \; .$$

It may be shown from Eqs. (18)–(21) that $\Phi_w(0,0) = -\pi\, Ze\,\omega_p^2/2v\,\Omega_0$, i.e., $\phi_1(0,0) = \phi_2(0,0) = 0$, if damping can be neglected ($\gamma \rightarrow 0$). The value of $\Phi_w(0,0) = \phi_0(0,0)$ represents a model-independent contribution to Φ from the poles $\omega = \pm i\kappa v$ in the complex ω plane, corresponding to the extreme long-wavelength response ($k \rightarrow 0$) of the medium. The function ϕ_0 is symmetric with regard to a reflection in the $\tilde{z} = 0$ plane so that its mean gradient at the origin is zero. Both $\partial\phi_2(0,\tilde{z})/\partial\tilde{z}$ and $\partial\phi_0(0,\tilde{z})/\partial\tilde{z}$ diverge logarithmically at $\tilde{z} \rightarrow \pm 0$. Their sum has a finite discontinuity at the origin that cancels a discontinuity in the $\tilde{z}$ derivative of ϕ_i there.

Only the term $\phi_1(\rho,\tilde{z})$ has a nonzero mean $\tilde{z}$ gradient at the origin and, thus, contains the retarding effect of the medium on the particle. It may be shown that $F_1(0_-)$, the retarding force on a unit test charge located just behind the ion, in terms of Eq. (20) is given by

$$F_1(0_-) \equiv \frac{\partial}{\partial\tilde{z}}\phi_1(0,\tilde{z})\Big|_{\tilde{z}\rightarrow 0_-} = \frac{Ze\,\omega_p^2}{v^2} \ln\left|\frac{\tilde{v}^2}{\tilde{v}^2 - \nu^2}\right| \; . \tag{22}$$

Similarly, if the test charge is located just in front of the ion, the retarding force becomes

$$F_1(0_+) \equiv \frac{\partial}{\partial\tilde{z}}\phi_1(0,\tilde{z})\Big|_{\tilde{z}\rightarrow 0_+} = \frac{Ze\,\omega_p^2}{v^2} \ln\left|\frac{\tilde{v}^2 + \nu^2}{\tilde{v}^2}\right| \; . \tag{23}$$

The arithmetic mean of these terms, multiplied by the charge Ze, yields the stopping power of the medium for the ion, viz.,

$$-\frac{dE}{dz} = \frac{Z^2e^2\omega_p^2}{2v^2} \ln\left|\frac{\tilde{v}^2+\nu^2}{\tilde{v}^2-\nu^2}\right| \; . \tag{24}$$

In Eqs. (22)–(24), $\tilde{v}^2 = v^2 - \beta^2$ and $\nu^4 = \tilde{v}^4 - \hbar^2\Omega_0^2/m^2$. For v much larger than β and $(\hbar\Omega_0/m)^{1/2}$, one retrieves

$$-\frac{dE}{dz} = \frac{Z^2e^2\omega_p^2}{v^2} \ln\left|\frac{2mv^2}{\hbar\Omega_0}\right| \; , \tag{25}$$

the Bethe[8] stopping power formula for fast ions proceeding through an electron gas characterized by the plasma frequency Ω_0.[18] This prescription of computing the stopping power of the medium from the mean force on the particle is well known.[19] Although we have (properly) omitted the contribution from ϕ_0 and ϕ_1 to the retarding force in the calculation displayed in Eqs. (22)–(24), it may be seen that the total force is continuous at the origin and possesses a finite discontinuity in slope there.

The electron density fluctuation function may be written

$$\delta n(\rho,\tilde{z}) = \delta n_1(\rho,\tilde{z}) + \delta n_2(\rho,\tilde{z}) \tag{26}$$

in terms of contributions from the poles at $\pm\omega_c$ and $\pm\omega_s$, respectively.

One finds for negligible damping that

$$\delta n_1(\rho, \pm\tilde{z}) = -\frac{Zm^2\omega_p^2}{\sqrt{2}\pi\hbar^2}\int_0^{q_c} \frac{qJ_0(\sqrt{2}\rho q)\sin(\sqrt{2}\xi_\pm\tilde{z})}{\delta^2\xi_\pm}\,dq \tag{27}$$

and

$$\delta n_2(\rho,\tilde{z}) = \frac{Zm^2\omega_p^2}{2^{3/2}\pi\hbar^2}\int_{q_c}^{\infty} qJ_0(\sqrt{2}\rho q)\exp(-\sqrt{2}\eta_-|\tilde{z}|) \times \frac{\eta_+C+\eta_-S}{\eta_+\eta_-(\eta_+^2+\eta_-^2)}\,dq \ . \tag{28}$$

In this approximation, the density is enhanced at the ion by the amount

$$\delta n(0,0) = \delta n_2(0,0) \simeq \frac{Zm\omega_p^2}{4\hbar v} = \frac{\pi n Ze^2}{\hbar v} \ , \tag{29}$$

where small terms due to collective effects containing ω_p and β are neglected. This result agrees with the exact calculation[20] of electron scattering on a point charge, Ze, in the limit $v \gg Ze^2/\hbar$.

Figure 3 shows plots of $\phi_0(0,\tilde{z})/Ze$ vs $\tilde{z}$ (curve A) and $[\phi_1(0,\tilde{z})+\phi_2(0,\tilde{z})]/Ze$ vs $\tilde{z}$ (curve B) for the material-parameter values given in the figure caption. For comparison with B the corresponding potential function computed in the local dielectric approximation of Eq. (4) is displayed as the dot-dash curve C. As discussed following Eq. (8), $\phi_0(0,\tilde{z})$ is symmetric with respect to the position of the ion at $\tilde{z}=0$. Note that in the domain $\tilde{z}>0$, the asymmetric potential function $(\phi_1+\phi_2)/Ze$ (curve B) has been scaled up by a factor of 100 so that single-particle fluctuations are easily seen. The sum-total wake potential, Eq. (17), is given by curve D. The slope at $\tilde{z}=0$ yields the stopping power, Eq. (24).

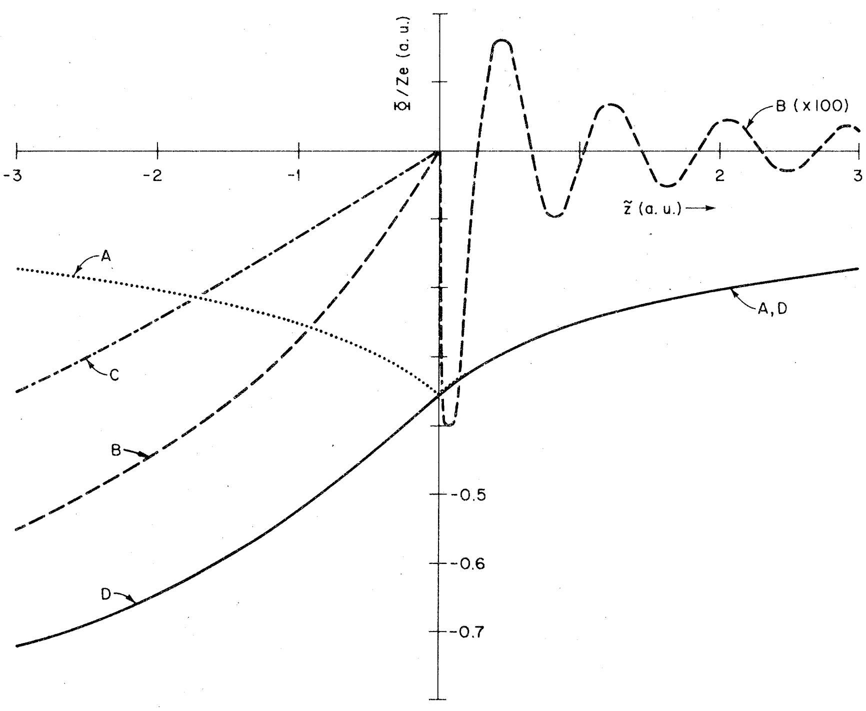

FIG. 3. Scalar electric potential in a medium near the track of a projectile, located at $\tilde{z}=0$, moving with velocity $v=4$ a.u. $=8.76\times10^8$ cm/sec in the positive $\tilde{z}$ direction through a medium characterized by $\omega_p=0.919$ a.u. $=25$ eV, $\beta=0.974$ a.u. $=2.13\times10^{10}$ cm/sec, and $\omega_g=\gamma=0$. These potential values were computed from Eqs. (17)–(21) with the use of the dielectric function of Eq. (15). Curve A shows $\phi_0(0,\tilde{z})/Ze$ vs $\tilde{z}$, and is symmetric with respect to reflection through the point $\tilde{z}=0$. Curve B depicts $[\phi_1(0,\tilde{z})+\phi_2(0,\tilde{z})]/Ze$ as a function of $\tilde{z}$. Note that in the region $\tilde{z}>0$ the function has been multiplied by 100 for the sake of clarity. Curve D displays the total wake potential, Eq. (17). For purposes of comparison, $[\Phi(0,\tilde{z})/Ze - h_0(0,\tilde{z})]$ computed from Eq. (4) has been displayed as curve C, showing the prediction of local dielectric theory.

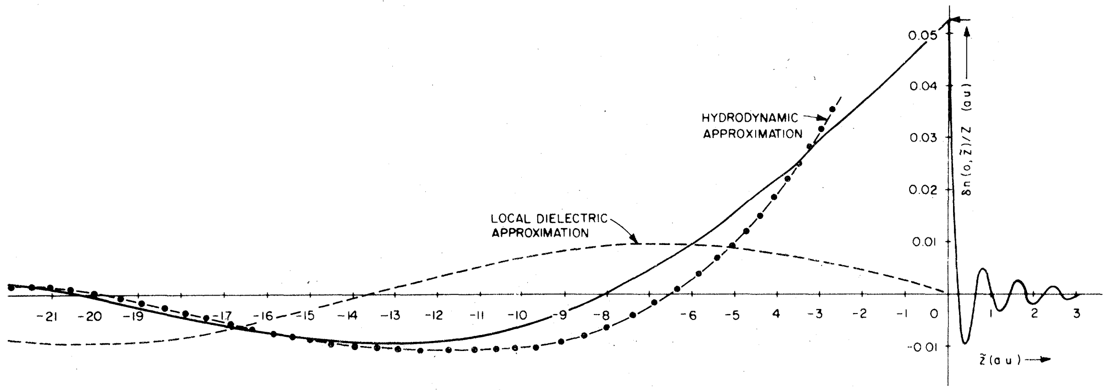

FIG. 4. Induced density fluctuations along the trajectory of a projectile for the same parameters chosen for Fig. 3. The solid curve was calculated from Eqs. (26)–(28). It shows a collective wake trailing the particle and the electron density enhancement, Eq. (29), at the origin. The value of $\delta n(0,0)$ is given to high accuracy by Eq. (29), which was derived neglecting collective effects completely. The bow wave and the periodic crispations superimposed on the trailing wake signify small-impact parameter collisions with the projectile. The dashed curve displays the results of calculating $\delta n(0,\tilde z)$ from Eq. (10) using the dielectric function, Eq. (3), without dispersion. When dispersion is included according to Eq. (13), without single-particle response, δn follows the dash-dot curve labeled "hydrodynamic approximation."

Figure 4 exhibits a plot of $\delta n(0,\tilde z)/Z$ vs $\tilde z$ computed from Eqs. (26)–(28) for the parameters used in preparing Fig. 3. The prominent peak at $\tilde z=0$ is predominantly due to single-particle density enhancement at the ion. At distances large compared to v/ω_p behind the ion, $\delta n(0,\tilde z)$ oscillates with wavelength $\sim 2\pi v/\omega_p$. The dashed curve represents the result of computing $\delta n(0,\tilde z)$ from Eq. (10) in the local dielectric approximation, Eq. (3); it oscillates for all $\tilde z<0$, but out of phase by $\pi/2$ compared to the solid curve. When merely dispersion is included according to Eq. (13) without single-particle response, $\delta n(0,\tilde z)$ follows the dash-dot curve referred to as the hydrodynamic approximation.

Figures 5–7 display the wake potential as $\Phi(\rho,\tilde z)/Ze$ in the $\rho,\tilde z$ plane as derived from Eq. (17) for the parameters chosen for Fig. 3 and the ion velocities indicated in multiples of the atomic unit $v_0=e^2/\hbar$. Figures 8–10 show the corresponding electron-density fluctuations according to Eqs. (26)–(28). One sees the distinctive oscillations of the wake potential in the region behind the particle, $\tilde z<0$, of wavelength $\simeq 2\pi v/\omega_p$. Preceding the particle, the bow wave with much smaller amplitude appears at $\tilde z>0$, of wavelength $\simeq 2\pi\hbar/mv$, as given for $\rho=0$ in the magnified view of Fig. 3. The bow waves, here clearly visible, form periodic paraboloidal disturbances with apexes slightly in front of the projectile and extending behind it with half angle of opening $\sim \arcsin(\beta/v)$. They signify the emission of plasmons by the ion, that eventually are damped into electron-hole pairs. Single-particle effects in the form of bow waves are contained only in a dielectric description such as Eq. (15) that gives asymptotically the proper single-particle behavior for large k.

These are new results. Heretofore, the equations for Φ, presented in complete form in Refs. 1 and 11, were discussed only in terms of simplified dielectric functions which did not contain single-particle descriptions and, thus, could not lead to the complete, rich wake structure given by Eq. (26) *et seq.*

Vager and Gemmell[21] proposed an empirical formula for the wake potential to account for measured distributions[22] for protons emerging along the beam direction from thin foils bombarded with (2 to 3.5) MeV $(\mathrm{HeH})^+$ ions. The experiment probes the wake potential close to the origin, near the initial separation given by the internuclear distance (~2 Å) of the ions. The formula results from Heisenberg broadening[18] of the local dielectric potential by replacing ρ^2 with $\rho^2+(\hbar/mv)^2$, where $2\pi\hbar/mv$ is the de Broglie wavelength of an electron in the medium viewed from the rest frame of the ion. In short, compared to our Eq. (4), the Eq. (5) in Ref. 21,

$$\Phi_{\mathrm{VG}}(\rho,\tilde z)=-\frac{Ze\,\omega_p}{v}\int_0^\infty \sin\left[\frac{\omega_p\zeta}{v}\right]\times\left[\rho^2+\left[\frac{\hbar}{mv}\right]^2+(\zeta+\tilde z)^2\right]^{-1/2}d\zeta\ , \tag{30}$$

is a potential that is Heisenberg-broadened in the ρ direction.[23] This can be seen by integrating Eq. (30), with the identity

$$(x^2+y^2)^{-1/2}=\int_0^\infty dt\,J_0(xt)\exp(-|y|t)\ , \tag{31}$$

to obtain

$$\Phi_{\mathrm{VG}}=Zeh_{\mathrm{VG}}(\rho,\tilde z)+\frac{2Ze\,\omega_p}{v}\sin\left[\frac{\omega_p\tilde z}{v}\right]\times K_0\left[\frac{\omega_p}{v}\left[\rho^2+\left[\frac{\hbar}{mv}\right]^2\right]^{1/2}\right]\Theta(-\tilde z)\ , \tag{32}$$

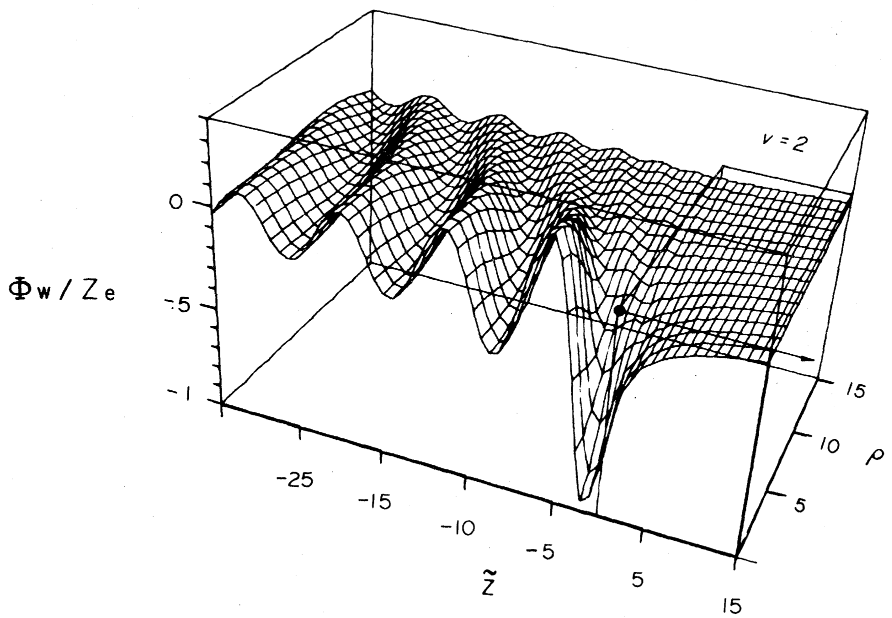

FIG. 5. Wake potential surface $\phi_w(\rho,\tilde{z})/Ze$, as calculated for a projectile moving with velocity v in a medium having properties as specified in the caption of Fig. 3. This particle is located at the origin of the $(\tilde{z}, \rho, \Phi)$ coordinate system as indicated by the dot and the arrow points in the direction of $\vec{v}$.

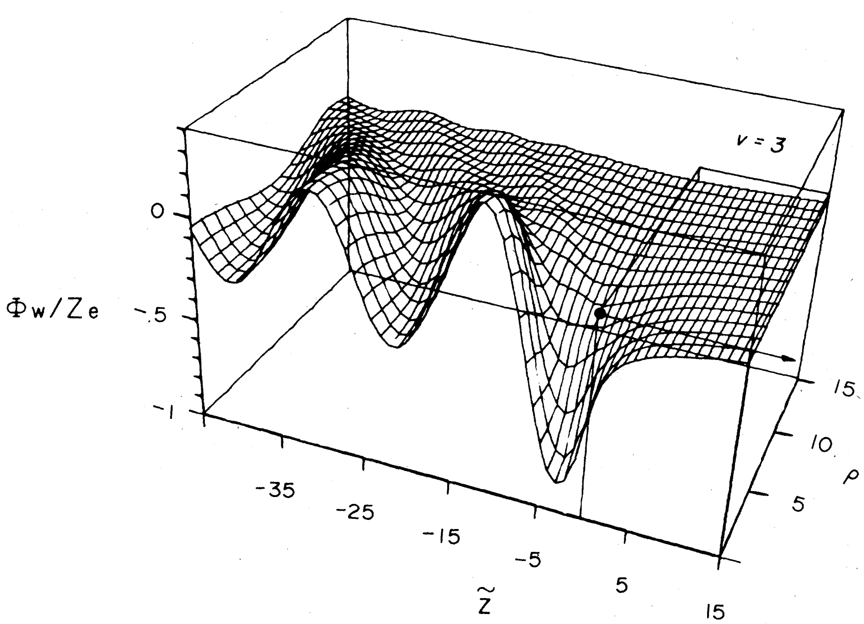

FIG. 6. Wake potential surface for the conditions of Fig. 5 except that $v=3$.

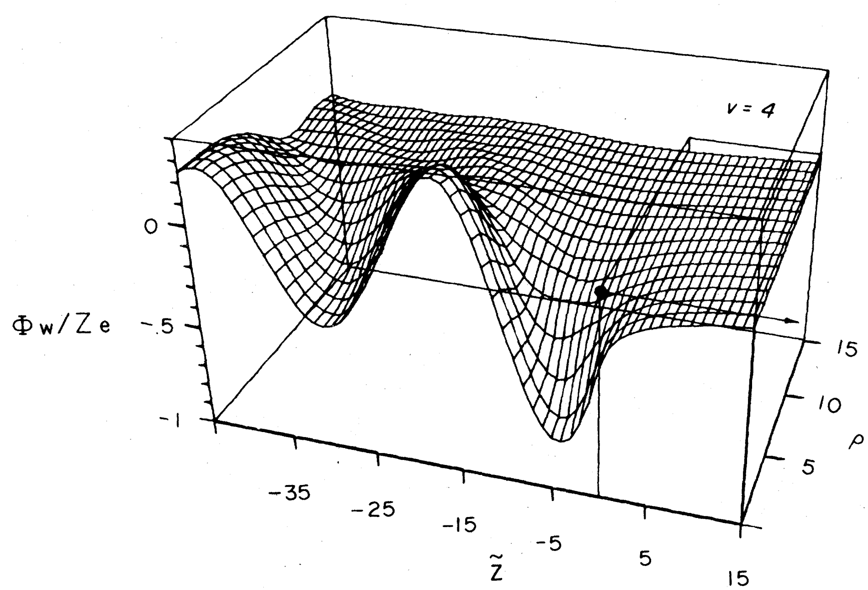

FIG. 7. Wake potential surface for the conditions of Fig. 5 except that $v=4$.

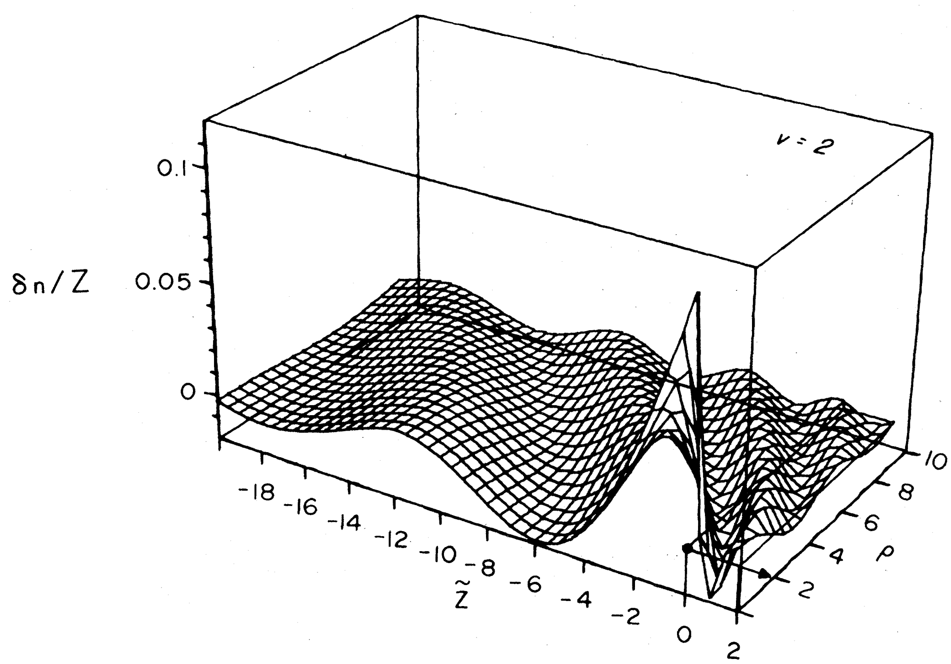

FIG. 8. Surfaces depicting electron density fluctuations $\delta n(\rho,\tilde{z})$ induced by a moving ion under conditions of Fig. 5. The density enhancement at the origin is clearly visible. The single-particle bow wave and the crispations superimposed on the collective wake have wavelength $\sim 2\pi\hbar/mv$. A series of wave fronts generated by the particle motion appear ahead of the particle. The crests of these waves extend to the side of and behind the particle, widening and blending smoothly to constitute disturbances with the limiting wavelength $2\pi v/\Omega_0$ characteristic of collective motion. The parameters are the same as those specified in Fig. 5. Note that the scales of $\tilde{z}$ and ρ have been expanded as compared to those of Fig. 5 to exhibit details.

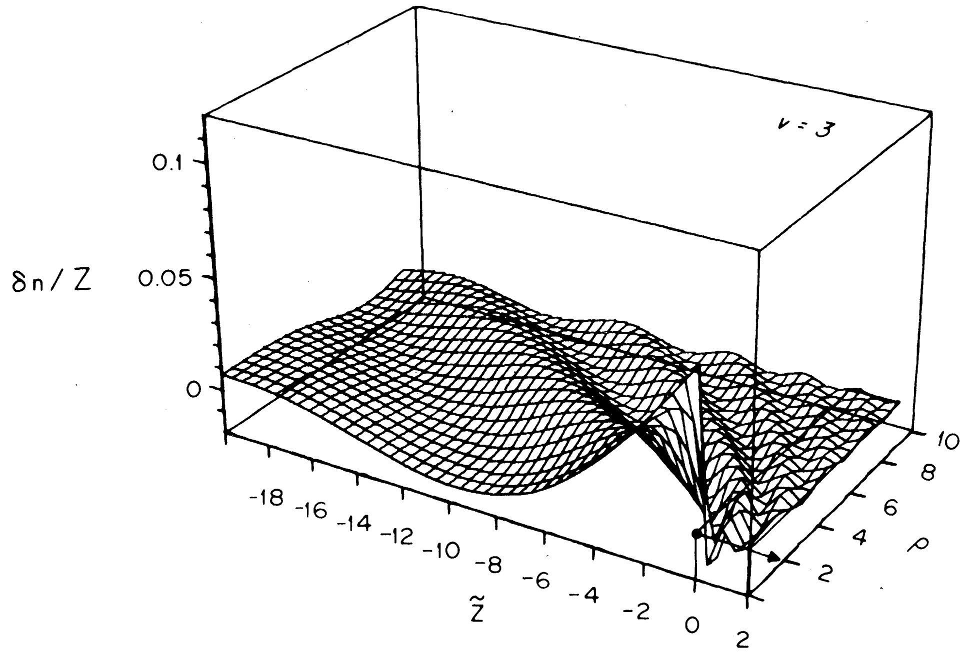

FIG. 9. Surface depicting electron-density fluctuations for the conditions of Fig. 5 except that $v=3$.

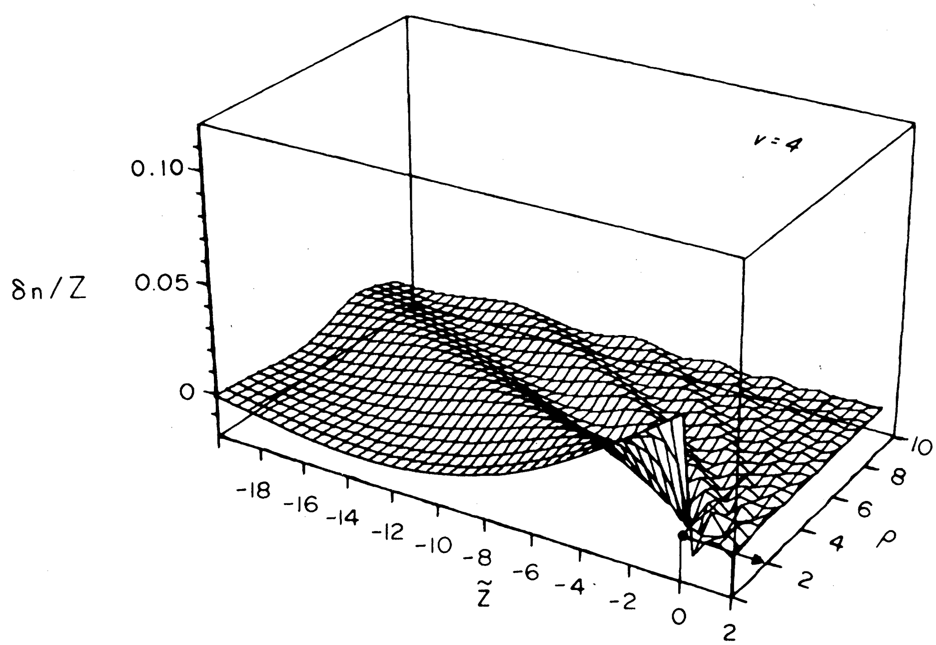

FIG. 10. Surface depicting electron-density fluctuations for the conditions of Fig. 5 except that $v=4$

where

$$h_{\rm VG}(\rho,\tilde{z})=\frac{1}{R}-\frac{\omega_p}{v}S_0\left[\frac{\omega_p}{v}\left[\rho^2+\left(\frac{\hbar}{mv}\right)^2\right]^{1/2},\ \frac{\omega_p\tilde{z}}{v}\right]\ . \tag{33}$$

Evidently, this type of heuristic quantum correction does not include Heisenberg broadening in the $\tilde{z}$ direction nor the bow wave component and, thus, leads to a result that differs merely in minor ways from our simplified form[1,9] quoted in Eq. (4). Only a complete dielectric description, as Eq. (15), reveals the full-wake phenomenon with bow waves, Eqs. (26)–(29), and yields the potential that gives the correct formula for the stopping power, Eq. (25).

As we indicated earlier,[11] for the effective, velocity-dependent charge number, $Z^*(v)$, of the moving ion,[24] the relative density fluctuation $|\delta n/n|$, in the collective part of the wake $[\tilde{z}\lesssim\frac{1}{2}\pi(v/\omega_p)]$, given by

$$\left|\frac{\delta n}{n}\right|=\left|\frac{e\nabla^2\Phi}{m\omega_p^2}\right|\lesssim Z^*(v)\left(\frac{v_0}{v}\right)^3\frac{\hbar\omega_p}{mv_0^2}\ ,\quad v>v_0\ , \tag{34}$$

is always smaller than one. That is, linear-response theory applies even for collective wake phenomena induced by ions with large atomic numbers.

The paraboloidal cones of boundary waves displayed in Figs. 5–10 deserve further comment. They are akin to Mach cones of acoustical waves generated in elastic media and to Vavilov-Cherenkov cones of the radiation fields generated in dielectric media by swift projectiles. But the waves discussed here differ from the known phenomena. They represent coherent charge-density fluctuations induced by the longitudinal electric field of moving ions in a Fermi liquid of charged particles. These density fluctuations consist of coherently emitted elementary excitations. In the linear average description used here, they are plasmons at large distances ($\gg v/\Omega_0$) from the track and quasiparticles (struck, dressed electrons) at points close ($\ll v/\Omega_0$) to the track. The energy flux in the shock front may be quite large for $Z\gg 1$ and $v>v_0$, according to the theory employed here. One must remember, however, that the plasmon is a quantum entity. Multiplasmon absorption by a single electron ejected from the valence band could conceivably result in the emission of a very energetic electron. But the probability for such high-order, compound processes is unknown and must be evaluated before one can make quantitative predictions about the significance of such high-energy products for the study of electronic shock waves. It seems likely that the overwhelming fraction of the decay products consists of a large number of low-energy electrons, each with energy $\approx\hbar\Omega_0$, corresponding to the single-particle decay of plasmon states.

III. ENERGY FLUCTUATIONS

The wake potential described by Eq. (1) represents a statistical average of a quantity that is subject to quantal fluctuations. A measure of these variations may be obtained by comparing Ω, the straggling of energy loss (or gain) of a test charge Q located at an arbitrary position in the wake, with $-\langle dE\rangle$, the expected value of its energy loss. We do not assume that the test charge is bound in the wake of the leading charge but only that it proceeds with equal velocity through the medium and remains at essentially the same location in a coordinate system in which the leading charge is at rest for a time long enough for the calculation sketched below to be valid. We have in mind an ionic dicluster formed when a swift molecular ion is incident on a solid. The energy loss may be written in terms of the force on the test charge exerted through a path length dR as

$$-\langle dE\rangle=-(Q^2\langle dE\rangle_0+QZe\,\langle dE\rangle_w)\ . \tag{35}$$

The mean energy loss for a unit charge due to the self-wake of the test particle is given by

$$-\langle dE\rangle_0=dR\,\frac{\partial}{\partial\tilde{z}}\Phi_0=dR\frac{2}{\pi v^2}\int_0^\infty\kappa\,d\kappa\int_0^\infty\frac{\omega\,d\omega}{k^2}\,{\rm Im}\left[\frac{-1}{\epsilon(k,\omega)}\right]\ . \tag{36}$$

The energy loss due to the wake of the leading ion at the position $\rho,\tilde{z}$ for a unit test charge, in terms of Eq. (1), is given by

$$-\langle dE(\rho,\tilde{z})\rangle_w=dR\,\frac{\partial}{\partial\tilde{z}}\Phi_w(\rho,\tilde{z})/Ze=dR\,\frac{2}{\pi v^2}\int_0^\infty\kappa\,d\kappa\int_0^\infty\frac{\omega\,d\omega}{k^2}J_0(\rho\kappa)\,{\rm Im}\left[\frac{-\exp(i\omega\tilde{z}/v)}{\epsilon(k,\omega)}\right]\ . \tag{37}$$

The total force, $-\langle dE/dR\rangle$, is due to the action of electronic motion induced in the medium through the scalar electric potential, Φ_0, set up by the test charge and through the wake potential Φ trailing the swift ion. The force is the result of the development, in time, of the wave function of the medium under the perturbing influence of the ion and the test charge.

The effect of the medium in terms of elementary collision processes entails the quantum of energy $\hbar\omega$ and the momentum $\hbar\vec{\kappa}$ perpendicular to $\vec{v}$. The probability, $d^2p/d\kappa\,d\omega$, that the test charge absorbs a quantum of frequency ω and wave vector $\vec{\kappa}$ while traversing the path length dR becomes

$$\frac{d^2p}{d\kappa\, d\omega} = dR\frac{2Q}{\pi \hbar v^2}\frac{\kappa}{\kappa^2+\omega^2/v^2}\left[ZeJ_0(\rho\kappa)\,\mathrm{Im}\left(\frac{-\exp(i\omega\tilde{z}/v)}{\epsilon(k,\omega)}\right)+Q\,\mathrm{Im}\left(\frac{-1}{\epsilon(k,\omega)}\right)\right]. \tag{38}$$

Note that only if both ρ and $\tilde{z}$ are zero is Eq. (38) positive definite. It must have the possibility of being negative, since it may describe energy gain in certain regions of the wake.

The differential probability $d^2p/d\omega\, d\kappa$ is similar to the complex space- and time-dependent Van Hove correlation function,[25] which is obtained by Fourier-transforming a positive-definite probability distribution function that depends on energy and momentum transfer. This type of correlation function reflects the essential quantum properties of the system.[18] Equation (38) may also be regarded as a kind of Wigner distribution function, since it describes momentum and energy transfers to the medium at an arbitrary position.

To obtain Ω^2 we need only multiply the integrands of Eqs. (36) and (37) by $\hbar\omega$, as was shown on general grounds by Bohr.[26] Thus,

$$\Omega^2(\rho,\tilde{z}) = \langle (dE)^2\rangle - \langle dE\rangle^2 = |Q^2\Omega_0^2 + Q\, Ze\,\Omega_w^2(\rho,\tilde{z})| \tag{39}$$

where the usual straggling in energy loss for a unit test charge is given by

$$\Omega_0^2 = dR\,\frac{2\hbar}{\pi v^2}\int_0^\infty \kappa\, d\kappa \int_0^\infty \frac{\omega^2\, d\omega}{k^2}\,\mathrm{Im}\left(\frac{-1}{\epsilon(k,\omega)}\right), \tag{40}$$

i.e., is caused by the wake set up by the test charge itself. The contribution of the wake induced by the leading ion to the straggling in the energy loss of the test charge at $\rho,\tilde{z}$ becomes, for $Q=e$,

$$\Omega_w^2(\rho,\tilde{z}) = dR\,\frac{2\hbar}{\pi v^2}\int_0^\infty \kappa\, d\kappa \int_0^\infty \frac{\omega^2\, d\omega}{k^2} J_0(\kappa\rho)\,\mathrm{Im}\left(\frac{-\exp(i\omega\tilde{z}/v)}{\epsilon(k,\omega)}\right). \tag{41}$$

It is understood that Ω^2 by definition must be positive definite, hence the absolute value sign on the right-hand side of Eq. (39). In the limiting case $Q \ll Ze$, both the energy loss and the straggling of the test charge calculated from Eq. (39) without the absolute value sign may become negative if it is located, e.g., in the

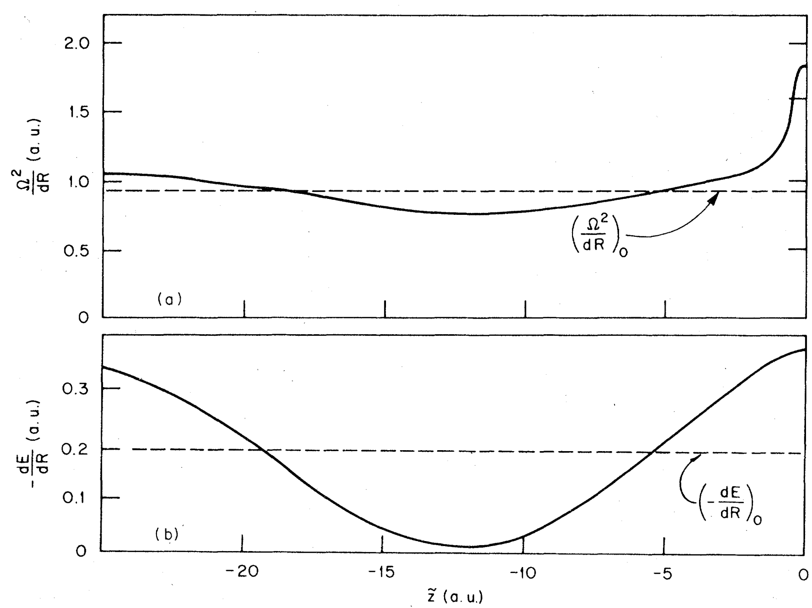

FIG. 11. Total energy straggling per unit pathlength, $\Omega^2(0,\tilde{z})/dR$ [(a), solid curve], of a charge $Q=e$ behind a moving proton under the conditions of Fig. 3 is only slightly larger than the constant quantity, Ω_0^2/dR [(a), dotted line] due to the test-charge wake in the absence of the leading proton. The total stopping power, $-\langle dE(0,\tilde{z})/dR\rangle$ [(b), solid curve] of a charge $Q=e$ in the proton wake varies strongly with $\tilde{z}$ and can approach zero, as compared to the constant $-dE/dR_0$ [(b), dashed line] of the test charge without a leading proton. The parameters chosen were the same as those used for Fig. 3.

region

$$-\frac{3\pi}{2}\frac{v}{\omega_p} \lesssim \tilde{z} \lesssim -\frac{\pi}{2}\frac{v}{\omega_p} \quad ; \quad 0 \leq \rho \leq v/\omega_p \ .$$

Figure 11(a) displays Eq. (39) for a test charge $Q = e$ along the trajectory ($\rho = 0$) of a proton ($Z = 1$). The difference between Ω^2/dR (solid curve) and the $\tilde{z}$ independent Ω_0^2/dR (dashed line) is seen to be $<10\%$ at all distances equal to or larger than typical internuclear separations in molecular ions ($\sim$2 a.u.). By comparison, Fig. 11(b) shows that the stopping power, $-\langle dE(0,\tilde{z})/dR \rangle$, for the test charge along the leading-ion track varies strongly with $\tilde{z}$ relative to the constant value, $-\langle dE/dR \rangle_0$, in the absence of a wake and, in fact, can approach the value zero. We conclude that under typical conditions of experimental interest, energy fluctuations in the wake have only a small effect on the energy loss and straggling of projectiles moving in the coherent wakes that trail swift ions in solids. This is to be expected since the trailing part of the wake consists mainly in small displacements of a relatively large number of electrons and hence carries small momenta ($<< \hbar k_F$). In addition the quantal energy content of the trailing wake should be narrowly concentrated about the plasmon energy. The leading ion plows its way through the electron gas leaving only gentle perturbations that persist in the neighborhood of the track. These perturbations may affect the trailing ion appreciably but should give rise to minimal fluctuations in its motion compared with fluctuations experienced in its direct interaction with the undisturbed medium. Similarly, we expect that dewaking of an electron in a wake-bound state trailing a swift ion will originate primarily from interactions of the wake-bound electron with electrons in the ground state of the solid[11] and that negligible contributions will arise due to interaction with the wake of the leading ion. This implies the integrity of the wake potential, which indeed has been confirmed through observations of the alignment of diclusters by the wake force,[3] the Coulomb-explosion patterns of clusters,[27] and the wake splitting of atomic states under resonant coherent excitation in crystal channels.[28]

V. SUMMARY

We have shown that a swift charged particle induces excitations in an extended matter medium. In the region behind the particle, they are predominantly collective in character. In the forward hemisphere of directions, quasiparticle excitations make up bow waves preceding the particle. These constitute knock-on electrons which have experienced small-impact-parameter collisions with the particle. In domains very close to the particle ($R < \hbar/mv$), both the wake potential and the wake density undergo marked variations along the particle track. The former determines the stopping power of the medium for the particle, and the latter the electron density at the projectile.

Energy straggling of particles moving in the wake of leading ions is shown to be somewhat larger than that experienced by isolated particles. But the increments are sufficiently small for normally occurring ion clusters so as to affirm the wake as a well-defined physical phenomenon in many-electron systems.

A swift ion creates paraboloids of multiple electronic shock waves of some complexity. It is conceivable that this rich spatial structure of electron-density fluctuations may have interesting manifestations in experiment and important consequences for the behavior of matter under high-intensity ion-beam bombardment.

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