ELECTRONIC STOPPING POWER FOR FAST IONS CARRYING ELECTRONS*

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The influence of an electron bound to a fast light ion on the impact parameter dependent electronic energy transferred in a single collision to a neutral atom was calculated within the perturbation formalism, using sum rules. The random stopping power, calculated analytically from this theory was shown to have the Bethe form. Analytical results were obtained for the dipole approximation. The present results were compared with other theoretical results.

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1. Introduction

The impact parameter dependent electronic energy losses and the stopping power have been of interest and of theoretical and practical importance since the early works [1–2]. Theoretical results for random stopping for partially stripped ions [3–5] show good agreement with experimental data. Much work was devoted to the impact parameter dependent energy transfer for bare ions [6–17], employing the first order Born approximation, many electron ground state and sum rules [6–9], wave packet theory [10], the harmonic oscillator model [11-12], the dipole approximation [13–14], the electron density treatment [10, 15–17], classical electrodynamics [18] and higher order perturbation treatment [19]. Numerical calculations based on semiclassical approximation were published [20]. In Refs [9, 21] some approximate formulae used in computer simulations [22–23] were presented.

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In this report we show results for the impact parameter dependent electronic energy transfer $\Delta E(b)$ in a single collision of a fast, light ion carrying bound electrons frozen in a ground state with an atom. The random stopping power $S_r(v)$, for such ion, calculated analytically from $\Delta E(b)$ through integration over impact parameter b, was shown to have the Bethe form. The dipole region contribution to the $S_r(v)$ was incorporated in a fitting parameter ω_0 , replacing in the Bethe formula the mean excitation energy I. The properties of the ground state of target atom were taken into account shell by shell, by means of the Thomas Reiche Kuhn sum rule.

The results of the present calculations were compared with other theoretical results for binary collision of helium and hydrogen ions, carrying electrons in their ground state, with carbon and aluminum atoms. This comparison showed that the present model, which does not take into account ion-inelastic processes, can provide approximate information on the $\Delta E(b)$.

We use atomic units throughout this work.

2. Calculation procedure

We start from considering of a light ion of atomic number Z_i moving along a straight line with velocity v and with impact parameter b in respect to a target atom placed in the origin. The ion is supposed to carry N_i electrons bound in the ground state and described by the spatial density $\rho_i(r)$. The target atom of atomic number Z_a, is described by the Hartree Fock Hamiltonian H_0 , and the atomic ground state $|0_a\rangle$, and the atoms are treated to be free in the lattice site. The reaction of the free electrons of the medium to the disturbance is described in terms of a scalar dielectric response function $\varepsilon(k,\omega)$ [24–25]. The excitation and exchange of the electrons of the ion are not taken into account in this treatment. This electrons are called to be frozen in the ground state.

The total potential $V(r,b,v,t)$ produced by an ion, accompanied by electrons frozen in the ground state on the ion, is given by:

$$V(r,b,v,t) = \left(Z_i|\boldsymbol{R}|^{-1} - N_i \int d^3r' \rho_i(r')|\boldsymbol{R}+\boldsymbol{r}'|^{-1}\right), \qquad (1)$$

where, $\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}t - \boldsymbol{r}$, and $\boldsymbol{r}$ is the position of a target atom electron. The total potential at the position of atomic electron, screened dynamically by reaction of the medium, represented by a dielectric response function $\varepsilon(k,\omega)$, is obtained from Eq. (1) after making an appropriate Fourier transform [24–25],

$$V(r,b,v,\omega) = Z_i(\pi v)^{-1} \int d^3q \exp\left(i\boldsymbol{q}(\boldsymbol{r}-\boldsymbol{b})\right) \delta\left(q_z - \frac{\omega}{v}\right) \frac{Z(q)}{q^2\varepsilon(q,\omega)}, \qquad (2)$$

where $Z(q)$, the ionic form factor, is here given by,

$$Z(q) = 1 - Z_i^{-1} \left\langle 0_i \middle| \sum_i^{N_i} \exp(iqr_i) \middle| 0_i \right\rangle . \tag{3}$$

Within the first order time dependent theory the average energy $\Delta E(b,v)$ transferred from the ion to the target atom in a binary collision is given by:

$$\Delta E(b,v) = \sum_n \omega_{n0} |f_{n0}|^2 , \tag{4}$$

where $\omega_{n0} = \omega_n - \omega_0$, $H_0|n_a\rangle = \omega_n|n_a\rangle$,

$$f_{n0} = \left\langle n_a | V(r,b,v,\omega_{n0}) | 0_a \right\rangle . \tag{5}$$

We start from calculation of the random stopping power defined as the integral from $\Delta E(b,v)$, Eq.(4), over impact parameter b, $S_r = \int d^2b \Delta E(b,v)$, to yield the $S_r(v)$ in the following form:

$$S_r(v) = 2Z_i^2 v^{-2} \sum_n \int_{q<2v} d^3q \delta \left(q_z - \frac{\omega_{n0}}{v} \right) \frac{Z^2(q)}{q^2 |\varepsilon(q,\omega_{n0})|^2} . \tag{6}$$

In the Bethe treatment for bare ions [1–5], and for high velocity dressed ions [4], we can divide the integration over q at a momentum $q_0 = \omega_0/v$, into two regions: the region where the dipole approximation can be applied and the sum rule region. This parameter q_0 is finally cancelled out by adding the two components. The dipole term, when set to zero, can be used for the definition of the lower limit of integration q_0 in the sum rule term. It was also shown [8], that for high velocity the contribution coming from the dipole term is incorporated in ω_0, if we take $\omega_0 > 2\omega_b$, where ω_b is the binding energy. This choice allows us to reproduce the Bethe form for the $S_r(v)$ at high velocity. From this moment on we divide all Z_a electrons of the atom into groups of n_j electrons nearly of the same binding energy ω_j and with $q_j = \omega_j/v$. We can fit $S_r(v)$, given by the sum rule term of Eq.(6) to Ziegler's empirical stopping power [28–29] through an appropriate selection of $\{\omega_j\}$ parameters. In the following, for short notation, we will use index 0 instead of j. The upper limit Q of integration over q, in Eq. (6) for S_r comes from kinematical considerations.

After replacement of $\{\omega_{n0}\}$ in the δ-function of Eq.(2) and subsequently in Eq.(5) by ω_0 the interaction potential is given by a function of coordinates only and we can perform summation in Eq. (4) over all excited and ionized

states for the group of n_0 electrons by using the familiar sum rule [26] with the result:

$$\Delta E(b) = \sum_n \omega_{n0} |\langle 0_a | V(r, b, v, \omega_0) | 0_a \rangle|^2 = \tfrac{1}{2} \langle 0_a | | \nabla V(r, b, v, \omega_0)|^2 | 0_a \rangle , \tag{7}$$

where the gradient ∇V is taken in the space coordinates of all n_0 electrons. The integration over impact parameter b yields the random stopping S_r , of Eq.(6) in the form,

$$S_r(v) = 2Z_i^2 v^{-2} n_0 \int_{q<2v} d^3q \delta \left(q_z - \frac{\omega_0}{v} \right) Z^2 \frac{(q)}{q^2 |\varepsilon(q, \omega_0)|^2} . \tag{8}$$

The S_r of Eq. (8) can be calculated analytically provided we use $\varepsilon(k, \omega) = 1$, and the hydrogen like ionic form factor defined as, $Z(q) = 1 - Z_i^{-1} N_i [(1 + (q a_i/2)^2]^{-2}$, $a_i = 1/Z_i$. With the lower limit of integration for the sum rule term given by $q_0 = \omega_0/v$, and the upper limit $Q = 2v$, the random stopping power $S_r(v)$ can be obtained after elementary integration as,

$$S_r(v) = \frac{4\pi Z_i^2}{v^2} n_0 \left(\ln \frac{2v^2}{\omega_0} + a \left(\frac{a}{2} - 1 \right) [A(y) - A(z)] + a^2 [B(y) - B(z)] \right) ,$$

$$A(y) = (1 + y^2)^{-1} - \ln(1 + y^2) , \qquad B(y) = \frac{(1 + y^2)^{-3}}{6} + \frac{(1 + y^2)^{-2}}{4} ,$$

$$y = v a_i , \qquad z = \omega_0 \frac{a_i}{2v} , \qquad a = \frac{N_i}{Z_i} , \qquad a_i = \frac{1}{Z_i} , \tag{9}$$

n_0 is the number of atomic electrons on the energy shell ω_0.

The potential of Eq. (2), with the restrictions imposed on the limits of integration over q, can be written as

$$V(r, b, v, \omega) = -\frac{2Z_i}{v} \exp \left(\frac{iz\omega}{v} \right) f_0 ,$$

$$f_m = \int_0^Q dq\, q^{m+1} J_m(qs) \frac{Z(k)}{k^2 \varepsilon(k\omega)} ,$$

$$k^2 = q^2 + \frac{\omega^2}{v^2} , \quad Q^2 + \frac{\omega^2}{v^2} = 4v^2 , \quad s = |r - b| , \tag{10}$$

where $J_m(x)$ is the Bessel function of the first kind and m-th order.

After substitution of the potential, Eq. (10), to Eq. (7) the impact parameter dependent energy transfer can then be obtained in the form amenable for numerical calculations:

$$\Delta E(b) = 2Z_i^2 v^{-2} n_0 \langle 0_a | \left(\frac{\omega_0}{v}\right)^2 |f_0|^2 + |f_1|^2 | 0_a \rangle . \tag{11}$$

The analytical results for the potential V of Eq. (10) can be obtained provided we use small-q form for the dielectric response function $\varepsilon(q,\omega) = 1 + q_{\mathrm{TF}}^2/q^2$ (q_{TF} is the Thomas–Fermi screening wave vector), the hydrogen-like ionic form factor, and provided we extend the integration over q to infinity. The result is

$$V(r,b,v,\omega) = \frac{-2Z_i}{v} \exp \frac{i\omega z}{v} \{K_0(Cs)(1-\xi) + \xi[K_0(As) + \eta s K_1(As)]\}$$

$$\xi = \alpha \left[1 - \left(\frac{k_{\mathrm{TF}} a_i}{2}\right)^2\right]^{-2}; \quad \eta = \frac{\left[4a_i^{-2} - k_{\mathrm{TF}}^2\right]}{2A};$$

$$A^2 = \frac{\omega_0^2}{v^2} + 4a_i^{-2}; \quad C^2 = \frac{\omega_0^2}{v^2} + k_{\mathrm{TF}}^2; \quad \alpha = \frac{N_i}{Z_i}. \tag{12}$$

In this case the impact parameter dependent energy transfer $\Delta E(b)$ is obtained by taking a squared modulus of the potential gradient, Eq. (12), and taking the average over the atomic ground state. The result is

$$\Delta E(b) = 2\left(\frac{Z_i}{v}\right)^2 n_0 \left(\frac{\omega_0}{v}\right)^2 \{g_1^2 + g_2^2\},$$

$$g_1 = (1-\alpha) K_0\left(\frac{b\omega_0}{v}\right) + \alpha[K_0(Ab) + \eta b K_1(Ab)],$$

$$g_2 = (1-\alpha) K_1\left(\frac{b\omega_0}{v}\right) + \alpha\delta[K_0(Ab) + \eta b K_0(Ab)],$$

$$A^2 = \left(\frac{\omega_0}{v}\right)^2 + \left(\frac{2}{a_i}\right)^2, \quad \alpha = \frac{N_i}{Z_i}, \quad \eta = \frac{2}{A a_i^2}, \quad \delta = \left[1 + \left(\frac{2v}{\omega_0 a_i}\right)^2\right]^{0.5}. \tag{13}$$

$K_n(x)$ is the Bessel function of the second kind and n-th order. For a bare ion $N_i = 0$, and for $\varepsilon(k,\omega) = 1$, the Eq. (13) is reduced to the familiar dipole approximation result.

The result of Eq. (11) and Eq. (13) can be compared with other approximate analytical result [6]

$$\Delta E(b) = \left[\frac{S_r}{4\pi}\right] \frac{2b}{b_a} K_1\left(\frac{2b}{b_a}\right)\left(\frac{2}{b_a}\right)^2, \tag{14}$$

where $b_a = (2\omega_0)^{-0.5}$, which has the same form as obtained for bare ions in Ref. [10] within the local electron density formalism. This result can be related also to the Oen and Robinson (OR) formula [21], not valid in the high velocity region, but widely applied for its simplicity:

$$\Delta E(b) = 0.045\left[\frac{S_r}{4\pi}\right] \exp\left(\frac{-0.3b}{a_{\mathrm{TF}}}\right)\left(\frac{2}{a_{\mathrm{TF}}}\right)^2, \tag{15}$$

where $a_{\mathrm{TF}} = 0.88534(Z_i^{2/3} + Z_a^{2/3})^{-0.5}$, is the Thomas- Fermi screening radius. S_r is the random stopping power given by Eq. (8), or determined experimentally.

3. Discussion

In order to find the effect caused by bound electrons on the energy loss we have determined and drawn results of $S_r(v)$ based on Eqs (8)–(9), and of $\Delta E(b)$ based on the Eqs (4), (13)–(15). Since $S_r(v)$, Eqs (8)–(9), differs from the Ziegler's empirical random stopping power $S_z(v)$ [28–29], we fitted S_r to S_z in the case of bare ions by a proper selection of $\{\omega_0\}$ set. The ω_0's separate the dipole and sum rule regions for given groups of electrons n_0 's. As an input data for the fitting procedure we used the binding energies $\{\omega_b\}$ taken from Ref. [27].

In the random case in this velocity region the function defined as $Z^2_{\mathrm{eff}} = S_r(\mathrm{He}^+)/S_r(p^+)$, is nearly a constant. This behaviour is in contradiction to that of the effective charge, which tends to saturation due to the electron exchange. At present Z^2_{eff} is determined by the velocity independent ion form factor.

In the estimation of $\Delta E(b)$ we carried out summation over all energy shells of the atom. The contribution of the outermost valence electrons is dominant for distant collisions and contribution of inner shell electrons is larger for close collisions.

In Fig. 1 the $\Delta E(b)$, calculated on the basis of Eqs (11)–(15), are drawn for proton and hydrogen atoms colliding with Al atoms. The SCA calculation for the inner-shell energy transfer (denoted by s) for 1.0 MeV protons, presented in Ref. [20], are overestimated by Eq. (11), with $q_{\mathrm{TF}} = 0$, nearly by a factor of 2 in the available b region. For large b, however, results of Eq. (11) follow the dipole approximation, Eq. (13). The Oen and Robinson formula, Eq. (15), approaches rather the total energy transfer (denoted by t) taken from Ref. [20] for large b, and underestimates close collisions.

The $\Delta E(b)$ given by Eq. (11)–(15), for He and He ions in a collision with C atoms are presented in Fig. 2, for ion velocity v=20.7. In this case, the approximation of Eq. (14), underestimates the $\Delta E(b)$ of Eq. (11) for large impact parameters. For small b the tendency is opposite.

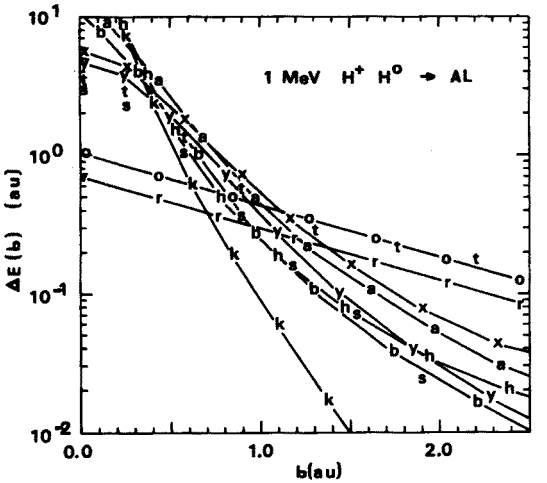

Fig. 1. The $\Delta E(b)$ for 1.0 MeV (v=6.3 au) hydrogen ions in collision with Al atom. Results for p^+ and H^0 ions are shown by pairs of curves (1, 2), respectively. (x, y) — Eq. (11), (a, b) — Eq. (14), (o, r) — Eq. (15), (h, k) — Eq. (13). SCA for 1.0 MeV p^+ in Al, Ref. [20]: symbols s and t indicate inner-shell and total energy transfers, respectively.

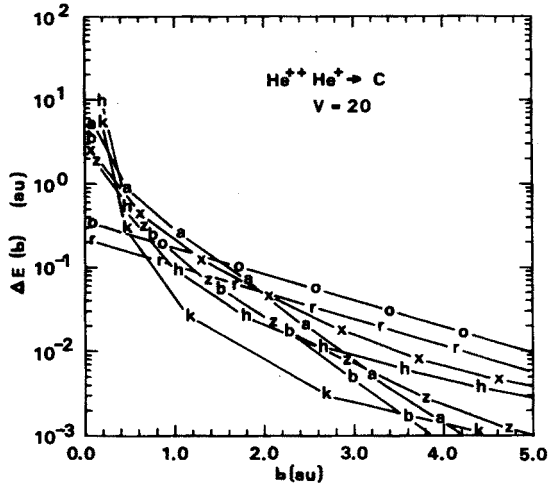

Fig. 2. The $\Delta E(b)$ for helium ions, v=20.7 colliding with C atom. As in Fig. 1 results for He^{++} and He^+ ions are shown by pairs of curves (1, 2), respectively. (x, y) — Eq. (11), (a, b) — Eq. (14), (o, r) — Eq. (15), (h, k) — Eq. (13).

We can conclude that the decrease of $\Delta E(b)$ for ions carrying electrons is much faster than for bare ion. Due to the present shell-wise treatment,

the effective charge is no longer a constant. We can define impact parameter b dependent square of the effective charge as, $Z^2_{\rm eff}(b) = \Delta E_{\rm ion}(b)/\Delta E_{p+}(b)$. In the Oen and Robinson case, where the electron distribution is described within the statistical model $Z^2_{\rm eff}(b)$ is a constant quantity. In the present model the $Z^2_{\rm eff}(b)$, which is a decreasing function of impact parameter b, reflects efficiency of inner-shell excitations for small b, and outermost-shells excitations for large b.

4. Conclusions

In conclusion, it seems that Eqs (11)–(15) provide a basis for rapid determination of the $\Delta E(b)$ for swift light ions carrying electrons in a frozen charge state. They can be used in simulation codes applied for high velocity transmission and surface scattering. Due to shell-wise treatment the influence of bound electrons appears to be impact parameter dependent. The projectile inelastic contribution however demands further study.

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