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EFFECT OF ELECTRON SHELL NONSPHERICITY OF AN EXCITED ION ON ITS STOPPING IN ELECTRON GAS

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The effect of nonsphericity of electron shells of ions, arising in their excitation in the course of passage through matter, on their stopping parameters is considered. The quantitative calculations are carried out within the framework of the dielectric theory for the stopping effective charge of fast nonrelativistic Li^+ ions in their passage through a carbon target. A substantial difference in stopping effective charges between ions with uniform, elongated, and compressed (relative to the direction of motion) electron shell distributions is established.

INTRODUCTION

The excitation of fast ions in their passage through matter has a strong effect on the distribution of the ion fractions of an ion beam and its stopping parameters [1–5]. To illustrate, the effective charge of an ion, which characterizes the stopping power of the given medium with respect to this ion in some or other specified ("frozen") state, depends on the degree of screening of the nuclear charge of the ion by the electrons of its shell, hence on the degree and character of its excitation. Based on the binary ion–atom collision model, Tsuchida and Kaneko [6] have recently paid attention to the possible dependence of the effective charge of an excited ion on the shape of the angular distribution of its electron cloud. We have extended the investigation started by the authors of [6] to the processes of stopping of fast ions in solids and plasma, and in order to take account of the collective response of the electrons of the medium to the passing charge, we have resorted, instead of the binary ion–atom collision model, to the dielectric theory of stopping [7] in its best known, Brandt–Kitagawa version [8]. The analysis is conducted using the general theory of alignment of the angular momenta of atoms and ions in collisions. This allows us to study, using the density matrix apparatus, the effect of the angular anisotropy of the electron cloud of an ion on its effective charge, as applied not only to "pure", but also to mixed states.

FORMALISM

We consider the stopping of an ion with charge $q = Z_1 - N$, where Z_1 is the charge of its nucleus and N is the number of bonded electrons, in the interval between two successive collision events causing a change in its charge or excitation state. Following the generally adopted terminology, we will refer to such an ion as an ion "frozen" in a certain state. Let $\mathbf{v}$ be the velocity of the ion and $\epsilon(\mathbf{k}, \omega)$ be the dielectric function of the medium. The ion charge density $\rho_{\text{ion}}(\mathbf{r}, t)$ in the coordinate system of the target has the form

$$\rho_{\text{ion}}(\mathbf{r}, t) = Z_1 \delta(\mathbf{r} - \mathbf{v}t) - \rho_e(\mathbf{r} - \mathbf{v}t), \tag{1}$$

where $\rho_e(\mathbf{r}')$ is the charge density of the electron shell of the ion normalized in accordance with the condition

$$\int \rho_e(\mathbf{r}')\,d^3r' = N.$$

The electric field $\mathbf{E}(\mathbf{r},t)$ induced by the motion of the ion acts on the ion itself to cause its stopping with force $\mathbf{F}_{\text{stopping}}(t)$ whose magnitude, i.e., the stopping power of the medium, $S_{\text{ion}} \equiv -(\frac{dE}{dx}) = |\mathbf{F}_{\text{stopping}}(t)|$, is calculated by the formula

$$F_{\text{stopping}}(t) = -e\frac{\mathbf{v}}{v}\int \rho_{\text{ion}}(\mathbf{r},t)\mathbf{E}(\mathbf{r},t)\,d^3r. \quad (2)$$

The distribution of the electric field strength will be found from the Maxwell equations

$$\mathbf{D} = \hat{\epsilon}\,\mathbf{E}, \quad \nabla\mathbf{D} = 4\pi e\rho_{\text{ion}}. \quad (3)$$

To this end, we will go over from the $(\mathbf{r},t)$- to the $(\mathbf{k},\omega)$-representation,

$$\rho_{\text{ion}}(\mathbf{k},\omega) \equiv \int \rho_{\text{ion}}(\mathbf{r},t)e^{-i(\mathbf{kr}-\omega t)}d^3r\,dt = 2\pi[Z_1 - \rho_e(\mathbf{k})]\delta(\omega - \mathbf{kv}), \quad (4)$$

where

$$\rho_e(\mathbf{k}) = \int \rho_e(\mathbf{r})e^{-i\mathbf{kr}}\,d^3r \quad (5)$$

is the form factor of the electron cloud of the passing ion. According to expression (3), in the $(\mathbf{k},\omega)$-representation we have

$$\begin{aligned} \mathbf{D}(\mathbf{k},\omega) &= -\frac{i\mathbf{k}}{k^2}\,4\pi e\rho_{\text{ion}}(\mathbf{k},\omega), \\ \mathbf{E}(\mathbf{k},\omega) &= \frac{1}{\epsilon(\mathbf{k},\omega)}\mathbf{D}(\mathbf{k},\omega) = -2\pi\frac{i\mathbf{k}}{k^2}\,4\pi e\frac{[Z_1 - \rho_e(\mathbf{k})]}{\epsilon(\mathbf{k},\omega)}\,\delta(\omega - \mathbf{kv}). \end{aligned} \quad (6)$$

Hence we find

$$\mathbf{E}(\mathbf{r},t) = \frac{1}{(2\pi)^4}\int \mathbf{E}(\mathbf{k},\omega)e^{i(\mathbf{kr}-\omega t)}\,d^3k\,d\omega = -\frac{4\pi e}{(2\pi)^3}\int \frac{i\mathbf{k}}{k^2}[Z_1 - \rho_e(\mathbf{k})]\frac{1}{\epsilon(\mathbf{k},\mathbf{kv})}e^{i\mathbf{k}(\mathbf{r}-\mathbf{v}t)}\,d^3k. \quad (7)$$

Substituting expressions (1) and (6) into (2), we obtain the expression for the stopping power of the medium in the form of an integral in the three-dimensional momentum space,

$$S_{\text{ion}} = \frac{e^2}{2\pi^2 v}\int \frac{\mathbf{vk}}{k^2}[Z_1 - \rho_e(\mathbf{k})]^2\frac{i}{\epsilon(\mathbf{k},\mathbf{kv})}\,d^3k. \quad (8)$$

In an isotropic medium, the dielectric function $\epsilon(\mathbf{k},\omega)$ is independent of the direction of the vector $\mathbf{k}$: $\epsilon(\mathbf{k},\omega) = \epsilon(k,\omega)$. In such a medium, the population of the excited states of the passing ion and the form of the angular distribution of its electron cloud in these states are characterized by axial symmetry about the direction of motion of the ion beam and also by "forward–backward" symmetry about this direction by virtue of the certain parity of the states of the ion. The degree of anisotropy of this distribution is directly related to the degree of alignment of the angular momentum $\mathbf{J}$ of the ion relative to the symmetry axis, the main alignment parameter $A_{20}(J,J)$ characterizing the extent of the quadrupole deformation of the electron cloud being governed by the relative population $W(JM) = W(J,-M)$ of the magnetic sublevels $|JM\rangle$ of the state under consideration [9],

$$A_{20}(J,J) = \left[\frac{5}{(2J+3)J(J+1)(2J-1)}\right]^{1/2}\sum_M[3M^2 - J(J+1)]\cdot W(JM), \quad \sum_M W(JM) = 1.$$

In view of these considerations, the general form of the angular distribution of the charge of electrons in an ion, in both the coordinate and the momentum representation, is given by the formulas

$$\rho_e(\mathbf{r}) = \rho_e(r, \cos^2\theta_r), \quad \rho_e(\mathbf{k}) = \rho_e(k, \cos^2\theta_k).$$

Then we turn to formula (4) and, using the relation

$$\omega = \mathbf{kv} = kv \cdot \cos\theta_k,$$

go over, in calculating the integral in expression (7), from the angular variable θ_k to the equivalent variable ω,

$$d^3k = k^2\,dk \sin\theta_k\,d\theta_k\,d\phi_k = -k^2\,dk\,d(\cos\theta_k)\,d\phi_k = -k^2\,dk\frac{d\omega}{kv}d\phi_k$$

with the appropriate limits of integration

$$(\theta_k)_{\min} = 0 \to \omega = kv, \quad (\theta_k)_{\max} = 180^\circ \to \omega = -kv.$$

And finally, using the general Kramers–Kronig formulas [10]

$$\mathrm{Re}[\epsilon(k,-\omega)] = \mathrm{Re}[\epsilon(k,\omega)], \quad \mathrm{Im}[\epsilon(k,-\omega)] = -\mathrm{Im}[\epsilon(k,\omega)], \tag{9}$$

we obtain the final formula for the stopping power of an isotropic medium with respect to the ion passing though it,

$$S_{\text{ion}} = \frac{2e^2}{\pi v^2}\int_0^\infty \frac{dk}{k}\int_0^{kv}\left[Z_1 - \rho_e\left(k, \left(\tfrac{\omega}{kv}\right)^2\right)\right]^2 \mathrm{Im}\left[-\frac{1}{\epsilon(k,\omega)}\right]\omega\,d\omega. \tag{10}$$

With the expression in the square brackets replaced by the charge $Z_p = 1$, the same formula gives the stopping power of the medium with respect to the passing proton, S_p. By definition, their ratio is the square of the effective charge of the ion "frozen" in the charge state q,

$$q_{\text{eff}} = \sqrt{\frac{S_{\text{ion}}}{S_p}} = \sqrt{\frac{\int_0^\infty \frac{dk}{k}\int_0^{kv}\left[Z_1 - \rho_e\left(k, \left(\frac{\omega}{kv}\right)^2\right)\right]^2 \mathrm{Im}\left[-\frac{1}{\epsilon(k,\omega)}\right]\omega\,d\omega}{\int_0^\infty \frac{dk}{k}\int_0^{kv}\mathrm{Im}\left[-\frac{1}{\epsilon(k,\omega)}\right]\omega\,d\omega}}.$$

Omitting in formulas (9), (10) the variable $\left(\frac{\omega}{kv}\right)^2$ in the expression $\rho_e\left(k, \left(\frac{\omega}{kv}\right)^2\right)$, we can take the factor $[Z_1 - \rho_e(k)]^2$ outside the integral sign $\int_0^{kv}\ldots\omega\,d\omega$ and thus turn back to the usual formulas of the dielectric theory of stopping of ions, where the electron shell of the ion is taken to be spherically symmetric [8, 11, 12].

Where the velocities of the passing ion are high, we calculate the dielectric function of the medium using the model of collective plasma oscillations of a degenerate electron gas [13], where the thermal spread of the electrons that smears the Fermi limit is disregarded,

$$\epsilon(k,\omega) = 1 + \frac{\omega_p^2}{\omega_g^2 + \frac{3}{5}k_F^2k^2 + \frac{1}{4}k^4 - \omega(\omega + i\gamma)}.$$

Here the parameters of the plasmon frequency $\omega_p = \sqrt{\frac{4\pi e^2 n_e}{m_e}}$ and Fermi momentum $k_F = (3\pi^2 n_e)^{1/3}$ are governed by the number density n_e of the electrons in the medium under consideration, the parameter ω_g is introduced to take account of the energy gap in the spectra of dielectrics and semiconductors, and γ is responsible for the damping of plasma oscillations. In the limit as $\gamma \to 0$, the integrand in formulas (9), (10) assumes the form

$$\mathrm{Im}\left[-\frac{1}{\epsilon(k,\omega)}\right] = \frac{\pi\omega_p^2}{2A(k)}\delta[\omega - A(k)], \tag{11}$$

where we have introduced, following the work [8], the additional notation to ease the writing of the subsequent formulas,

$$A(k) = \sqrt{\Omega_0^2 + \frac{3}{5}k_F^2k^2 + \frac{1}{4}k^4}, \quad \Omega_0^2 = \omega_p^2 + \omega_g^2. \tag{12}$$

The roots of the equation

$$\sqrt{\Omega_0^2 + \frac{3}{5}k_F^2k^2 + \frac{1}{4}k^4} = \omega \tag{13}$$

at $\omega = kv$ define the limits of integration

$$k_\pm = \sqrt{2\left(v^2 - \frac{3}{5}k_F^2\right) \pm 2\sqrt{\left(v^2 - \frac{3}{5}k_F^2\right)^2 - \Omega_0^2}} \tag{14}$$

with respect to the variable k in the expressions for the stopping power of the medium and the effective charge of the ion that follow from formulas (9), (10):

$$S_{\text{ion}} = \frac{\omega_p^2}{v^2}\int\limits_{k_-}^{k_+}\frac{dk}{k}\left[Z_1 - \rho_e\left(k, \left(\tfrac{A(k)}{kv}\right)^2\right)\right]^2, \quad q_{\text{eff}} = \sqrt{\frac{\int_{k_-}^{k_+}\frac{dk}{k}\left[Z_1 - \rho_e\left(k, \left(\frac{A(k)}{kv}\right)^2\right)\right]^2}{\ln\frac{k_+}{k_-}}}. \tag{15}$$

CALCULATIONS: EFFECTIVE CHARGE OF EXCITED Li^+ IONS IN A CARBON TARGET

Let us consider as an example the passage of the helium-like Li^+ ion in the $1s2p{:}^1P_1$ singlet state (its excitation energy amounts to 62 eV [14]) through a carbon target. The form of the angular anisotropy in the distribution of the charge of the electrons in such an ion is governed by the alignment of its total angular momentum $J = 1$ (in the case under consideration, it coincides with the orbital angular momentum L of the ion). The measure of alignment is the parameter $A_{20}(1,1)$. When the quantization axis is selected along the direction of the passing flow, this parameter is related to the relative population $W(M)$ of the different states $1s2p{:}^1P_{1,M}$ by formula (8),

$$A_{20}(1,1) = \sqrt{2}(W_1 - W_0),$$

and its limiting values are $A_{20}(1,1)_{\min} = -\sqrt{2}$ (the case of population of the "pure" state $1s2p{:}^1P_{1,M=0}$) and $A_{20}(1,1)_{\max} = \frac{1}{\sqrt{2}}$ (the case of population of the states $1s2p{:}^1P_{1,M=\pm1}$, each with a weight of 50%).

The space distribution of the electrons in the general case of mixed state $1s2p{:}^1P_1$ is found by the known rules [9]

$$\rho_e(\mathbf{r}) = \frac{1}{4\pi}\left[R_{1s}^2(r) + R_{2p}^2(r)\left(1 - \sqrt{2}A_{20}(1,1)\,P_2(\cos\theta_r)\right)\right],$$

where $R_{1s}(r)$ and $R_{2p}(r)$ are the radial wave functions of the electrons in the corresponding states of the ion and $P_2(\cos\theta)$ is a Legendre polynomial. The calculation of its correspondent momentum distribution (5) reduces to the calculation of the radial integrals

$$I^{(\lambda=0)}(k) = \int\limits_0^\infty\left[R_{1s}^2(r) + R_{2p}^2(r)\right]j_0(kr)r^2\,dr, \quad I^{(\lambda=2)}(k) = \int\limits_0^\infty R_{2p}^2(r)\,j_2(kr)r^2\,dr,$$

$$\rho_e(k, \cos^2\theta_k) = I^{(\lambda=0)}(k) + A_{20}(1,1)\sqrt{2}\,P_2(\cos\theta_k)I^{(\lambda=2)}(k),$$

where $j_\lambda(kr)$ are spherical Bessel functions. To calculate them, we use the hydrogen-like functions $R_{1s}(r) = Z^{3/2} \cdot 2e^{-Zr}$ and $R_{2p}(r) = \frac{(Z-1)^{5/2}}{2\sqrt{6}} r\, e^{-\frac{1}{2}(Z-1)r}$, assuming that, owing to the partial screening of the nucleus by the $1s$-electron, the $2p$-electron is in the Coulomb field of the charge $(Z-1)$.

The parameters of the plasmon frequency, $\omega_p = \sqrt{\frac{4\pi e^2 n_e}{m_e}}$, and the Fermi momentum, $k_F = (3\pi^2 n_e)^{1/3}$, that are needed for calculations (11)–(15) ($\omega_g = 0$ at that) will be found proceeding from the average number density of electrons, n_e, in a solid-state carbon target,

$$n_e = 0.052, \quad \omega_p = 0.810, \quad k_F = 1.160$$

(all in atomic units). The calculation results are presented in Fig. 1.

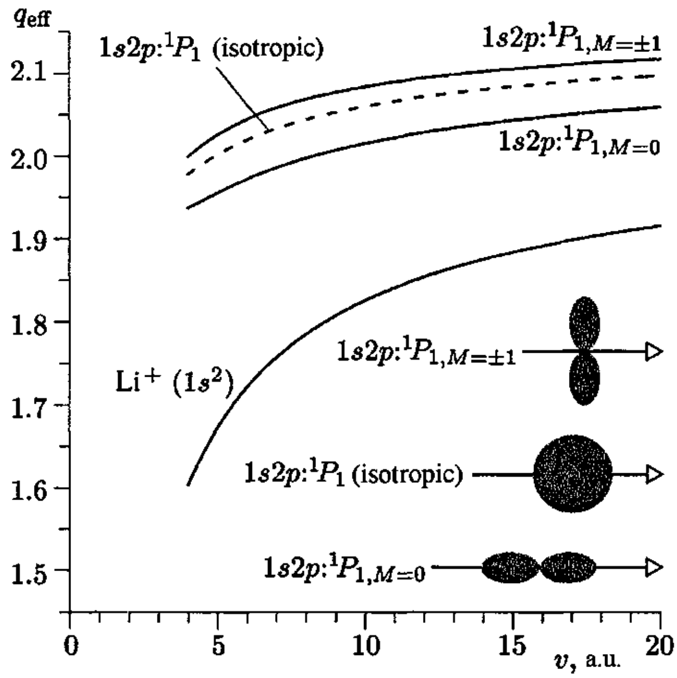

Fig. 1

Fig. 1. Effective charge of the $\rm Li^+$ ion in the excited state $1s2p{:}^1P_1$ in the passage through a carbon target. Bottom curve — electron cloud configuration maximally extended along the direction of motion of the ion ($M = 0$; $A_{20} = -\sqrt{2}$), top curve — electron cloud configuration maximally compressed along the direction of motion of the ion ($M = \pm 1$; $A_{20} = 1/\sqrt{2}$), dashed curve — the case of spherically symmetric charge distribution.

In the velocity interval v = 4–20 a.u. (which corresponds to $\rm Li^+$ ion energies from 3 to 70 MeV) the effective charge of the ion rises monotonically with its velocity, no matter what the form of the angular distribution of the density of its electrons. When the electron cloud of the ion is extended along the direction of its motion, the stopping of the ion is weakened in comparison with the case where all of its three states $1s2p{:}^1P_1$ with $M = 0, \pm 1$ are equally populated. In the opposite case the ion is more strongly stopped, the deviation from the case where the distribution of the electron density of the ion is isotropic being less significant. On the whole, the discrepancy between the magnitudes of the stopping powers of targets,

$$S_{\rm ion} = S_p\, (q_{\rm eff})^2,$$

corresponding to the maximally extended and the maximally compressed form of the distribution of the electron cloud of the $\rm Li^+$ ion in the state $1s2p{:}^1P_1$ amounts, in the above ion velocity interval, to some 10%.

CONCLUSION

The general theory proposed in this work allows one to take account of the nonsphericity of the electron shell of an ion in studying its stopping in a degenerate electron gas. The calculations carried out within the framework of the dielectric theory of stopping, as applied to the passage of nonrelativistic ions through solid-state targets, provide a quantitative estimate of the scale of the effect studied, which proves to be of the same order of magnitude as that obtained earlier by Tsuchida and Kaneko [6] within the framework of the binary ion–atom collision model. The final conclusion of these authors about the importance of using the theoretical results concerning the effect of excitation of ions on their stopping in computer simulation of the passage of ions through matter is thus additionally substantiated.

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