Relaxation and Backscattering of Light Ions in a Semi-Infinite Medium

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Relaxation and backscattering of light ions of moderate energy ($\lesssim 1$ keV) in solid walls are investigated applying the normal Boltzmann equation to a semi-infinite medium, thereby satisfying the exact boundary conditions at the wall surface. Since momentum and energy relax on different scales, Boltzmann's equation is solved in a two scale procedure, treating momentum and energy relaxation separately. Matching the two regions self-consistently yields the ion distribution function and with that macroscopic quantities, e.g. the range distribution and the spectral reflexion coefficient. The application of the method is demonstrated for a simple test model with constant nuclear scattering cross section and no electronic losses.

I. Introduction

In recent years, relaxation and backscattering of particles at solid walls attracted increasing interest. Beside the wide industrial application of ion implantation technique for surface coating or doping of semiconductors, the interaction of a hot plasma with the liner, the limiter — or divertor plates of a tokamak is an important problem of modern fusion technology. Within the context of tokamak physics, one is primarily interested in scattering of light ions of moderate energy ($E_0 \sim 1$ keV).

Due to ion neutralisation, it raises serious difficulties to measure the spectral (energy- and angle-dependent) reflexion coefficient for ions in the energy regime $E \lesssim 1$ keV [1–3].

Numerical simulation codes [4, 5] lack the deep physical insight of an analytical investigation of the problem.

Previous analytical approaches studying the problem start from the model of random binary collisions, e.g. [4], to which they apply the so-called "backward Boltzmann equation" [6–10]. This equation requires an infinite homogeneous medium and therefore yields results only approximately correct for small reflexion coefficients. (Attempts to extend the results of the backward Boltzmann equation to include multiple crossing [10] suffer from the fact that they must assume the angular distribution for the reflected particles.) Moreover, the existing methods solving the backward Boltzmann equation do not evaluate the microscopic distribution function but macroscopic profiles, e.g. range-distributions.

It follows from the preceding that present theories are not satisfactory for light ions due to the high values of the reflexion coefficient and the inability to describe the backscattering microscopically — a necessary requirement to formulate the boundary conditions for the plasma at the wall.

We therefore aim at developing a method to solve the unrestricted Boltzmann equation in a semi-infinite medium accounting correctly for the physically prescribed boundary conditions. This is a difficult task because of the strong anisotropy of the distribution function near the surface, varying strongly over one mean free path. Well-known methods in neutron transport theory [11] treat only the problem of momentum relaxation. Modified theories [12, 13] account for energy exchange, they however turn out to be unsuitable for describing the energy relaxation in a cold medium. Therefore we consider it the central task of our investigation to develop the solution of the Boltzmann equation accounting for energy relaxation and for momentum exchange selfconsistently. Our solution reduces the calculation of the complete distribution of the ions inside and in front of the wall to known numerical methods. For a simple test model even a complete analytical solution is derived.

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II. The Basic Equation

On basis of the model of random binary collisions we start from the stationary force-free Boltz-

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mann equation in plane geometry

$$\mu v \frac{\partial f(v,\mu,z)}{\partial z} = \left(\frac{\delta f}{\delta t}\right)_n + \left(\frac{\delta f}{\delta t}\right)_{el} . \tag{1}$$

Here, $f(v, \mu, z)$ denotes the distribution function of the ions. v is the magnitude of the ion velocity and μ designates the cosine of the angle with the z-direction ($\mu = v_z/v$). The target covers the range $z > 0$, the target surface is located at $z = 0$. The collision terms $(\delta f/\delta t)_n$ and $(\delta f/\delta t)_{el}$ describe the effect of nuclear (elastic) and electronic (inelastic) collisions, respectively.

The nuclear collisions are treated by means of Boltzmann's collision integral in the standard procedure [14]. In doing so we use the Lorentz approximation, which neglects terms of higher order in m/m_0 (m and m_0 are the masses of the ion and the target atom, respectively). The thermal energy of the target material ($\lesssim 0.1$ eV) is neglected in comparison to the kinetic energy of the ions (~ 100 eV). Further, we allow for a linear anisotropy of the nuclear scattering cross-section. Thus we get [15]

$$\begin{aligned}\left(\frac{\delta f}{\delta t}\right)_n = &- n_0(z)\, v\, q_t(v)\,(f - f^0 - \mu f^1) \\ &- n_0(z)\, v\, q\, \mu f^1 \\ &+ \frac{m}{m_0}\frac{n_0(z)}{v^2}\frac{\partial}{\partial v}\{q(v)\, v^4 f^0(v,z)\} ,\end{aligned} \tag{2}$$

where

$$\begin{aligned} f^0 &= \tfrac{1}{2}\int_{-1}^{1} f(v,\mu,z)\,\mathrm{d}\mu \quad \text{and} \\ f^1 &= \tfrac{3}{2}\int_{-1}^{1} \mu f(v,\mu,z)\,\mathrm{d}\mu \end{aligned} \tag{3}$$

designate the isotropic and linearly anisotropic part of the distribution function, respectively. $n_0(z)$ is the target density, q_t the total and q the momentum transfer cross section for nuclear scattering.

The electronic collisions are described by a Fokker-Planck collision operator. Here, we make use of the fact that in the energy range $E_0 \lesssim 1$ keV the characteristic mean free path of electronic collisions is much greater than that for angular scattering. Therefore we can include electronic collisions consistently in our Lorentz approximation [15]. Doing this, we have to account only for the effect of these collisions on the isotropic part of the distribution function. Due to the zero temperature (0.1 eV $\ll$ 100 eV) of the target atoms the diffusion term also vanishes and the energy loss is described by

$$\left(\frac{\delta f}{\delta t}\right)_{el} = \frac{n_0(z)}{v^2}\frac{\partial}{\partial v}\left\{\frac{s_{el}(v)}{m} v^2 f^0(v,z)\right\}, \tag{4}$$

where $s_{el}(v)$ is the stopping power for electronic collisions.

We now normalize the physical quantities through the relations $v = v_c V$; $n_0(z) = n_c N_0(z)$; $q(v) = q_c Q(V)$; $q_t(v) = q_c Q_t(V)$; $s_{el}(v) = s_c S_{el}(V)$ with characteristic values v_c, n_c, q_c and s_c, to be chosen such that V, N_0, Q and S_{el} have order 1. Further, we introduce the new spatial variable

$$x = \int_0^z N_0(z')\,\mathrm{d}z'/\lambda_m \tag{5}$$

and the characteristic relaxation lengths

$$\lambda_m = \frac{1}{n_c q_c}$$

for momentum relaxation,

$$\lambda_{\varepsilon n} = \frac{m_0}{m}\frac{1}{n_c q_c} = \frac{m_0}{m}\lambda_m$$

for energy relaxation due to nuclear collisions,

$$\lambda_{\varepsilon el} = \frac{m v_c^2}{n_c s_c}$$

for energy relaxation due to electronic collisions,

$$\lambda_\varepsilon = \left(\frac{1}{\lambda_{\varepsilon n}} + \frac{1}{\lambda_{\varepsilon el}}\right)^{-1}$$

for total energy relaxation. (6)

With this, the kinetic equation becomes

$$\begin{aligned}\mu\frac{1}{\lambda_m}\frac{\partial f}{\partial x} = &- \frac{1}{\lambda_m} Q(f - f^0) \\ &+ \frac{1}{\lambda_{\varepsilon n}}\frac{1}{V^3}\frac{\partial}{\partial V}\{Q\, V^4 f^0\} \\ &+ \frac{1}{\lambda_{\varepsilon el}}\frac{1}{V^3}\frac{\partial}{\partial V}\{S_{el}\, V^2 f\} .\end{aligned} \tag{7}$$

To prepare the evaluation of this equation, we define the distribution function

$$F(V,\mu,x) = Q(V)\, V^4\left(1 + \frac{\lambda_{\varepsilon n}}{\lambda_{\varepsilon el}}\frac{S_{el}(V)}{V^2 Q(V)}\right) f(V,\mu,x) \tag{8}$$

and replace the velocity V by

$$u = \int_{\tilde{V}}^{\infty} \left[3\,Q^2(V')\,V' \left(1 + \frac{\lambda_{\varepsilon n}}{\lambda_{\varepsilon el}} \frac{S_{el}(V')}{V'^2 Q(V')} \right) \right]^{-1} \mathrm{d}V' . \tag{9}$$

This transformation yields for the energy relaxation a simple heat conduction equation. Thus we get

$$\frac{\mu}{Q(u)} \frac{1}{\lambda_m} \frac{\partial F(u,\mu,x)}{\partial x} + \frac{1}{\lambda_m} F(u,\mu,x) \tag{10}$$
$$= \frac{1}{\lambda_m} (F^0 + \mu F^1) - \frac{1}{\lambda_m} \frac{Q}{Q_t} \mu F^1$$
$$- \frac{1}{\lambda_{\varepsilon n}} \frac{1}{3Q^2(u)} \frac{\partial F^0(u,x)}{\partial u} .$$

III. Solution of the Kinetic Equation

For solving the kinetic equation, we make use of the different scale lengths of momentum and energy relaxation in our problem: An ion-beam impinging on the wall surface will isotropize within a sheath of thickness λ_m practically without loosing energy. On the other hand, the energy is exchanged on the scale $(\lambda_\varepsilon \lambda_m)^{1/2} = \lambda_m/\varepsilon$, $\varepsilon = \sqrt{\lambda_m/\lambda_\varepsilon} \ll 1$, where the distribution function is nearly isotropic.

Mathematically, this provides the basis of an asymptotic two-scale theory. We develop this theory by neglecting terms of order ε^2. In the "inner" (momentum relaxation) region, we account for the complete anisotropy of the distribution function and neglect energy exchange. In the "outer" (energy relaxation) region we expand $f(u, \mu, x)$ in terms of Legendre polynomials. The results will be matched in a selfconsistent manner to yield a unified solution of the equation.

We may therewith distinguish four parts of our solution;

a) solution of (10) on the inner scale λ_m,
b) solution of (10) on the outer scale λ_m/ε,
c) matching of the inner and outer solution,
d) derivation of the macroscopic quantities from the ion distribution function.

a) *Momentum Relaxation*

We introduce the inner variable $x_m = Q(u)x$, and the distribution function

$$\hat{F}_m(u,\mu,x_m) = F(u,\mu,x) - (1 - Q/Q_t)\mu \hat{F}^0_m(u,x_m)\,x_m . \tag{11}$$

Neglecting the last term in (10) ($\sim \varepsilon^2$) we get

$$\mu\,(\partial \hat{F}_m/\partial x_m) + \hat{F}_m(u,\mu,x_m) = \tfrac{1}{2} \int_{-1}^{1} \hat{F}_m(u,\mu',x_m)\,\mathrm{d}\mu' . \tag{12}$$

The lower index m indicates the momentum relaxation zone. The ion velocity u enters only as a parameter, since there is no energy exchange in this region.

Following the method of Case [11], we solve this integro differential equation by expanding $\hat{F}_m(u,\mu,x_m)$ in terms of the eigenfunctions of (12). Making the ansatz

$$\hat{F}^\nu_m(u,\mu,x_m) = \varphi_\nu(u,x_m)\,\psi_\nu(u,\mu)$$

one finds the eigenfunctions

$$\varphi_\nu(u,x_m) \propto \exp[-x_m/\nu] \tag{13a}$$

and

$$\psi_\nu(u,\mu) = h(u)\left[\frac{\nu}{2} \mathscr{P} \frac{1}{\nu - \mu} + \lambda(\nu)\,\delta(\nu - \mu) \right], \tag{13b}$$

with the normalization

$$\int_{-1}^{1} \psi_\nu(u,\mu)\,\mathrm{d}\mu = h(u) . \tag{14}$$

Here $\mathscr{P}$ denotes the principle value. The spectrum of the eigenvalues ν is established by the normalization condition (14). In the range $\nu \in [-1, 1]$, (14) determines the function $\lambda(\nu)$. So we have a continuous part of the spectrum here. Outside the interval $[-1, 1]$, there are two additional discrete eigenvalues $\nu_\pm = \pm\infty$. The corresponding eigenfunctions are

$$\hat{F}^{\nu_+}_m(u,\mu,x_m) = \frac{1}{2} h(u)$$

and

$$\hat{F}^{\nu_-}_m(u,\mu,x_m) = \frac{x_m - \mu}{2} h(u) . \tag{15}$$

It can be shown [11] that for functions defined in the interval $\mu \in [0, 1]$ already the eigenmodes with positive eigenvalues ($\nu \in [0, 1]$ and ν_+) form a complete set. This applies to the boundary condition at the surface of our semi-infinite medium. In addition to this boundary condition at the target surface, we require a certain asymptotic ($x_m \to \infty$) behaviour of the distribution function to guarantee the matching of the momentum-relaxation zone

with the energy-relaxation region. Under these aspects we write

$$F_m(u,\mu,x_m) = a(u)\frac{1}{2} + w(u)\frac{x_m-\mu}{2} + \int_0^1 d\nu \left\{ A(u,\nu)\left[\frac{\nu}{2}\mathscr{P}\frac{1}{\nu-\mu} + \lambda(\nu)\,\delta(\nu-\mu)\right] \cdot \exp\left[-\frac{x_m}{\nu}\right]\right\}, \quad (16)$$

where the current distribution $w(u)$ must be determined by the matching procedure of the momentum and the energy relaxation zone. The other expansion coefficients $a(u)$ and $A(u,\nu)$ are determined by the boundary condition at the surface $x_m = 0$. We choose here the condition for a monoenergetic ion beam

$$F_m(V,\mu>0,x_m=0) = \delta(V-V_0)\,\delta(\mu-\mu_0). \quad (17)$$

Any arbitrary boundary condition may be constructed by linear superposition.

Methods of functional-analysis [11] yield the expansion coefficients

$$a(u) = a_1\frac{1}{3Q(V_0)}\,\delta(u) + a_2 w(u) \quad \text{and}$$

$$A(u,\nu) = A_1(\nu)\frac{1}{3Q(V_0)}\cdot\delta(u) + A_2(\nu)\,w(u) \quad \text{with}$$

$$a_1 = 3\frac{\mu_0}{X(-\mu_0)},$$

$$a_2 = \frac{3}{2}\int_0^1 \frac{\mu^2}{X(-\mu)}\,d\mu,$$

$$A_1(\nu) = \frac{X(-\nu)}{\nu\,\Lambda^+(\nu)\,\Lambda^-(\nu)}\,\frac{\mu_0}{X(-\mu_0)} \cdot\left(\frac{\nu}{2}\mathscr{P}\frac{1}{\nu-\mu_0} + \lambda(\nu)\,\delta(\nu-\mu_0)\right),$$

$$A_2 = -\frac{1}{6}\,\frac{X(-\nu)}{\Lambda^+(\nu)\,\Lambda^-(\nu)}. \quad (18)$$

The functions $X(\nu)$, $\Lambda^+(\nu)$, $\Lambda^-(\nu)$ and $\lambda(\nu)$ are defined in [11] and listed in the appendix.

b) Energy Relaxation

To describe the energy relaxation we introduce the outer variable $x_\varepsilon = \varepsilon x$ and expand $F(u,\mu,x)$ in (10) in terms of Legendre-polynomials

$$F(u,\mu,x) = \sum_{l=0}^{\infty} F_\varepsilon^l(u,x_\varepsilon)\,P_l(\mu). \quad (19)$$

The lower index ε indicates the energy relaxation solution. Again neglecting terms of order ε^2, only the coefficients F^0 and F^1 remain, since one can prove generally

$$F_\varepsilon^n \sim \varepsilon^n F_\varepsilon^0. \quad (20)$$

Introducing this into (10) we arrive after some calculations [15] at

$$\frac{\partial^2(QF_\varepsilon^1)}{\partial x_\varepsilon^2} = \frac{\partial(QF_\varepsilon^1)}{\partial u}, \quad (21)$$

$$F_\varepsilon^0(u,x_\varepsilon) = \sqrt{\frac{m_0}{m}}\int_{x_\varepsilon}^{\infty} Q(u)\,F_\varepsilon^1(u,x')\,dx'. \quad (22)$$

To determine $F_\varepsilon^1(u,x_\varepsilon)$ from (21) in a semi-infinite medium, we must prescribe an "initial" condition at $u=0$ and a "boundary" condition at $x_\varepsilon = 0$.

The initial condition is

$$F_\varepsilon^1(u=0,x_\varepsilon) = 0, \quad (23)$$

since according to (9) $u\to 0$ corresponds to $v\to\infty$. The boundary condition must be constructed by matching the inner and outer solution. At the moment we abbreviate it in the form

$$Q(u)\,F_\varepsilon^1(u,x_\varepsilon=0) = \omega(u) \quad (24)$$

which yields

$$F_\varepsilon^1(u,x_\varepsilon) = \frac{x_\varepsilon}{2\sqrt{\pi}}\,\frac{1}{Q(u)} \cdot\int_0^u \omega(\xi)\,\frac{\exp[-x_\varepsilon^2/4(u-\xi)]}{[u-\xi]^{3/2}}\,d\xi, \quad (25)$$

$$F_\varepsilon^0(u,x_\varepsilon) = \frac{m_0}{m}\,\frac{1}{\sqrt{\pi}} \cdot\int_0^u \omega(\xi)\,\frac{\exp[-x_\varepsilon^2/4(u-\xi)]}{\sqrt{u-\xi}}\,d\xi.$$

c) Matching of the Inner and Outer Solutions

In order to get a unique and uniformly valid solution, we must match the inner and outer solu-

tions. This demands that the asymptotic expansions in ε of the inner and outer solutions are identical up to the order ε. Therefore we write (16) in the outer — and (25) in the inner variable and expand in ε. Comparing the corresponding contributions in ε^0 and ε^1, i.e. the expressions for F^0 and F^1, we obtain two relations, which determine the boundary distributions $w(u)$ and $\omega(u)$:

$$\omega(u) = -\,Q(u)\frac{w(u)}{2} \tag{26}$$

and

$$w(u) = -\,\alpha\,\delta(u) - \frac{\beta}{\sqrt{\pi}}\int_0^u \frac{Q(\xi)\,w(\xi)}{\sqrt{u-\xi}}\,\mathrm{d}\xi \tag{27}$$

with

$$\alpha = -\frac{2}{3}\frac{\mu_0}{X(-\mu_0)\,Q(V_0)}\left[\int_0^1 \frac{\mu^2}{X(-\mu)}\,\mathrm{d}\mu\right]^{-1},$$

$$\beta = \frac{2}{3}\sqrt{\frac{m_0}{m}}\left[\int_0^1 \frac{\mu^2}{X(-\mu)}\,\mathrm{d}\mu\right]^{-1}.$$

Equation (27) is a weakly singular Volterra integral equation, which has a unique solution $w(u)$ for arbitrary α, β, $Q(u)$. Supposing we have solved this equation, we can construct the total distribution function:

$$\begin{aligned} F(u,\mu,x) = \frac{j_0}{2\pi}\Bigg\{&\int_0^1 \mathrm{d}\nu\left[A(u,\nu)\left(\frac{\nu}{2}\,\mathscr{P}\frac{1}{\nu-\mu} + \lambda(\nu)\,\delta(\nu-\mu)\right)\exp\left(-\frac{Q_t(u)\,x}{\nu}\right)\right] \\ &- \sqrt{\frac{m_0}{m}}\frac{1}{2\sqrt{\pi}}\int_0^u Q(\xi)\,w(\xi)\,\frac{\exp\left(-\dfrac{m}{m_0}\dfrac{x^2}{4(u-\xi)}\right)}{\sqrt{u-\xi}}\,\mathrm{d}\xi \\ &- \sqrt{\frac{m_0}{m}}\frac{1}{4\sqrt{\pi}}\frac{x\,\mu}{Q(u)}\int_0^u Q(\xi)\,w(\xi)\,\frac{\exp\left(-\dfrac{m}{m_0}\dfrac{x^2}{4(u-\xi)}\right)}{(u-\xi)^{3/2}}\,\mathrm{d}\xi\Bigg\}. \end{aligned} \tag{28}$$

Here, j_0 denotes the particle current density incident on the target-surface. This complicated expression reduces to a much simpler form if we are interested in the distribution of the reflected ions only:

$$\begin{aligned} &F(u,\mu<0,x=0) \\ &= \frac{j_0}{2\pi}\left\{\frac{1}{2}\frac{\mu_0}{(\mu_0-\mu)\,X(\mu)\,X(-\mu_0)\,Q(V_0)}\,\delta(u)\right. \\ &\qquad \left. + \frac{1}{2\,X(\mu)}\,w(u)\right\}. \end{aligned} \tag{29}$$

This formula follows from (28) by a limiting process. Equation (29) allows the following interpretation: The first term in (29) gives the contribution of the socalled "Albedo problem" for an incident beam $\delta(u)\,\delta(\mu-\mu_0)$. This problem is concerned with the reflexion of particles from a semi-infinite medium neglecting energy loss altogether. The second term represents the solution of the "Milne problem", describing the scattering of an ion current of distribution $w(u)$ approaching the surface from an infinite distance through the medium. This current distribution is produced in the energy relaxation zone of our model: An ion whose energy is changed ($u_0 = 0 \to u_1$) in the energy relaxation zone is effectively described in the momentum relaxation region by a negative Milne current contribution at u_0 and a positive one at u_1. The negative current contribution at the energy of the incident particles ($u = 0$) corresponds to the term $\alpha\,\delta(u)$ in (27) which corrects the pure albedo contribution (first term of (29)).

d) Reflexion Coefficients and Range Distribution

The reflexion coefficients can be evaluated from the limiting distribution (29). Defining the microscopic reflexion coefficient

$$R(u,\mu,v_0,\mu_0) = -\frac{j_-(u,\mu)}{\mu_0\,j_0}$$

with

$$\begin{aligned} &j_-(u,\mu)\,\mathrm{d}u\,\mathrm{d}\mu \\ &= 2\pi\,\mu\,v\,f(v,\mu<0,x=0)\,v^2\,\mathrm{d}v\,\mathrm{d}\mu \end{aligned}$$

we get

$$R(u,\mu,v_0,\mu_0) = -\frac{3}{2}\frac{\mu}{(\mu_0-\mu)X(\mu)X(-\mu_0)}\delta(u) - \frac{3}{2}\frac{\mu Q(u)}{\mu_0 X(\mu)}w(u). \quad (30)$$

From this, the "spectral" and "total" coefficients are found by integration:

$$R(u,v_0,\mu_0) := \int_{-1}^{0} R(u,\mu,v_0,\mu_0)\,\mathrm{d}\mu = \delta(u) + \frac{Q(u)}{\mu_0}w(u) \quad (31)$$

and

$$R(v_0,\mu_0) := \int_0^{u_b} R(u,v_0,\mu_0)\,\mathrm{d}u = 1 + \frac{1}{\mu_0}\int_0^{u_b} Q(u)w(u)\,\mathrm{d}u. \quad (32)$$

Here, u_b corresponds to a spherical surface binding energy.

To determine the range distribution we must evaluate the divergence of the ion current. In the random binary collision model all ions crossing a lower energy limit E_l are trapped in the solid. We thus get after some calculations

$$\frac{\partial j}{\partial x} = -\frac{\partial}{\partial x}\left\{\sqrt{\frac{m}{m_0}}\frac{j_0}{2\sqrt{\pi}}x\int_0^{u_l}\mathrm{d}u \cdot \int_0^{u} Q(\xi)w(\xi)\frac{\exp\left[-\frac{m}{u u_0}\frac{x^2}{4(u-\xi)}\right]}{(u-\xi)^{3/2}}\mathrm{d}\xi\right\}, \quad (33)$$

where u_l corresponds to E_l.

IV. Results for a Simplified Testmodel

In our formulas (30)—(33) the function $w(u)$ is still unknown and must be determined from (27), which, in general, needs a numerical treatment [e.g. 16]. However, for a simple test model with constant nuclear scattering cross section and no electronic losses, we can give analytical results to illustrate the qualitative features of the solution. The special assumptions of this test model were chosen to keep the problem analytically tractable. They do not describe all physical properties correctly: The assumption of a constant scattering cross section implies a nuclear stopping power $S_n(E) \sim E$ whereas one usually assumes $S_n(E) \sim E^{1/3}$ for low and $S_n(E) = \text{const}$ for higher energies. The neglect of electronic losses in the test model, forced by the constant cross section [15], also is not close to reality in the keV range. Note, however, that the electronic losses in our general formalism are readily accounted for by a simple scale transformation.

For constant nuclear scattering-cross section, we solve (27) by Laplace transformation applying the convolution theorem. We find

$$w(u) = -\frac{\alpha}{3}\left\{\frac{\mathrm{d}}{\mathrm{d}u}G(\beta\sqrt{u}) + \delta(u)\right\} \quad (34)$$

with the function

$$G(z) = e^{z^2}\operatorname{erfc}(z). \quad (35)$$

With this the reflexion coefficients (30)—(32) are readily determined. The range distribution (33) is evaluated to be

$$\frac{\mathrm{d}j}{\mathrm{d}x} = \frac{\alpha}{3}j_0\sqrt{\frac{m}{m_0}}\exp\left(-\frac{m}{m_0}\frac{x^2}{4\sqrt{u_l}}\right)\cdot\left\{\beta G\left(\beta\sqrt{u_l} + \sqrt{\frac{m}{m_0}}\frac{x}{2\sqrt{u_l}}\right) - \frac{1}{\sqrt{\pi u_l}}\right\}. \quad (36)$$

Figures 1 and 2 show the spectral and total reflexion coefficient, respectively. Figure 1 indicates a strong peaking of high energetic ions for grazing incidence.

Due to the assumptions of the test model the total reflexion coefficient shown in Fig. 2 is inde-

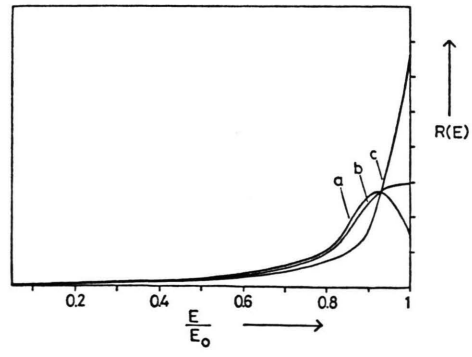

Fig. 1. Spectral reflexion coefficient in arbitrary units. The curves a, b, c correspond to 0°, 30°, and 60° incidence from the surface normal, respectively. The mass ratio is $m_0/m = 64$.

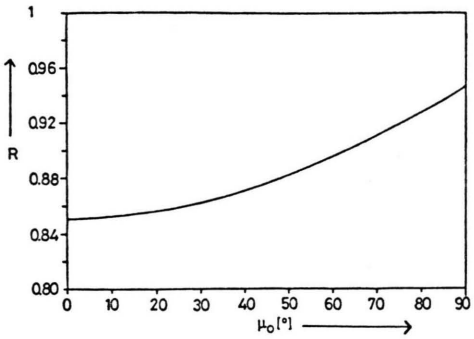

Fig. 2. Total reflexion coefficient as a function of the angle of the incidence. The mass ratio is $m_0/m = 64$.

pendent of the initial ion energy, and its relatively high value illustrates the fact that our test-model does not account for increasing cross section at low energies and for electronic losses.

The range distribution is shown in Figure 3. We see a Gaussian shape with a maximum at a distance of $x_\varepsilon = 0(1)$ from the target surface. This is to be expected from the random walk picture of the ion motion in the medium. Deviations from the Gauss-profile near the surface $x = 0$ are due to the exact boundary conditions.

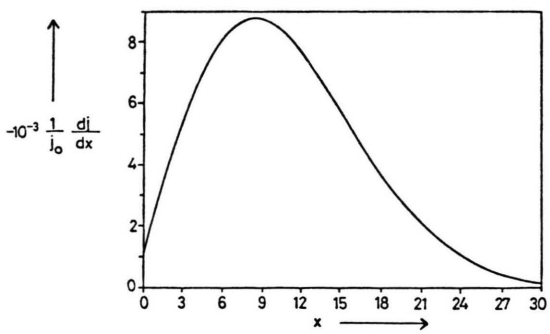

Fig. 3. Range distribution of the ions. The parameters are: $\mu_0 = 1$, $m_0/m = 64$, and $E_l = 1/40\ E_0$.

V. Summary and Discussion

Applying the full Boltzmann equation to the model of random binary collisions we developed a kinetic approach which is suitable to describe light ion scattering at moderate energies. The method is based on the different relaxation lengths for momentum and energy transfer and results in an asymptotic two scale analysis to first order in $\varepsilon = \sqrt{\lambda_m/\lambda_\varepsilon}$. It yields the complete distribution function of the ions in a semi-infinite medium, accounting for the correct boundary conditions at the target surface.

There are essentially two requirements entering our analysis: the different scale-lengths of momentum and energy relaxation and the "linearly anisotropic" nuclear scattering cross section. For typical ion-target combinations like protons on copper the first condition is justified up to energies of $E_0 \sim$ 2 keV. (For higher energies the electronic losses become dominant so that the momentum and energy relaxation lengths approach comparable values.)

The assumption of a linearly anisotropic scattering cross section is much less restrictive than one might expect, as can be seen from the following arguments: Within the Lorentz approximation, the energy exchange anyhow depends only on the isotropic and linearly anisotropic parts of the scattering cross section. So our description of the energy relaxation region and of the matching procedure is completely unaffected by this assumption. Only from the momentum relaxation region an effect might occur. One can show, however, that the part of the distribution function which is influenced by deviations from a linearly anisotropic cross section is damped out exponentially within the first mean free path. So the asymptotic form of the solution (see (15)) again is not influenced.

We have demonstrated the application of our procedure for a test model. In this special case the evaluation of (27) could be performed analytically. The results for the spectral resp. total reflexion coefficient and for the range distribution shown in Figs. 1—3 illustrate typical features of ion scattering at solid walls. Quantitatively there are still deviations from experimental results which can be explained by the special assumptions of the test model (see discussion in Section IV). Therefore our procedure should be applied to realistic cross sections including electronic energy losses. This requires a numerical solution of the coupling equation (27). The corresponding calculations are in progress.

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Appendix

The central function, to which $\Lambda^-(z)$, $\Lambda^+(z)$, $\lambda(z)$ and $X(\mu)$ are related, is the "Dispersion function"

$$\Lambda(z) = 1 - \frac{z}{2}\int_{-1}^{1} \frac{d\mu}{z-\mu}, \quad z \in \mathbb{C}\backslash[-1,1].$$

$\Lambda^-(z)$ and $\Lambda^+(z)$ are the limiting values of this function on the real interval $[-1, 1]$:

$$\Lambda^{\pm}(z) = \lim_{\varepsilon \to 0} \Lambda(z \pm i\varepsilon), \quad z \in [-1,1], \quad \varepsilon \in \mathbb{R}.$$

$\lambda(z)$ and $X(z)$ are constructed from these values:

$$\lambda(z) = \tfrac{1}{2}[\Lambda^+(z) + \Lambda^-(z)], \quad z \in [-1,1];$$

$$X(z) = \frac{1}{1-z} \cdot \exp\left\{\frac{1}{2\pi i}\int_0^1 \frac{d\mu}{\mu - z} \ln\left[\frac{\Lambda^+(\mu)}{\Lambda^-(\mu)}\right]\right\},$$

$$z \in \mathbb{C}\backslash[0,1].$$

For $z \in [-1, 0]$, $X(z)$ is tabulated in [11].

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