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ANALYTICAL DIFFERENTIAL CROSS SECTIONS FOR ION-ATOM HIGH-ENERGY ELASTIC SCATTERING

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A general approach to high energy elastic scattering of ions on atoms is presented. Differential cross sections for the scattering of particles with similar masses are obtained in analytical form. The cross sections are doubly-differential (i. e. with respect to the scattering angle and to the energy transferred during the collision) and were obtained by using the binary encounter approximation and assuming an inverse-power r^{-s} central force potential for interaction between the colliding particles. Numerical calculations are performed for $H^+ - H^+$ and $H^+ - H(1s)$ collisions and the results are compared with quantum mechanical calculations and experimental data. The cross sections are a good approximation for the ion-atom systems with impact energies greater than 1 keV.

1. Introduction

The central force, r-dependent (r being the interparticle distance) potentials for interaction between atoms and molecules have played a significant role in atomic and molecular physics. Such a simple representation of the interparticle interactions is often successful in describing particle collisions including calculations of the cross sections for elastic scattering of atoms and ions[1]. The great convenience of the potentials results from the fact that they lead to simple (often analytical) yet reliable expressions for the collision integrals, scattering cross sections, etc. A typical central force potential has the form

$$U(r) = U^{rep}(r) + U^{att}(r), \tag{1}$$

where $U^{rep}(r)$ and $U^{att}(r)$ represent repulsive and attractive parts, respectively.

The potential of the form (1) is used in this work for evaluation of the differential cross sections for high-energy elastic scattering of atomic particles. Such collisions are suitable for treatment within the framework of the classical binary encounter approximation[2)] (the binary encounter approximation has been fairly successful even in some typical quantum mechanical problems, such as interaction of low-energy electrons with atoms and ions[2−5)]). The classical treatment of the scattering is valid, even for potentials of infinite range, in a large range of the scattering angle χ. This is seen when uncertainty principle arguments are used to estimate the critical angle χ_{cr} for validity of the classical analysis[3)]. These arguments lead to the criterion $\chi > \chi_{cr} \gg \hbar K$, where $\hbar$ is the reduced Planck constant and K is the angular momentum of the colliding system. The systems considered in the present work consist of atomic particles of high impact energy so that $\hbar K$ is very small and χ_{cr} is a small fraction of a degree. In addition, the assumptions of high impact energy and equal (or almost equal) masses of the colliding particles allow for several simplifications in the mathematical description of the problem.

In a high energy scattering, the most important part of the interaction takes place at the close distances where the interaction is strong and repulsive. Thus one can neglect, as a first order approximation, the contribution of the long-distance forces i. e. the term $U^{att}(r)$ in Eq. (1). Consequently, the central force $F_s(r)$ can be characterized by a constant a_s (positive for repulsive interaction) and an exponent s:

$$F_s(r) = -\frac{\partial U_s(r)}{\partial r} = \frac{a_s}{r^s}; \quad s \geq 2, \tag{2}$$

with the interaction potential of the form:

$$U(r) = U^{rep}(r) = a_s (s-1)^{-1} r^{1-s}. \tag{3}$$

The purpose of this work is to evaluate analytical formulae for the differential cross sections, using the potential (3) for elastic scattering of ions on atoms, assuming similar masses of the particles and that the incident ion is much faster than the target atom. These cross sections are in relatively good agreement with experimental data at least for scattering in small angles (experimental data for large angles are not available). Analytical cross sections are of a great convenience in modelling collisional processes in gases and plasmas (e. g. analysis of the kinetic phenomena in the interstellar and interplanetary media). Solutions of such models are very time-consuming and methods for time-effective calculating of collisional rates (which requires cross sections) of an acceptable accuracy are very desirable.

The following differential cross sections are considered:

1. The differential cross section q' for the binary collision in which the incident particle is scattered into angles χ and $0 \leq \Phi \leq 2\pi$ with simultaneous change in energy equal to ΔE (geometry of the scattering is shown in Fig. 1).

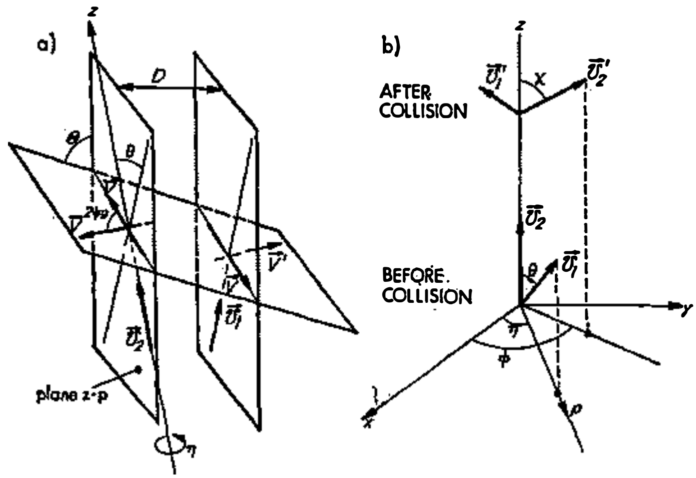

Fig. 1. Geometry of binary collision.

a) Geometrical quantities characterizing the binary encounter: $0 \leq \vartheta \leq \pi$, $0 \leq \eta \leq \pi$, $0 \leq \psi_g \leq 2\pi$, $0 \leq \Theta \leq 2\pi$ and $0 \leq D \leq \infty$. The quantities Θ and D can be expressed, for a given interaction potential, in terms of the angles ϑ, ψ_g, χ and ΔE. As a consequence, the set of quantities ϑ, η, ψ_g, Θ and D can be replaced by a set of quantities ϑ, η, ψ_g, χ and ΔE. The latter set is used in the present analysis.

b) Orientation in space of the velocities of the colliding particles as seen in the z-p plane: $\vec{v}_1$ and $\vec{v}_2$ the velocities before the encounter; $\vec{v}_1'$ and $\vec{v}_2'$ are the velocities after the encounter.

Note that angle ϑ is on the figure denoted by θ.

2. The differential cross section q'' for scattering of the incident particle into angles χ and $0 \leq \Phi \leq 2\pi$ with simultaneous change in energy $\Delta E_1 \leq \Delta E \leq \Delta E_2$.
3. The differential cross section q''' for scattering of the incident particle into angles $0 \leq \Phi \leq 2\pi$, $\chi_1 \leq \chi \leq \chi_2$ with simultaneous change in energy $\Delta E_1 \leq \leq \Delta E \leq \Delta E_2$.

Final formulae for the differential cross sections q' and q'' are obtained in analytical form and the cross section q''' is given in the form of a simple integral.

The approach of this work is quite general and the evaluated cross sections can be applied to any ion-atom system with similar masses of the colliding particles and with the energy of the incident ion much greater than the energy of the atom. Examples of numerical calculations are given for $H^+ - H^+$ and $H^+ - H(1s)$ systems (with impact energies equal to about 1 keV) for which both, quantum-mechanical calculations and experimental data are available in literature.

2. *The approach*

We consider an elastic collision of two particles (particle 1, called the target particle, and particle 2, called the incident particle); the collision is characterized by the particles' masses m_1 and m_2, respectively, and their velocities $\vec{v}_1$ and $\vec{v}_2$ (before the collision) and $\vec{v}_1'$ and $\vec{v}_2'$ (after the collision). All the vectors are defined in Fig. 1.

When the colliding particles are atoms or atomic ions, the interaction is a time--dependent, many-body problem. However, we assume here that the incident particle interacts with the target particle via a resultant time-averaged, distance--dependent central force. Then, using the binary encounter approximation[2], one can define the cross section σ for the elastic scattering of the incident particle into the direction specified by the scattering angles χ and Φ (Fig. 1) with a simultaneous change in energy ΔE. The direction of the velocity $\vec{v}_1$ is specified by the angles ϑ and η. The energies of the incident particle before and after the collision, E_2 and E_2' respectively, are

$$E_2' = \frac{1}{2} m_2 (v_2')^2 \text{ and } E_2 = \frac{1}{2} m_2 v_2^2, \ (\Delta E = E_2' - E_2). \tag{4}$$

Using the relationship $g = 1/\cos^2 \psi_g$ (where ψ_g is defined in Fig. 1), the general form of the cross section σ is[2]

$$\sigma (\vartheta, \eta \to \chi, \Phi; \Delta E) = \int \frac{V}{v_2} \frac{\partial F_s(g)}{\partial g} [W(g)]^{-1/2} \delta [h_\chi (g)] \delta [h_\Phi (\Phi)] \,\mathrm{d}g, \tag{5}$$

where

$$V = (v_1^2 + v_2^2 - 2 v_1 v_2 \cos \vartheta)^{1/2}, \tag{6}$$

$$W(g) = (4a^2 - 2b\Delta E) g^{-1} - (4a^2 + b^2) g^{-2} - (\Delta E)^2, \tag{7}$$

$$a = \mu v_1 v_2 \sin \vartheta,$$

$$b = \varkappa \left[E_2 - E_1 + \frac{1}{2} (m_1 - m_2) v_1 v_2 \cos \vartheta\right], \tag{8}$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2},$$

$$\varkappa = 4 \frac{m_1 m_2}{(m_1 + m_2)^2},$$

$$h_\chi (g) = \cos \chi - \left(1 + \frac{\Delta E}{E_2}\right)^{-1/2} \left[1 + \frac{1}{2} \frac{\Delta E}{E_2} - 2 \left(\frac{m_1}{m_1 + m_2}\right)^2 \left(\frac{V}{v_2}\right)^2 g^{-1}\right], \tag{9}$$

and

$$h_\Phi (\Phi) = \Phi - \eta - \arccos \left\{\left(1 + \frac{\Delta E}{E_2}\right)^{-1/2} (\sin \vartheta \sin \chi)^{-1} \left[\left(\frac{m_2 v_2}{m_1 v_1} + \cos \vartheta\right)\right.\right.$$

$$\left.\left.\left(1 - \left(1 + \frac{\Delta E}{E_2}\right)^{1/2} \cos \chi\right) + \frac{1}{2} \frac{m_2 v_2}{m_1 v_1} \left(1 + \frac{m_1}{m_2}\right) \frac{\Delta E}{E_2}\right]\right\} = 0. \tag{10}$$

The derivatives $\partial F_s(g)/\partial g$ in Eq. (5), have general form $\partial F_s(g)/\partial g = C_s G(g) \cdot H_s(g)$ and will be discussed in the next section. The value of the exponent s depends on the kind of particles taking part in the scattering and on the impact energy. In case of a collision of two charges, the assumption of Coulomb potential ($s = 2$) is well-justified. Collisions of neutral particles can sometimes be accurately described by using values of s between 5 and 0, or ∞. The latter case corresponds to collision of two rigid spheres with radii R_1 and R_2, respectively; $s = 0$ for $r \leq R_1 + R_2$, and $s = \infty$ for $r > R_1 + R_2$. In case of interaction of a proton with a hydrogen atom, it is reasonable to assume $s = 3$ at high impact energies (see Appendix). Taking the above into account, we consider in what follows the potentials with the exponent $s = 2$ (for $H^+ - H^+$ collision). $s = 3$ (for $H^+ - H$ collision) and $s = 5$ and 0, or ∞ (possibly for H — H collision).

We use below the relationship

$$\int_a^b f(x)\,\delta\,[p(x)]\,\mathrm{d}x = \sum_r f(x_r)\left[\left|\frac{\partial p(x)}{\partial x}\right|_{x=x_r}\right]^{-1}, \tag{11}$$

which is valid for any two analytic functions $f(x)$ and $p(x)$[7] and where x_r are the solutions of $p(x) = 0$ in (a, b). We also use the binomial theorem

$$(1 + x)^m = \sum_{k=0}^{\infty} \binom{m}{k} x^k, \tag{12}$$

where $\binom{m}{k}$ is the symbolic notation for »binomial coefficients« in which m is non-integer. Integrating Eq. (5) and introducing notation

$$\lambda = \frac{\Delta E}{E_2} \tag{13}$$

and

$$\gamma = \frac{E_2}{E_1}, \tag{14}$$

one obtains:

$$\sigma(\vartheta, \eta \to \chi, \Phi; \lambda) = (\gamma^{1/2} + \gamma^{-1/2} - 2\cos\vartheta)^2\, C_s G(g')\, H_s(g') \times$$
$$\times\, [4\,(2E_2\gamma)^{1/2}\,(1 - \cos\chi)^{5/2}]^{-1}\,[Z(\vartheta, \chi, \lambda)]^{-1/2}\,\delta\,[h_\Phi(\Phi)], \tag{15}$$

where

$$g' = \frac{1}{2}(1 - \cos\chi)^{-1}\,(1 - 2\gamma^{-1/2})\cos\vartheta + \gamma^{-1}, \tag{16}$$

$$Z(\vartheta, \chi, \lambda) = \sin^2\vartheta - \frac{1}{2}\,[(\gamma - 1)\,\lambda + (1 - \cos\chi)\,(1 + 2\gamma^{1/2}\cos\vartheta + \gamma) +$$
$$+ \frac{1}{4}(1 - \cos\chi)^{-1}\,(1 - 2\gamma^{1/2}\cos\vartheta + \gamma)\,\lambda^2] \tag{17}$$

and

$$h_\Phi(\Phi) = \Phi - \eta - \arccos\{(\sin\vartheta\sin\chi)^{-1}[(\gamma^{1/2} + \cos\vartheta)(1 - \cos\chi) + \gamma^{1/2}\lambda]\}. \quad (18)$$

Whe assumed in the above that $m_1 = m_2$ and we kept only the first two terms in the expansion (12) with $x = \lambda$. This results from the fact that $\lambda \ll 1$ in elastic collisions.

The limits λ_l and λ_u for validity of expression (15) are given by roots of the equation $Z(\Theta, \chi, \lambda) = 0$, i. e., by

$$\lambda_{l,u} = 2(1 - 2\gamma^{1/2}\cos\vartheta + \gamma)^{-1}[(1-\gamma)(1-\cos\chi) \pm \sin\vartheta \times$$
$$\times [2(1-\cos\chi)(1 - 2\gamma^{1/2}\cos\vartheta + \gamma) - 4(1-\cos\chi)^2\gamma]^{1/2}]. \quad (19)$$

Within these limits of λ, the scattering angle χ is always

$$\chi \leq \arccos\left[\frac{1}{2}(1 + 2\gamma^{-1/2}\cos\vartheta - \gamma^{-1})\right]. \quad (20)$$

Taking the above into account, the range of the energy exchanged during a collision is:

$$0 \leq \lambda \leq \min\{\lambda_u, \gamma^{-1}\}, \quad \text{if} \quad \lambda \geq 0, \quad (21)$$

and

$$\max[\lambda_l, -1] \leq \lambda \leq 0, \quad \text{if} \quad \lambda < 0. \quad (22)$$

If the energy E_2 of the incident particle is given in eV, then the units of the binary cross section (15) are $cm^2 eV^{-1} rad^{-1}$. Now, one can define three important differential cross sections:

1. The cross section q', in $cm^2 eV^{-1} rad^{-2}$, for scattering of the incident particle into an angle $0 \leq \Phi \leq 2\pi$ and an angle χ with simultaneous change in energy equal to ΔE:

$$q'(\vartheta, \chi; \Delta E) = \int_0^{2\pi} \sigma(\vartheta, \eta \to \chi, \Phi; \Delta E)\,d\Phi. \quad (23)$$

2. The cross section q'', in $cm^2 rad^{-1}$, for scattering of the incident particle into an angle $0 \leq \Phi \leq 2\pi$ and an angle χ with simultaneous change in energy $\Delta E_1 \leq \Delta E \leq \Delta E_2$:

$$q''(\vartheta, \chi; \Delta E_1 \leq \Delta E \leq \Delta E_2) = \int_{\Delta E_1}^{\Delta E_2}\int_0^{2\pi} \sigma(\vartheta\,\eta \to \chi, \Phi; \Delta E)\,d\Phi\,\Delta E. \quad (24)$$

3. The total elastic scattering cross section q'', in cm^2, for scattering of the incident particle into angles $0 \leq \Phi \leq 2\pi$ and $\chi_1 \leq \chi \leq \chi_2$ with simultaneous change in energy $\Delta E_1 \leq \Delta E \leq \Delta E_2$:

$$q'''(\vartheta, \chi_1 \leq \chi \leq \chi_2; \Delta E_1 \leq \Delta E \leq \Delta E_2) =$$
$$= \int_{\chi_1}^{\chi_2} \int_{\Delta E_1}^{\Delta E_2} \int_0^{2\pi} \sigma(\vartheta, \eta \to \chi_1 \leq \chi \leq \chi_2; \ \Delta E_1 \leq \Delta E \leq \Delta E_2) \, d\Phi \, d\Delta E \, d\chi. \tag{25}$$

The cross sections q', q'' und q''' are independent of the angle η; this is a result of averaging over the angle Φ (there is a z-axis symmetry of the collision in the central force potential).

The cross sections q' and q'' can be obtained in analytical form. Using relationship (23) one has

$$q'(\vartheta, \chi; \lambda) = D'_s R(\chi, \vartheta) \, [Z(\vartheta, \chi, \lambda)]^{-1/2}, \tag{26}$$

where conditions (21) an (22) must be met, and where

$$D'_s = \frac{C_s}{4(2\gamma)^{1/2} E_2}, \tag{27}$$

and

$$R(\vartheta, \chi) = G(g') H_s(g')(1 - \cos\chi)^{-5/2} \cdot (\gamma^{1/2} + \gamma^{-1/2} - 2\cos\vartheta)^2. \tag{28}$$

The final form of the cross section q'' is

$$q''(\vartheta, \chi; \lambda_1 \leq \lambda \leq \lambda_2) = D''_s R(\vartheta, \chi) \, Z_1(\vartheta, \chi), \tag{29}$$

where

$$D''_s = \frac{C_s}{4(2\gamma)^{1/2}}, \tag{30}$$

$$Z_1(\vartheta, \chi) = a_1^{-1/2} \left[\operatorname{arsin}\left(\frac{2a_1\lambda_2 + a_2}{a_3}\right) - \operatorname{arsin}\left(\frac{2a_1\lambda_1 + a_2}{a_3}\right) \right], \tag{31}$$

$$a_1 = \frac{1 - 2\gamma^{1/2}\cos\vartheta + \gamma}{8(1 - \cos\chi)}, \tag{32}$$

$$a_2 = \frac{\gamma - 1}{2}, \tag{33}$$

and

$$a_3 = 2\sin\vartheta(1 - \cos\chi) \left[\frac{1 - 2\gamma^{1/2}\cos\vartheta + \gamma}{2(1 - \cos\chi)} - \gamma \right]^{1/2}. \tag{34}$$

The cross section q''' can be found from

$$q''' = \int_{\chi_1}^{\chi_2} q'' \, d\chi, \tag{35}$$

where the condition (20) must be fulfilled.

3. Interaction potentials

In case of the central force potential $U(r)$ one has[8]:

$$g = \cos^{-2}\left\{ \int_{r_{min}}^{\infty} Dr^{-2} \left[1 - \left(\frac{D}{r}\right)^2 - \frac{2U(r)}{\mu V^2}\right]^{-1/2} \mathrm{d}r \right\}, \tag{36}$$

where D is the collision impact parameter, r is the distance between the reduced mass μ and the center of the force and r_{min} is the distance of closest approach. Solution of Eq. (36) with respect to D^2 gives

$$\frac{\partial F_s(g)}{\partial g} = 2D \frac{\partial D}{\partial g}. \tag{37}$$

Introducing

$$y = D/r \text{ and } y_{min} = D/r_{min} = D/(A_s)^{1/(s-1)}, \tag{38}$$

where $A_s = 2a_s/(mV^2)$, $(m = m_1 = m_2)$, the expression (36) can be rewritten as

$$g = \cos^{-2} \{ \int_0^Y [1 - y^2 - 2(s-1)^{-1} y_{min}^{1-s} y^{s-1}]^{-1/2} \mathrm{d}y \}, \tag{39}$$

where Y is the least positive root of the expression in the square brackets. Since

$$2D \frac{\partial D}{\partial g} = A^{2/(s-1)} \frac{\partial \, [y^2_{min}(g)]}{\partial g}, \tag{40}$$

$y_{min}(g)$ must be known. It can be determined from relationship (39) for a given value of the exponent s. When $s = 2$, the derivative (37) had simple form

$$\frac{\partial F_2(g)}{\partial g} = C_2 G(g) H_2(g), \tag{41}$$

with

$$C_2 = 4\,[2a_2/(mV^2)]^2, \quad G(g) = [4g^3(1 - g^{-1})]^{-1/2}$$

and

$$H_2(g) = 1/[4G(g)]. \tag{42}$$

When $s = 3$

$$\frac{\partial F_3(g)}{\partial g} = C_3 G(g) H_3(g) \tag{43}$$

with

$$C_3 = 2a_3/(mV^2) \text{ and } H_3(g) = \frac{\pi^2}{2} \arccos(g^{-1/2}) \left\{\frac{\pi^2}{4} - [\arccos(g^{-1/2})]^2 \right\}^{-2}. \tag{44}$$

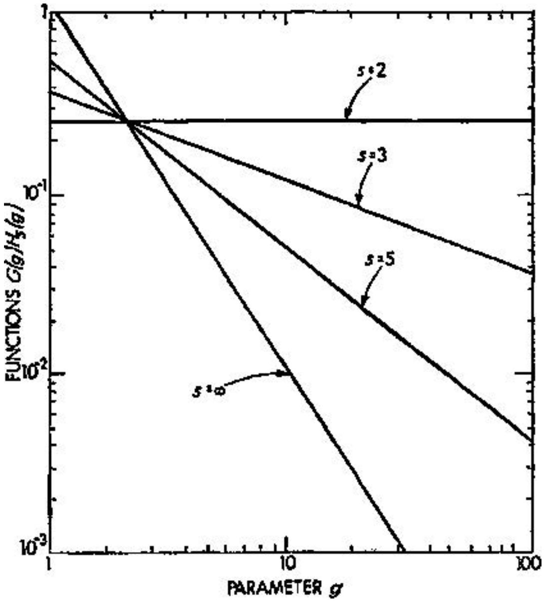

Fig. 2. Functions $G(g)\,H_s(g)$ for various values of the exponent s defined in Eq. (2).

In case when $s = 5$, the integral in Eq. (39) can be expressed by an elliptic integral. Taking $y^4_{min} = 2\cot^2(2\beta_1)$ and $y^2 = (1 - \tan^2\beta_1)\cos^2\beta_2$, the integral can be transformed to

$$I = (1 - 2\sin^2\beta_1)^{1/2} \int\limits_0^{\pi/2} (1 - \sin^2\beta_1 \sin^2\beta_2)^{-1/2}\, \mathrm{d}\beta_2, \tag{45}$$

which is the complete elliptic integral $K(k)$ with $k^2 = \sin^2\beta_1$. The modulus k is determined from the integrand in Eq. (39) by replacing y^2 by a new variable z and finding the roots z_1, z_2 and z_3 ($z_1 > z_2 > z_3$) of the expression in square brackets. Then, the expression can be given as $(z - z_1)(z - z_2)(z - z_3)$ and

$$k^2 = \frac{z_1 - z_2}{z_1 - z_3} = \frac{1}{2}\left[1 - \left(1 + \frac{2}{y^4_{min}}\right)^{-1/2}\right]. \tag{46}$$

Since $k < 1$, the complete elliptic integral $K(k)$ can be expanded into a quickly converging series[9]:

$$K(k) = \frac{\pi}{2} \sum_{n=0}^{\infty} \left[\frac{(2n-1)!!}{2^n n!}\right]^2 k^{2n}, \tag{47}$$

where the sum over n is close to unity because $k^2 < 1/2$ always. Therefore, we assume in what follows that $K(k) = \pi/2$. Taking this into account

$$\frac{\partial F_5(g)}{\partial g} = C_5 G(g)\, H_5(g), \tag{48}$$

with

$$C_5 = [2a_5/(mV^2)]^{1/2}$$

and
$$H_5(g) = \frac{2^{7/2}}{\pi^2} \arccos(g^{-1/2}) \left\{ 1 - \left[\frac{2}{\pi} \arccos(g^{-1/2}) \right]^4 \right\}^{-3/2}. \tag{49}$$

In case of a collision between two rigid spheres ($s = 0, \infty$) of radii R_1 and R_2 one has

$$\frac{\partial F_\infty(g)}{\partial g} = C_\infty G(g) H_\infty(g), \tag{50}$$

with

$$C_\infty = (R_1 + R_2)^2 \text{ and } H_\infty = 2g^{-1/2}(1 - g^{-1})^{1/2}. \tag{51}$$

4. *Potential constants*

The constants a_s can be found from theoretical considerations[1]. Also, if a theoretical or measured cross section is known (usually this is the singly-differential cross section per unit solid angle $\partial Q/\partial \Omega\,(\chi)$), one can compare this cross section with the related cross section q'' averaged over the angle ϑ and energy. As a result of such a comparison one obtains the value of the constant a_s. It should be added that the value of q'' for $H^+ - H$ interactions used for the comparison with the measured cross sections should be taken with ΔE_2 corresponding to an elastic collision, i. e., ≤ 10.2 eV (thus we neglect momentum transfer combined with charge exchange).

The constant a_s for proton-proton interaction is $a_2 = e^2 = 2.31 \cdot 10^{-19}$ gcm$^3 \cdot$ $\cdot$ s^{-2} = 1 a. u. Determination of a_s from the procedure discussed above can be done in the case of the proton-hydrogen atom interaction by using the singly-differential cross section measured by Houver et al.[10]. This gives $a_3 = 2.23 \cdot 10^{-27}$ g cm^4 s^{-2} = 1.83 a. u.; this value can be used in the entire energy range (700—2000 eV) discussed here. Experimental differential cross sections for H-H elastic scattering are not available, so that the constant a_5 must be found from a theory.

5. *Results and discussion*

As said before, experimental data for the doubly-differential cross sections for the elastic scattering of the heavy particles are not available. Therefore, we compare our singly-differential cross section q'' with the available measurements and quantum-mechanical calculations for the hydrogenic species. This can be made quite easily by taking values of $q''(\chi, \vartheta = \pi/2)$ instead of q'' averaged over the angle ϑ (since $v_2 \gg v_1$, the value of $q''(\chi, \vartheta = \pi/2)$ is close to the averaged value of q'').

The present results are in good agreement with the classical Rutherford formula[11]:

$$\frac{\partial \Omega}{\partial \Omega}(\chi) = \frac{e^4}{4}\left(E_2^2 \sin^4 \frac{\chi}{2}\right)^{-1}, \tag{52}$$

for $H^+ - H^+$ interaction (Fig. 3). In this case the quantum-mechanical differential cross section[6] (the Mott cross section) differs from the classical cross section (52) by an interference term resulting from the indistinguishability of the colliding particles. If the impact energy is much lower (as it is in our case) than about 25 keV (918 a. u.) then this term rapidly oscillates with the variation in the scattering angle causing that the average value of the term is practically zero. The small discrepancy between the Rutherford formula and the present calculations results from the mathematical simplification of the model discussed in previous sections.

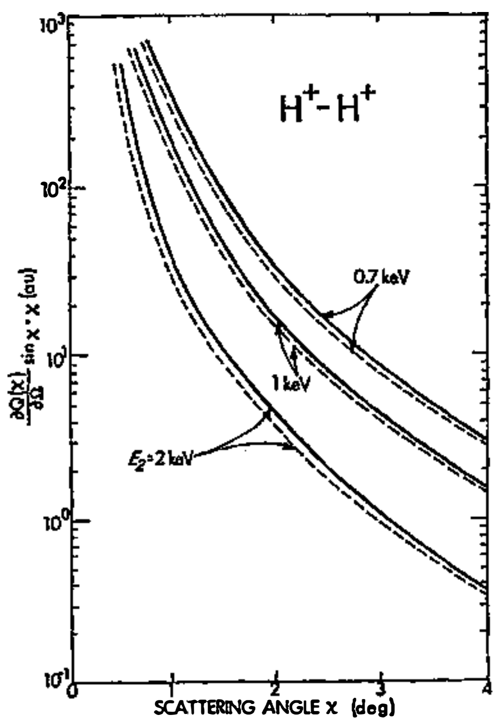

Fig. 3. Comparison of the differential cross section $g''(\chi, \vartheta = \pi/2)$ (solid line) with the Rutherford formula (Eq. (52)) (broken line) for $H^+ - H^+$ interaction. E_2 is the energy of the incident particle.

Experimental data[10] for the differential cross sections for $H^+ - H$ scattering are shown in Figs. 4—6 together with the present results and quantum-mechanical calculations of Gaussorgues et al.[12]. These results seem to indicate that the approach of the present work gives reasonable estimates of the differential cross sections

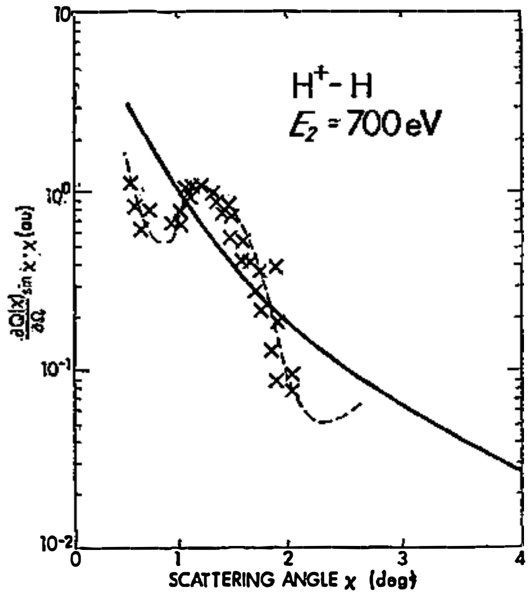

Fig. 4. Comparison of the differential cross section $q''(\chi, \vartheta = \pi/2)$ (solid line) with the result of theoretical calculations of Gaussorgues et al.[12] (broken line) and measurements of Houver et al.[10] for H^+ — H (1s) elastic scattering at $E_2 = 700$ eV.

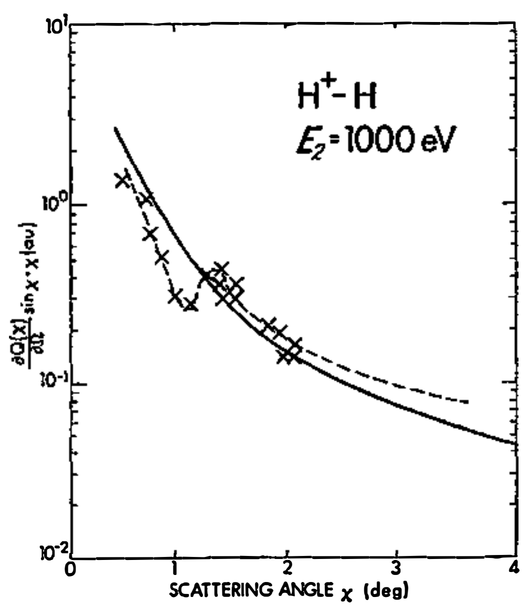

Fig. 5. Comparison of the differential cross section $q''(\chi, \vartheta = \pi/2)$ (solid line) with the results of theoretical calculations of Gaussorgues et al.[12] (broken line) and measurements of Houver et al.[10] for H^+ — H (1s) elastic scattering at $E_2 = 1000$ eV.

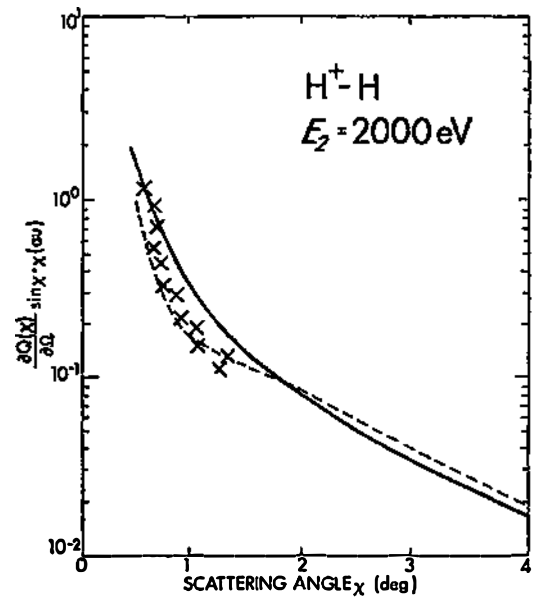

Fig. 6. Comparison of the differential cross section $q''(\chi, \vartheta = \pi/2)$ (solid line) with the results of theoretical calculations of Gaussorgues et al.[12] (broken line) and measurements of Houver et al.[10] for $H^+ - H$ (1s) elastic scattering at $E_2 = 2000$ eV.

for $H^+ - H$ scattering at high impact energies, at least for small angles (but not smaller than about 0.2—0.3°, because of the *glory* effect). It is difficult to estimate the accuracy of our cross sections for H-H scattering because of lack of corresponding experimental data. The accuracy of the present cross sections for scattering into large angles ($\chi \gg 1°$) in case of H^+-H and H-H systems also cannot be assessed because experimental data for large values of χ are not available.

The main advantage of the approach presented here is that the differential cross sections q' and q'' are given in simple analytical forms and the cross section q''' is given in form of an integral that can easily be calculated by standard numerical methods. The major weakness of this approach results from the fact that we use the repulsive inverse-power interaction potential in the entire range of the interparticle distance. This assumption causes the disappearance of the *rainbow* effect[8] (see Figs. 4—6), however this effect is not strong at high impact energies. Also, the *glory* effect, making the cross sections infinite at $\chi \to 0$, is still present in our model. This results from the fact that our differential cross section is defined in the standard way as an intensity of scattering per unit solid angle at a given angle χ[8].

Numerical calculations show that using the rigid-sphere potential ($s = 0, \infty$) leads to differential cross sections which are comparable with the cross sections shown in Figs. 3—6 only at χ equal to about 1—2°. The discrepancy becomes large at other values of the scattering angle and the cross sections based on the rigid-sphere potential are inaccurate.

Taking the above into account one can summarize the properties of the singly-differential cross sections (it seems that the doubly-differential cross sections evaluated above have similar properties) of the present work for $H^+ - H^+$ and $H^+ - H(1s)$ scattering in the central force potential $\sim r^{-s}$:

1. $H^+ - H^+$: the approach of the present work yields results in very good agreement, when Coulomb potential ($s = 2$) is used, with quantum-mechanical calculations.

2. $H^+ - H(1s)$: the present approach (with $s = 3$) is an acceptable first order approximation in the discussed energy range, at least for scattering in small angles. However, the central force potential r^{-s} is not able to reproduce the *rainbow* effect (this effect is weak at high impact energies).

3. The results shown in Figs. 4—6 indicate that the analytical cross sections evaluated in this work should be a good approximation for scattering with energies greater than about 1 keV, for ion-atom systems other than hydrogenic and perhaps for some atom-atom systems.

4. Using the rigid-sphere potential for the discussed collisions is inappropriate.

The results of this work seem to suggest that more accurate yet analytical differential cross sections may be obtained, within the framework of the binary encounter approximation, for the interactions discussed above and for systems other than hydrogenic as well. However, in such case a central force potential more realistic than r^{-s} would have to be used for ion-neutral and neutral-neutral systems. One such potential may be the simple screened Coulomb potential[13,14)]

$$U(r) = r^{-1} \exp(-r/p), \tag{53}$$

where the screening parameter p can be fit to accurate *ab initio* calculations of the ${}^2\Sigma_g$ and ${}^3\Sigma_u$ potentials of H_2^+ and ${}^1\Sigma_g$ and ${}^3\Sigma_u$ potentials of H_2. Another potential that seems to be even more appropriate is[15)]

$$U(r) = A_s r^{-s} + A_t r^{-t} \exp(-\omega r), \tag{54}$$

where the terms on the right-hand side represent, static and dynamic multipole interaction, respectively. The potential (54) would probably reproduce the *rainbow* structure in the differential cross sections. In order to obtain analytical forms of the cross sections, the potential (54) would have to be divided into three regions of interaction:

$$U(r) = \begin{cases} A_s r^{-s}, \\ B_1 + B_2 \exp(-\omega r), \\ A_t r^{-t}. \end{cases} \tag{55}$$

Ending, some remarks should be made about comparing of the differential cross sections in the center-of-mass and laboratory systems. Since the interaction potentials used in the present work are spherically symmetric, the scattering angular distribution does not depend on the azimuthal angle Φ. In such a case, and when the masses of the colliding particles are equal, the element of solid angle $d\Omega_{CM}$ ($d\Omega = \sin\chi \, d\chi \, d\varphi$) in the center-of-mass system is related to the corresponding element $d\Omega_L$ in the laboratory system as

$$d\Omega_{CM} = [8(1 + \cos\chi_{CM})]^{1/2} \, d\Omega_L, \tag{56}$$

while the scattering angles χ are related as

$$\tan\chi_L = \frac{\sin\chi_{CM}}{\cos\chi_{CM} + 1}. \tag{57}$$

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Appendix

The exponent $s = 3$ has been chosen for $H^+ - H$ interaction potential because of mathematical convenience allowing to evaluate the analytical cross sections. This value of the exponent is also supported (as a first order approximation of the central force potential) by acceptable physical arguments discussed below (atomic units are used).

The repulsive, short-range potential $V(r)$ for interaction between a completely stripped incident ion and a target atom can be obtained by application of a variational minimization and maximization principle[16] to the Thomas-Fermi-Dirac (TFD) statistical model of the atom[17]. Then the short-range potential can be given[16] as

$$V_A(r) = Z_i \left[\frac{Z_a \varphi(r)}{r} + \frac{Z_a - N_a}{r_0} - \frac{1}{32\pi^2} \right], \tag{A1}$$

where r is the interparticle distance, r_0 is the size (radius) of the spherically symmetric atom, Z_i and Z_a are the charge number of the ion and atomic number of the atom, respectively, N_a is the number of the atomic electrons and $\varphi(r)$ is the TFD screening function obtained from numerical solution of the Thomas-Fermi equation[17].

The potential (A1) is similar to the Firsov ion-atom potential[18]

$$V_F(r) = Z_i \frac{Z_a \varphi(r)}{r}, \tag{A2}$$

which is a good approximation for the interparticle distance smaller than a couple of the Bohr radii. This is however satisfactory for our purposes because the main part of the interaction occurs in this region.

The potentials (A1) and (A2) give the same interparticle force

$$F_{A,F}(r) = - Z_i Z_a \left[r^{-1} \frac{d\varphi(r)}{dr} - r^{-2} \varphi(r) \right]. \tag{A3}$$

Analytical form of the TFD screening function $\varphi(r)$ can be obtained by using the Kerner's argument[19] that the product $r\varphi(r)$ is so slowly varying that it can be treated as a constant. Consequently, Kerner proposed an accurate fit to the screening function in the form

$$\varphi(r) = (1 + cr)^{-1}, \tag{A4}$$

where $c = 1.525$. Introducing Eq. (A4) into Eq. (A3) one obtains

$$F_{A,F}(r) = \left(\frac{c+1}{c + r^{-1}} \right) r^{-3}. \tag{A5}$$

The most important region of the interaction at the impact energies considered in this work is at $1 < r < 3$. At these distances the expression in the parenthesis in Eq. (A5) varies slowly with r. Thus, comparison of Eq. (A5) with Eq. (2) allows to conclude that $s = 3$ is an acceptable approximation for central force repulsive potential in $H^+ - H$ collision. One may expect that the TFD statistical theory should be more accurate when the number of atomic electrons is much greater that one. However, various analysis of TFD calculations for small atoms (including hydrogen) suggest[20,21] that assumption of $s = 3$ is a reasonable first order approximation for the $H^+ - H$ interaction. The choice of the exponent $s = 3$ for the ion-atom short-range interaction is also supported by the results obtained by Marchi and Smith[22] for the $He^+ - He$ repulsive potential.

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ANALITIČKI DIFERENCIJALNI UDARNI PRESJECI ZA ION-ATOM VISOKOENERGETSKO ELASTIČNO RASPRŠENJE

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Prikazana je teorija visokoenergetskog raspršenja iona na atomima. Dobivena je analitička formula koja određuje diferencijalni udarni presjek pri raspršenju čestica podjednakih masa. Dvostruko-diferencijalni udarni presjek (obzirom na kut raspršenja i na energiju transferiranu u sudaru) određen je primjenom aproksimacije binarnih sudara uz pretpostavku da je potencijal interakcije oblika r^{-s}. Numerički računi provedeni su za $H^+ - H^+$ i $H^+ - H(1s)$ sudare, a dobiveni rezultati uspoređeni su s rezultatima kvantno-mehaničkog računa i s eksperimentalnim podacima. Udarni presjek je dobra aproksimacija za sistem ion-atom s impaktnom energijom iznad 1 keV.