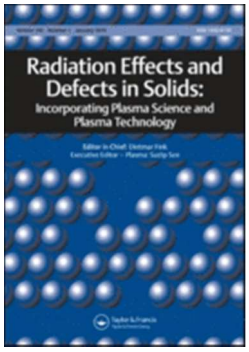

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RESEARCH ARTICLE

Classical-trajectory calculations of the electronic stopping cross-section for low-energy H and H^+ projectiles by H_2-molecules.

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(*April 4, 2013*)

A model that enables the classical-trajectory simulation of the interaction between an atomic particle and a target containing one or more electrons is devised. It makes use of the so-called Gaussian kernel approximation (GKA) and *ad hoc* potentials. In this way, the most relevant quantum properties of the electron can be preserved and, at the same time, still using classical mechanics to solve the response of the electronic system to the presence of a moving, heavy charge. As a first step to assessing the proposed model we calculate the electronic stopping cross section for 1keV to 20 keV Protons and Hydrogen impinging upon atomic and molecular Hydrogen targets. The results show a fairly good agreement between experiments and previous theoretical calculations over the entire bombarding energy studied in this paper.

Keywords: stopping power; classical Monte-Carlo; Molecular-Dynamics; numerical simulation;

***PACS*:** 34.50.Bw; 34.10.+x; 02.70.Ss; 07.05.Tp

1. Introduction

The interaction of ions and atomic species with atomic, molecular and solid targets is an important issue in a number of scientific and technological problems (*1*). It is not a surprise, therefore, that a huge amount of experimental and theoretical works have been accumulated on this subject matter over the years. In spite of this, however, the problem posed by the interaction between a moving ion and an atom or a molecule remains without being solved by exact analytical procedures and, so far, these cases can be handled only by resorting to approximate methods.

Among these approaches, computer-simulations have proven to be attractive alternatives. This is so, to a large extent, because they are capable of attacking a number of cases starting from simple assumptions. Computer simulations are grouped into quantum or classical. In quantum simulations the interaction process is solved by solving the Schrödinger equation, whereas, in classical ones the motion of all particles in the system, including electrons, are described by the Newton equations. Obviously, quantum approaches are more accurate than classical calculations but, the latter have not completely abandoned because classical simulations are both conceptually and numerically simpler than the quantum counterpart.

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Computer simulations of systems containing one classical electron appear to be fairly accurate (*2*). However, when more than one electron are present a difficulty appears. This comes from the well-known fact that two classical electrons orbiting around a nucleus is an unstable system. Several attempts at solving such a difficulty have been proposed. The so-called Heisenberg core (*3–5*) cleverly solved such a problem. However, as pointed out in Ref.(*6*), the Heisenberg-core leads to bound states where electrons occupy a sort of crystalline structure and have no internal motion. The Author of such a paper resolved this shortcoming by using the energy-bounded approach, which basically consisted in using a *constraint* potential that prevents autoionization without forcing electrons to stay at rest.

Following a similar approach, calculations of the ionization and capture cross-sections of targets containing more than one electron were recently reported (*7, 8*). There, stability against autoionization is achieved by assuming that electrons are represented by density distributions. In order to numerically perform such calculations however, they use two approaches: one relies on the so-called *Gaussian kernel approximation* (GKA) whereas in the other, called *average collective repulsion* (ACR), the electron-electron repulsion is obtained by taking an average over the positions occupied by each electron on different trajectories, see Ref. (*8*) for details. Remarkably, the so-calculated cross-sections exhibited a superb agreement with experimental data.

Encouraged by these results, we calculate the stopping cross-sections H_2 for 1 to 20 keV H^+ and H projectiles using the GKA. Differences exist, however, between the present calculations and those in Ref.(*8*). In the first place, we introduce a *quantum potential* which mimics the kinetic energy associated with the *spatial extent* of the electron and, secondly, a *binding potential* is also used, as it is necessary in order to account for the bonding states that may occur between two approaching nuclei. The present calculations, however, are expected to work well only within a range of energy going, approximately, from 1 to 25 keV/nucleus. A lower limit applies since we ignore the recoiling of the target nuclei and the use of the so-called straight-line approximation for the projectile trajectory. The upper limit stems from ours using of the GKA even for the electron-nuclei interaction, which precludes large energy transfers between projectile and electrons and so, the stopping cross sections so calculated would underestimate data for bombarding energies greater than, say, 25 keV.

This paper is organized as follows: in Section 2 we outline the theoretical assumptions used in the present calculations. The results of the computer simulations are presented in Section 3, where they are also compared with previous similar theoretical calculations and experimental data. Finally, Section 4 contains a summary and the concluding remarks. It must be mentioned that, unless otherwise stated, atomic units are used throughout this paper.

2. Theoretical background

We assume that the electron can be described by a Gaussian-distributed "fluid" , i.e. the Gaussian kernel approximation (GKA) in Ref. (*8*). As a consequence, if one has a set of M-electrons, the probability of finding one electron at $(\mathbf{r}, d\mathbf{r}^3)$ is given by expression

$$\rho(\mathbf{r},t) = \sum_{i=1}^{M} \frac{1}{(\sqrt{2\pi}\sigma_i)^3} \exp\left[-\frac{(\mathbf{r}-\mathbf{r}_i)^2}{2\sigma_i^2}\right]. \qquad (1)$$

Within this approximation, the center of the Gaussian peak $\mathbf{r}_i$ and its width σ_i are the variables which describe the i-th electron. Furthermore, since such electrons are assumed to be *distinguishable*, each Gaussian will be linked to the same electron all along calculations.

In order to obtain the equation governing the dynamics of such Gaussians, we have to write the corresponding kinetic and potential energy of the electrons in Eq.(1) in the field of nuclear charges and those of the electrons themselves.

In the first place, one can use the fluids' continuity equation to find the velocity field of each Gaussian in Eq.(1), the result being $\mathbf{v}_i = \dot{\mathbf{r}}_i + (\mathbf{r} - \mathbf{r}_i)\dot{\sigma}_i/\sigma_i$, where $\dot{\mathbf{r}}_i = d\mathbf{r}_i/dt$, and $\dot{\sigma}_i = d\sigma_i/dt$. Accordingly, the mean kinetic energy of the electrons thus becomes

$$T = \frac{1}{2}\sum_i \left(\dot{\mathbf{r}}_i^2 + 3\dot{\sigma}_i^2\right), \tag{2}$$

Secondly the Coulomb energy of a negatively charged distribution given by Eq.(1) in the presence of point-like nuclear charges can be readily obtained. For computational purposes however we can approximate them by the expression

$$V^{(C)} = -\sum_{i,n} \frac{Z_n}{\sqrt{r_{i,n}^2 + \alpha_C\,\sigma_i^2}} + \sum_{i,j<i} \frac{1}{\sqrt{r_{i,j}^2 + \alpha_C\,\sigma_{i,j}^2}}\,. \tag{3}$$

In the equation above Z_n denotes the atomic number of nucleus n-th, $r_{i,j} = |\mathbf{r}_i - \mathbf{r}_j|$ and $r_{i,n} = |\mathbf{r}_i - \mathbf{R}_n|$, where $\mathbf{R}_n$ is the vector position of the n-th nucleus. Similarly, $\sigma_{i,j} = \sqrt{\sigma_i^2 + \sigma_j^2}$, and $\alpha_C = \sqrt{\pi/2}$.

In addition to the Coulomb, we must introduce a *quantum potential* in order to provide our classical particles with most relevant quantum properties, namely the one arising from the uncertainty principle that prevents electrons from falling into the atomic nucleus and that of Pauli's exclusion principle. With such a purpose, we assume the following approximation

$$V^{(Q)} = V_1^{(Q)} + V_2^{(Q)}\,, \tag{4}$$

where,

$$V_1^{(Q)} = C_1^{(Q)} \sum_i \sigma_i^{-2}\,, \tag{5}$$

and,

$$V_2^{(Q)} = C_2^{(Q)} \sum_{i,j<i} g_{i,j} \left\{ r_{i,j}^2 + (\sigma_i - \sigma_j)^2 + \right.$$
$$\left. \tau^2 \left[(\dot{\sigma}_i - \dot{\sigma}_j)^2 + (\mathbf{v}_i - \mathbf{v}_j)^2 \right] \right\}^{-3/2}\,, \tag{6}$$

where

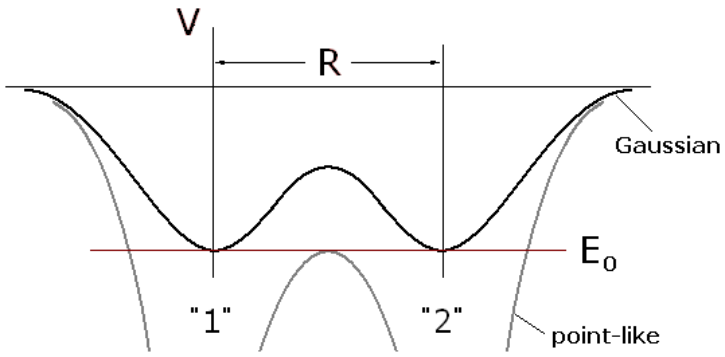

Figure 1. Potential energy of a Gaussian (black line) and that of a point-like (gray line) electron in the field of two, equal nuclear charges, i.e. "1" and "2". E_0 denotes the total energy of the electron.

$$g_{i,j} = \begin{cases} 1 & \text{if} \quad i-j \bmod 2 = 0 \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

mod being the modulo function, i.e. x mod a = the remainder of the division of x by a. Notice that $C_1^{(Q)}$, $C_2^{(Q)}$ and τ are the three parameter entering the proposed quantum potential.

Observe that $V_1^{(Q)}$ approximates the expectation value of the kinetic energy, namely $\frac{1}{2}\Delta$, for a quantum state described by a Gaussian wave function. Similarly, the potential $V_2^{(Q)}$ accounts for the Pauli's exclusion principle. In fact, $V_2^{(Q)}$ tends to infinity when two Gaussians approach to the same point in the position-velocity space though, function $g_{i,j}$ ensures that this potential applies to electrons which have the same parity. That is to say, odd electrons are assumed to have all the same spin and different from those of the even ones.

It is clear that the advantage of using the Gaussian approximation stems from the fact that the electron may have zero kinetic-energy, that is to say has no motion, and at the same time it may remain without falling into the nuclear field. Unfortunately however, this approach has an undesirable consequence which can be explained by using the sketch in Fig.1. There, one can readily see that, as the nuclei get closer than, say, R, a point-like electron, with total energy E_0, is free to move along the two nuclei, whereas a Gaussian electron, with same energy, will remain sitting over nuclei "1" or "2" without moving at all. It is obvious that Gaussian electrons will have a reduced probability of transitioning to and from an approaching atom and, expectedly, this may have noticeable consequences on the stopping calculations.

In order to approximately solve this problem we introduce the following *binding potential*

$$V^{(b)} = -C^{(b)} \sum_i \sum_{n,m<n} \sqrt{Z_n\, Z_m} \times \frac{f_b\left(R_{n,m}/\sigma_i\right)}{\sqrt{\left|\mathbf{r}_i - \frac{1}{2}(\mathbf{R}_n + \mathbf{R}_m)\right|^2 + \alpha_C\, \sigma_i^2}}, \tag{8}$$

where,

$$f_b(x) = \begin{cases} 16\,x^2\,(x_{cut}-x)^2\,/x_{cut}^4 & \text{if} \quad 0 \le x < x_{cut} \\ 0 & \text{otherwise} \end{cases} \tag{9}$$

In the expression above x_{cut} is the cut-off coefficient, which together with $C^{(b)}$ constitute the two, free parameters entering the binding potential.

One can easily realize that $V^{(b)}$ lowers the potential energy between two approaching atoms, giving rise to the formation of bonds and increasing the possibility of electronic transitions during collision. Similarly, function f_b forces the binding potential to become different form zero only within a limited range of internuclear separations. That is, $V_b = 0$ for $R_{n,m} = 0$ and $R_{n,m} > x_{cut}\sigma_i$.

It is worth observing that the binding potential (8) is similar to those introduced by Tersoff (*9*) and Brenner (*10*) in order to account for chemical bonds in Molecular Dynamics simulations. Actually, expression (8) is more general than those in the previously mentioned reference because $V^{(b)}$ also includes the electrons, but the proposed binding potential, however, is far from being so studied as those in Refs. (*9, 10*). Actually, expression (9) has been checked only for two approaching Hydrogen therefore, it may not necessarily work for different nuclei.

Having arrived at this point, it must be noticed that we started assuming Gaussians, however, in writing the potential functions (3-8) we have used an heuristic approach rather than adhering to the model of Gaussian electrons. Therefore, to be consistent with this fact, in the following we wont use the term Gaussian any more and refer to them just as "particles" or, simply, electrons.

Once we have the kinetic and potential functions, the problem of the interaction of a atomic projectile with an atomic or molecular target can be readily solved. To this end, we wrote a computer code which, apart from handling the various procedures necessary to simulate the collision process, carries out the integration of the Newton's equation of motion, i.e. Eqs.(1-8), by using the ordinary differential equation integration routine (ODEINT) from Ref.(*11*).

In the first place, the computer code sets-up the target and the projectile by furnishing them with the proper number of particles. Then, particles are allowed to move with a certain frictional force so that they will find a minimum of the potential energy. In this part of the calculation projectile is at rest and well separated from target so that projectile and target interactions are negligible.

Secondly, the equations of motion of all the particles in the system are numerically solved. In this way, the code determines the position of all the particles in the system during the range of time that is relevant to the stopping process. As was already mentioned, projectile is obliged to moving along a straight line at constant velocity, whereas the target nuclei are kept at rest during passage of the projectile. Figure 2 shows a schematics of the model calculation.

Finally, integration stops when projectile is moving away form target and the state of all electrons can be unambiguously determined, that is, electrons should be either ionized, captured or bound to the target. At this point, one *history* of the computer simulation has finished. Then, the energy transferred to the electrons, i.e. ΔE, is obtained by taking the difference between the total energy of the particles at the end and that at the beginning of the history. It should be mentioned that before launching a new history both projectile and target are randomly rotated around one of their nucleus, if more than one. As a consequence, all these histories constitute independent events and so, by repeating K-times such histories we can obtain the mean energy-loss of the projectile as the arithmetic mean $Q(p) = K^{-1}\sum \Delta E_k$, where K stands for the number of histories and p is the impact parameter. Similarly,

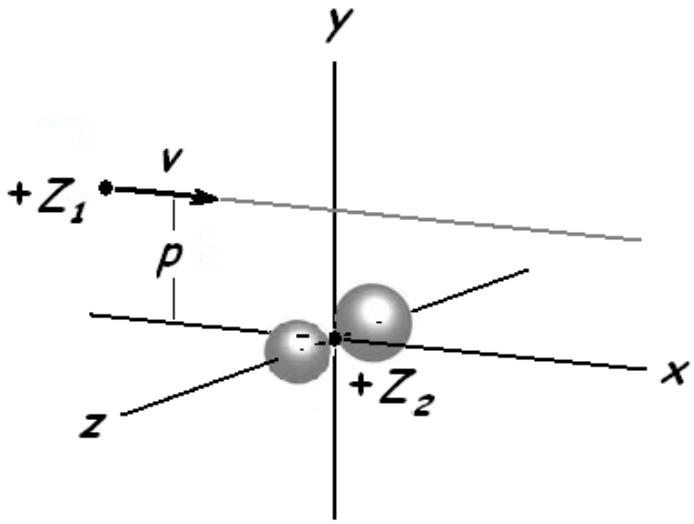

Figure 2. Schematics view of the collision between a $+Z_1$ charged nucleus interacting with a $+Z_2$ nuclear charge surrounded by two spherical clouds representing the electrons. p denotes the impact parameter and v the projectile velocity.

the electronic stopping cross-section thus becomes

$$S_e = \pi \int_0^\infty dp^2\, Q(p)\ . \tag{10}$$

This integral is performed by numerical means, i.e. by sampling p over the relevant range of impact parameters, where the number of points in the sample depends on the statistical uncertainty one would like to achieve, which is typical of the order of five percent.

The results of calculating the electronic stopping cross-section using the procedure described here will be discussed in the following section.

3. Results

Before going into stopping calculations however, we have to find a sensible set of values for the parameters entering the model. To this end, we use the standard least-square minimization procedure and, in the first place, parameters $C_1^{(Q)}$ and $C_2^{(Q)}$ are calculated by fitting the successive ionization potential data to those calculated using the present model. To be more precise, the successive ionization potentials of $Z_2 = 1$,.. 5 atoms are calculated and fit to experimental data in Ref.(*12*). The results of such a fitting yield $C_1^{(Q)}= 0.305$ and $C_2^{(Q)}= 0.653$. A comparison of our calculations with data is depicted in Fig.3. As one can see, the proposed model reproduce the ionization energies remarkably well. In fact, calculations deviate from data less than five percent, all along the twenty five experimental results used in the fitting.

Next, we set $x_{cut} = 6$ and calculate $C^{(b)}$ and α_b by fitting the potential energy curves for H_2^+ and H_2 molecules in Ref.(*13*). The results of such calculations produce $C^{(b)}= 0.2$. Figure 4 shows the energy curves in Ref.(*13*) and those of the present calculations. As one can readily see, the agreement with data is fairly good. For the two cases, the binding energy and the internuclear separation at the

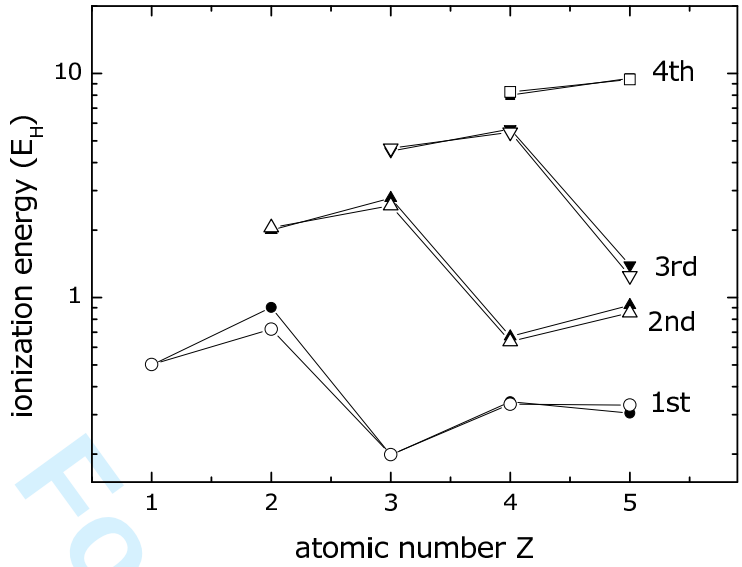

Figure 3. Successive ionization energies for Z=1-5 atoms. Full symbols: experimental data from Ref.(*12*); open symbols: calculations in this work.

Table 1. Calculated values of the binding energy and internuclear separation at the minimum of the potential energy. Reference values from Ref.(*13*) appear enclosed in square brackets.

Molecule	H_2^+	H_2
Binding energy (E_H)	0.11 [0.103]	0.17 [0.166]
Equilibrium distance (a_0)	1.8 [2.00]	1.6 [1.40]

minimum energy are described with a fair degree of accuracy. In Table 3 we show the binding energies and the equilibrium positions for the H_2^+- and H_2-molecule obtained using our model and, for a comparison, those in Ref. (*13*) are also shown enclosed within brackets. As one can see, the binding energy and the equilibrium distance obtained in this paper and those in Ref.(*13*) are fairly similar. The worst case is that of the equilibrium distance for the Hydrogen molecule which differs from calculations by approximately 14%.

With regard to parameter τ we have set it to unity all along the present calculations, however, since we limited ourselves to low velocities such a parameter is rather irrelevant in this paper. Actually, we may conclude that, within the range of bombarding energy considered in the present calculations, τ has nearly no effects on the stopping calculations.

Going to the stopping cross section calculations, firstly, we compare our results with the theoretical calculations in Ref. (*14*). Notice that the results in such a publication can be regarded as reference values, because they were obtained using quantum simulations.

Figure 5 shows the results of the stopping according to Ref.(*14*) and those in this paper. Remarkably, our classical model compare reasonably well with such quantum-based calculations. In fact, our results appear to reproduce satisfactorily well the main features of the stopping cross section for the three colliding pairs. Curiously however, discrepancy is notoriously large for the case of H^+ on atomic Hydrogen and for bombarding energies larger than 5 keV. In this case, our results are observed not to increase as faster as those in Ref. (*14*), i.e. dotted line in Fig.5. Such a deviation however is hard to understand, since the lack of a long range potential, as that of Coulomb, leads to fast neutral particles to have smaller stopping than charged ones at same velocity.

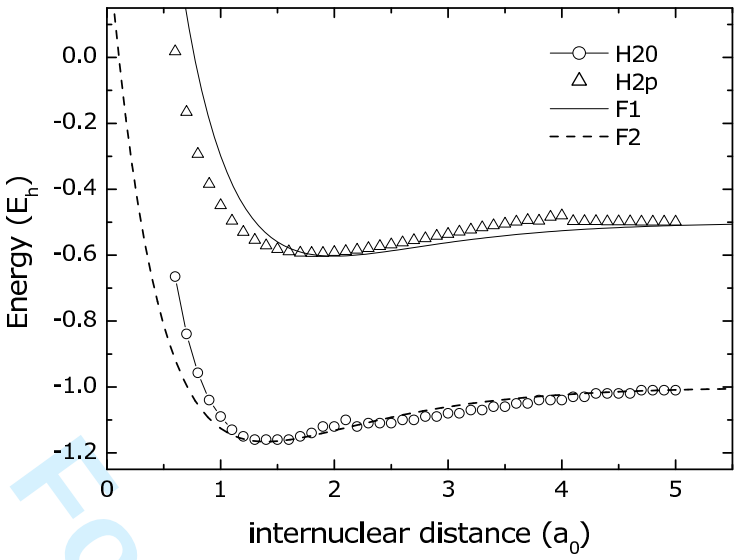

Figure 4. Potential energy of H_2^+ and H_2 molecules. Continuous lines: theoretical results from Ref.(*13*). Open symbols: results of the present calculations.

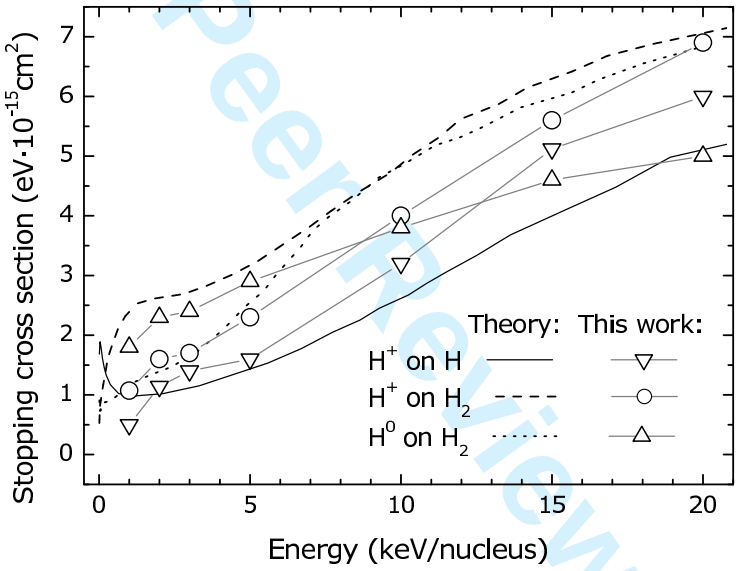

Figure 5. Theoretically calculated stopping cross sections. Lines: Cabrera-Trujillo et al. (*14*). Calculations in this paper are denoted by open symbols.

A comparison of our calculations with experimental data in figure 6 shows that, for neutral Hydrogen, the stopping obtained from our classical model reproduce experiments remarkably well. The results for protons, however, though not too different from data, show a different slope. This is quite reasonable though, since, at the bombarding energies in such a figure, the neutral fraction of Hydrogen in a H_2 gas is of the order of 80% or larger (*15*). Therefore, atomic Hydrogen are supposedly the dominant species in the beam and so, measurements, within such a bombarding range, should be determined by the stopping of atomic Hydrogen.

Finally, it is important mentioning that one of the worst case, computationally speaking, i.e. that of 1 keV H^0 on H_2, the code needs approximately 3000 histories in order to produce a stopping cross section with a 5% relative error, and this takes of the order of 500 seconds, total time, running on a desktop PC equipped with a x86 family, 2.2GHz processor. The computer code was written in FORTRAN 77, compiled and run using MS-Developer Studio (*20*), and the resulting executable

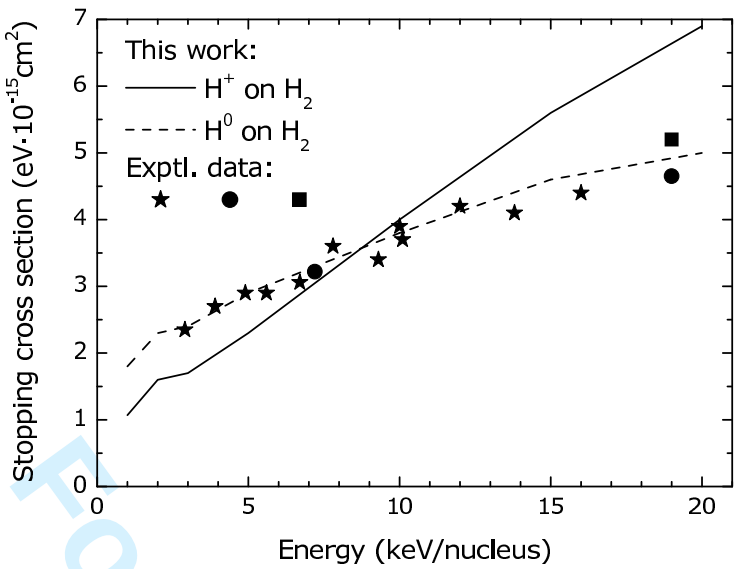

Figure 6. Stopping cross section. Small symbols: experimental results from Refs. (*17*) (★), (*18*) (•), and (*19*) (■) . Calculations in this paper are denoted by lines.

file has a size of the order of 240 kB.

4. Summary and Conclusions

A model calculation is proposed that allows one to numerically simulate, using classical mechanics, the interaction between 1 - 20 keV H^+ and H^0 projectiles and atomic and molecular Hydrogen targets. It is based on the assumption that electrons are Gaussian distributions of charge and three *ad hoc* potentials which, to some extent, account for the uncertainty and Pauli exclusion principles, and a binding potential.

It should be noticed that, although the present model was initially conceived for Gaussian electrons, we have actually followed a heuristic approach rather than sticking strictly to Gaussian electrons. As a consequence, the basics assumptions in this model are not the Gaussian electrons, but the expressions used for the kinetic and potential energies in Eqs.(2-9).

The results in this paper show that this approach appears to be capable of reproducing the successive ionization energies of multi-electronic atoms, and the potential energies of the ground state for the H_2^+ and H_2 molecules with an acceptable degree of accuracy. We also calculate the stopping cross section atomic and molecular Hydrogen for 1 to 20 keV protons and atomic Hydrogen projectiles. The results show a fairly good agreement with previous theoretical study of the same colliding pairs as well as with experimental data. The proposed approach is theoretically simple and very efficient in terms of computer resources. Consequently, we dare suggest that this approach constitutes a promising alternative for computer simulating the collision between atomic or molecular particles, carrying several electrons, by using the classical dynamics equations.

Acknowledgement

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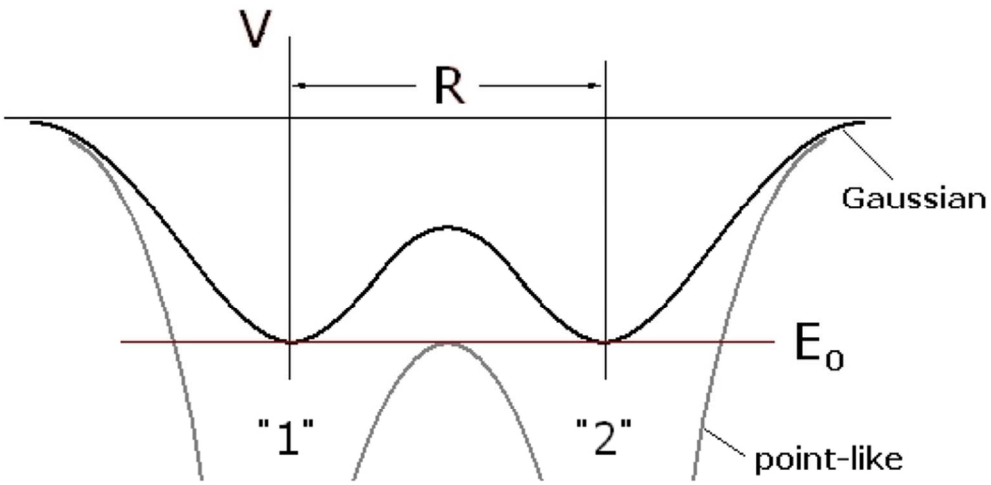

Potential energy of a Gaussian (black line) and that of a point-like (gray line) electron in the field of two, equal nuclear charges, i.e. ``1'' and ``2''. E_0 denotes the total energy of the electron.
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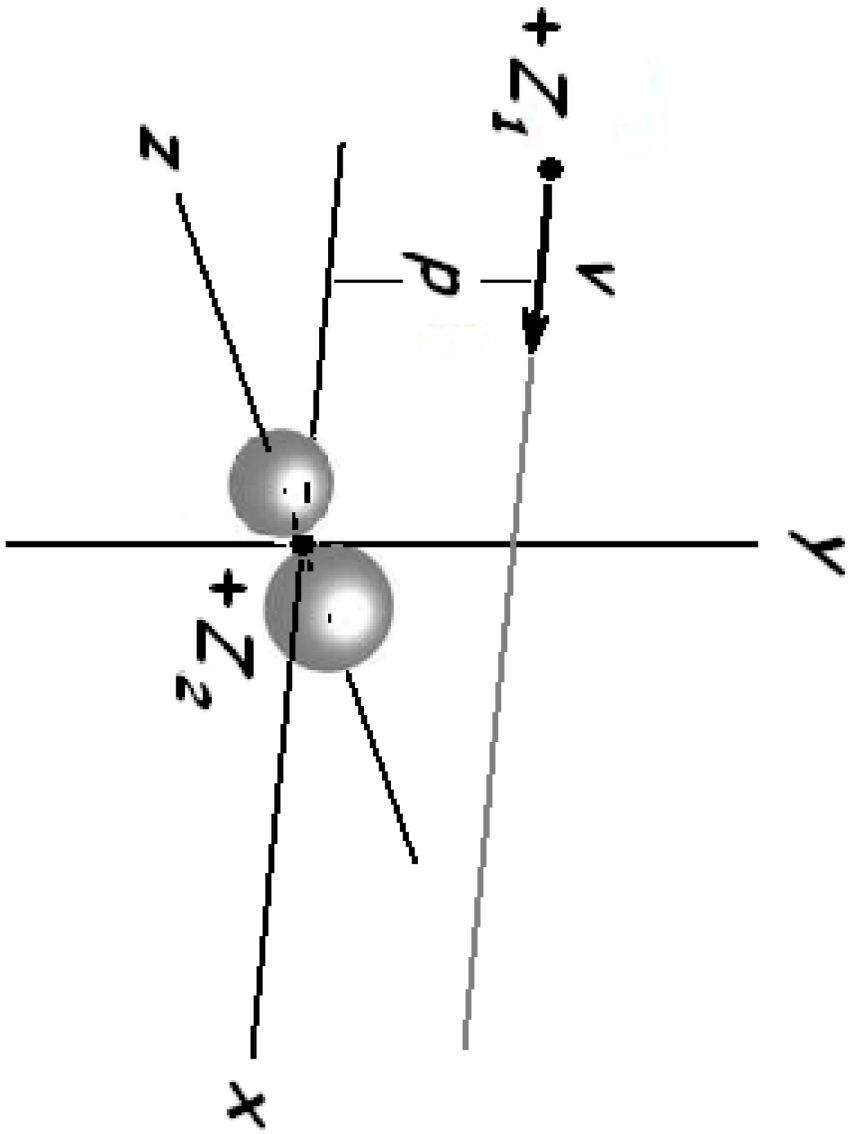

Schematics view of the collision between a +Z$_1$ charged nucleus interacting with a +Z$_2$ nuclear charge surrounded by two spherical clouds representing the electrons. p denotes the impact parameter and v the projectile velocity.
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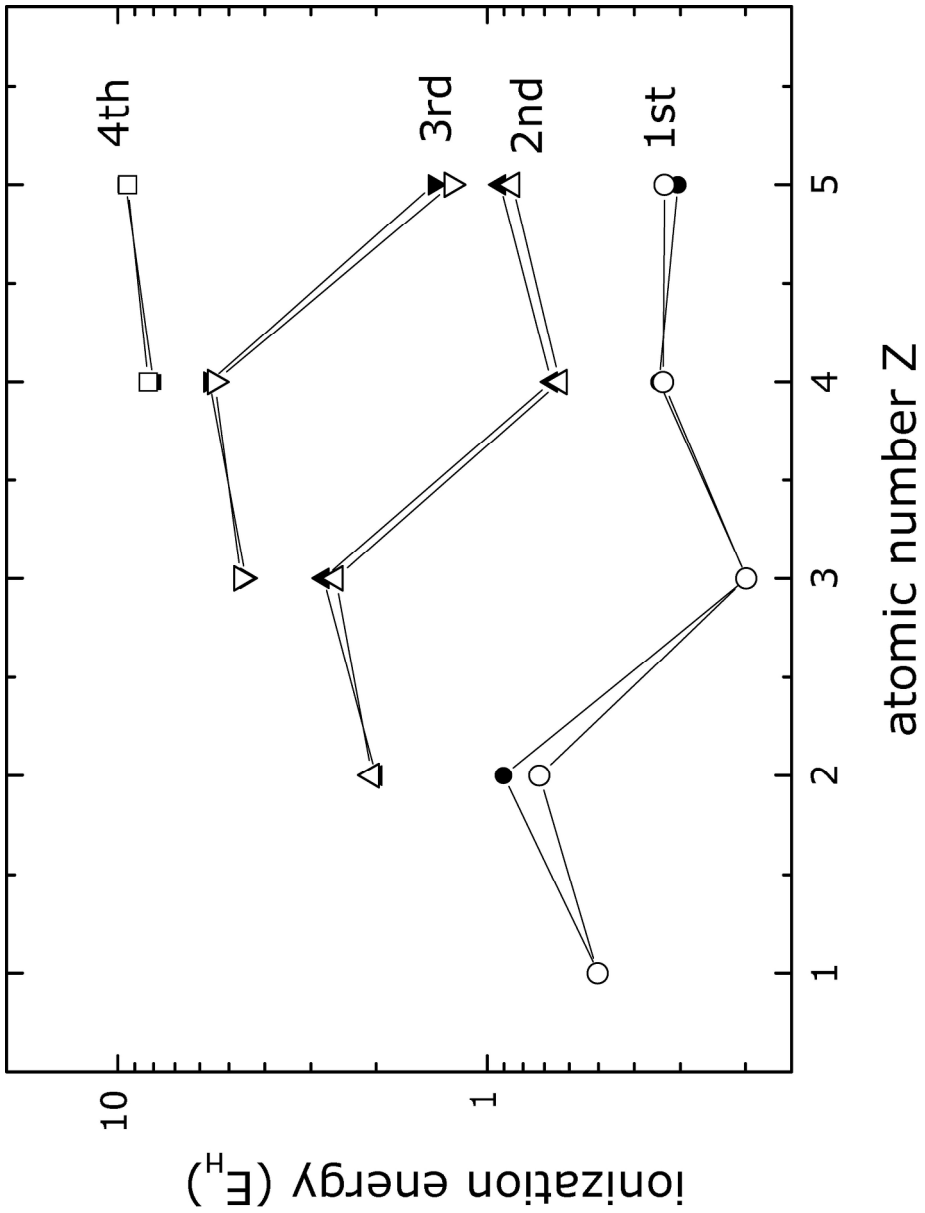
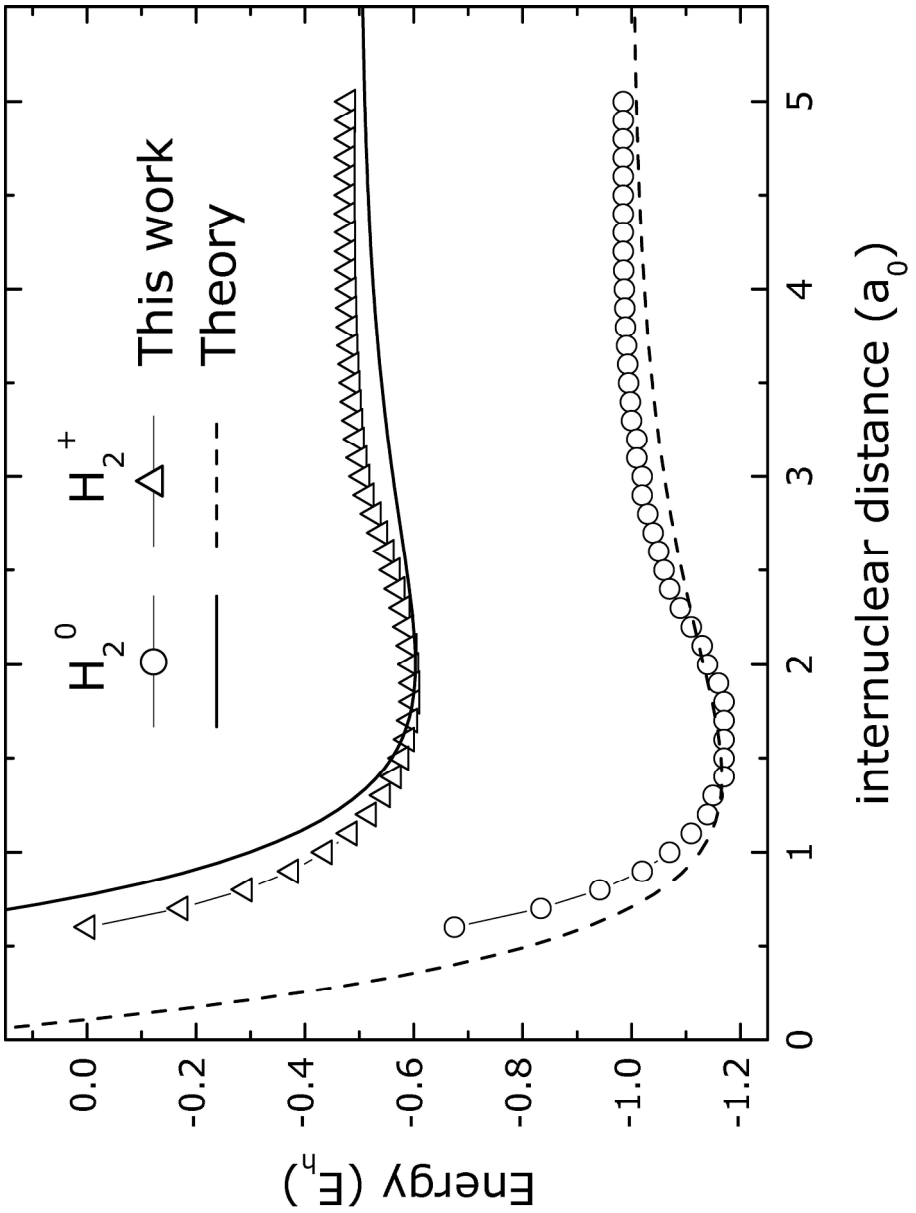
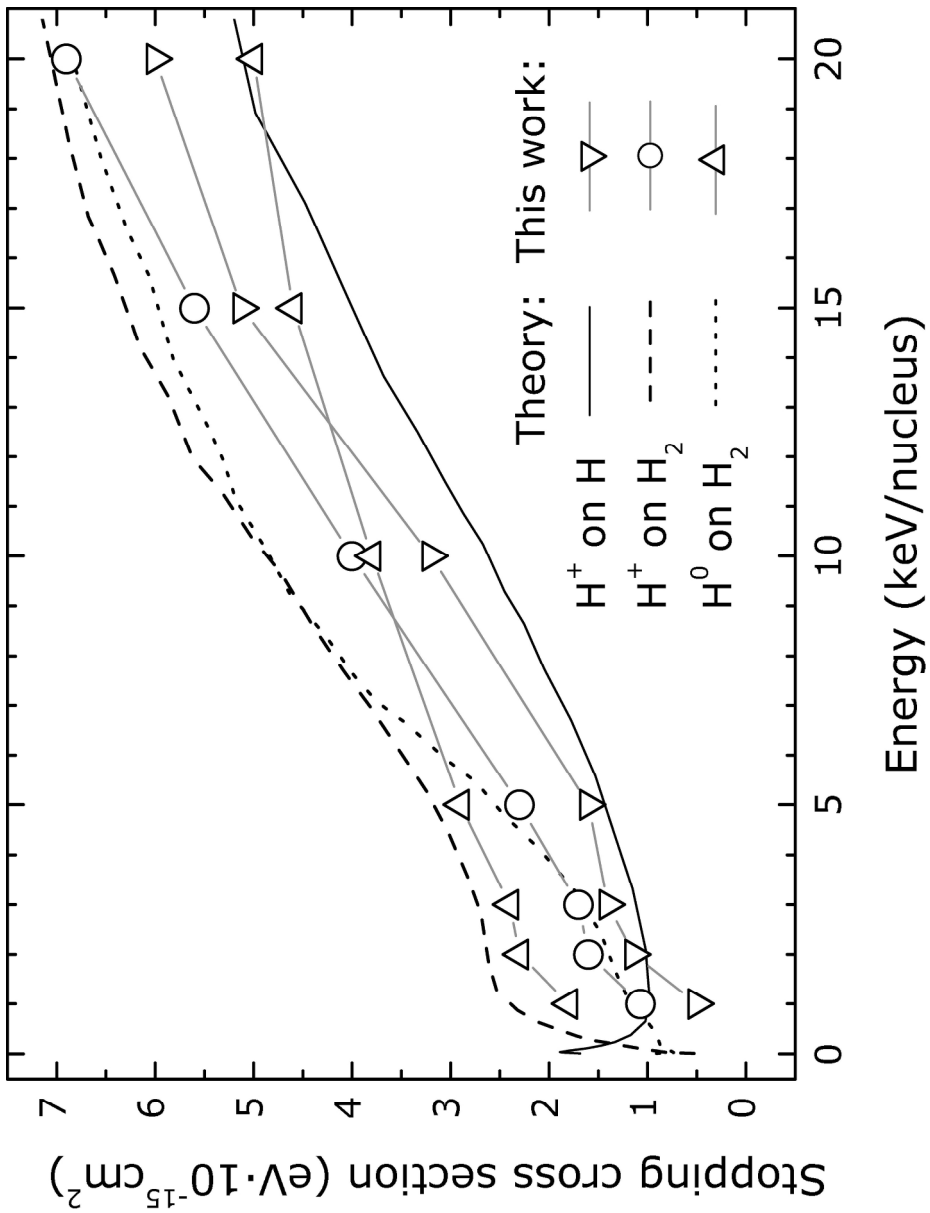


Successive ionization energies for Z=1-5 atoms. Full symbols: experimental data from Ref.\cite{CRC}; open symbols: calculations in this work.
221x291mm (300 x 300 DPI)



Potential energy of H$^+_2$ and H$_2$ molecules. Continuous lines: theoretical results from Ref.\cite{Sharp71}. Open symbols: results of the present calculations.
228x303mm (300 x 300 DPI)



Theoretically calculated stopping cross sections. Lines: Cabrera-Trujillo et al. \cite{CT2003}. Calculations in this paper are denoted by open symbols.
220x288mm (300 x 300 DPI)