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LETTER TO THE EDITOR

Role of projectile continuum states in the ionization of atomic hydrogen by high-energy ion impact

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Abstract. Ionization of atomic hydrogen in collisions with H^+ and He^{2+} ions is studied by a large-scale coupled-channel calculation. It is demonstrated that high-lying continuum states of the projectile, which have been disregarded in previous calculations, contribute significantly to the ionization of the target atom. The portion of the ionization into these projectile continuum states amounts to 13% of the total ionization cross section in the case of H^+ impact even in the MeV region, and the question is raised as to the normalization procedure of experimental values to the Born cross section there. The partial cross section of the ionization into the target continuum satisfies the Z^2 scaling rule (where Z is the projectile charge) at high energies while the component into the projectile continuum states has a weaker dependence on the charge. As a result the ratio of the total ionization cross sections by He^{2+} and H^+ impact deviates from the Z^2 scaling by 4–5 % above the collision energy of 500 keV u^{-1} in close agreement with the experimental findings of Shah and Gilbody.

The coupled-channel method based on atomic orbital (AO) expansion has been widely applied to ion–atom collisions in the intermediate-energy region where the projectile velocity is comparable to the average velocity of the bound electron (Fritsch and Lin 1991). In this approach the contribution of continuum states is taken into account through discretized pseudo-continuum states which are constructed by diagonalizing the atomic Hamiltonian of the target or the projectile in terms of a set of square-integrable basis functions. In most cases these pseudostates are used for improving the convergence of the basis set expansion rather than for calculating ionization cross sections directly.

We need a larger number of positive-energy pseudostates of the atomic Hamiltonian in order to calculate ionization cross sections, but a sufficiently large number of positive-energy states have not been used in previous calculations so far. Fritsch and Lin (1983) used a scaled-charge basis set for proton–hydrogen-atom collisions. They included only s and p orbitals which have ten (on each centre) positive-energy states. Shakeshaft (1978) employed a slightly larger set of basis functions adding d orbitals for the same process. In these calculations continuum states on both the target and projectile are used in the energy region lower than 200 keV. Winter and Alston (1992) extended the calculation to higher energies supplementing the contribution of the f and g orbitals by the Born partial amplitudes for p+He^+ collision, but they did not include a continuum state on the projectile. Ermolaev (1990a, b) also used only target continuum states to investigate high-energy proton–hydrogen-atom collisions. Hitherto the influence of projectile continuum states on ionization of target atoms has not been studied in the high energy region.

All of these calculations are based on the Slater-type orbital (STO) expansion. Although real bound states can be represented as a linear combination of a finite number of Slater-type orbitals, it has a shortcoming that two-centre matrix elements cannot be evaluated analytically (McCarroll 1961). One has to perform numerical integration at least in one dimension. The convergence of the integral becomes quickly worse as the number of nodes of the wavefunction increases or the collision energy becomes higher. Thus the Slater-type basis function is not practically suitable for highly excited states nor high-lying continuum states, especially at high energies.

Recently Toshima and Eichler (1991, 1992) extended the coupled-state calculations to high-energy proton–hydrogen-atom collisions and succeeded in producing the Thomas peak without relying on the perturbation theory for the first time. Their method is based on the Gauss-type orbital (GTO) expansion in which all the matrix elements can be evaluated analytically. They showed that very high-lying continuum states of both the target and projectile contribute significantly to the Thomas mechanism (Thomas 1927) and new features of the two-centre effect of the double continua were reported. The high-lying continua play a decisive role as an intermediate state in the Thomas double-scattering mechanism. In this letter we show that it is not a characteristic of the Thomas mechanism but a general feature of high-energy ion–atom collisions that high-lying continua of the projectile are selectively populated at high energies. The enhanced population of the high-lying continuum states can be expected to affect the direct ionization process.

We study the ionization processes

$$\mathrm{H}^+ + \mathrm{H}(1\mathrm{s}) \rightarrow \mathrm{H}^+ + \mathrm{H}^+ + \mathrm{e} \tag{1}$$

$$\mathrm{He}^{2+} + \mathrm{H}(1\mathrm{s}) \rightarrow \mathrm{He}^{2+} + \mathrm{H}^+ + \mathrm{e} \tag{2}$$

by the coupled-channel method in the framework of the impact parameter treatment. The projectile is assumed to travel along a classical straight trajectory with a constant velocity $\boldsymbol{v}$. The Schrödinger equation describing the collision process (atomic units are used unless otherwise stated)

$$\left(H - \mathrm{i}\frac{\partial}{\partial t}\right)\Psi(\boldsymbol{r}_\mathrm{T}, t) = 0 \tag{3}$$

are solved introducing an expansion

$$\Psi(\boldsymbol{r}, t) = \sum_{i=1}^{N_\mathrm{T}} a_i(t)\psi_i^\mathrm{T}(\boldsymbol{r}_\mathrm{T}, t) + \sum_{i=N_\mathrm{T}+1}^{N} a_i(t)\psi_i^\mathrm{P}(\boldsymbol{r}_\mathrm{P}, t) \tag{4}$$

in terms of the target functions

$$\psi_i^\mathrm{T}(\boldsymbol{r}_\mathrm{T}, t) = \varphi_i^\mathrm{T}(\boldsymbol{r}_\mathrm{T})\,\mathrm{e}^{-\mathrm{i}E_i^\mathrm{T} t} \tag{5}$$

and the projectile functions

$$\psi_i^\mathrm{P}(\boldsymbol{r}_\mathrm{P}, t) = \varphi_i^\mathrm{P}(\boldsymbol{r}_\mathrm{P})\,\mathrm{e}^{-\mathrm{i}E_i^\mathrm{P} t}\,\mathrm{e}^{\mathrm{i}\boldsymbol{v}\cdot\boldsymbol{r}_\mathrm{T}}\,\mathrm{e}^{-\mathrm{i}v^2 t/2}. \tag{6}$$

Here, r_T, r_P are the electron coordinates measured from the target and projectile nucleus, respectively, and φ_i^T, φ_i^P are the eigenfunctions of the target and projectile Hamiltonian with eigenvalues E_i^T and E_i^P. The atomic eigenfunctions of each centre are now further expanded in Gauss-type basis functions as

$$\varphi_{nlm}(r) = \sum_{\nu} c_{\nu}^{(n\ell)} \, e^{-\alpha_\nu r^2} \, r^\ell Y_{\ell m}(\hat{r}) \tag{7}$$

where the non-linear parameters α_ν are generated as a modified geometrical progression. The coefficients $c_\nu^{n\ell}$ are determined so as to diagonalize the atomic Hamiltonian of the target or the projectile (Toshima and Eichler 1991, 1992).

On each atomic system we have constructed 80–87 eigenstates which consist of all the bound states from $n = 1$ to 2 for the hydrogen atom (from $n = 1$ to 3 for the singly-charged helium ion) and positive-energy pseudostates covering from the ionization threshold to the energy of 2000 eV depending on the collision velocity. The angular momenta of the electronic states cover the range of $0 \leqslant \ell \leqslant 4$, and the maximum value is enlarged up to 6 when the convergence of the basis functions is checked.

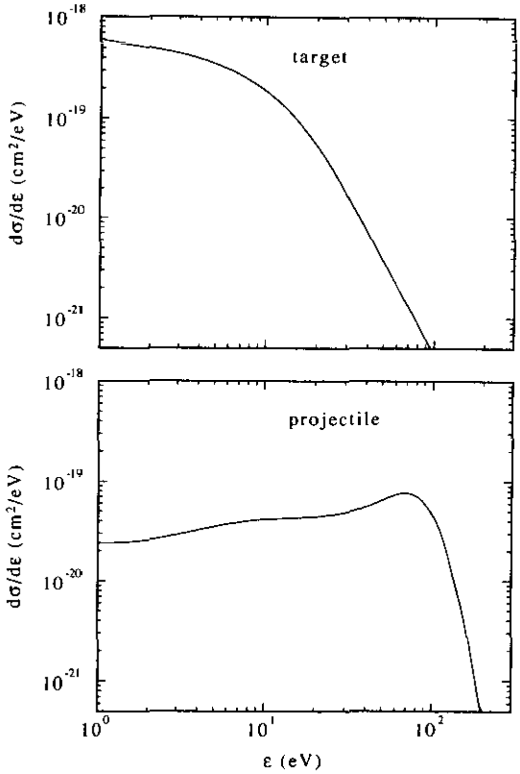

Figure 1. The energy distribution of the s ejected electron for the collision $H^+ + H(1s)$ at a collision energy of 200 keV. The upper graph is for the target continuum and the lower is for the projectile continuum.

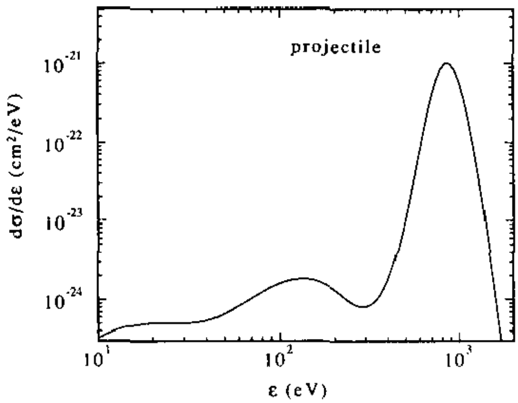

Figure 2. The energy distribution of the s ejected electron in the projectile continuum for the collision $H^+ + H(1s)$ at a collision energy of 1.5 MeV.

The energy distributions of the ejected s electrons of the process (1) are given in figure 1 for a collision energy of 200 keV and in figure 2 for a collision energy of 1.5 MeV. The energy distribution of the electrons with $\ell \neq 0$ is similar to figures 1 and 2. The energy distribution of the electron in the target continuum decreases monotonically as the electron energy increases in harmony with the results of Mukoyama *et al* (1985). On the other hand, the distribution for the projectile continuum extends to much larger electron energy. At a collision energy of 200 keV, it is flat up to 100 eV and goes down sharply above this energy. At a collision energy of 1.5 MeV, a very sharp peak exists around 850 eV in accordance with the finding of Toshima and Eichler (1991) in the calculation of the Thomas peak. The energies of 100 and 850 eV coincide with the energy of the electron that has the same velocity as the respective incident projectile. These high-velocity electrons are different from the peak component of the charge transfer to continuum states (CTC) since the latter have small relative kinetic energy if they are seen from the projectile nucleus.

Table 1. Partial cross sections for ionization into the target and the projectile continuum states of the coupled-channel calculations and the Born cross sections into the target continuum states in units of cm^2 for p+H(1s) collisions. $a(b)$ denotes $a \times 10^b$.

E (keV)	Target	Projectile	Total	Born
200	7.25(−17)	1.46(−17)	8.70(−17)	7.71(−17)
500	3.34(−17)	5.75(−18)	3.92(−17)	3.65(−17)
1000	2.00(−17)	3.05(−18)	2.30(−17)	2.01(−17)
1500	1.40(−17)	2.26(−18)	1.62(−17)	1.41(−17)
2000	1.10(−17)	1.54(−18)	1.25(−17)	1.10(−17)

Table 1 lists the partial ionization cross sections to the target and the projectile continuum states of the process (1). The portion of ionization into the projectile continuum states decreases very slowly above 500 keV as the collision energy increases. Even at 1.5 MeV it has a contribution of 13 % of the total ionization cross section. The partial cross sections for ionization into the target continuum states only are very close to the Born cross sections above 1 MeV. This excellent agreement shows that the discretized pseudo-continuum states used in this calculation can be regarded as a complete set for the present problem, since real continuum states of the hydrogen atom are used for the Born approximation summing up over all the partial waves of the ionized electron. In the analysis of the experiment of Shah and Gilbody (1981), they normalized their measured values to the Born cross section at 1.5 MeV. The present calculation implies that this nomalization procedure is not justified even in the MeV region.

Table 2. Partial cross sections for ionization into the target and the projectile continuum states of the coupled-channel calculations in units of cm^2 for $He^{2+} + H(1s)$ collisions. $a(b)$ denotes $a \times 10^b$.

E (keV u^{-1})	Target	Projectile	Total
200	2.49(−16)	4.97(−17)	2.98(−16)
500	1.34(−16)	1.50(−17)	1.49(−16)
1000	8.03(−17)	8.28(−18)	8.86(−17)
1500	5.61(−17)	6.64(−18)	6.28(−17)
2000	4.40(−17)	4.81(−18)	4.88(−17)

Table 3. The ratio of ionization cross sections $\sigma(He^{2+})/4\sigma(H^{+})$. The experimental data are from Shah and Gilbody (1981) and the Glauber cross sections are from McGuire (1982).

E (keV u^{-1})	Present	Expt	Glauber
200	0.857	0.895	0.851
500	0.950	0.954†	0.946
1000	0.963	—	0.975
1500	0.967	—	0.981
2000	0.973	—	0.983

† Interpolated value.

Table 2 gives the partial cross sections for the process (2). We see a similar contribution of the projectile continuum states but the portion is smaller than for the proton impact. The partial cross sections into the target continuum states satisfy the scaling rule of Z^2 (where Z is the projectile charge) very well, as the Born cross sections do. It is interesting to see that this scaling holds even at 500 keV u^{-1} where the Born cross section deviates from the partial cross section of the coupled-channel method. Because of the contribution of the projectile continuum states the total cross sections do not satisfy the scaling law. Though absolute measurement of ionization cross sections of atomic hydrogen has not been performed yet, the relative ratio $\sigma(He^{2+})/4\sigma(H^{+})$ can be determined accurately. The energy dependence of the cross section ratio is given in table 3, where we see that the ratio changes little in the wide energy range from 500 keV u^{-1} to 2000 keV u^{-1}. The value 0.95 agrees well with the measured value of Shah and Gilbody (1981) at 500 keV u^{-1}. Since the present coupled-channel cross sections obey the Z^2 rule above 500 keV if we do not include the projectile continuum states, this deviation of 5% is solely due to the contribution of the projectile continuum states. The ratio of the Glauber cross sections (McGuire 1982) has an energy dependence similar to the coupled-channel results, but the details are rather different between them. Firstly, Glauber ionization cross sections are always smaller than the Born value (McGuire 1982) while the present coupled-channel cross sections are larger for H^+ impact. Secondly, only the continuum states of the target atom are explicitly taken into account in the Glauber approximation. It is not clear how these two theoretical approaches are related in the Z dependence of the ionization cross sections. Precise absolute measurement is desired in order to clarify the discrepancy in the details of the theoretical predictions.

In summary it is shown that high-lying continuum states contribute to the ionization process of atomic hydrogen even in the MeV region. The component of ionization into the projectile continuum states is responsible for the deviation from the Z^2 scaling law at collision energies above 500 keV u^{-1}.

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