

# Numerical treatment of ion collisions with water molecules

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**Synopsis** A lattice treatment has been implemented to study collisions of multiply charged ions with H<sub>2</sub>O within the independent electron approximation. The method has been applied to calculate ionization and electron capture probabilities for collisions of H<sup>+</sup>, He<sup>2+</sup>, Li<sup>3+</sup> and C<sup>6+</sup> with H<sub>2</sub>O, at energies  $20 \leq E \leq 300$  keV/u.

In a previous work[1], we applied a lattice method to solve the time-dependent Schrödinger equation (TDSE) that appears in the semiclassical description of ion-atom collisions:

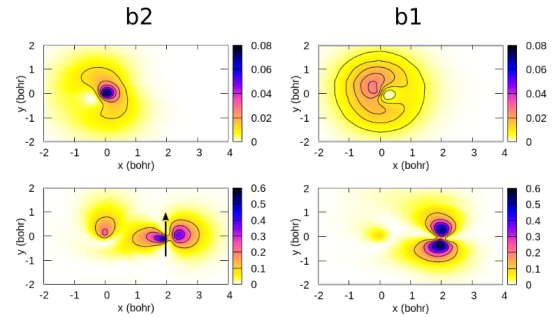
$$\hat{H} - i \frac{d}{dt} \Psi(\vec{r}, t) = 0, \quad (1)$$

where  $\hat{H}$  is the clamped-nuclei Born-Oppenheimer electronic hamiltonian of the quasimolecule formed during the collision and  $\Psi$  is the electronic wavefunction. In that work we employed a modified version of the code GridTDSE code [2], originally designed to study the time evolution of nuclear wavepacket. In the lattice method the wavepacket is represented by a vector  $\vec{\Psi}$  that stores the values of  $\Psi$  on the points of a 3D cartesian grid at each value of  $t$ . The generalization to ion-molecule collisions is straightforward at high collision energies, by employing the Franck-Condon approximation that assumes that the nuclei of the molecular target remain fixed at their equilibrium positions,  $\vec{R}_e$ , during the collision. The generalization to many-electron systems involves the use of the independent electron approximation where each electron moves in an effective potential  $\hat{V}_{\text{ef}}(\vec{r}_i; \vec{R}_e)$  that includes the electron interaction with the core formed by the nuclei and the other electrons and  $\hat{H} = \hat{T} + \hat{V}_{\text{ef}} - Z/r_Z$ , where  $Z$  is the charge of the ion.

The lattice method was applied to study electron-loss in H<sup>+</sup> + H<sub>2</sub>O collisions in Ref. [3]. In the present work we consider the application of this method to collisions of He<sup>2+</sup>, Li<sup>3+</sup> and C<sup>6+</sup> with H<sub>2</sub>O. We have also calculated the electron capture probabilities as explained in Ref. [1].

The application of our numerical method re-

quires large computing resources, but it is very useful to support close-coupling and classical-trajectory-Monte-Carlo calculations. It also allows us to follow the time evolution of the electronic wavepacket, as illustrated in Fig. 1 for electron capture in Li<sup>3+</sup> + H<sub>2</sub>O collisions. The snapshots of the figure have been taken at the point of closest approach  $Y = 0$ . and at  $Y = 27.6 a_0$ , where the molecule has left the box.



**Figure 1.** Contour plots of the electron density on the  $XY$  plane for the collisions Li<sup>3+</sup> + H<sub>2</sub>O (1b<sub>2</sub>, 1b<sub>1</sub>). In the calculation the Li<sup>3+</sup> is fixed at the origin and the molecule follows a rectilinear trajectory  $\vec{R} = \vec{b} + \vec{v}t$  with  $v = 1.8$  a.u.,  $b = 2.0 a_0$ ,  $\vec{v} \parallel \vec{Y}$  and  $\vec{b} = b\hat{X}$ . During the collision the molecular plane is parallel to the  $XZ$  plane and the snapshots have been taken at  $Y = 0$ . (bottom panels) and  $Y = 27.6 a_0$ . (top panels).

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## References

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- [2] Suarez J *et al* 2009 *Comput. Phys. Commun.* **180** 2025
- [3] Errea L F *et al* 2015 *Chem. Phys.* **462** 17

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