Multiresolution Approach for Laser-Modified Collisions of Excited Atoms and Ions

Javier Domínguez[1], Predrag S. Krstić[1] and R. Cabrera -Trujillo[2]
[1] *Institute for Advanced Computational Science*, Stony Brook University, Stony Brook, New York, USA.
[2] *Instituto de Ciencias Físicas*, Universidad Nacional Autónoma de México, México.

Abstract

We expand the time-evolution functionality of the Multiresolution ADaptive Numerical Environment for Scientific Simulation (MADNESS), band-limited, gradient-corrected, symplectic propagator approach to solve numerically the time-dependent Schrödinger equation for a single-electron ion-atom collisions in a strong femtosecond laser field. We apply this method to H$^+$+ H($2s$) collision system in the range of 100 ev - 25 keV collision energies modified by the presence of a 800 nm laser field of terawatt intensity. We calculate the $n = 1 - 6$ state charge exchange and $n = 3 - 6$ state excitation cross-sections, as well as the total ionization laser-free cross-section, comparing our results with existing theoretical, and experimental data reported in the literature. The presence of the laser field increase the charge exchange and excitation crosssections by a factor of 15 for collision energies $1 - 15$ keV [1].

Theory

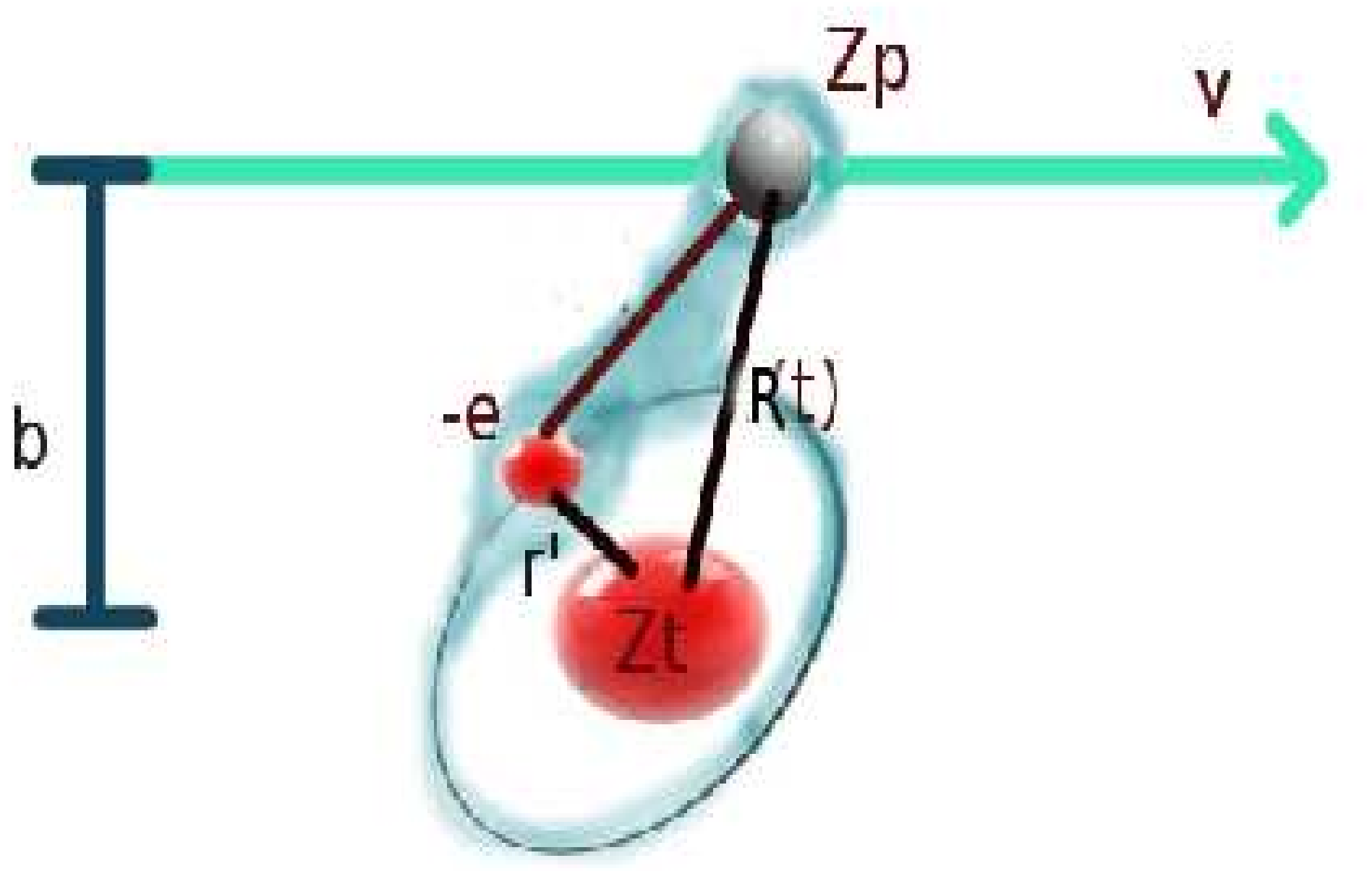
The electronic Hamiltonian,

$$\mathbf{H} = -\frac{1}{2}\nabla^2 - \frac{1}{|\vec{r}|} - \frac{1}{|\vec{r} - \vec{R}(t)|} - \vec{r}\cdot\vec{\mathcal{E}}(t), \qquad (1)$$

$\vec{R}(t)$ is the classical, predefined trajectory.

High collision energies

$E_p > 1$ keV.

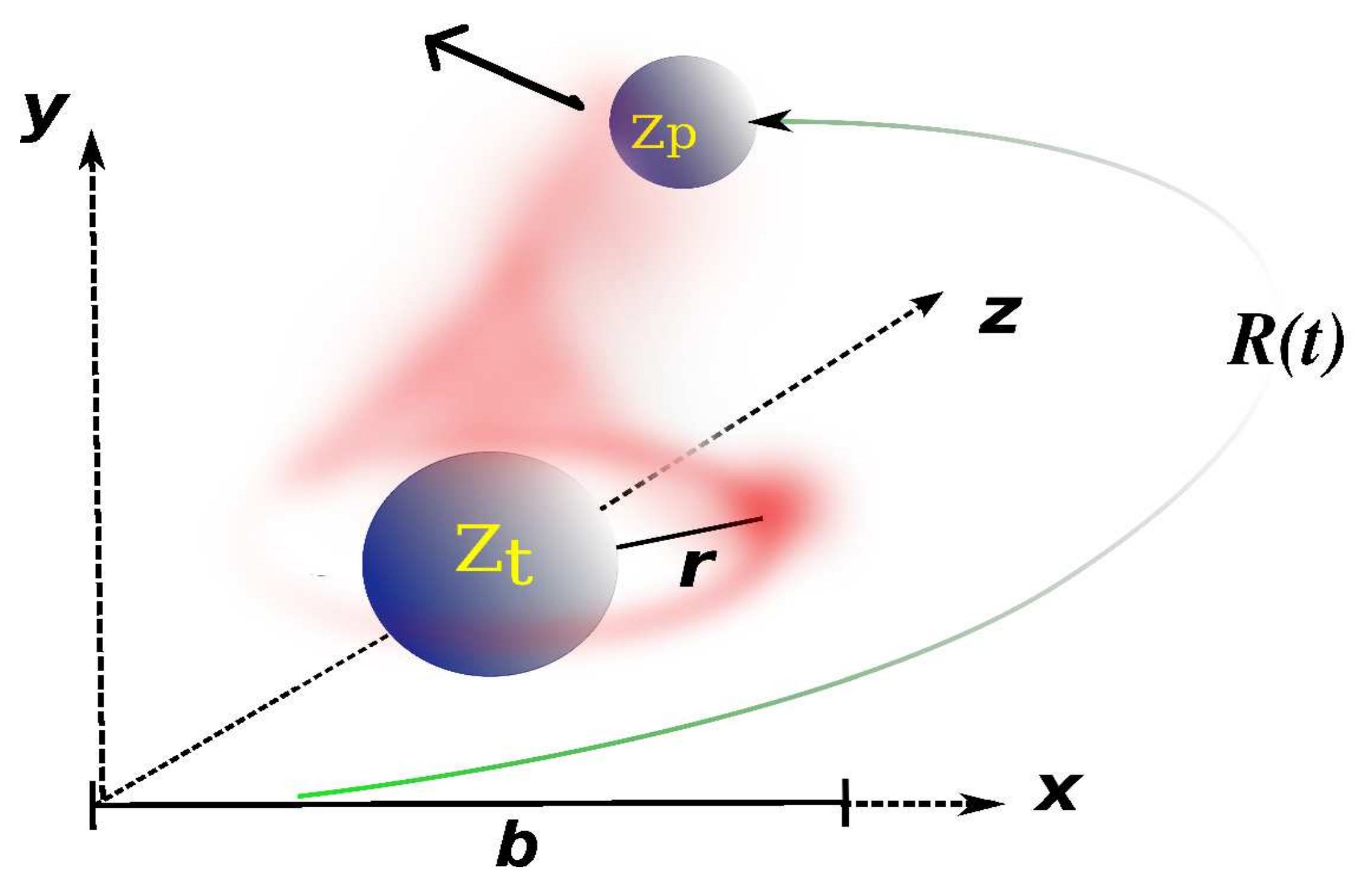


Low collision energies

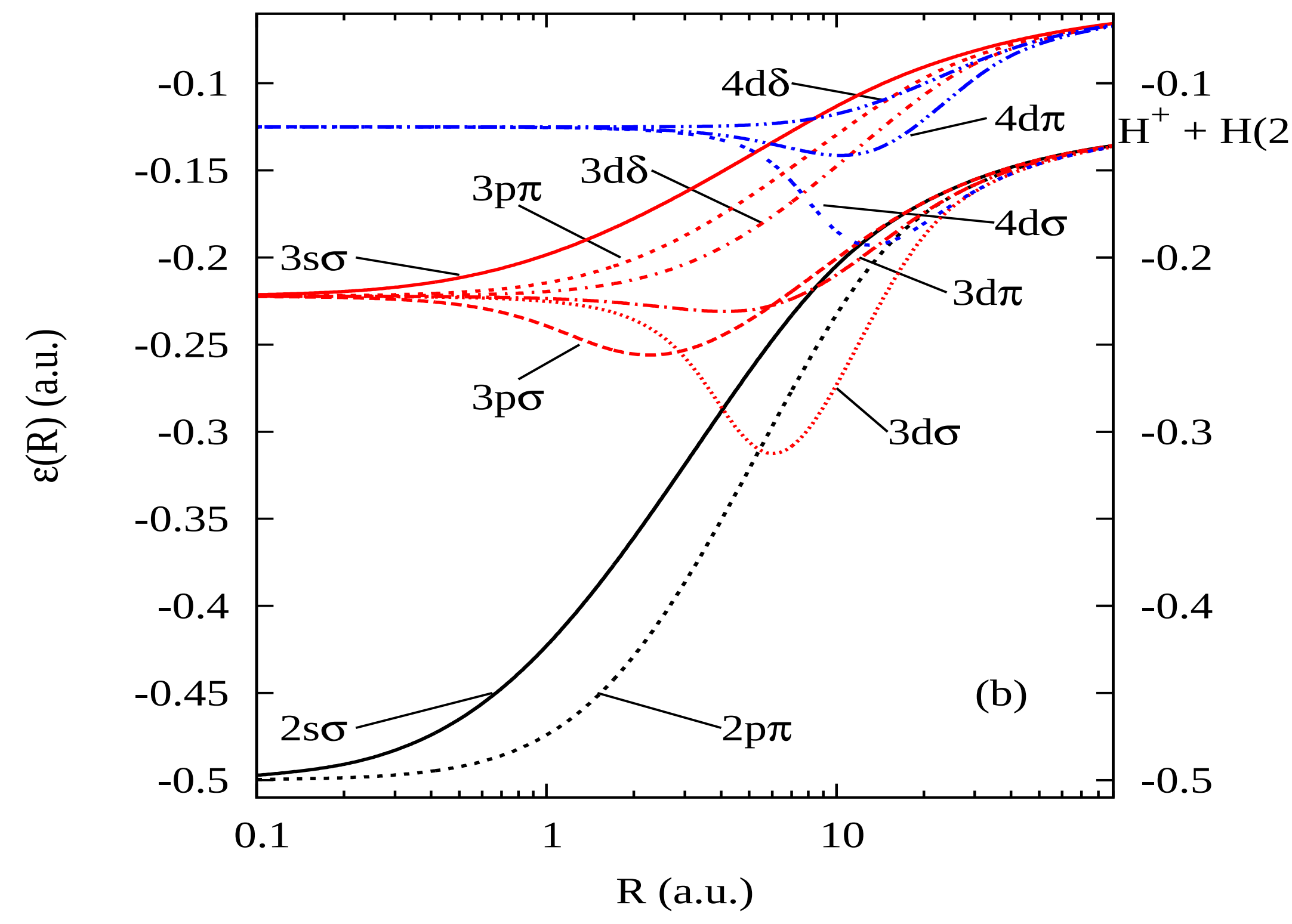
$E_p \le 1$ keV.

Hamiltonian for ion-atom interaction.

$$\mathcal{H}(R,P) = \frac{P^2}{2\mu} + \frac{1}{|\vec{R}(t)|} + \epsilon_{2s\sigma}(R). \qquad (2)$$



Potential energy curves



Laser model

The laser pulse is modeled as

$$\vec{\mathcal{E}}(t) = \mathcal{E}_0 \exp\left[-\left(\frac{\omega t}{2n_{\rm cy}}\right)^2\right]\cos(\omega t + \phi)\,\hat{k} \quad (3)$$

The initial time is $t_0 = -z_0/v_p$; $n_{\rm cy} = 2$, the number of cycles; $\mathcal{E}_0 = 0.1$ a.u ($I = 3.15 \times 10^{14}$ W/cm^2), the amplitude of the electric field; $\omega = 0.0569$ a.u. ($E_{ph} \sim 1.55$ eV), laser frequency; and $\phi = -\pi/2$, the RCLP [2].

ion-atom collision dynamics

We use the time-dependent implementation of MADNESS for the dynamics, by applying the fourth-order propagator operator as [3]

$$U(dt,t) = e^{-\frac{i}{6}\mathbf{V}(t+dt)dt}e^{-\frac{i}{2}\mathbf{T}dt}e^{-\frac{2i}{3}\mathbf{V}(t+\frac{dt}{2})dt} e^{-\frac{i}{2}\mathbf{T}dt}e^{-\frac{i}{6}\mathbf{V}(t)dt} + O(dt^5).$$

Here, **T** and **V** are the kinetic and potential energies, respectively. The complete dynamics of the ion-atom collision is obtained as $\Psi(\vec{r}, t + dt) = U(dt,t)\Psi(\vec{r},t)$. TDSE is limited by the condition $dt \propto \Delta x^2$ [4,5].

Implementation parameters

z_0	-200 a.u.	initial position
$\{x,y,z\}$	500 a.u.	lateral dimension
b	[0.5,100] a.u.	imp. param. range
Δb	0.5 a.u.	b-step
k	8	scaling functions
ϵ	1×10^{-4}	tolerance
ξ	0.25	cut parameter

At t_0, we obtain the energy of H($2s$) as $E_{2s} = -1.248$ a.u. The nl-electron capture and nl-excitation probabilities are calculated as

$$P_{nl}(E_p, b) = \sum_m \left|\int_V \phi^*_{nlm}(\vec{r})\Psi(E_p, b, t_f)dV\right|^2,$$

where $\phi_{nlm}(\vec{r})$ are the stationary hydrogenic orbitals calculated by MADNESS. For the electron capture probability, we consider a translation factor as $\phi_{nlm}(\vec{r}) = \phi_{nlm}(\vec{r} - \vec{R})\exp(i\vec{v}_p(t_f)\cdot\vec{r})$, where $\vec{v}_p(t_f)$ is the projectile velocity. We get the n-state cross-section as

$$\sigma_{nl}(E_p) = 2\pi\sum_l \int_0^{b_{\rm max}} P_{n,l}(E_p, b)bdb. \qquad (4)$$

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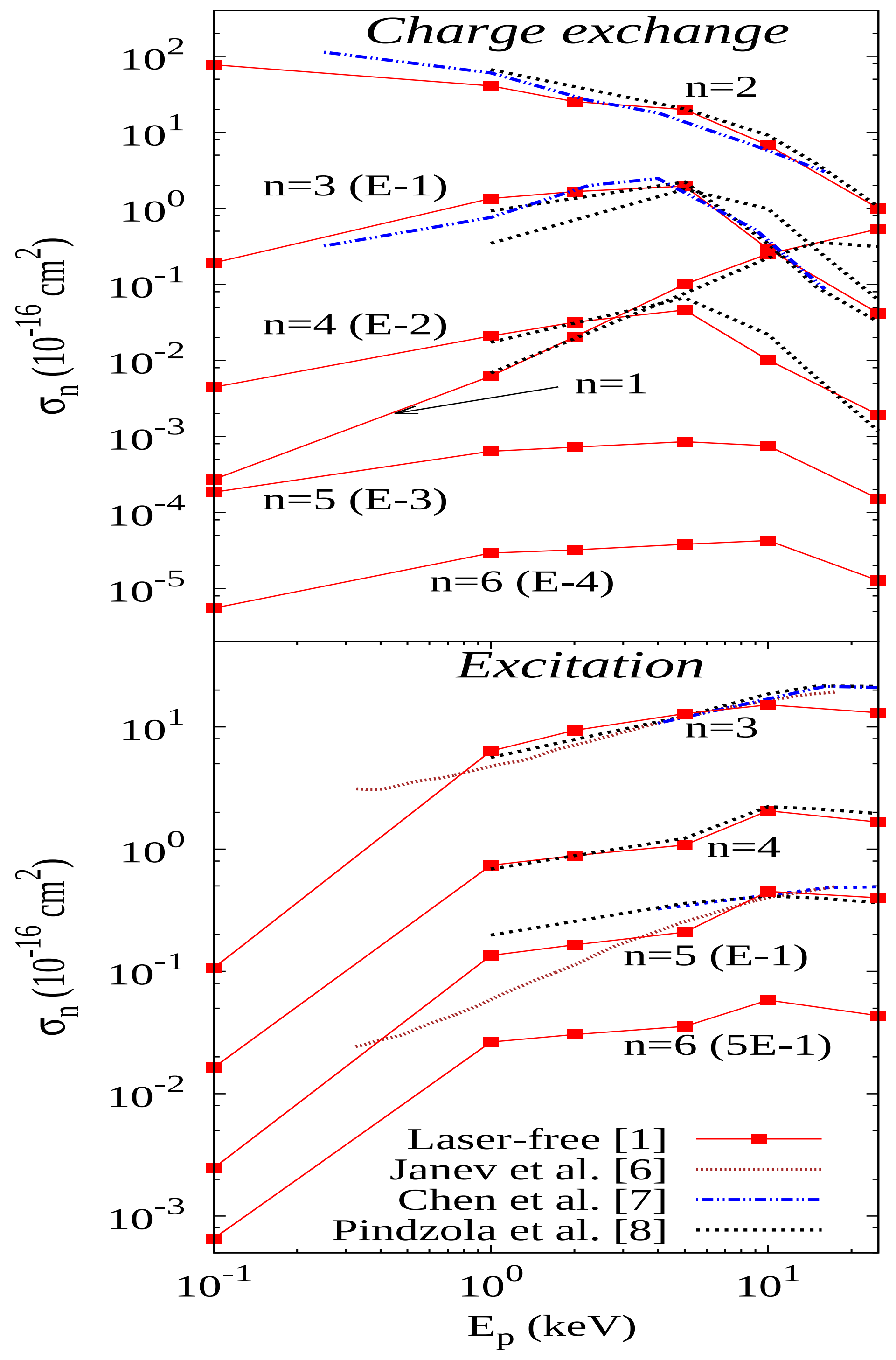
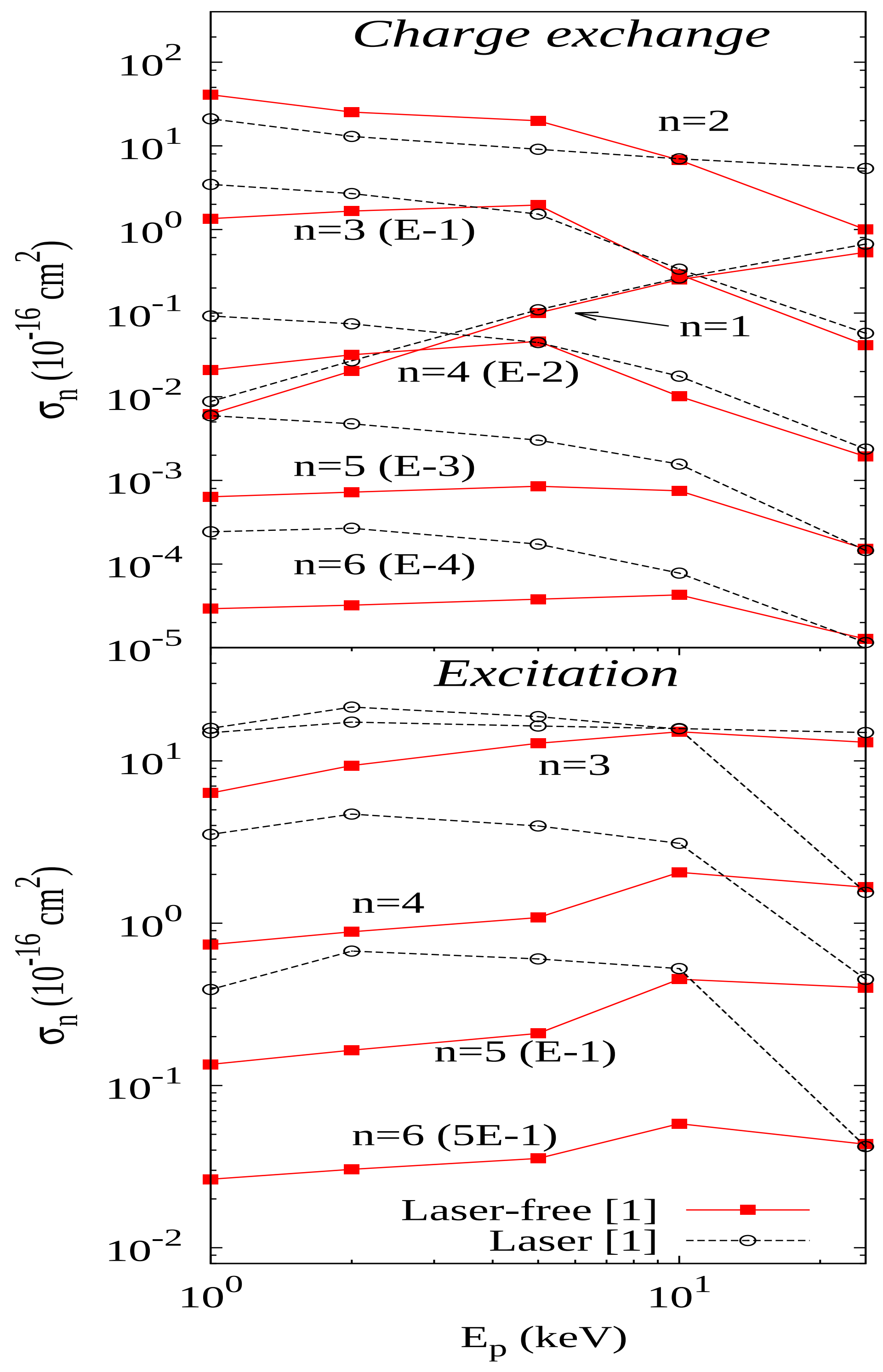
Laser-free results



Laser modified



Conclusions

We have successfully applied, for the first time, **MADNESS–TDSE** to obtain a **benchmark** data of laser-assisted **collisions** of H$^+$ with initially excited H($2s$), in the energy range $0.1 - 25$ keV. Our laser-free results agree well with the literature data. The laser increases the state-to-state cross-sections for the charge exchange and excitation processes by an order of magnitude.

References

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