Entanglement generation in electron molecule inelastic scattering process

Martin Mendez y Federico M. Pont
Grupo de Teoría de la Materia Condensada (GTMC). Instituto de Física Enrique Gaviola (IFEG).
Facultad de Matemática, Astronomía, Física y Computación (FAMAF). Universidad Nacional de Córdoba (UNC).
martinmendez@unc.edu.ar, pont.federico@unc.edu.ar

Motivation and Goal

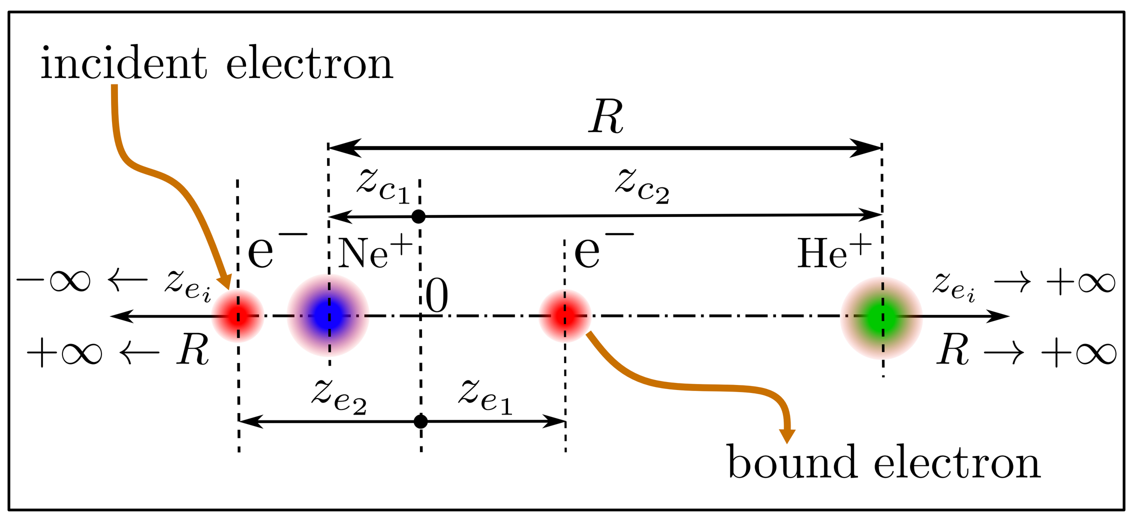
Collision processes are at the very core of many fields of physics,such as plasma physics, astrophysics, environmental science and radiation damage. On this work we discuss the generation and dynamics of entanglement during an inelastic collision (inter coulombic electron capture, ICEC) between an electron and a molecule, which may be dissociated after the collision. We computed the fully coupled electron-nuclear dynamics to describe the process.

Previous works addressed charge transfer and ionization processes using quantum information measures as witnesses of the dynamics. Here we compute quantum correlations developed during the inelastic process, quantified using several quantities such as quantum and shannon mutual information, shannon differential entropy and von Neumann entropy. We focus also on the correlations before, during and after the collision is over, and analyze the amount of the newly generated correlations that survive after the collision.

Model

3D Hamiltonian

$$\hat{H}_{\text{tot}} = \hat{T} + \hat{V}_{\text{conf}} + \hat{V}_{\text{int}}$$



$$\hat{V}_{\text{conf}} = \sum_i \frac{m_i(\omega_i)^2}{2}\left[(x_i)^2 + (y_i)^2\right]$$

Transversal harmonic Confinement

$$\hat{V}_{\text{int}} = \sum_{i,j\wedge i\neq j} \frac{q_i q_j \exp(-\alpha_{ij}|\hat{\mathbf{r}}_j - \hat{\mathbf{r}}_i|)}{|\hat{\mathbf{r}}_j - \hat{\mathbf{r}}_i|}$$

Yukawa interaction potential

Strong confinement potential and equivalent one-dimensional model

$$\Psi(\mathbf{r}_{e_1}, \mathbf{r}_{e_2}, \mathbf{r}_{c_{12}}) = \psi(z_{e_1}, z_{e_2}, z_{c_{12}}) \prod_{i=\{e_1,e_2,c_{12}\}} \chi_0^{(i)}(x_i, y_i)$$

$$\left\langle \Psi \middle| \hat{V}_{ij} \middle| \Psi \right\rangle = \iiint \prod_k dz_k \|\psi(z_{e_1}, z_{e_2}, z_{c_{12}})\|^2 V_{\text{eff}}^{(ij)}(|z_{ij}|)$$

$$\hat{H} = \sum_i \left[\frac{(\hat{\mathbf{p}}_i)^2}{2m_i} + \hbar\omega_i\right] + \sum_{i,j\wedge i\neq j} V_{\text{eff}}^{(ij)}(|z_{ij}|)$$

$$V_{\text{eff}}^{(ij)}(|z_{ij}|) = \frac{\pi^{3/2} q_i q_j}{2\left(\sqrt{2}l_c\right)} \exp\left[\left(\frac{|z_{ij}|}{\sqrt{2}l_c}\right)^2 + \left(\frac{\sqrt{2}l_c}{2l_{\alpha_{ij}}}\right)^2\right] \operatorname{erfc}\left(\frac{|z_{ij}|}{\sqrt{2}l_c} + \frac{\sqrt{2}l_c}{2l_{\alpha_{ij}}}\right)$$

Entropies

Shannon differential entropy

$$S_{z_i}^{\text{Sh}}(t) = \int \rho(z_i,t)\log_2[\rho(z_i,t)]dz_i$$

$$S_{z_i,z_j}^{\text{Sh}}(t) = \iint \rho(z_i,z_j,t)\log_2[\rho(z_i,z_j,t)]dz_i dz_j$$

von Neumann entropy

$$S_i^{\text{vN}}(t) = -\sum_{\alpha=1}^{N} \lambda_\alpha^{(i)}(t)\log_2\left(\lambda_\alpha^{(i)}(t)\right)$$

where i, j, k can be $\{e_1, e_2, c_{12}\}$ but different from each other

von Neumann conditional entropy

$$S_{\alpha_1|\alpha_2}^{\text{vN}}(t) = S_{\alpha_1,\alpha_2}^{\text{vN}}(t) - S_{\alpha_2}^{\text{vN}}(t)$$

$$S_{\alpha_1,\alpha_2|\alpha_3}^{\text{vN}}(t) = S_{\alpha_1,\alpha_2,\alpha_3}^{\text{vN}}(t) - S_{\alpha_3}^{\text{vN}}(t)$$

$$S_{e|N}^{\text{vN}}(t) = -S_{e|e}^{\text{vN}}(t) = S_e^{\text{vN}}(t) - S_N^{\text{vN}}(t)$$

$$S_{N|e}^{\text{vN}}(t) = 0$$

$$S_{e,e|N}^{\text{vN}}(t) = -S_N^{\text{vN}}(t)$$

$$S_{e,N|e}^{\text{vN}}(t) = -S_e^{\text{vN}}(t)$$

Negative values of the CEs are a sufficient (not necessary) condition for the presence of entanglement [45]. The negative value obtained in Eq. (33) indicate the presence of entanglement between electrons (both taken as one part) and the nuclei coordinate, while Eq. (34) indicate the presence of entanglement between one electron and the nuclei-electron compound. The sign of Eq. (31) is not defined *a priori*; however, we will show that for the system and processes considered here, $S_e^{\text{vN}}(t) > S_N^{\text{vN}}(t)$ for all t (see Figs. 4–6), and thus the entanglement between electrons is confirmed $[S_{e|e}^{\text{vN}}(t) < 0]$.

Mutual informations

The QMI measures correlations (quantum and classical) between subsystems. It is non-negative (due to sub-additivity of VNE). QMI exceeds the bound of classical MI, because quantum systems can be supercorrelated.

The SMIs represent the degree of correlations between two continuos particle densities. It quantifies the interdependence between two particles, providing insight into how much information one conveys about the other. It can be interpreted as a measure of deviations from a Hartree reference state.

$$I_{e,e}^{\text{vN}}(t) : I_{e,e|N}^{\text{vN}}(t) = 2S_{e|N}^{\text{vN}}(t) - S_{e,e|N}^{\text{vN}}(t) = 2S_e^{\text{vN}}(t) - S_N^{\text{vN}}(t)$$

$$I_{e,N}^{\text{vN}}(t) : I_{e,N|e}^{\text{vN}}(t) = S_{e|e}^{\text{vN}}(t) + S_{N|e}^{\text{vN}}(t) - S_{e,N|e}^{\text{vN}}(t) = S_N^{\text{vN}}(t)$$

$$I_{e,e}^{\text{Sh}}(t) = 2S_e^{\text{Sh}}(t) - S_{e,e}^{\text{Sh}}(t)$$

$$I_{e,N}^{\text{Sh}}(t) = S_e^{\text{Sh}}(t) + S_N^{\text{Sh}}(t) - S_{e,N}^{\text{Sh}}(t)$$

Methods

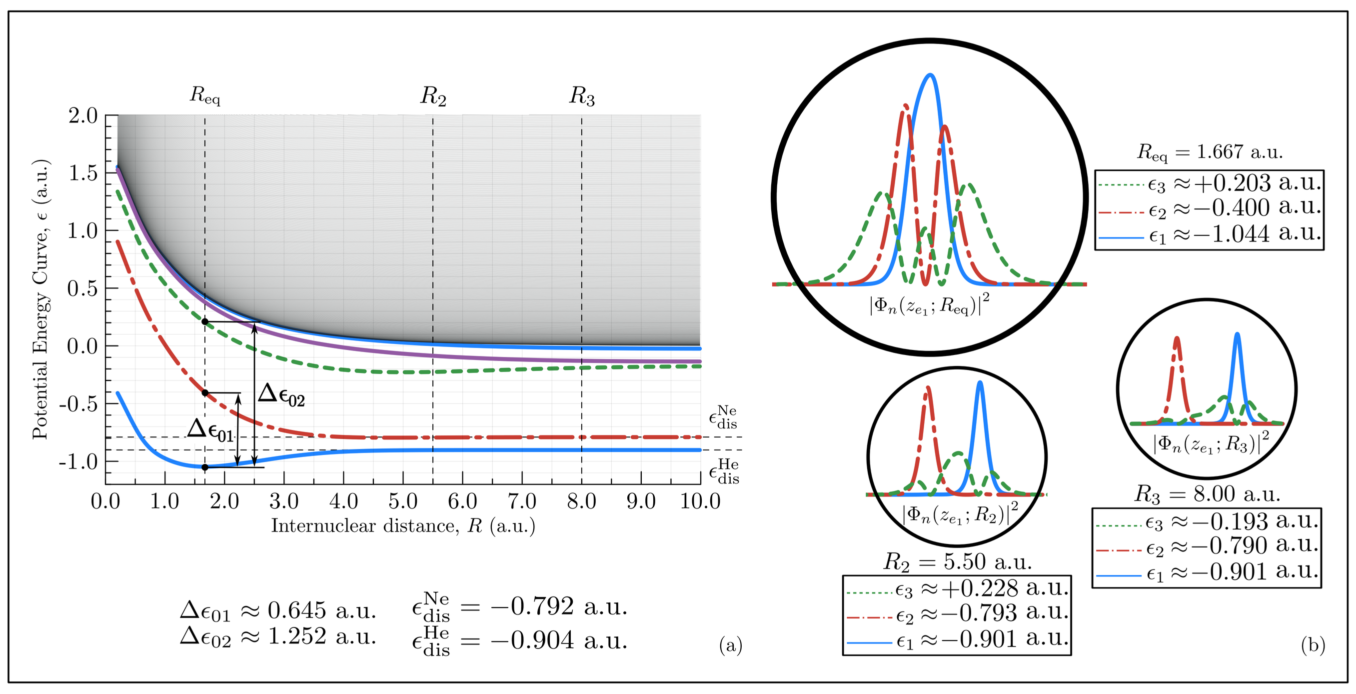
PECs calculation

$$\hat{H}_{\text{NeHe}^+}(R)\Phi_n(z_{e_1};R) = \epsilon_n(R)\Phi_n(z_{e_1};R)$$

$$\hat{W}_{\pm}^{(z_i)} = i\eta(z_i \mp z_{i\text{CAP}})^2\Theta(z_i \mp z_{i\text{CAP}}) \text{ CAPs}$$

Symmetrized electronic spatial wave function

$$\psi_{\text{symm}}^{\text{init}} = \frac{1}{\sqrt{2}}[\phi_i(z_{e_1})\Phi_0(z_{e_2};R) + \phi_i(z_{e_2})\Phi_0(z_{e_1};R)]$$



Probability density

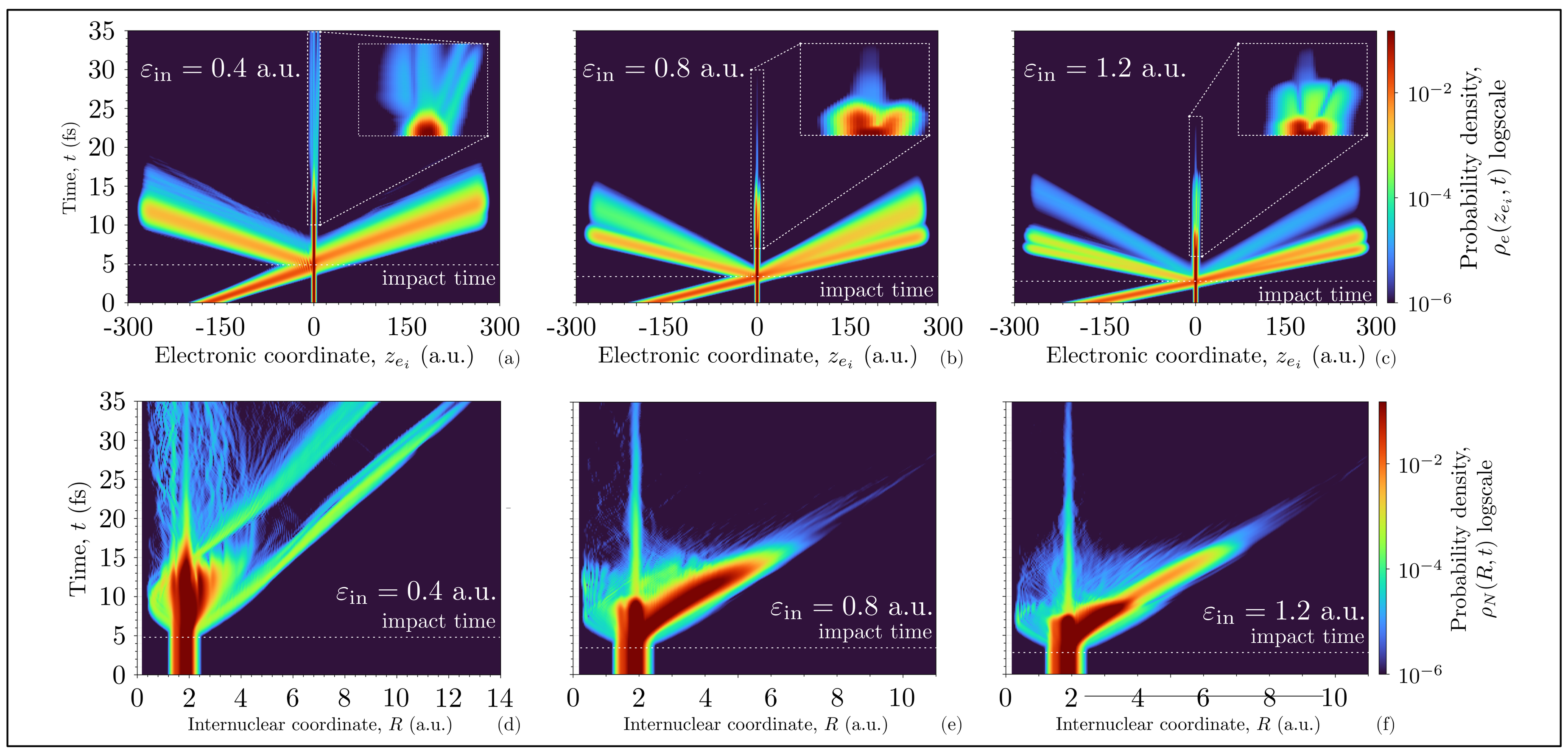
$$\rho(z_i,z_j,t) = \int |\psi(z_{e_1},z_{e_2},z_{c_{12}},t)|^2 dz_k$$

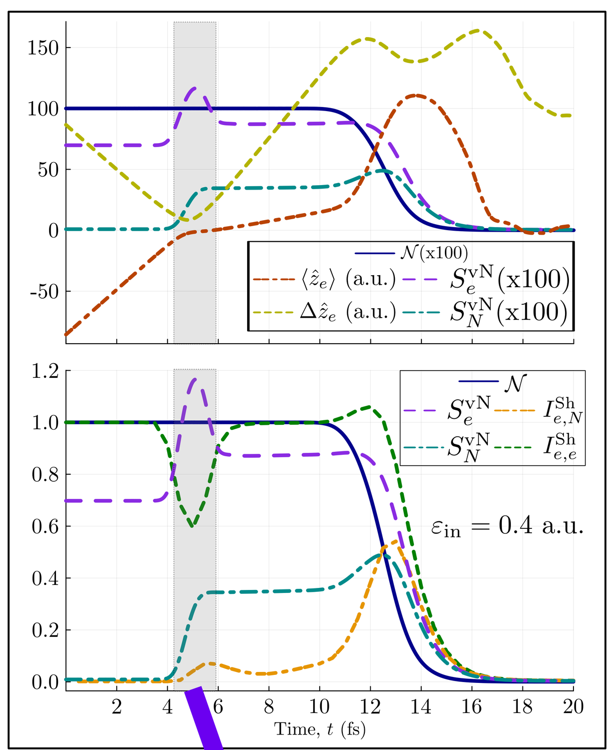
$$\rho(z_i,t) = \iint |\psi(z_{e_1},z_{e_2},z_{c_{12}},t)|^2 dz_j dz_k$$

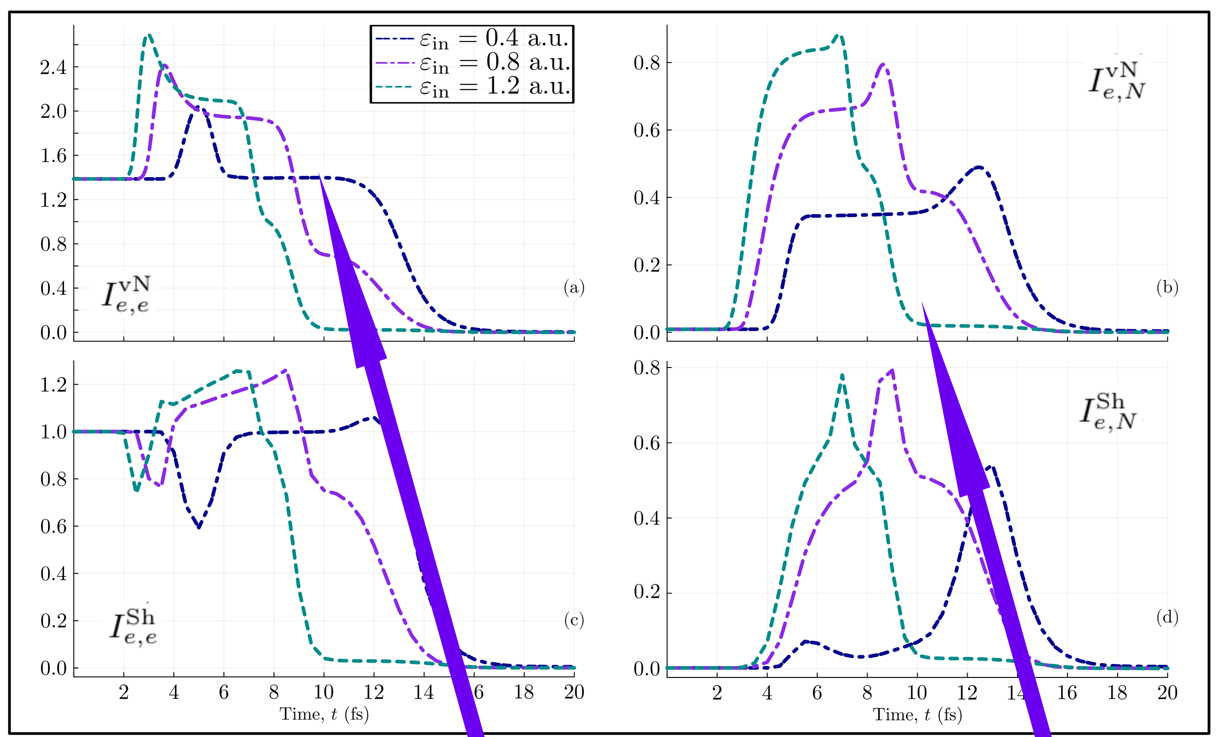
Density operator

$$\hat{\rho}_i(t) = \text{Tr}_{j,k}(\hat{\rho}(t))$$

$$\hat{\rho}_i(t)\left|\lambda_\alpha^{(i)}(t)\right\rangle = \lambda_\alpha^{(i)}(t)\left|\lambda_\alpha^{(i)}(t)\right\rangle$$



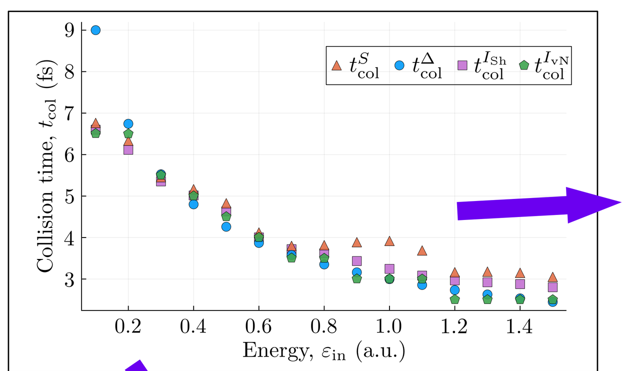




No extra conditional information between electrons after collision without inelastic scattering

Correlations between electron and nuclei are build up in every collision, even without inelastic scattering

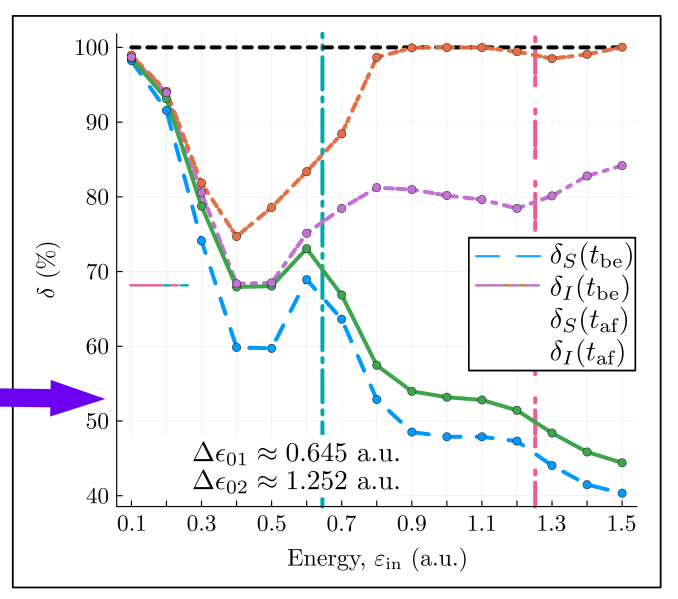
Time of collision



Time of collision is taken as the maximum of the conditional information

$$\delta_S(t) = \frac{S_e^{\text{vN}}(t)}{S_e^{\text{vN}}(t_{\text{col}})}.$$

Entanglement relative to the maximum generated



Conclusions

The correlations and entanglement dynamics were studied and matched to the different stages of an electron-molecule collision process named ICEC. The processes includes capture and emission of an electron and may dissociate the molecule. The time of collision is defined from maximal values of entanglement measures. Amount of entanglement retained after the collision is over is measured. Entanglement and correlations between electrons (incoming and bound) are sustained only if inelastic collisions are present. However, the corr. between electron and nuclei build up in all cases even for elastic scatt. (vibrational).

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