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Consistent Coupled Mean-Field Description of Electron Removal Processes in He^+-Ne and He^+-Ar Collisions

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Introduction

- Objective: ion-atom collisions with active target *and* projectile electrons
- Idea: combine mean-field calculations for both types of electrons
- Crucial point: account for non-orthogonality of propagated orbitals

Theory

Mean-field description of the many-electron problem

- Target electrons

$$i\partial_t\psi_i^T(\boldsymbol{r},t) = \hat{h}_T(t)\psi_i^T(\boldsymbol{r},t) \quad i=1,\dots,N_T$$
$$\hat{h}_T(t) = -\frac{1}{2}\Delta + \left(-\frac{Q_T}{r_T} + v_{ee}^T(r_T,t)\right) + \left(-\frac{Q_P}{r_P} + v_H^P(r_P)\right)$$
$$v_{ee}^T(r_T,t) = \left(1 - -\frac{P_{\rm net}^{\rm loss}(t) + P_0^{\rm loss}(t) - 1}{N_T - 1}\right) v_{ee}^{T,0}(r_T).$$

$v_{ee}^{T,0}(r_T)$: Accurate atomic ground-state Hartree plus exchange potential obtained from the optimized potential method (OPM) [1]
$v_H^P(r_P)$: electrostatic potential of a H-like $1s$ orbitals
$P_{\rm net}^{\rm loss}, P_0^{\rm loss}$: probabilities for net-electron and zero-electron removal from the target $\rightarrow$ time-dependent term accounts for the increasing attraction of the target potential as electrons are removed *during* the collision (target response)

- Projectile electron

$$i\partial_t\psi_i^P(\boldsymbol{r},t) = \hat{h}_P(t)\psi_i^P(\boldsymbol{r},t) \quad i\equiv N_P = 1$$
$$\hat{h}_P(t) = -\frac{1}{2}\Delta + -\frac{Q_P}{r_P} + \left(-\frac{Q_T}{r_T} + v_H^T(r_T)\right).$$

$v_H^T(r_T)$: Accurate ground-state Hartree potential of the target atom obtained from the optimized potential method (OPM) [1]

- Problem: use of different Hamiltonians $\hat{h}_T, \hat{h}_P$ leads to non-orthogonal propagated target and projectile orbitals!

Solution of the single-particle equations

The Basis Generator Method (**BGM**) [2]:
expansion of the orbitals $\psi_i^T(\boldsymbol{r},t)$ and $\psi_i^P(\boldsymbol{r},t)$ in *dynamically adapted* basis sets

$$\psi_i^{T(P)}(\boldsymbol{r},t) = \sum_{\mu=0}^{M_{T(P)}}\sum_{v=1}^{V_{T(P)}} c_{\mu v}^{i,T(P)}(t)\chi_v^{\mu,T(P)}(\boldsymbol{r},t)$$
$$\chi_v^{\mu,T(P)}(\boldsymbol{r},t) = [W_{P(T)}(r_{P(T)})]^\mu\varphi_v^{T(P)}(\boldsymbol{r}) \qquad \mu=0,\dots,M_{T(P)}$$
$$W_{P(T)}(r_{P(T)}) = \frac{1}{r_{P(T)}}(1-\exp(-r_{P(T)}))$$

- $\varphi_v^{T(P)}(\boldsymbol{r})$: eigenfunctions of the undisturbed target (projectile) Hamiltonian $(1s\cdots 4f)$ $\rightarrow$ account for single-particle elastic and excitation channels
- $\{\chi_v^{\mu,T(P)}(\boldsymbol{r},t), \mu=1\cdots 8\}$: pseudostates $\rightarrow$ account for single-particle rearrangement channels (transfer to the other center and ionization)

Analysis of the single-particle solutions

- Calculate overlap integrals $S_{ij}(t_f) = \langle\psi_i(t_f)|\psi_j(t_f)\rangle$ at final time $t=t_f$
- Construct normalized N-electron wave function

$$\Psi(x_1,\dots,x_N;t_f) = \frac{\det(\phi_1(x_1,t_f),\dots,\phi_N(x_N,t_f))}{\sqrt{N!\det(S_{11}(t_f),\dots,S_{NN}(t_f))}}$$

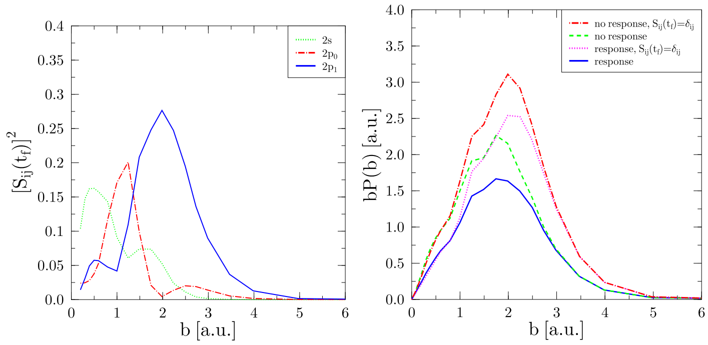
- One-particle density

$$n(\mathbf{r},t_f) = N\sum_{s_1,\dots s_N}\int|\Psi(\mathbf{r},s_1,x_2,\dots x_N;t_f)|^2 d^3r_2,\dots d^3r_N$$
$$= \sum_{i,j=1}^{N} S_{ij}^{-1}(t_f)\psi_j^*(\mathbf{r},t_f)\psi_i(\mathbf{r},t_f)$$

- Average electron numbers ('net probabilities') are calculated in channel representation instead of performing integrals over n in configuration space

$$P_{\rm net}^{T,P} = \sum_{i,j=1}^{N}\sum_{k=1}^{K_T,K_P} c_k^{i(T,P)} S_{ij}^{-1} c_k^{j*(T,P)}\Big|_{t=t_f}$$
$$c_k^{i(T,P)} = \langle\varphi_k^{(T,P)}|\psi_i\rangle\big|_{t=t_f}$$
$$P_{\rm net}^{\rm rec} = N_T - P_{\rm net}^T$$
$$P_{\rm net}^{\rm free} = N - P_{\rm net}^T - P_{\rm net}^P$$

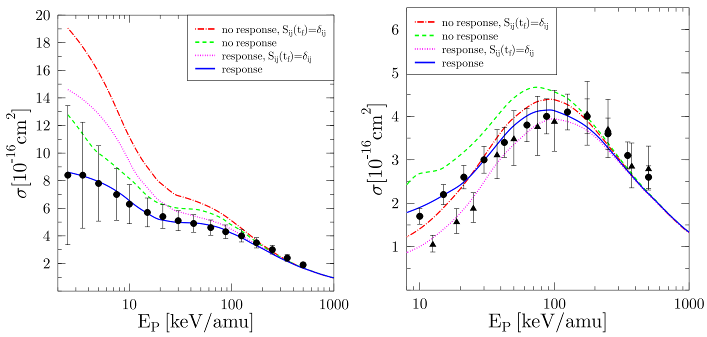
Results



(a) Overlaps $|S_{ij}(t_f)|^2$ of propagated target ($2s, 2p0, 2p_1$) and projectile ($1s$) states (target response model)

(b) Impact-parameter-weighted net electron loss probabilities

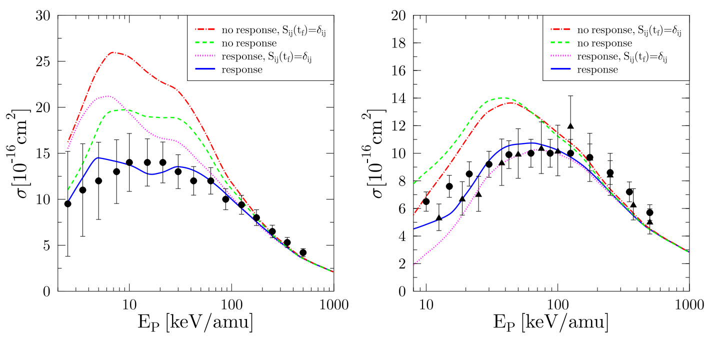
Figure 1: Impact-parameter dependent quantities for He^+-Ne collisions at $E_P = 10$ keV/amu



(a) Net recoil ion production

(b) Net free electron production

Figure 2: Total cross sections for net recoil ion and net free electron production as functions of impact energy for He^+-Ne collisions. Lines: present theoretical results; lines labeled $S_{ij}(t_f) = \delta_{ij}$: previous results from Ref. [3]. Symbols: experimental data from Ref. [4] (circles) and Ref. [5] (triangles)



(a) Net recoil ion production

(b) Net free electron production

Figure 3: Total cross sections for net recoil ion and net free electron production as a function of impact energy for He^+-Ar collisions. Lines: present theoretical results. Symbols: experimental data from Ref. [4] (circles) and Ref. [5] (triangles)

References

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