New classical CTMC approaches to $A^{q+} + \text{He}$ processes

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Abstract. Any small perturbations in the classical stable Helium atom may produce unphysical autoionization that prevents its classical dynamical study. Previous attempts have required barrier potentials to limit the electron energy. As a first approach we consider two sets of $N$ classical electron trajectories, whose evolution obey the Hamilton equations in the full Hamiltonian. Each classical electron of one set feels the average repulsion due to the classical electrons of the other set. Smoothing of the evaluation of the classical electronic repulsion is proposed assuming that each electron can be described by Gaussian functions centred on the position of the corresponding electrons.

1. Introduction

Previous attempts to describe classically (CTMC) two electron systems [1, 2, 3] have required new potential energy terms that depend on both space and momentum coordinates.

To minimize the non central components of repulsive forces that appear just before the onset of unphysical autoionization, we included two sets of $N$ classical electrons that simulate the corresponding quantal electronic densities, averaging repulsive forces that act over each electronic trajectory. We have also implemented time dependent model potentials in target and projectile centers in a different approach. Both methods are highlighted here.

2. Averaged Collective Repulsion approach (ACR)

We use two coupled sets of $N$ classical electron trajectories which evolve collectively because of the repulsion term according to the Hamilton equations [4], under the Hamiltonian:

$$H_i = \frac{p_i^2}{2m} - \frac{Z_T}{r_i^T} - \frac{Z_P}{r_i^P} + \frac{1}{N} \sum_{j}^{N} \frac{1}{|r_i - r_j|}$$

for each trajectory $i$ of one set with $j$ running over all trajectories of the other set and where $T$ and $P$ refers to target and projectile.

2.1. Gaussian kernel approximation

Evaluation of the repulsion potential is performed between electrons described by Gaussian functions centered on the positions of the corresponding classical trajectories at each time in a
kernel representation \[5\]. For example, the repulsive potential felt by the electron \(i\) of the set 1 due to the whole set of electrons 2 is:

\[
V_{i1}^{\text{rep}}(r_{i1}) = \frac{1}{(2\pi)^3 3^2 \sigma^3 N} \sum_{j2} \int d\mathbf{r} \, e^{-\frac{(\mathbf{r}-\mathbf{r}_{j2(1)})^2}{2\sigma^2}} \frac{1}{|r_{i1} - r|}
\]

(2)

where \(r_{i1}\) and \(r_{j2}\) are the positions of the electronic trajectories and \(\sigma\) is the smoothing parameter.

2.2. Dynamics

We have tested the stability of the He atom against small electrostatic perturbations obtaining stability with respect to autoionization.

To carry out a collision, we first generate a microcanonical distribution with an effective charge. Then an electrostatic model potential generated by the previous microcanonical distribution is obtained and finally, spacial and momentum coordinates of the classical trajectories that define the actual initial distribution are generated using the tranformation given by C.O. Reinhold and C.A. Falcon (1986) \[6\] under the generated model potential.

![Figure 1. Representation of the target distance (module) of a collision at impact parameter \(b = 2\text{a.u.}\) and velocity \(v = 1\text{a.u.}\) with two sets of \(N=250\) and a smoothing parameter \(\sigma = 0.28\).](image)

At the end of the collision, a number of trajectories will be captured by the projectile, a different number will remain in the target and the rest will be ionized as can be seen in figure 1. As each electron of the first set is correlated to each electron of the second set and vice versa, an \(N^2\) statistics is performed to obtain the probabilities for each process.

3. Dynamic Screening

In an alternative way we have modified and extended to the projectile the dynamic screening model developed by V. J. Montemayor and G. Schiwietz (1989) \[3\] which consisted of independent pairs of trajectories evolving on time dependent central model potentials with magnitudes that depend on the bond energy of the other electron in each pair according to:

\[
H = H_0 + V_{ee,1}^A(\mathbf{r}_1, E_{0,2}) + V_{ee,2}^A(\mathbf{r}_2, E_{0,1}) + V_{ee,1}^B(\mathbf{r}_1, E_{0,2}) + V_{ee,2}^B(\mathbf{r}_2, E_{0,1})
\]

(3)

where \(H_0\) is the sum of the monoelectronic Hamiltonians and \(V_{ee,i}^{(A,B)}\) are time-dependent model potentials of the form, for \(i \neq j\):

\[
V_{ee,i} = N_c(E_{0,j}) \frac{1 - (1 + \alpha r_i) e^{-2\alpha r_i}}{r_i}
\]

(4a)

\[
N_c(E_{0,j}) = \begin{cases} 
0 & \text{for } E_{0,j} \geq 0 \\
 g(\mu)^2 & \text{for } I_{1s^2} < E_{0,j} < 0 \\
1 & \text{for } E_{0,j} < I_{1s^2}
\end{cases}
\]

(4b)
\[ g(\mu) = \frac{1.25^{1.25/2}}{(\mu^2 + 1.25 - 1)^{1.25/2}} \]  
\[ \mu(E) = \frac{|-E|}{|E_{lim}|} + \frac{1}{2} - \frac{|-E|}{|E_{lim}|} - \frac{1}{2} \]  
\[ E_{0,j} = -\frac{Z}{r_j} + \frac{p_j^2}{2}(+V_{ee,j}) \]  

\( I_{ls^2} \) is the ionization potential. \( E_{lim} \) is a constant that refers to the point where the model potential drops smoothly. Here we use \( N_c \) as the time-dependent screening parameter varying between 1 and 0, unlike [3] where this variation was included in the parameter \( \alpha \). Collisions were carried out using a microcanonical distribution in a model potential initial conditions [6].

4. Results and Conclusions

Our ACR results for the collisions He(1s^2)+H^+ are illustrated in figures 2 for single capture and ionization, and in figures 3 for double processes compared with previous theoretical and experimental results. Our calculations fairly agree with experimental values of single capture with a good convergence at high energies, and only slightly underestimate those of single ionization in figure 2b, although they present the correct shape as also happens with the results from independent pairs of electronic trajectories using a gaussian kernel approximation for the repulsion. Double process results (figure 3) overestimate the experimental data but improve the previous Heisemberg Core CTMC calculations [11]. Dynamic screening results for single ionization and double processes are above the experimental ones except for single capture. To understand this behaviour a further study is required.

We have developed a new method using an average of repulsion terms between the two set of electrons that represent the quantum electronic cloud of Helium atom. A Gaussian kernel
approximation has been employed to eliminate unphysical ionization. We have also extended the dynamic screening method to the projectile modifying the time dependent parameter. We have obtained good results for single processes while double processes overestimate experimental data with both methods. Further work on the optimization of the time-dependent model parameters and new calculations employing larger statistics must be performed.

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