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Double Charge Transfer in Alpha Particle Collisions with He Atoms

M. S. PINDZOLA

Department of Physics, Auburn University, Auburn, AL, USA

ABSTRACT: A time-dependent lattice method is used to calculate the double charge transfer cross section in alpha particle collisions with He atoms at 100.0 keV/amu. The large scale calculations on a small 6D lattice yields a double charge transfer cross section twice as large as experimental measurements.

1. INTRODUCTION

A time-dependent lattice (TDL) method was originally developed to study excitation, ionization, and charge transfer in proton collisions with H atoms [1, 2]. The TDL method was then extended to investigate excitation and charge transfer in proton collisions with laser excited Li atoms [3, 4]. The TDL method was also applied to study charge transfer in proton collisions with He atoms [5] and alpha particle collisions with H atoms[6]. Recently the TDL method was applied to calculate single charge transfer in C^{6+} collisions with H and He atoms [7] in support of astrophysical interest in ion-atom interactions present in the solar wind.

In this paper we extend the one-active electron TDL method to handle two-active electrons by moving from 3 dimensions to 6 dimensions. A basic two-active electron ion-atom system is found in alpha particle collisions with He atoms. Recent molecular orbital close-coupling calculations for single and double charge transfer in slow alpha particle collisions with He[8] provides a summary of all experimental and theoretical studies for this system. Our first large scale calculations for double charge transfer in alpha particle collisions with He atoms involves a fast alpha particle with the two electrons represented on a fairly small 6 dimensional lattice.

The rest of the paper is organized as follows: in section 2 we review the time-dependent lattice method, in section 3 we calculate the double charge transfer cross section in alpha particle collisions with He atoms and compare with experimental measurements, while in section 4 we conclude with a brief summary. Unless otherwise stated, we will use atomic units.

2. THEORY

For charge transfer in bare ion collisions with two-active electron atoms, the time- dependent Schrodinger equation in the frame of reference of the projectile is given by:

$$i\,\frac{\partial P(x_1,y_1,z_1,x_2,y_2,z_2)}{\partial t} = \sum_{i=1}^{2}\left(T(\vec{r_i})\right)P(x_1,y_1,z_1,x_2,y_2,z_2,t)$$

$$+\sum_{i=1}^{2}\left(U(\vec{r_i})\right)P(x_1,y_1,z_1,x_2,y_2,z_2,t)$$

$$+V(\vec{r_i},\vec{r_2})P(x_1,y_1,z_1,x_2,y_2,z_2,t)$$

$$+\sum_{i=1}^{2}\left(W(\vec{r_i},t)\right)P(x_1,y_1,z_1,x_2,y_2,z_2,t). \tag{1}$$

The electron kinetic energy operator is given by:

$$T(\vec{r_i}) = -\frac{1}{2}\left(\frac{\partial^2}{\delta x_i^2}+\frac{\partial^2}{\delta y_i^2}+\frac{\partial^2}{\delta z_i^2}\right) \tag{2}$$

The electron-electron interaction operator is given by:

$$V(\vec{r_1},\vec{r_2}) = \frac{1}{\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}} \tag{3}$$

For the stationary alpha particle:

$$U(\vec{r_i}) = \frac{-2}{\sqrt{x_i^2+y_i^2+z_1^2}}. \tag{4}$$

For the moving Heatom:

$$W(\vec{r_i},t) = \frac{-2}{R_i(t)}\,, \tag{5}$$

where for straight line trajectories:

$$R_i(t) = \sqrt{(x_i-b)^2+\left(y_i-(y_{io}+vt)\right)^2+z_i^2}\,, \tag{6}$$

b is an impact parameter, $y_{i0}<0$ is a starting position, and v is the projectile speed.

The ground state for double capture to the alpha particle is obtained by relaxation in imaginary time (τ=it) of the equation given by:

$$-\frac{\partial P(x_1,y_1,z_1,x_2,y_2,z_2,\tau)}{\partial \tau} = \sum_{i=1}^{2}\left(T(\vec{r_i})\right)P(x_1,y_1,z_1,x_2,y_2,z_2,\tau)$$

$$+\sum_{i=1}^{2}\left(U(\vec{r_i})\right)P(x_1,y_1,z_1,x_2,y_2,z_2,\tau) \tag{7}$$

$$+V(\vec{r_i},\vec{r_2})P(x_1,y_1,z_1,x_2,y_2,z_2,\tau).$$

The ground state for the moving He atom is obtained by relaxation in imaginary time of the equation given by:

$$-\frac{\partial P(x_1,y_1,z_1,x_2,y_2,z_2\tau)}{\partial\tau}=\sum_{i=1}^{2}\left(T(\vec{r_i})\right)P(x_1,y_1,z_1,x_2,y_2,z_2,\tau)$$

$$+\sum_{i=1}^{2}\left(W(\vec{r_i},t=0)\right)P(x_1,y_1,z_1,x_2,y_2,z_2,\tau) \qquad (8)$$

$$+V(\vec{r_i},\vec{r_2})P(x_1,y_1,z_1,x_2,y_2,z_2,\tau)\ .$$

In both cases the initial state, $P(x_1, y_1, z_1, x_2, y_2, z_2, \tau=0)$, is set equal to the product of two analytic Hydrogenic ground states, while the final state, $P_{grnd}(x_1, y_1, z_1, x_2, y_2, z_2)$, is given by:

$$P_{grnd}(x_1, y_1, z_1, x_2, y_2, z_2)=P(x_1, y_1, z_1, x_1, y_2, z_2, \tau\rightarrow\infty). \qquad 9$$

The initial condition for the solution of the time-dependent equation in real time (Eq. (1)) is given by:

$$P(x_1, y_1, z_1, x_2, y_2, z_2, t=0)=P_{grnd}(x_1, y_1, z_1, x_2, y_2, z_2), \qquad (10)$$

where $P_{grnd}(x_1, y_1, z_1, x_2, y_2, z_2)$ is the ground state of the moving He atom. Asymptotic wavefunctions, $P(x_1, y_1, z_1, x_2, y_2, z_2, t\rightarrow\infty)$, are obtained by time propagating Eq. (1) until the projectile has moved well past the target. The probability of double capture is given by:

$$C_{grnd}(\text{v,b}) = \left|\int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}dy_1\int_{0}^{\infty}dz_1\int_{-\infty}^{\infty}dx_2\int_{-\infty}^{\infty}dy_2\int_{0}^{\infty}dz_2\times P_{grnd}^{*}(x_1,y_1,z_1,x_2,y_2,z_2)\times P(x_1,y_1,z_1,x_2,y_2,z_2,t\rightarrow\infty)\ \right|^2, \qquad (11)$$

where $P_{grnd}(x_1, y_1, z_1, x_2, y_2, z_2)$ is the ground state for double capture to the alpha particle. We note that the collision Hamiltonian has reflection symmetry with respect to the $z_1 = z_2 = 0$ plane. The double capture cross section for a specific velocity is given by:

$$\sigma_{double}=2\,\pi\,\sum_m\int_0^{\infty}C_{grnd}(v,b)bdb \qquad (12)$$

3. RESULTS

The double charge transfer cross section for alpha particle collisions with He atoms at an incident energy of 100.0 keV/amu is calculated using the TDL method. A lattice of 72×144×36×72×144×36 points is used with a uniform grid spacing of $\Delta x_1= \Delta y_1 =\Delta z_1 =\Delta x_2=\Delta y_2 =\Delta z_2 =0.20$. Thus the lattice extends from -7.2 to+7.2 in the x_i directions, from -14.4 to +14.4 in the y_i directions, and from 0.0 to + 3.6 in the z_i directions. The lattice is partitioned over 46, 656 cores on a massively parallel supercomputer.

Relaxation of the lattice using Eq.(7) or Eq. (8) yields the He ground state with an energy of -76.0 eV. A time spacing of $\Delta t = 0.01$ and 200 time steps is used to obtain the He ground state at the initial position of the projectile and at the position of the alpha particle. Relaxation on a larger lattice with a finer grid spacing would bring the energy into closer agreement with the experimental energy of -79.0 eV.

Propagation on the lattice using Eq. (1) begins at $y_1 = y_2 = -7.2$ with a velocity of v = 2.0 corresponding to an incident energy of 100.0 keV/amu. A time spacing of $\Delta t = 0.005$ and 2880 time steps moves the He atom projectile across the lattice to a position of $y_i = +21.6$, beyond the boundary at $y_i = +14.4$.

TDL calculations for alpha particle collisions with He atoms are carried out using 8 impact parameters ranging from b = 0.0 to b = 2.0 and at an incident velocity of v = 2.0 corresponding to a projectile energy of 100.0 keV/amu. The probabilities for double capture to the ground state of He obtained using Eq. (11) are presented in Table 1. The double capture cross section obtained using Eq. (12) is found to be 27 Mb, which is twice as large as the experimental measurement of 13.5Mb [9].

Table 1
Alpha particle + He collisions at a projectile energy of 100 keV/amu (v = 2.0)

Impact Parameter b	*Double Capture Probability $C_{grnd}(v, b)$*
0.0	0.3350
0.2	0.2700
0.4	0.1560
0.6	0.0818
0.8	0.0434
1.0	0.0229
1.4	0.0052
2.0	0.0003

4. SUMMARY

A time-dependent lattice method has been used to calculate the double charge transfer cross section in alpha particle collisions with He atoms at 100.0 keV/amu. The large scale calculations on a small 6 dimensional lattice yields a double charge transfer cross section twice as large as experimental measurements.

With the development of larger and faster massively parallel supercomputers, we plan to extend the 6 dimensional lattice to more points and thus larger distances over which the projectile and target can interact. Future calculations will check cross section convergence at high projectile energies and will allow studies to proceed to lower projectile energies where the double capture cross sections are an order of magnitude larger.

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