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Single and Double Charge Transfer in Flatland

M. S. PINDZOLA AND T. G. LEE

Department of Physics, Auburn University, Auburn, AL 36849

ABSTRACT: The time-dependent Schrodinger equation is solved in a two dimensional flatland space for the single charge transfer to the ground state for both p + H and α + H collisions at an incident energy of 10 keV/amu. The total ground state single capture probability is found to be almost 1500 times larger for the p + H collision. The time-dependent Schrodinger equation is also solved in a four dimensional flatland space for the double charge transfer to the ground state for both α + He and Li^{3+} + He collisions at an incident energy of 50 keV/amu. The total ground state double capture probability is found to be almost 15 times larger for the α + He collision.

1. INTRODUCTION

Charge transfer in p + H collisions by direct solution of the time-dependent Schrodinger equation was first studied in a two dimensional Cartesian flatland [1]. With the development of parallel supercomputers, charge transfer in bare ion collisions with one active electron atoms and ions by direct solution of the time-dependent Schrodinger equation was subsequently studied in a full three dimensional Cartesian space. Calculations have been made for p + H [2–4], α + H [5], Be^{4+} + H [6], p + He^{+} [7], α + Li^{2+} [7], and p + Li [8, 9] collisions.

Double charge transfer in bare ion collisions with two active electron atoms and ions by direct solution of the time-dependent Schrodinger equation has yet to be studied in either a four dimensional Cartesian flatland space or the full six dimensional Cartesian space. Only a study of the single ionization in $\bar{p}$ + He collisions has used a four dimensional Cartesian flatland space to solve the time-dependent Schrodinger equation to better understand ejected electron correlation effects [10].

In this paper the time-dependent Schrodinger equation is solved in a two dimensional flatland space for the single charge transfer to the ground state for both p + H and α + H collisions. The time-dependent Schrodinger equation is also solved in a four dimensional flatland space for the double charge transfer to the ground state for both α + He and Li^{3+} + He collisions. Details of the numerical methods are presented in Section II, single and double charge transfer results are presented in Section III, and a brief summary of future plans is given in Section IV. Unless otherwise stated, all quantities are given in atomic units.

2. THEORY

2.1. Two Dimensional Flatland

The time-dependent Schrodinger equation for a bare ion projectile colliding with a H atom is given by:

$$i\frac{\partial \Psi(\vec{r},t)}{\partial t} = \left(-\frac{1}{2}\nabla^2 - \frac{Z_t}{|\vec{r}\,|} - \frac{Z_p}{|\vec{r}-\vec{R}(t)|} \right) \Psi(\vec{r},t), \tag{1}$$

where Z_t = 1, Z_p is the projectile charge, and $\vec{R}(t)$ is the time-dependent projectile ion position vector. As a first approximation we consider a two dimensional (2D) Cartesian flatland space in which the time-dependent equation is given by:

$$i\frac{\partial P(x,y,t)}{\partial t}=T(x,y)P(x,y,t)+V(x,y,t)P(x,y,t), \tag{2}$$

where

$$T(x,y)=-\frac{1}{2}\frac{\partial^2}{\partial x^2}-\frac{1}{2}\frac{\partial^2}{\partial y^2}-\frac{Z_t}{\sqrt{c_t+x^2+y^2}} \tag{3}$$

and

$$V(x,y,t)=-\frac{Z_p}{\sqrt{c_p+(x-b)^2+\left(y-(y_s+vt)\right)^2}}. \tag{4}$$

The projectile follows a straight-line trajectory given by:

$$\vec{R}(t)=b\hat{i}+(y_s+vt)\hat{j}, \tag{5}$$

where b is the impact parameter, $y_s < 0$ is the starting position, and v is the projectile velocity. The coefficients c_t and c_p in Eqs. (3)-(4) are used to soften the singularity of the potentials and allow the energy of the 2D flatland atoms to resemble full 3D atoms.

The ground state of any H-like atom may be obtained by relaxation of the time-dependent Schrodinger equation in imaginary time (τ). In 2D Cartesian flatland space the time-dependent equation is given by:

$$-\frac{\partial \bar{P}(x,y,\tau)}{\partial \tau}=\bar{T}(x,y)\bar{P}(x,y,\tau), \tag{6}$$

where

$$\bar{T}(x,y)=-\frac{1}{2}\frac{\partial^2}{\partial x^2}-\frac{1}{2}\frac{\partial^2}{\partial y^2}-\frac{Z}{\sqrt{\bar{c}+(x-x_o)^2+(y-y_o)^2}} \tag{7}$$

and (x_0, y_0) is the position of a H-like atom with nuclear charge Z. For calculations of single charge transfer the projectile frame of reference is used. The target H atom ground state wavefunction, $\bar{P}^{H}_{target}(x,y)$, is found by relaxation of Eqs.(6)-(7) with $Z = Z_t = 1$, $\bar{c} = c_t$, $x_0 = b$, and $y_0 = y_s$ for each projectile trajectory. To obtain single charge transfer cross sections the projectile H-like atom ground state wavefunction, $\bar{P}^{H-like}_{projectile}(x,y)$, is found by relaxation of Eqs.(6)-(7) with $Z = Z_p$, $\bar{c} = c_p$, $x_0 = 0$, and $y_0 = 0$.

With the initial condition:

$$P(x,y,t=0)=\bar{P}^{H}_{target}(x,y), \tag{8}$$

the time-dependent Schrodinger equation is propagated forward in real time (t) using Eqs. (2)-(4). The ground state single capture scattering probability for a given projectile velocity and impact parameter is given by:

$$S(v,b)=\left|\int dx\int dy\bar{P}^{*H-like}_{projectile}(x,y)P(x,y,t\to\infty)\right|^2. \tag{9}$$

The single capture cross section for a given projectile velocity is given by:

$$\sigma(v) = 2\int S(v,b)\,db, \tag{10}$$

and has the dimensions of length.

2.2. Four Dimensional Flatland

The time-dependent Schrodinger equation for a bare ion projectile colliding with a He atom is given by:

$$i\frac{\partial \Psi(\vec{r}_1,\vec{r}_2,t)}{\partial t} = \sum_{i=1}^{2}\left(-\frac{1}{2}\nabla^2 - \frac{Z_t}{|\vec{r}_i|}\right)\Psi(\vec{r}_1,\vec{r}_2,t) + \frac{1}{|\vec{r}_1-\vec{r}_2|}\Psi(\vec{r}_1,\vec{r}_2,t) - \sum_{i=1}^{2}\left(\frac{Z_p}{|\vec{r}_i-\vec{R}(t)|}\right)\Psi(\vec{r}_1,\vec{r}_2,t), \tag{11}$$

where $Z_t = 2$, Z_p is the projectile charge, and $\vec{R}(t)$ is the time-dependent projectile ion position vector. As a first approximation we consider a four dimensional (4D) Cartesian flatland space in which the time-dependent equation is given by:

$$i\frac{\partial P(x_1,y_1,x_2,y_2,t)}{\partial t} = \sum_{i=1}^{2} T_i(x_i,y_i)\,P(x_1,y_1,x_2,y_2,t) + U(x_1,y_1,x_2,y_2)\,P(x_1,y_1,x_2,y_2,t), \\ +\sum_{i=1}^{2} V_i(x_i,y_i,t)\,P(x_1,y_1,x_2,y_2,t) \tag{12}$$

where

$$T_i(x_i,y_i) = -\frac{1}{2}\frac{\partial^2}{\partial x_i^2} - \frac{1}{2}\frac{\partial^2}{\partial y_i^2} - \frac{Z_t}{\sqrt{c_t + x_i^2 + y_i^2}}, \tag{13}$$

$$T_i(x_i,y_i) = -\frac{1}{2}\frac{\partial^2}{\partial x_i^2} - \frac{1}{2}\frac{\partial^2}{\partial y_i^2} - \frac{Z_t}{\sqrt{c_t + x_i^2 + y_i^2}}, \tag{14}$$

and

$$V_i(x_i,y_i,y) = -\frac{Z_p}{\sqrt{c_u + (x_1-x_2)^2 + (y_1-y_2)^2}}. \tag{15}$$

The projectile follows a straight-line trajectory given by:

$$\vec{R}(t) = b\hat{i} + (y_s + vt)\,\hat{j}, \tag{16}$$

where b is the impact parameter, $y_s < 0$ is the starting position, and v is the projectile velocity. The coefficients c_t, c_u, and c_t in Eqs.(13)-(15) are used to soften the singularity of the potentials and allow the energy of the 4D flatland atoms to resemble full 6D atoms.

The ground state of any He-like atom may be obtained by relaxation of the time-dependent Schrodinger equation in imaginary time (τ). In 4D Cartesian flatland space the time-dependent equation is given by:

$$-\frac{\partial \bar{P}(x_1,y_1,x_2,y_2,\tau)}{\partial \tau} = \sum_{i=1}^{2}\bar{T}_i(x_i,y_i)\,\bar{P}(x_1,y_1,x_2,y_2,\tau) + U(x_1,y_1,x_2,y_2,\tau), \tag{17}$$

where

$$\bar{T}(x_i, y_i) = -\frac{1}{2}\frac{\partial^2}{\partial x_i^2} - \frac{1}{2}\frac{\partial^2}{\partial y_i^2} - \frac{Z}{\sqrt{\bar{c} + (x_i - x_o)^2 + (y_i - y_o)^2}} \tag{18}$$

and (x_0, y_0) is the position of a He-like atom with nuclear charge Z. For calculations of double charge transfer the projectile frame of reference is used. The target He atom ground state wavefunction, $\bar{P}^{He}_{target}(x_1, y_1, x_2, y_2)$ is found by relaxation of Eqs. (17)-(18) with $Z = Z_t = 2$, $\bar{c} = c_t$, $x_0 = b$, and $y_0 = y_s$ for each projectile trajectory. To obtain double charge transfer cross sections the projectile He-like atom ground state wavefunction, $\bar{P}^{He-like}_{projectile}(x_1, y_1, x_2, y_2)$, is found by relaxation of Eqs. (17)-(18) with $Z = Z_p$, $\bar{c} = c_p$, $x_0 = 0$, and $y_0 = 0$.

With the initial condition:

$$P(x_1, y_1, x_2, y_2, t = 0) = \bar{P}^{He}_{target}(x_1, y_1, x_2, y_2), \tag{19}$$

the time-dependent Schrodinger equation is propagated forward in real time (t) using Eqs. (12)-(14). The ground state double capture scattering probability for a given projectile velocity and impact parameter is given by:

$$S(v,b) = \left| \int dx_1 \int dy_1 \int dx_2 \int dy_2 \bar{P}^{*H-like}_{projectile}(x_1, y_1, x_2, y_2) P(x_1, y_1, x_2, y_2, t \to \infty) \right|^2. \tag{20}$$

The double capture cross section for a given projectile velocity is given by:

$$\sigma(v) = 2\int S(v,b)\, db, \tag{21}$$

and has the dimensions of length.

3. RESULTS

3.1. Two Dimensional Flatland

For p + H and $\alpha + H$ collisions, we employed a $(384)^2$ point numerical lattice. The x and y coordinates were spanned from –38.4 to +38.4 in each direction using a uniform mesh spacing of $\Delta x = \Delta y = 0.20$. Only the y coordinate was partitioned over N_y parallel core processors. A low order finite difference method was used to represent the two kinetic energy operators, with message passing along the y coordinate. We also used a further parallelization over N_b impact parameters, with no message passing. Thus, the total number of parallel core processors needed for a given projectile velocity is $N_y N_b$. A run with $N_y = 12$ and $N_b = 5$ requires the use of 60 core processors.

For p + H collisions we choose $Z_t = Z_p = 1$ and $c_t = c_p = 0.80$ to give a ground state energy of H equal to –0.50, following relaxation on the lattice using Eqs. (6)-(7). For $\alpha + H$ collisions we choose $Z_t = 1$, $Z_p = 2$, $c_t = 0.80$, and $c_p = 0.40$ to give a ground state energy of He^+ equal to -2.00, following relaxation on the lattice using Eqs. (6)-(7).

The 2D one electron wavefunction was propagated in time using Eqs. (2)-(4) with a starting value of $y_s = -25.6$ in Eq.(5) and 24 impact parameters ranging from $b = 0.20$ to $b = 8.0$. For an incident energy of 10 keV/amu the projectile speed is $v = 0.64$. An exponential masking function was used to absorb any spurious wave reflection at the lattice boundaries. Ground state single capture scattering probabilities, $S(v, b)$ from Eq. (9), as a function of impact parameter are shown in Figure 1 for p + H collisions and in Figure 2 for $\alpha + H$ collisions. The single capture into the H atom ground state for p + H collisions is much more probable than single capture into the He^+ atomic ion ground state for $\alpha + H$ collisions. The total single capture cross sections obtained using Eq. (10) are 1.8 x 10^{-8} cm for p + H collisions, 1.2 x 10^{-11} cm for $\alpha + H$ collisions, and a ground state ratio of 1500.

It is interesting to note, that previous full three dimensional Cartesian space single capture cross sections at 10.0 keV/amu found 7.9 x 10^{-16} cm^2 for p + H collisions [3], 1.3 x 10^{-18} cm^2 for α collisions [5], and a ground state ratio of 600.

3.2. Four Dimensional Flatland

For α + He and Li^{3+} + He collisions, we employed a $(384)^4$ point numerical lattice. The x_1, y_1, x_2, and y_2 coordinates were spanned from –38.4 to +38.4 in each direction using a uniform mesh spacing of $\Delta x_1 = \Delta y_1 = \Delta x_2 = \Delta y_2 = 0.20$. Each coordinate was partitioned over N_c parallel core processors. A low order finite difference method was used to represent the four kinetic energy operators, with message passing along the x_1, y_1, x_2, and y_2 coordinates. We also used a further parallelization over N_b impact parameters, with no message passing. Thus, the total number of parallel core processors needed for a given projectile velocity is $N^4_c\, N_b$. A run with $N_{x1} = N_{y1} = N_{x2} = N_{y2}$= 12 and N_b = 5 requires the use of 103,680 core processors.

For α + He collisions we choose $Z_t = Z_p = 2$, $c_t = c_p = 0.41$, and $c_u = 0.1$ to give a ground state energy of He equal to -2.90, following relaxation on the lattice using Eqs. (17)-(18). For Li^{3+} + He collisions we choose $Z_t = 2$, $Z_p = 3$, $c_t = 0.41$, $c_p = 0.28$, and $c_u = 0.1$ to give a ground state energy of Li^{+} equal to -7.28, following relaxation on the lattice using Eqs. (17)-(18). The ground state energies for He and Li^{+} match experimental values [11].

The 4D two electron wavefunction was propagated in time using Eqs. (12)-(15) with a starting value of $y_s = -19.2$ in Eq. (16) and 12 impact parameters ranging from $b = 0.20$ to $b = 3.0$. For an incident energy of 50 keV/amu the projectile speed is $v = 1.42$. An exponential masking function was used to absorb any spurious wave reflection at the lattice boundaries. Ground state double capture scattering probabilities, $S(v, b)$ from Eq. (20), as a function of impact parameter are shown in Figure 3 for α + He collisions and in Figure 4 for Li^{3+} + He collisions. The double capture into the He atom ground state for α + He collisions is more probable than double capture into the Li^{+} atomic ion ground state for Li^{3+} + He collisions. The total double capture cross sections obtained using Eq. (21) are 7.4 x 10^{-10} cm for α + He collisions, 4.9 x 10^{-11} cm for Li^{3+} + He collisions, and a ground state ratio of 15.

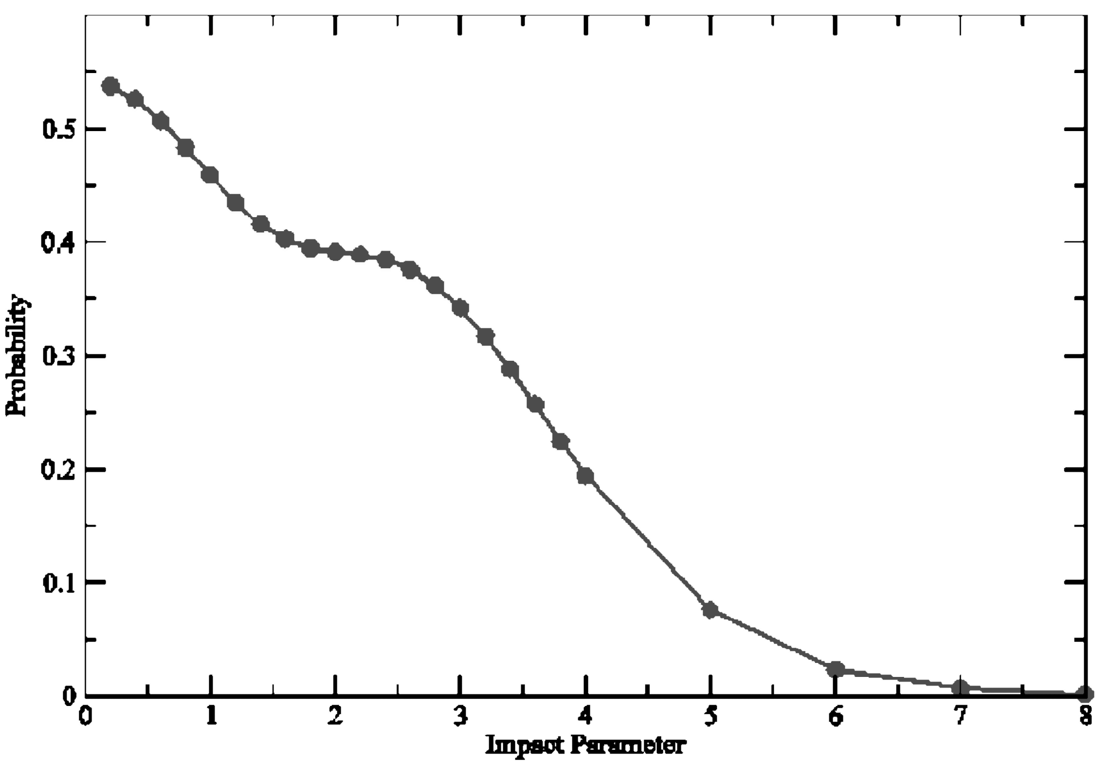

Figure 1: Ground state single capture probabilities in p + *H* collisions at an incident energy of 10.0 keV/amu

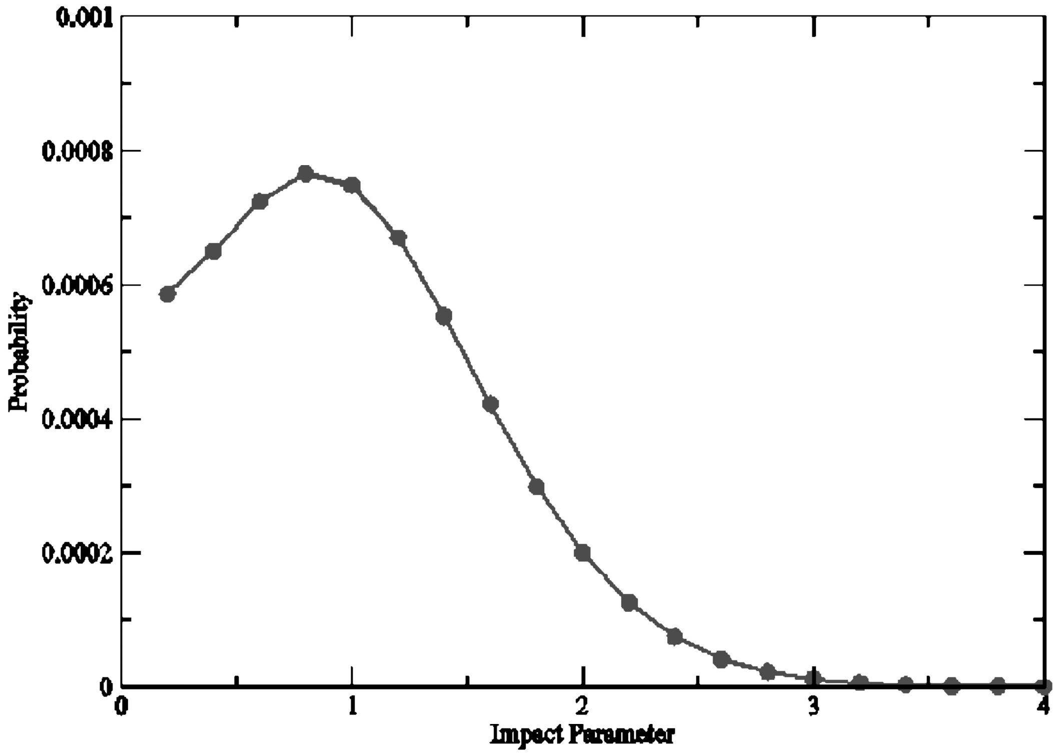

Figure 2: Ground state single capture probabilities in α + *H* collisions at an incident energy of 10.0 keV/amu

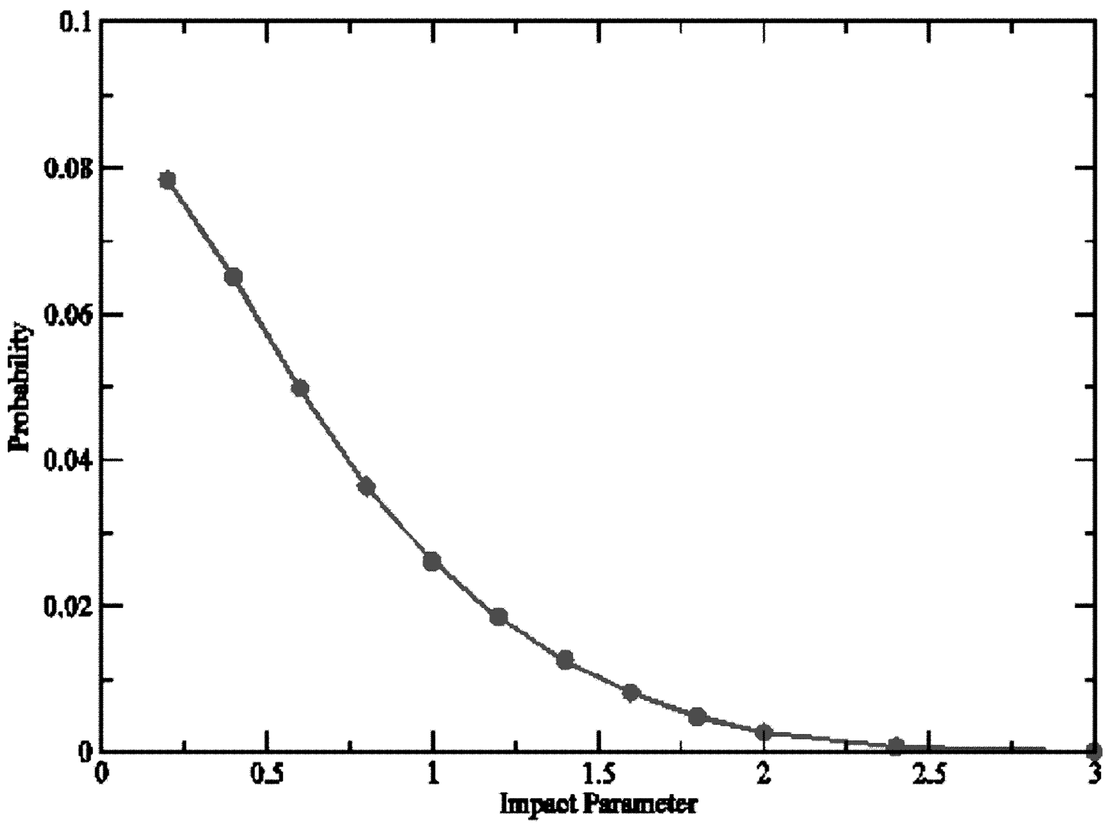

Figure 3: Ground state double capture probabilities in α + He collisions at an incident energy of 50.0 keV/amu

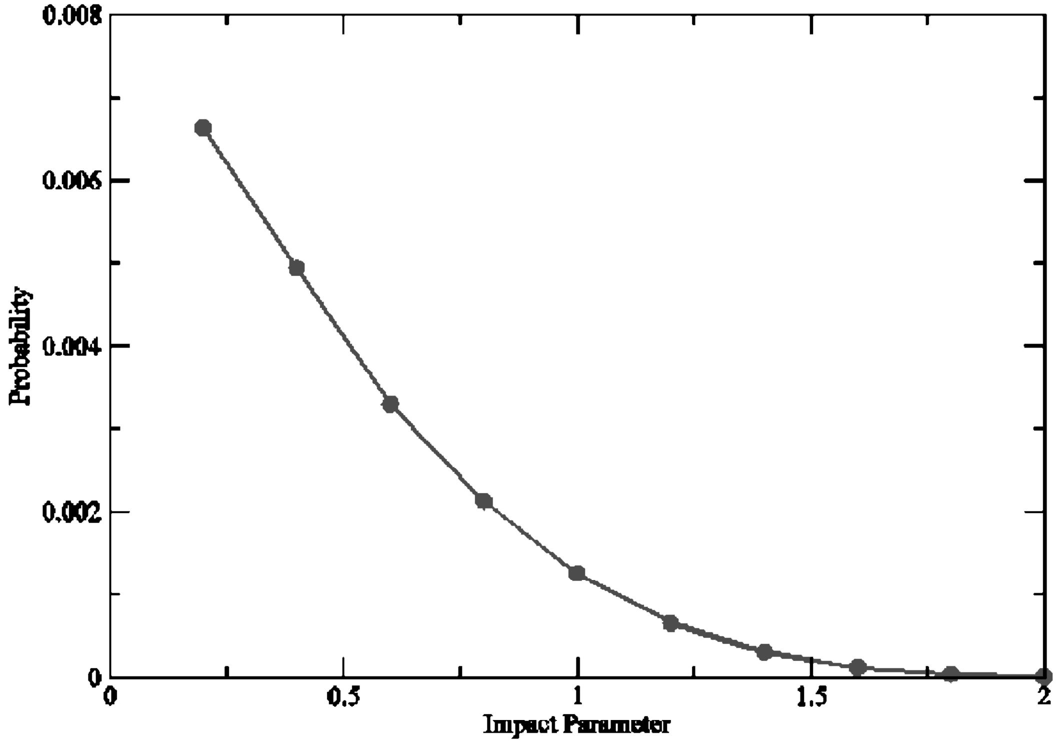

Figure 4: Ground state double capture probabilities in Li^{3+} + He collisions at an incident energy of 50.0 keV/amu

4. SUMMARY

In the future, we plan to continue the 2D flatland calculations for p + H and α + H collisions to determine single charge transfer into both ground and excited states at a variety of incident energies. It will be interesting to see how the 2D/3D cross section ratios compare for p and α projectiles. We also plan to continue the 4D flatland calculations for α + He and Li^{3+} + He collisions to determine double charge transfer into both ground and excited states at a variety of incident energies. Hopefully, the 4D cross section ratios can be used as guide for accessing the convergence of future truly large scale 6D cross section calculations.

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