Single and Double Charge Transfer in Flatland

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ABSTRACT: The time-dependent Schrödinger equation is solved in a two dimensional flatland space for the single charge transfer to the ground state for both $p + H$ and $\alpha + H$ 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 Schrödinger equation is also solved in a four dimensional flatland space for the double charge transfer to the ground state for both $\alpha + He$ and $Li^2+ + He$ 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 $\alpha + He$ collision.

1. INTRODUCTION

Charge transfer in $p + H$ collisions by direct solution of the time-dependent Schrödinger 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 Schrödinger equation was subsequently studied in a full three dimensional Cartesian space. Calculations have been made for $p + H$ [2–4], $\alpha + H$ [5], $Be^+ + H$ [6], $p + He^+$ [7], $\alpha + Li^+$ [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 $p + He$ 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 $\alpha + H$ 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 $\alpha + He$ and $Li^2+ + He$ 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:

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

where $Z_r = 1$, $Z_p$ 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:
where
\[
T(x,y) = -\frac{1}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{2} \frac{\partial^2}{\partial y^2} - \frac{Z_i}{\sqrt{c + x^2 + y^2}} \tag{3}
\]
and
\[
V(x,y,t) = -\frac{Z_p}{\sqrt{c + (x-b)^2 + (y-(y_s + vt))^2}}. \tag{4}
\]

The projectile follows a straight-line trajectory given by:
\[
\vec{R}(t) = b \hat{i} + (y_s + vt) \hat{j}. \tag{5}
\]

The ground state of any H-like atom may be obtained by relaxation of the time-dependent Schrödinger equation in imaginary time (\(\tau\)). In 2D Cartesian flatland space the time-dependent equation is given by:
\[
-\frac{\partial \tilde{P}(x,y,\tau)}{\partial \tau} = \tilde{T}(x,y) \tilde{P}(x,y,\tau), \tag{6}
\]
where
\[
\tilde{T}(x,y) = -\frac{1}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{2} \frac{\partial^2}{\partial y^2} - \frac{Z}{\sqrt{c + (x-x_0)^2 + (y-y_0)^2}} \tag{7}
\]
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, \(\tilde{P}^H_{\text{target}}(x,y)\), is found by relaxation of Eqs.(6)-(7) with \(Z = Z_t = 1, \ c = c, \ x_0 = b, \) and \(y_0 = y_s\) for each projectile trajectory. To obtain single charge transfer cross sections the projectile H-like atom ground state wavefunction, \(\tilde{P}^{H-\text{like projectile}}(x,y)\), is found by relaxation of Eqs.(6)-(7) with \(Z = Z_p, \ c = c_p, \ x_0 = 0, \) and \(y_0 = 0\).

With the initial condition:
\[
P(x,y,t = 0) = \tilde{P}^H_{\text{target}}(x,y), \tag{8}
\]
the time-dependent Schrödinger 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:
\[
S(v,b) = \int dx \int dy \tilde{P}^{H-\text{like projectile}}(x,y) P(x,y,t \rightarrow \infty). \tag{9}
\]

The single capture cross section for a given projectile velocity is given by:
\[ \sigma(v) = 2 \int S(v,b) \, db, \]  

(10)

and has the dimensions of length.

### 2.2. Four Dimensional Flatland

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

\[ i \frac{\partial \psi(\vec{r}_i,\vec{r}_f,t)}{\partial t} = \sum_{i=1}^{2} \left( -\frac{1}{2} \nabla^2 - \frac{Z_t}{|\vec{r}_i|} \right) \psi(\vec{r}_i,\vec{r}_f,t) + \frac{1}{|\vec{r}_i - \vec{r}_f|^2} \psi(\vec{r}_i,\vec{r}_f,t) - \sum_{i=1}^{2} \left( \frac{Z_p}{|\vec{r}_i - \bar{R}(t)|} \right) \psi(\vec{r}_i,\vec{r}_f,t), \]  

(11)

where \( Z_t = 2 \), \( Z_p \) is the projectile charge, and \( \bar{R}(t) \) 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:

\[ i \frac{\partial P(x_i,y_i,x_j,y_j,t)}{\partial t} = \sum_{i=1}^{2} T_i(x_i,y_i) P(x_i,y_i,x_j,y_j,t) + U(x_i,y_i,x_j,y_j) P(x_i,y_i,x_j,y_j,t), \]  

(12)

where

\[ T_i(x_i,y_i) = -\frac{1}{2} \frac{\partial^2}{\partial x_i^2} - \frac{1}{2} \frac{\partial^2}{\partial y_i^2} - \frac{Z_t}{\sqrt{c_i + x_i^2 + y_i^2}}, \]  

(13)

\[ T_i(x_i,y_i) = -\frac{1}{2} \frac{\partial^2}{\partial x_i^2} - \frac{1}{2} \frac{\partial^2}{\partial y_i^2} - \frac{Z_t}{\sqrt{c_i + x_i^2 + y_i^2}}, \]  

(14)

and

\[ V_i(x_i,y_i,y) = -\frac{Z_p}{\sqrt{c_i + (x_i - x_j)^2 + (y_i - y_j)^2}}. \]  

(15)

The projectile follows a straight-line trajectory given by:

\[ \bar{R}(t) = b \hat{i} + (y_i + vt) \hat{j}, \]  

(16)

where \( b \) is the impact parameter, \( y_i < 0 \) is the starting position, and \( v \) is the projectile velocity. The coefficients \( c_i, c_j, \) and \( c \) 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 Schrödinger equation in imaginary time (\( \tau \)). In 4D Cartesian flatland space the time-dependent equation is given by:

\[ - \frac{\partial \bar{P}(x_i,y_i,x_j,y_j,\tau)}{\partial \tau} = \sum_{i=1}^{2} \bar{T}_i(x_i,y_i) \bar{P}(x_i,y_i,x_j,y_j,\tau) + U(x_i,y_i,x_j,y_j,\tau), \]  

(17)

where
\[ \bar{T}(x_i, y_i) = -\frac{1}{2} \frac{\partial^2}{\partial x_i^2} - \frac{1}{2} \frac{\partial^2}{\partial y_i^2} - \frac{Z}{\sqrt{c + (x_i - x_o)^2 + (y_i - y_o)^2}} \]  

(18)

and \((x_o, y_o)\) 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, \(\bar{P}_{\text{target}}^{\text{He}}(x_1, y_1, x_2, y_2)\) is found by relaxation of Eqs. (17)-(18) with \(Z = Z_t = 2\), \(c = c_t\), \(x_o = b\), and \(y_o = y_f\) for each projectile trajectory. To obtain double charge transfer cross sections the projectile He-like atom ground state wavefunction, \(\bar{P}_{\text{projectile}}^{\text{He-like}}(x_1, y_1, x_2, y_2)\), is found by relaxation of Eqs. (17)-(18) with \(Z = Z_p\), \(c = c_p\), \(x_o = 0\), and \(y_o = 0\).

With the initial condition:

\[ P(x_1, y_1, x_2, y_2, t = 0) = \bar{P}_{\text{target}}^{\text{He}}(x_1, y_1, x_2, y_2), \]

(19)

the time-dependent Schrödinger 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:

\[ S(v, b) = \left| \int dx_1 \int dy_1 \int dx_2 \int dy_2 \bar{P}_{\text{projectile}}^{\text{He-like}}(x_1, y_1, x_2, y_2) P(x_1, y_1, x_2, y_2, t \rightarrow \infty) \right|^2. \]

(20)

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

\[ \sigma(v) = 2 \int S(v, b) \, db, \]

(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 \(\text{He}^+\) 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 \(y_f = -25.6\) 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 \(\text{He}^+\) atomic ion ground state for \(\alpha + H\) collisions. The total single capture cross sections obtained using Eq. (10) are \(1.8 \times 10^{-8}\) cm for \(p + H\) collisions, \(1.2 \times 10^{-11}\) 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 $7.9 \times 10^{-16}$ cm$^2$ for p + H collisions [3], $1.3 \times 10^{-18}$ cm$^2$ for $\alpha$ collisions [5], and a ground state ratio of 600.

### 3.2. Four Dimensional Flatland

For $\alpha$ + 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 $N_c N_b$. 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 $\alpha$ + 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 $\alpha$ + He collisions and in Figure 4 for Li$^{3+}$ + He collisions. The double capture into the He atom ground state for $\alpha$ + 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 $7.4 \times 10^{-10}$ cm for $\alpha$ + He collisions, $4.9 \times 10^{-11}$ 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](image)
Figure 2: Ground state single capture probabilities in $\alpha + H$ collisions at an incident energy of 10.0 keV/amu

Figure 3: Ground state double capture probabilities in $\alpha + \text{He}$ 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 \( \alpha + H \) 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 \( \alpha \) projectiles. We also plan to continue the 4D flatland calculations for \( \alpha + \text{He} \) and \( \text{Li}^{3+} + \text{He} \) 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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References