Photoionization of Ne^{8+}

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Article

- **"Single and Double Photoionization of Ne^{8+}",**
  M. S. Pindzola, S. A. Abdel-Naby, F. Robicheaux, and J. Colgan
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FLASH

FLASH

FLASH INFOSCREEN
FLASH ACCELERATOR PAGES

FLASH, the Free-Electron LASer in Hamburg, started user operation in summer 2005 as the first free-electron laser for VUV and soft X-ray radiation. Currently it covers a wavelength range from 4.2 nm to about 45 nm in the first harmonic with GW peak power and pulse durations between 50 fs and 200 fs. It is operated in the "self-amplified spontaneous emission" (SASE) mode and offers five beamlines for users.

TDCC Method for Atoms

The time-dependent Schrodinger equation for a two-electron atomic ion is given by:

$$i\frac{\partial\Psi(\vec{r_1},\vec{r_2},t)}{\partial t} = H(\vec{r_1},\vec{r_2},t)\Psi(\vec{r_1},\vec{r_2},t)$$

where

$$\begin{aligned} H(\vec{r_1},\vec{r_2},t) &= \sum_{i=1}^{2}\left(-\frac{1}{2}\nabla_i^2-\frac{Z}{r_i}\right)+\frac{1}{|\vec{r_1}-\vec{r_2}|} \\ &\quad +E(t)\cos\omega t\sum_{i=1}^{2} r_i\cos\theta_i \end{aligned}$$

Expanding in coupled spherical harmonics:

$$\Psi(\vec{r_1},\vec{r_2},t) = \sum_{l_1,l_2}\frac{P_{l_1l_2}^{LS}(r_1,r_2,t)}{r_1r_2}\sum_{m_1,m_2}C_{m_1m_20}^{l_1l_2L}Y_{l_1m_1}(\theta_1,\phi_1)Y_{l_2m_2}(\theta_2,\phi_2)$$

The time-dependent close-coupled equations are given by:

$$\begin{aligned} i\frac{\partial P_{l_1l_2}^{LS}(r_1,r_2,t)}{\partial t} &= T_{l_1l_2}(r_1,r_2)P_{l_1l_2}^{LS}(r_1,r_2,t) \\ &\quad +\sum_{l_1',l_2'}V_{l_1l_2,l_1'l_2'}^{L}(r_1,r_2)P_{l_1'l_2'}^{LS}(r_1,r_2,t) \\ &\quad +\sum_{L',l_1',l_2'}W_{l_1l_2,l_1'l_2'}^{LL'}(r_1,r_2,t)P_{l_1'l_2'}^{L'S}(r_1,r_2,t) \end{aligned}$$

where $T_{l_1l_2}(r_1,r_2)$ is a sum over one-body kinetic and nuclear operators, $V_{l_1l_2,l_1'l_2'}^{L}(r_1,r_2)$ is a two body coupling operator, and $W_{l_1l_2,l_1'l_2'}^{LL'}(r_1,r_2,t)$ is a sum over one-body radiation field operators.

TDCC Method for Atoms

The time-dependent radial wavefunctions, $P^{LS}_{l_1 l_2}(r_1, r_2, t)$, are represented on a two dimensional radial lattice:

$$r_1 = 0.10, 0.20, 0.30, ..., 100.0$$

$$r_2 = 0.10, 0.20, 0.30, ..., 100.0$$

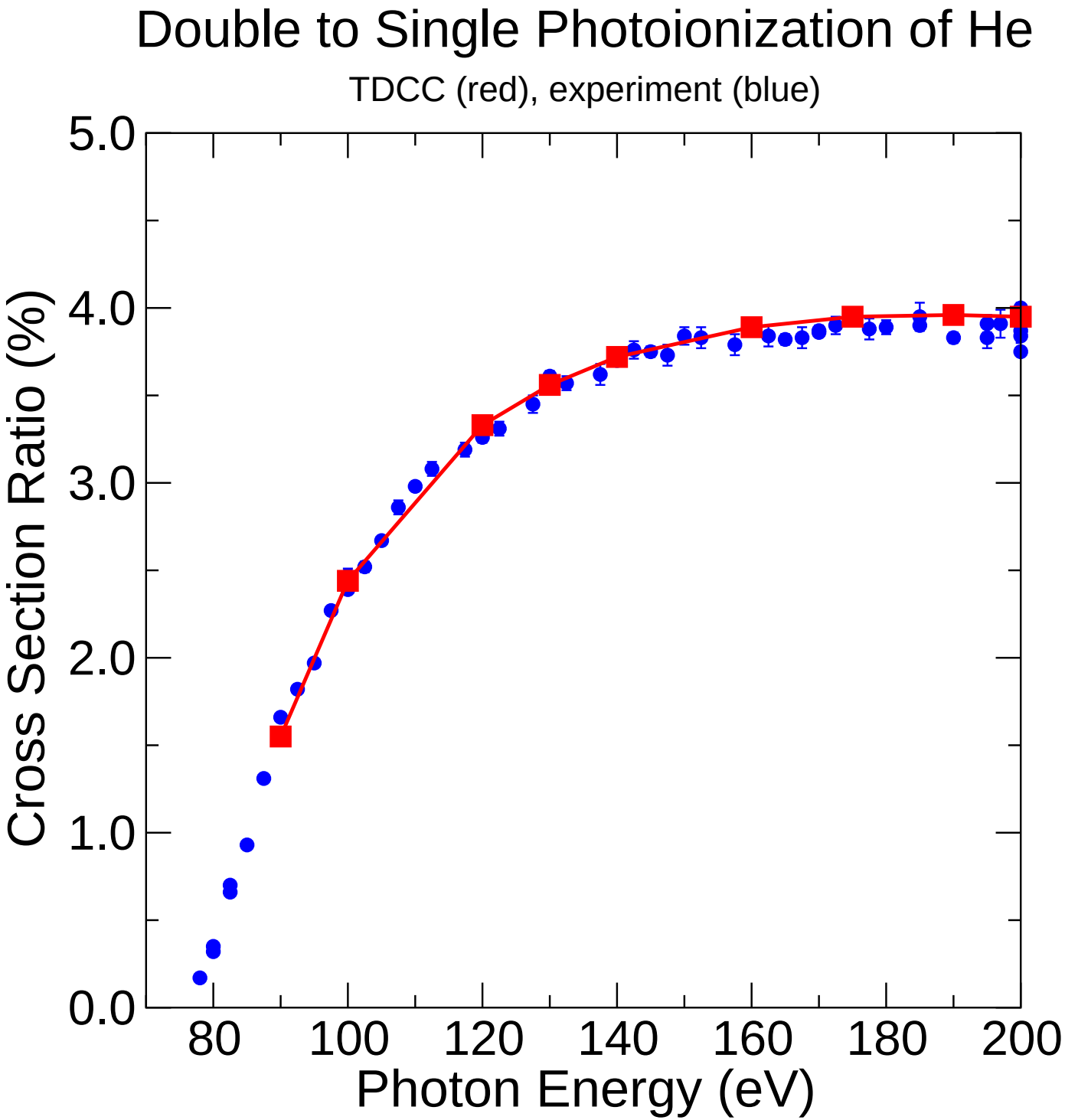
With 10 radial points for each core, the calculation uses 10,000 cores. The use of second derivatives in the Hamiltonian requires message passing between each core and its nearest neighbors.

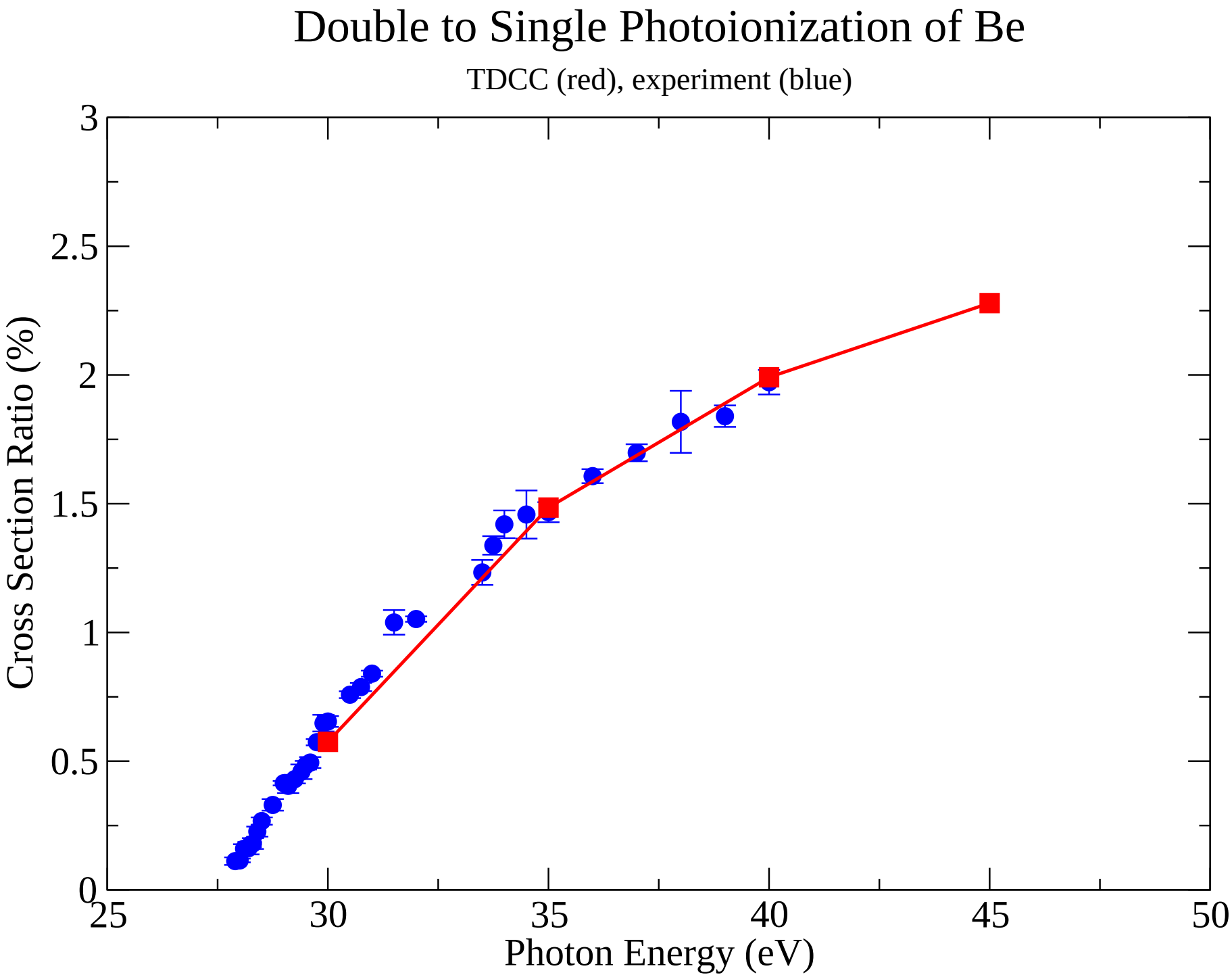
The number of coupled channels are given by:

$$^1S = ss, pp, dd, ff, gg, hh, ii$$

$$^1P = sp, ps, pd, dp, df, fd, fg, gf, gh, hg, hi, ih$$

Time propagation is for 10-15 oscillation periods. For $\Delta t = 0.001$ the total number of time steps is close to 50,000.


Double to Single Photoionization of He
TDCC (red), experiment (blue)
Cross Section Ratio (%)
0.0
1.0
2.0
3.0
4.0
5.0
80
100
120
140
160
180
200
Photon Energy (eV)


Double to Single Photoionization of Be
TDCC (red), experiment (blue)
Cross Section Ratio (%)
Photon Energy (eV)
0
0.5
1
1.5
2
2.5
3
25
30
35
40
45
50

RTDCC Method for Atoms

The time-dependent Dirac equation for a two-electron atomic ion is given by:

$$i\frac{\partial\vec{\Psi}(\vec{r}_1,\vec{r}_2,t)}{\partial t} = \bar{H}(t)\vec{\Psi}(\vec{r}_1,\vec{r}_2,t)$$

where

$$\bar{H}(t) = \begin{pmatrix} H(\vec{r}_1,\vec{r},t) & c\vec{\sigma}\cdot(\vec{p}_1+\vec{A}_1(t)) & c\vec{\sigma}\cdot(\vec{p}_2+\vec{A}_2(t)) & G(\vec{r}_1,\vec{r}_2) \\ c\vec{\sigma}\cdot(\vec{p}_1+\vec{A}_1(t)) & H(\vec{r}_1,\vec{r}_2,t)-2c^2 & G(\vec{r}_1,\vec{r}_2) & c\vec{\sigma}\cdot(\vec{p}_2+\vec{A}_2(t)) \\ c\vec{\sigma}\cdot(\vec{p}_2+\vec{A}_2(t)) & G(\vec{r}_1,\vec{r}_2) & H(\vec{r}_1,\vec{r}_2,t)-2c^2 & c\vec{\sigma}\cdot(\vec{p}_1+\vec{A}_1(t)) \\ G(\vec{r}_1,\vec{r}_2) & c\vec{\sigma}\cdot(\vec{p}_2+\vec{A}_2(t)) & c\vec{\sigma}\cdot(\vec{p}_1+\vec{A}_1(t)) & H(\vec{r}_1,\vec{r}_2,t)-4c^2 \end{pmatrix}$$

$$\vec{p}_i = -i\nabla_i$$

$$H(\vec{r}_1,\vec{r}_2,t) = \sum_{i=1}^{2}\left(-\frac{Z}{r_i}-U_i(t)\right)+C(\vec{r_1},\vec{r_2})$$

$$U_i(t) = -E(t)z_i\cos\omega t$$

$$\vec{A}_i(t) = \frac{E(t)}{\omega}\hat{z}_i\sin\left(\frac{\omega}{c}y_i-\omega t\right)+\frac{E(t)}{\omega}\hat{z}_i\sin\left(\omega t\right)$$

$$C(\vec{r}_1,\vec{r}_2) = \frac{1}{|\vec{r}_1-\vec{r}_2|}$$

$$G(\vec{r}_1,\vec{r}_2) = -\frac{\vec{\sigma}_1\cdot\vec{\sigma}_2}{|\vec{r}_1-\vec{r}_2|}$$

Expanding in coupled spin-orbit eigenfunctions:

$$\vec{\Psi}(\vec{r}_1,\vec{r}_2,t) = \begin{pmatrix} \sum_{j_1,j_2}\frac{PP^J_{\kappa_1\kappa_2}(r_1,r_2,t)}{r_1r_2}\sum_{m_1,m_2}C^{j_1j_2J}_{m_1m_2M}\Phi_{+\kappa_1,m_1}(\theta_1,\phi_1)\Phi_{+\kappa_2,m_2}(\theta_2,\phi_2) \\ i\sum_{j_1,j_2}\frac{QP^J_{\kappa_1\kappa_2}(r_1,r_2,t)}{r_1r_2}\sum_{m_1,m_2}C^{j_1j_2J}_{m_1m_2M}\Phi_{-\kappa_1,m_1}(\theta_1,\phi_1)\Phi_{+\kappa_2,m_2}(\theta_2,\phi_2) \\ i\sum_{j_1,j_2}\frac{PQ^J_{\kappa_1\kappa_2}(r_1,r_2,t)}{r_1r_2}\sum_{m_1,m_2}C^{j_1j_2J}_{m_1m_2M}\Phi_{+\kappa_1,m_1}(\theta_1,\phi_1)\Phi_{-\kappa_2,m_2}(\theta_2,\phi_2) \\ \sum_{j_1,j_2}\frac{QQ^J_{\kappa_1\kappa_2}(r_1,r_2,t)}{r_1r_2}\sum_{m_1,m_2}C^{j_1j_2J}_{m_1m_2M}\Phi_{-\kappa_1,m_1}(\theta_1,\phi_1)\Phi_{-\kappa_2,m_2}(\theta_2,\phi_2) \end{pmatrix}$$

RTDCC Method for Atoms

The time-dependent close-coupled equations are given by:

$$
\begin{aligned}
i\frac{\partial PP^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t)}{\partial t} &= (-\frac{Z}{r_1}-\frac{Z}{r_2})PP^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t) \\
&-c(\frac{\partial}{\partial r_1}-\frac{\kappa_1}{r_1})QP^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t) \\
&-c(\frac{\partial}{\partial r_2}-\frac{\kappa_2}{r_2})PQ^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t) \\
&-\sum_{J',M'}\sum_{\kappa_1',\kappa_2'} <(\kappa_1,\kappa_2)JM|U_1(t)+U_2(t)|(\kappa_1',\kappa_2')J'M'> PP^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&+ic\sum_{J',M'}\sum_{\kappa_1',\kappa_2'} <(\kappa_1,\kappa_2)JM|\vec{\sigma}\cdot\vec{A}_1(t)|(-\kappa_1',\kappa_2')J'M'> QP^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&+ic\sum_{J',M'}\sum_{\kappa_1',\kappa_2'} <(\kappa_1,\kappa_2)JM|\vec{\sigma}\cdot\vec{A}_2(t)|(\kappa_1',-\kappa_2')J'M'> PQ^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&+\sum_{J',M'}\sum_{\kappa_1',\kappa_2'} <(\kappa_1,\kappa_2)JM|C(\vec{r}_1,\vec{r}_2)|(\kappa_1',\kappa_2')J'M'> PP^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&+\sum_{J',M'}\sum_{\kappa_1',\kappa_2'} <(\kappa_1,\kappa_2)JM|G(\vec{r}_1,\vec{r}_2)|(-\kappa_1',-\kappa_2')J'M'> QQ^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t)
\end{aligned}
$$

$$
\begin{aligned}
i\frac{\partial QP^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t)}{\partial t} &= (-\frac{Z}{r_1}-\frac{Z}{r_2}-2c^2)QP^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t) \\
&+c(\frac{\partial}{\partial r_1}+\frac{\kappa_1}{r_1})PP^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t) \\
&+c(\frac{\partial}{\partial r_2}-\frac{\kappa_2}{r_2})QQ^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t) \\
&-\sum_{J',M'}\sum_{\kappa_1',\kappa_2'} <(-\kappa_1,\kappa_2)JM|U_1(t)+U_2(t)|(-\kappa_1',\kappa_2')J'M'> QP^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&-ic\sum_{J',M'}\sum_{\kappa_1',\kappa_2'} <(-\kappa_1,\kappa_2)JM|\vec{\sigma}\cdot\vec{A}_1(t)|(\kappa_1',\kappa_2')J'M'> PP^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&-ic\sum_{J',M'}\sum_{\kappa_1',\kappa_2'} <(-\kappa_1,\kappa_2)JM|\vec{\sigma}\cdot\vec{A}_2(t)|(-\kappa_1',-\kappa_2')J'M'> QQ^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&+\sum_{J',M'}\sum_{\kappa_1',\kappa_2'} <(-\kappa_1,\kappa_2)JM|C(\vec{r}_1,\vec{r}_2)|(-\kappa_1',\kappa_2')J'M'> QP^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&+\sum_{J',M'}\sum_{\kappa_1',\kappa_2'} <(-\kappa_1,\kappa_2)JM|G(\vec{r}_1,\vec{r}_2)|(\kappa_1',-\kappa_2')J'M'> PQ^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t)
\end{aligned}
$$

RTDCC Method for Atoms

$$
\begin{aligned}
i\frac{\partial PQ^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t)}{\partial t} &= (-\frac{Z}{r_1}-\frac{Z}{r_2}-2c^2)PQ^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t) \\
&+c(\frac{\partial}{\partial r_1}-\frac{\kappa_1}{r_1})QQ^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t) \\
&+c(\frac{\partial}{\partial r_2}+\frac{\kappa_2}{r_2})PP^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t) \\
&-\sum_{J',M'}\sum_{\kappa_1',\kappa_2'}<(\kappa_1,-\kappa_2)JM|U_1(t)+U_2(t)|(\kappa_1',-\kappa_2')J'M'>PQ^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&-ic\sum_{J',M'}\sum_{\kappa_1',\kappa_2'}<(\kappa_1,-\kappa_2)JM|\vec{\sigma}\cdot\vec{A}_1(t)|(-\kappa_1',-\kappa_2')J'M'>QQ^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&-ic\sum_{J',M'}\sum_{\kappa_1',\kappa_2'}<(\kappa_1,-\kappa_2)JM|\vec{\sigma}\cdot\vec{A}_2(t)|(\kappa_1',\kappa_2')J'M'>PP^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&+\sum_{J',M'}\sum_{\kappa_1',\kappa_2'}<(\kappa_1,-\kappa_2)JM|C(\vec{r}_1,\vec{r}_2)|(\kappa_1',-\kappa_2')J'M'>PQ^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&+\sum_{J',M'}\sum_{\kappa_1',\kappa_2'}<(\kappa_1,-\kappa_2)JM|G(\vec{r}_1,\vec{r}_2)|(-\kappa_1',\kappa_2')J'M'>QP^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t)
\end{aligned}
$$

$$
\begin{aligned}
i\frac{\partial QQ^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t)}{\partial t} &= (-\frac{Z}{r_1}-\frac{Z}{r_2}-4c^2)QQ^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t) \\
&-c(\frac{\partial}{\partial r_1}+\frac{\kappa_1}{r_1})PQ^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t) \\
&-c(\frac{\partial}{\partial r_2}+\frac{\kappa_2}{r_2})QP^{JM}_{\kappa_1\kappa_2}(r_1,r_2,t) \\
&-\sum_{J',M'}\sum_{\kappa_1',\kappa_2'}<(-\kappa_1,-\kappa_2)JM|U_1(t)+U_2(t)|(-\kappa_1',-\kappa_2')J'M'>QQ^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&+ic\sum_{J',M'}\sum_{\kappa_1',\kappa_2'}<(-\kappa_1,-\kappa_2)JM|\vec{\sigma}\cdot\vec{A}_1(t)|(\kappa_1',-\kappa_2')J'M'>PQ^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&+ic\sum_{J',M'}\sum_{\kappa_1',\kappa_2'}<(-\kappa_1,-\kappa_2)JM|\vec{\sigma}\cdot\vec{A}_2(t)|(-\kappa_1',\kappa_2')J'M'>QP^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&+\sum_{J',M'}\sum_{\kappa_1',\kappa_2'}<(-\kappa_1,-\kappa_2)JM|C(\vec{r}_1,\vec{r}_2)|(-\kappa_1',-\kappa_2')J'M'>QQ^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t) \\
&+\sum_{J',M'}\sum_{\kappa_1',\kappa_2'}<(-\kappa_1,-\kappa_2)JM|G(\vec{r}_1,\vec{r}_2)|(\kappa_1',\kappa_2')J'M'>PP^{J'M'}_{\kappa_1'\kappa_2'}(r_1,r_2,t)
\end{aligned}
$$

RTDCC Method for Atoms

The time-dependent radial wavefunctions, $PP^{JM}_{\kappa_1\kappa_2}(r_1, r_2, t)$, $QP^{JM}_{\kappa_1\kappa_2}(r_1, r_2, t)$, $PQ^{JM}_{\kappa_1\kappa_2}(r_1, r_2, t)$, $QQ^{JM}_{\kappa_1\kappa_2}(r_1, r_2, t)$ **are represented on a two dimensional radial lattice:**

$$r_1 = 0.01, 0.02, 0.03, ..., 10.0$$

$$r_2 = 0.01, 0.02, 0.03, ..., 10.0$$

With 10 radial points for each core, the calculation uses 10,000 cores. The use of first derivatives in the Hamiltonian requires message passing between each core and its nearest neighbors.

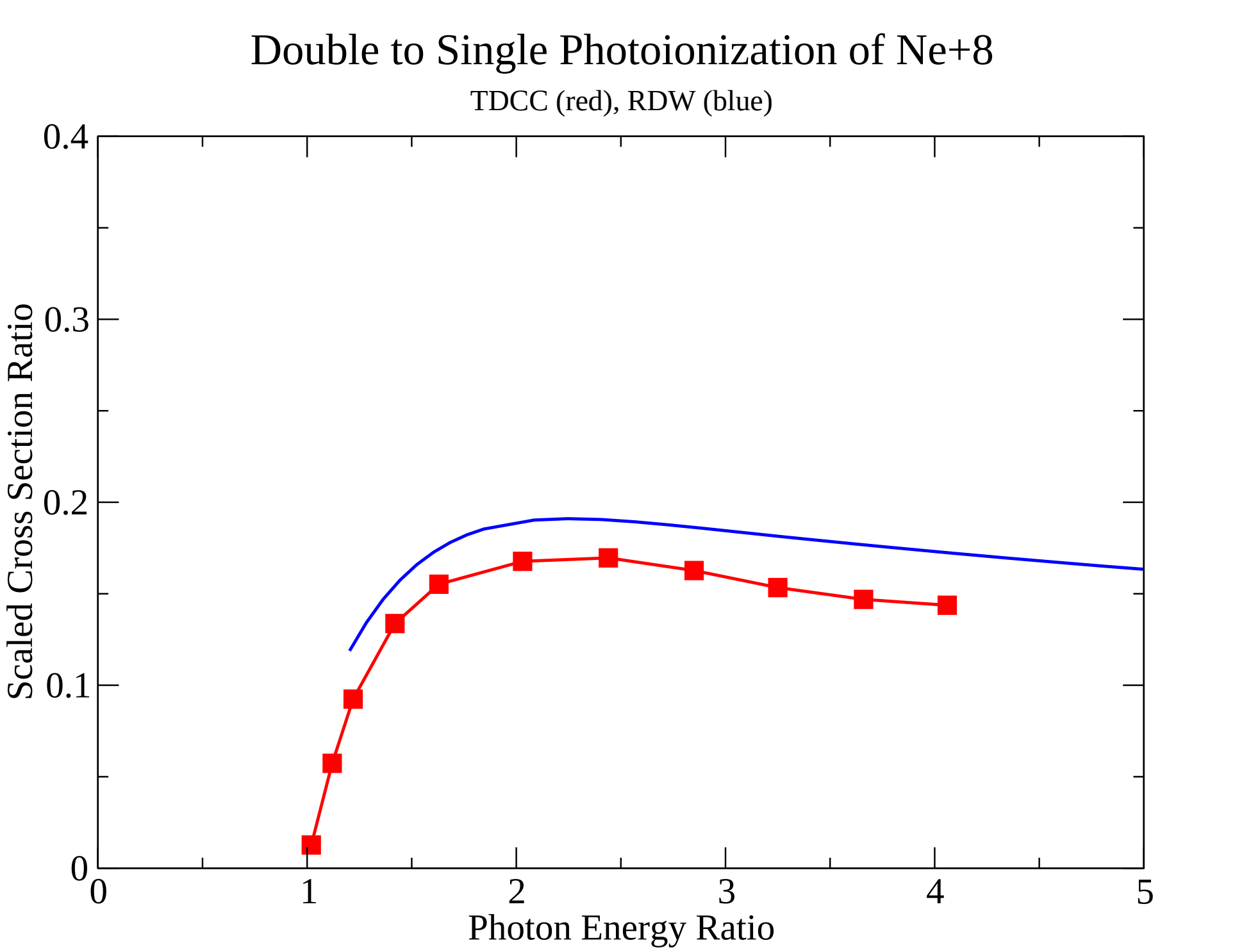
The number of coupled channels are given by:

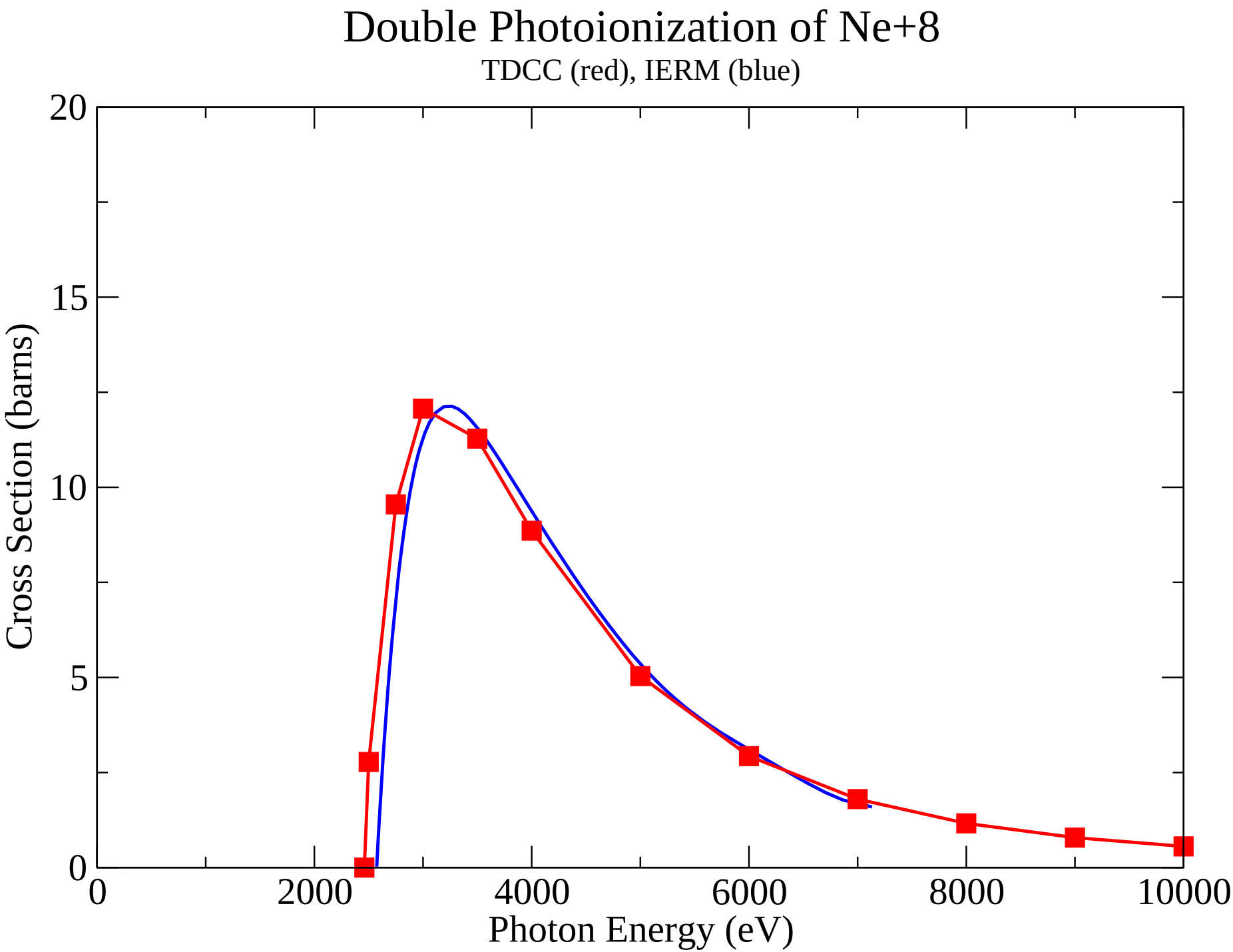
$$(JM = 00) = ss, \bar{p}\bar{p}, pp, \bar{d}\bar{d}, dd, \bar{f}\bar{f}$$

$$(JM = 10) = s\bar{p}, \bar{p}s, sp, ps, \bar{p}\bar{d}, \bar{d}\bar{p}, p\bar{d}, \bar{d}p, pd, dp, \bar{d}\bar{f}, \bar{f}\bar{d}, d\bar{f}, \bar{f}d$$

$$(JM = 20) = s\bar{d}, \bar{d}s, sd, ds, \bar{p}p, p\bar{p}, pp, \bar{p}\bar{f}, \bar{f}\bar{p}, p\bar{f}, \bar{f}p$$

Time propagation is for 10-15 oscillation periods. For $\Delta t = 0.00001$ **the total number of time steps is close to 50,000.**


Double to Single Photoionization of Ne+8
TDCC (red), RDW (blue)
Scaled Cross Section Ratio
Photon Energy Ratio
0
0.1
0.2
0.3
0.4
0
1
2
3
4
5


Double Photoionization of Ne+8
TDCC (red), IERM (blue)
Cross Section (barns)
Photon Energy (eV)
0
5
10
15
20
0
2000
4000
6000
8000
10000

Current Projects

- **Two-Photon Triple Ionization of Li**
- **Double Photoionization of H_2**
- **Double Photoionization of Li_2**