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Neutron-Impact Ionization of Atoms using the Time-Dependent Close-Coupling Method

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ABSTRACT: The time-dependent close-coupling method has been recently applied to calculate the neutron-impact atomic ionization cross sections for the He, C, F, and Ge atoms. For each atom we present single and double ionization cross sections of various inner and outer subshells. In general the single ionization cross section is larger than the double ionization cross section at low incident energies for all four neutral atom systems.

1. INTRODUCTION

Neutron-impact atomic ionization cross sections for the He, C, F, and Ge atoms have recently been calculated using the time-dependent close-coupling (TDCC) method[?, ?, ?]. Both the exterior complex scaling method[?] and the time-dependent close-coupling method[?] were found to yield cross sections for the single and double ionization of He that were in good agreement over an energy range from 0.0 to 150.0 keV.

The study of the neutron-impact ionization of atoms is motivated by attempts to directly observe the interaction of dark matter with atoms. One of the leading candidates for dark matter are weakly interacting massive particles (WIMPS). The WIMP-impact ionization of atoms would yield single and double ionization cross sections that would behave in a similar manner to those produced by neutron-impact ionization of atoms.

The rest of the paper is structured as follows: in section 2 we review the time-dependent close-coupling method for the neutron ionization of atoms, in section 3 we present TDCC neutron ionization cross sections for He, C, F, and Ge, and in section 4 we give a brief summary. Unless otherwise stated, all quantities are given in atomic units.

2. THEORY

2.1. Neutron-Atom Nuclear Collisions

Neutron-Atom nuclear cross sections are obtained from tabulated values for head-on collisions[?]. The cross sections are obtained by multiplying the head-on collision cross sections at 0.0 degrees by 4'.

The speed at which the target atom nucleus takes off is given by:

$$v_t = \frac{2m_n v_n}{m_n + m_t} \ , \tag{1}$$

where v_n is the incident neutron speed, m_n is the neutron mass, and mt is the target nuclear mass. For He atoms:

$$v_t = \frac{2}{5} v_n \ , \tag{2}$$

for C atoms:

$$v_t = \frac{2}{13} v_n \ , \tag{3}$$

for F atoms:

$$v_t = \frac{2}{20} v_n \ , \tag{4}$$

and for Ge atoms:

$$v_t = \frac{2}{73} v_n \ . \tag{5}$$

2.2. Neutron-Atom Atomic Collisions

The time-dependent close-coupled equations for the $P^{LM}_{l_1 l_2}$ (r_1, r_2, t) radial wavefunctions are given by:

$$\begin{aligned} i\frac{\partial P^{LM}_{l_1 l_2}(r_1, r_2, t)}{\partial t} &= (T_{l_1}(r_1) + T_{l_2}(r_2)) P^{LM}_{l_1 l_2}(r_1, r_2, t) \\ &+ \sum_{l_1', l_2'} V^{L}_{l_1 l_2, l_1' l_2'}(r_1, r_2) P^{LM}_{l_1' l_2'}(r_1, r_2, t) \ , \end{aligned} \tag{6}$$

where Tl_i (r_i) is the one-body interaction operator and $V^{L}_{l_1 l_2, l_1' l_2'}$ (r_1, r_2) is the two-body interaction operator. The one-body interaction operator is given by:

$$T_l(r) = -\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{2r^2} - \frac{Z}{r} + V_l^{HX}(r)| \ , \tag{7}$$

where V_l^{HX} (r) is a Hartree local exchange potential for the atomic core.

The total single ionization cross section is given by:

$$\begin{aligned} \sigma_{single}(n_1 l_1, E_n) &= \sigma_{nA}(E_n) \\ &\times 2 \sum_L \sum_{l_2} \int_0^\infty dk_2 |\hat{P}^L_{single}(n_1 l_1, k_2 l_2)|^2 \ , \end{aligned} \tag{8}$$

where $\sigma_{nA}(E_n)$ are the neutron-atom nuclear cross sections and $\hat{P}^L_{single}(n_1 l_1, k_2 l_2)$ are single ionization probability amplitudes found by projecting the solution of the time-dependent close-coupling equations onto products of single particle states, $P_{n_1 l_1}(r_1) P_{k_2 l_2}(r_2)$.

The total double ionization cross section is given by:

$$\begin{aligned} \sigma_{double}(E_n) &= \sigma_{nA}(E_n) \\ &\times \sum_L \sum_{l_1, l_2} \int_0^\infty dk_1 \int_0^\infty dk_2 |\hat{P}^L_{double}(k_1 l_1, k_2 l_2)|^2 \ , \end{aligned} \tag{9}$$

where $\hat{P}^{L}_{double}(k_1 l_1, k_2 l_2)$ are double ionization probability amplitudes found by projecting the solution of the time-dependent close-coupling equations onto products of single particle states, $P_{k_1 l_1}(r_1) P_{k_2 l_2}(r_2)$.

3. RESULTS

3.1. Neutron Collisions with the Helium Atom

A complete set of bound $P_{nl}(r)$ and continuum $P_{kl}(r)$ orbitals for He^+ were calculated by solving the radial Schrodinger equation.

The neutron nuclear cross sections for the Helium atom are given in Table 1[?]. We solved the time-dependent close-coupling equations using a 720 × 720 point radial lattice with a mesh spacing of $\Delta r_1 = \Delta r_2 = 0.20$ for the neutron atomic cross sections for the Helium atom.

The neutron atomic cross sections for the single and double ionization of the 2*s* subshell are given in Table 2 and Figure 1[?]. As seen in Figure 1 the single and double ionization cross sections have similar magnitudes. The single ionization cross section is larger than the double ionization cross section at the lower energies, but falls below at energies around 1250 keV.

3.2. Neutron Collisions with the Carbon Atom

Following a Hartree-Fock calculation[?] for the $1s^2 2s^2$ configuration of C^{2+}, a complete set of bound $P_{nl}(r)$ and $P_{kl}(r)$ orbitals for C^+ were calculated by solving the radial Schrodinger equation. For each l a local exchange potential is adjusted so that the single particle energies for the active subshells match calculations made in the Hartree-Fock Relativistic approximation[?].

The neutron nuclear cross sections for the Carbon atom are given in Table 3[?]. We solved the time-dependent close-coupling equations using a 480 × 480 point radial lattice with a mesh spacing of $\Delta r_1 = \Delta r_2 = 0.20$ for the neutron atomic cross sections for the Carbon atom.

For the ionization of the $2p^2$ subshell, the 3s orbital has a binding energy of -10.15 eV, the 2^p orbital has a binding energy of -24.90 eV, the 3d orbital has a binding energy of -6.48 eV, and the 4f orbital has a binding energy of -3.43 eV. The use of a 3s pseudo-orbital prevents the unphysical excitation of the 1s and 2s filled subshells. The neutron atomic cross sections for the single and double ionization of the 2p subshell are given in Table 4 and Figure 2. The single ionization cross section is larger than the double ionization cross section at low energies, but they come together at high energies.

For the ionization of the $2s^2$ subshell, the 2*s* orbital has a binding energy of -31.53 eV, while the 2*p*, 3*d*, and 4*f* orbitals have the same energies as before. The use of a 2*s* pseudo-orbital prevents the unphysical excitation of the 1*s* filled subshell. The neutron atomic cross sections for the single and double ionization of the 2*s* subshell are given in Table 5 and Figure 3. The single ionization cross section is larger than the double ionization cross section at all energies.

For the ionization of the $1s^2$ subshell, the 1*s* orbital has a binding energy of -316.60 eV, while the 2*p*, 3*d*, and 4*f* orbitals have the same energy as before. The 2*s* orbital is deleted from list since as a filled subshell it cannot be excited. The neutron atomic cross sections for the single and double ionization of the 1*s* subshell are given in Table 6 and Figure 4. The single ionization cross section becomes much larger than the double ionization cross section at high energies.

3.3. Neutron Collisions with the Fluorine Atom

Following a Hartree-Fock calculation[?] for the $1s^2 2s^2 2p^3$ configuration of F^{2+}, a complete set of bound $P_{nl}(r)$ and $P_{kl}(r)$ orbitals for F^+ were calculated by solving the radial Schrodinger equation. For each l a local exchange potential is adjusted so that the single particle energies for the active subshells match calculations made in the Hartree-Fock Relativistic approximation[?].

The neutron nuclear cross sections for the Fluorine atom are given in Table 7[?]. We solved the time-dependent close-coupling equations using a 480 × 480 point radial lattice with a mesh spacing of $\Delta r_1 = \Delta r_2 = 0.20$ for the neutron atomic cross sections for the Fluorine atom.

For the ionization of the $2p^5$ subshell, the 3*s* orbital has a binding energy of -12.90 eV, the 2*p* orbital has a binding energy of -37.48 eV, the 3*d* orbital has a binding energy of -6.35 eV, and the 4*f* orbital has a binding energy of -3.42 eV. The use of a 3*s* pseudo-orbital prevents the unphysical excitation of the 1*s* and 2*s* filled subshells. The neutron atomic cross sections for the single and double ionization of the 2*p* subshell are given in Table 8 and Figure 5. The single ionization cross section is much larger than the double ionization cross section at 3.0 MeV.

For the ionization of the $2s^2$ subshell, the 2*s* orbital has a binding energy of -31.53 eV, while the 2*p*, 3*d*, and 4*f* orbitals have the same energies as before. The use of a 2*s* pseudo-orbital prevents the unphysical excitation of the 1*s* filled subshell. The neutron atomic cross sections for the single and double ionization of the 2*s* subshell are given in Table 9 and Figure 6. The single ionization cross section is much larger than the double ionization cross section at 3.0 MeV.

For the ionization of the $1s^2$ subshell, the 1*s* orbital has a binding energy of -316.60 eV, while the 2*p*, 3*d*, and 4*f* orbitals have the same energy as before. The 2*s* orbital is deleted from list since as a filled subshell it cannot be excited. The neutron atomic cross sections for the single and double ionization of the 1*s* subshell are given in Table 10 and Figure 7. The single ionization cross section is much larger than the double ionization cross section at all energies.

3.4. Neutron Collisions with the Germanium Atom

Following a Hartree-Fock calculation[?] for the $1s^22s^22p^63s^23p^63d^{10}4s^2$ configuration of Ge^{2+}, a complete set of bound $P_{nl}(r)$ and $P_{kl}(r)$ orbitals for Ge^+ were calculated by solving the radial Schrodinger equation. For each *l* a local exchange potential is adjusted so that the single particle energies for the active subshells match calculations made in the Hartree-Fock Relativistic approximation[?].

The neutron nuclear cross sections for the Germanium atom are given in Table 11[?]. We solved the time-dependent close-coupling equations using a 480 × 480 point radial lattice with a mesh spacing of $\Delta r_1 = \Delta r_2 = 0.20$ for the neutron atomic cross sections for the Germanium atom.

For the ionization of the $4p^2$ subshell, the 5*s* orbital has a binding energy of -8.18 eV, the 4*p* orbital has a binding energy of -15.92 eV, the 4*d* orbital has a binding energy of -6.68 eV, and the 4*f* orbital has a binding energy of -3.50 eV. The use of pseudo-orbitals prevents the unphysical excitation of the 1*s*, 2*s*, 2*p*, 3*s*, 3*p*, 3*d*, and 4*s* filled subshells. The neutron atomic cross sections for the single and double ionization of the $4p^2$ subshell are given in Table 12 and Figure 8. The single ionization cross section is much larger than the double ionization cross section at the highest energy.

For the ionization of the $4s^2$ subshell, the 4*s* orbital has a binding energy of -23.78 eV, while the 4*p*, 4*d*, and 4*f* orbitals have the same energies as before. The neutron atomic cross sections for the single and double ionization of the $4s^2$ subshell are given in Table 13 and Figure 9. The single ionization cross section is larger than the double ionization cross section at the highest energy.

4. SUMMARY

In this paper we reviewed the TDCC calculations made for the neutron-impact ionization of atoms. Neutron-impact single and double ionization cross sections for the He, C, F, and Ge atoms have been made for incident energies ranging from 0.5 MeV to 4.0 MeV.

In the future we plan to carry out more TDCC calculations for the neutron-impact ionization of atoms. We look forward to furthur experimental results for the neutron-impact single and double ionization cross sections to check the theoretical predictions for the C, F, and Ge atoms.

Acknowledgments

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Table 1. Neutron + Helium Nuclear Cross Sections
($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$)

Energy	Cross Section
250.0 KeV	0.172 b
500.0 KeV	0.452 b
750.0 KeV	4.339 b
1000.0 KeV	13.245 b
1250.0 KeV	16.424 b
1500.0 KeV	14.263 b
1750.0 KeV	11.846 b
2000.0 KeV	10.137 b

Table 2. Neutron + Helium Atomic Cross Sections
($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$)

Energy	Single Ionization 2s Cross Section	Double Ionization 2s Cross Section
250.0 KeV	0.088 b	0.005 b
500.0 KeV	0.254 b	0.047 b
750.0 KeV	2.001 b	0.797 b
1000.0 KeV	4.618 b	3.159 b
1250.0 KeV	4.223 b	4.408 b
1500.0 KeV	2.699 b	3.993 b
1750.0 KeV	1.662 b	3.316 b
2000.0 KeV	1.067 b	2.766 b

Table 3. Neutron + Carbon Nuclear Cross Sections
($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$)

Energy	Cross Section
1.0 MeV	3.2321 b
2.0 MeV	1.9063 b
3.0 MeV	2.3600 b
4.0 MeV	6.3385 b

Table 4. Neutron + Carbon Atomic Cross Sections ($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$)

Energy	2p Single Ionization Cross Section	2p Double Ionization Cross Section
1.0 MeV	3.0779 b	0.3011 b
2.0 MeV	1.1902 b	0.3556 b
3.0 MeV	0.9072 b	0.5059 b
4.0 MeV	1.6120 b	1.2766 b

Table 5. Neutron + Carbon Atomic Cross Sections ($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$)

Energy	2s Single Ionization Cross Section	2s Double Ionization Cross Section
1.0 MeV	2.1106 b	0.0632 b
2.0 MeV	1.5754 b	0.1342 b
3.0 MeV	1.6655 b	0.2836 b
4.0 MeV	3.3312 b	0.9533 b

Table 6. Neutron + Carbon Atomic Cross Sections ($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$)

Energy	1s Single Ionization Cross Section	1s Double Ionization Cross Section
1.0 MeV	0.2982 b	0.0011 b
2.0 MeV	0.3303 b	0.0023 b
3.0 MeV	0.5742 b	0.0059 b
4.0 MeV	1.9208 b	0.0262 b

Table 7. Neutron + Fluorine Nuclear Cross Sections ($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$)

Energy	Cross Section
1.0 MeV	2.7043 b
2.0 MeV	1.0423 b
3.0 MeV	12.6543 b
4.0 MeV	6.5584 b

Table 8. Neutron + Fluorine Atomic Cross Sections ($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$)

Energy	2p Single Ionization Cross Section	2p Double Ionization Cross Section
1.0 MeV	1.6570 b	0.1404 b
2.0 MeV	0.9346 b	0.1050 b
3.0 MeV	12.3767 b	1.8065 b
4.0 MeV	6.2772 b	1.1681 b

Table 9. Neutron + Fluorine Atomic Cross Sections ($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$)

Energy	2s Single Ionization Cross Section	2s Double Ionization Cross Section
1.0 MeV	0.6306 b	0.0108 b
2.0 MeV	0.4632 b	0.0128 b
3.0 MeV	7.7601 b	0.3034 b
4.0 MeV	4.8344 b	0.2510 b

Table 10. Neutron + Fluorine Atomic Cross Sections ($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$)

Energy	1s Single Ionization Cross Section	1s Double Ionization Cross Section
1.0 MeV	0.0326 b	0.000025 b
2.0 MeV	0.0247 b	0.000029 b
3.0 MeV	0.4428 b	0.0007 b
4.0 MeV	0.3011 b	0.0006 b

Table 11. Neutron + Germanium Nuclear Cross Sections ($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$)

Energy	Cross Section
1.0 MeV	8.9133 b
2.0 MeV	10.3974 b
3.0 MeV	15.4943 b
4.0 MeV	23.1975 b

Table 12. Neutron + Germanium Atomic Cross Sections ($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$)

Energy	4p Single Ionization Cross Section	4p Double Ionization Cross Section
1.0 MeV	1.4120 b	0.0076 b
2.0 MeV	3.0451 b	0.0269 b
3.0 MeV	6.3022 b	0.0775 b
4.0 MeV	11.6604 b	0.1846 b

Table 13. Neutron + Germanium Atomic Cross Sections ($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$)

Energy	4s Single Ionization Cross Section	4s Double Ionization Cross Section
1.0 MeV	0.2245 b	0.0007 b
2.0 MeV	0.6144 b	0.0018 b
3.0 MeV	1.5241 b	0.0043 b
4.0 MeV	3.2600 b	0.0090 b

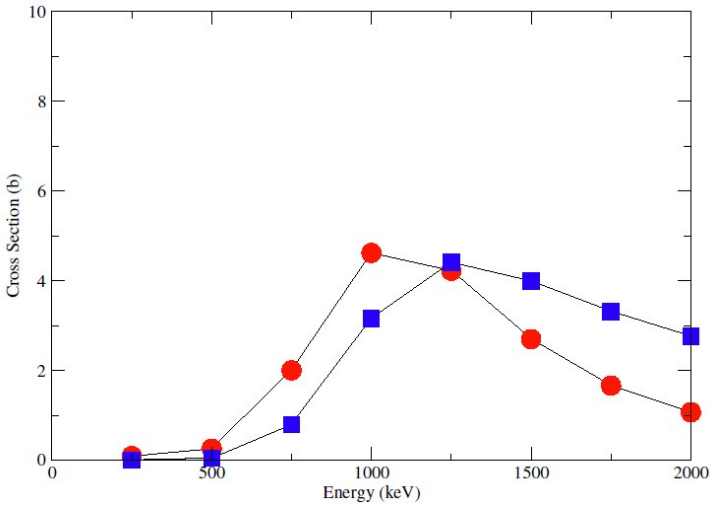

Figure 1. Neutron ionization of the 2*s* subshell of Helium. Solid line with circles(red): time-dependent close-coupling method for single ionization, solid line with squares(blue): time-dependent close-coupling method for double ionization ($1.0\ \text{b} = 1.0 \times 10^{-24}\ \text{cm}^2$).

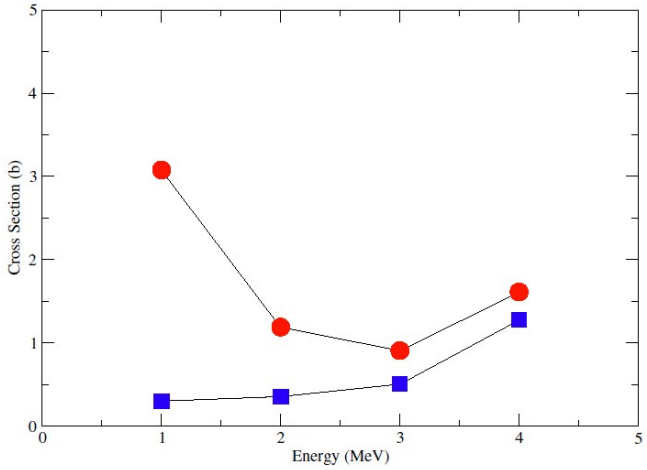

Figure 2. Neutron ionization of the 2*p* subshell of Carbon. Solid line with circles(red): time-dependent close-coupling method for single ionization, solid line with squares(blue): time-dependent close-coupling method for double ionization (1.0 b = 1.0 × 10^{-24} cm^2).

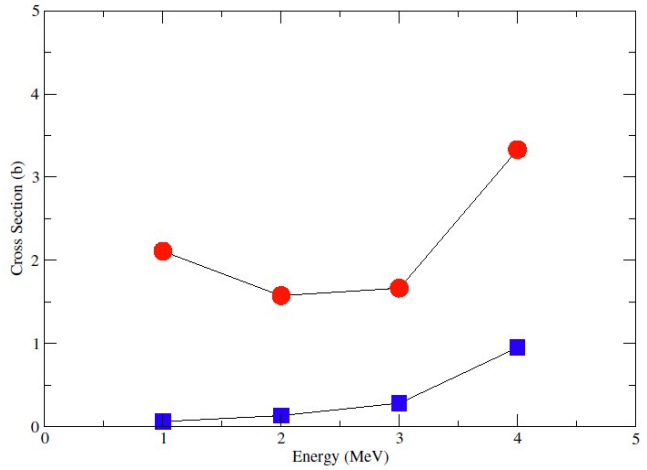

Figure 3. Neutron ionization of the 2*s* subshell of Carbon. Solid line with circles(red): time-dependent close-coupling method for single ionization, solid line with squares(blue): time-dependent close-coupling method for double ionization (1.0 b = 1.0 × 10^{-24} cm^2).

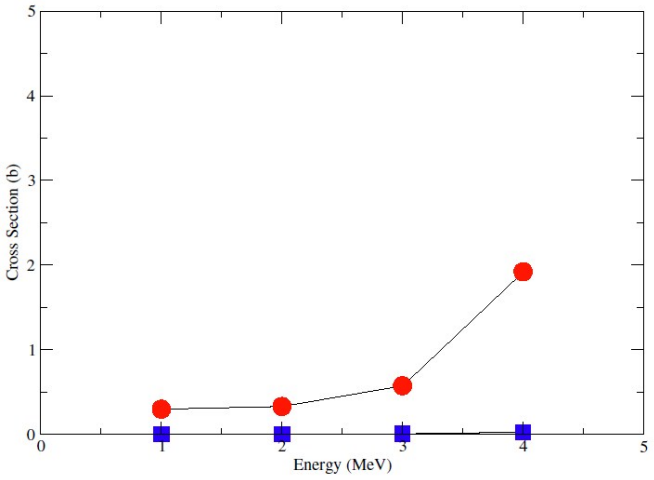

Figure 4. Neutron ionization of the 1s subshell of Carbon. Solid line with circles(red): time-dependent close-coupling method for single ionization, solid line with squares(blue): time-dependent close-coupling method for double ionization (1.0 b = 1.0 × 10^{-24} cm^2).

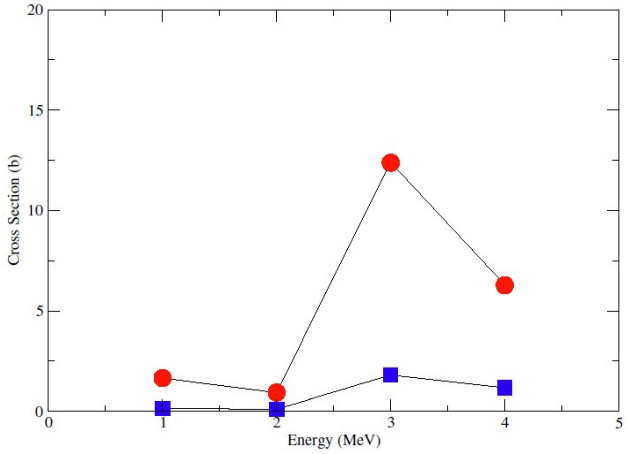

Figure 5. Neutron ionization of the 2*p* subshell of Fluorine. Solid line with circles(red): time-dependent close-coupling method for single ionization, solid line with squares(blue): time-dependent close-coupling method for double ionization (1.0 b = 1.0×10^{-24} cm^2).

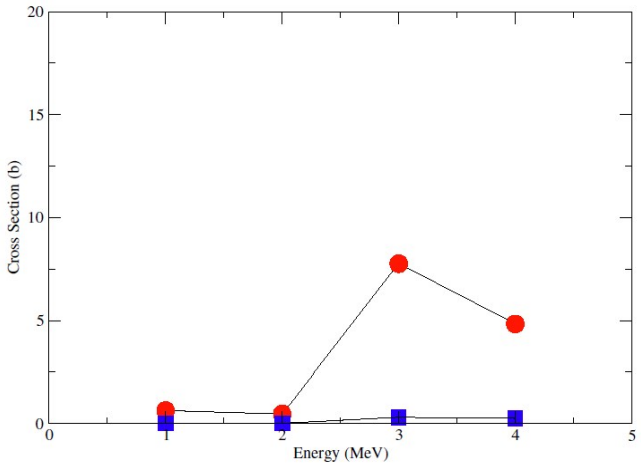

Figure 6. Neutron ionization of the 2*s* subshell of Fluorine. Solid line with circles(red): time-dependent close-coupling method for single ionization, solid line with squares(blue): time-dependent close-coupling method for double ionization (1.0 b = 1.0×10^{-24} cm^2).

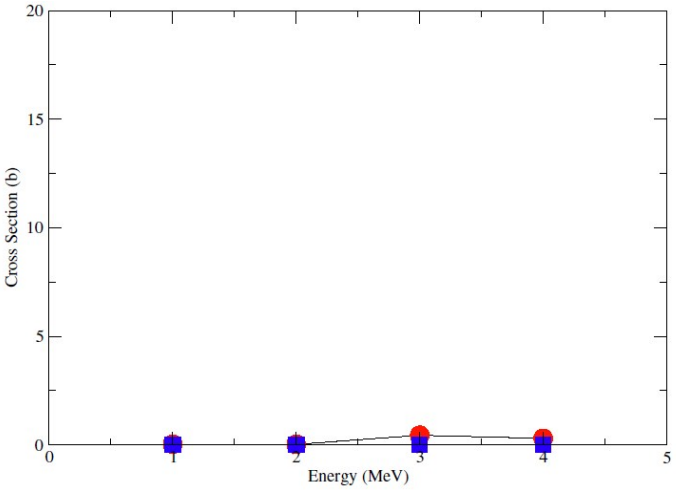

Figure 7. Neutron ionization of the 1*s* subshell of Fluorine. Solid line with circles(red): time-dependent close-coupling method for single ionization, solid line with squares(blue): time-dependent close-coupling method for double ionization (1.0 b = 1.0×10^{-24} cm^2).

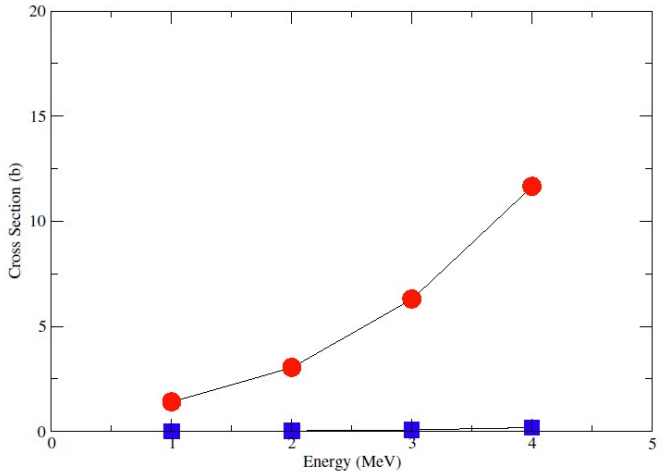

Figure 8. Neutron ionization of the 4*p* subshell of Germanium. Solid line with circles(red): time-dependent close-coupling method for single ionization, solid line with squares(blue): time-dependent close-coupling method for double ionization (1.0 b = 1.0 × 10^{-24} cm^2).

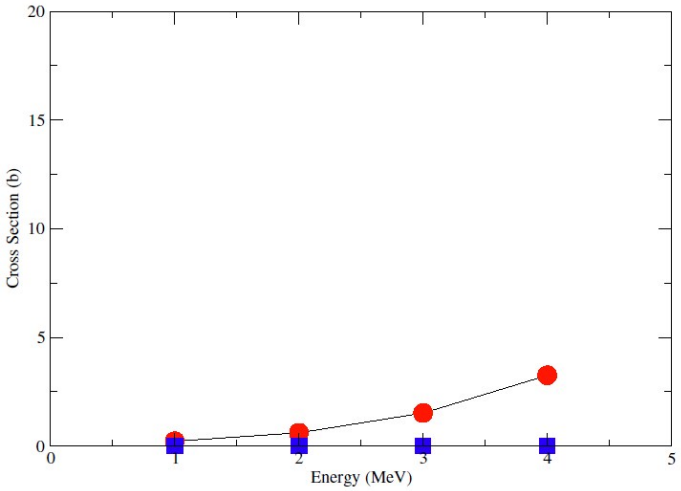

Figure 9. Neutron ionization of the 4*s* subshell of Germanium. Solid line with circles(red): time-dependent close-coupling method for single ionization, solid line with squares(blue): time-dependent close-coupling method for double ionization (1.0 b = 1.0 × 10^{-24} cm^2).

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