Neutron Ionization of Helium near the Neutron-Alpha Particle Collision Resonance

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Abstract.

Neutron-impact single and double ionization cross sections of the He atom are calculated near the neutron-alpha particle collision resonance. Calculations using the time-dependent close-coupling method for total and differential cross sections are made at 8 incident neutron energies ranging from 250 keV to 2000 keV. At the resonance energy peak the double ionization cross sections unexpectedly become larger than the single ionization cross sections. This finding appears to be related to the high velocity of the recoiling alpha particle, which makes it unlikely that the atomic electrons can recombine with the alpha particle nucleus, enhancing the double ionization cross section.

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1. Introduction

The existence of dark matter has been inferred from a number of cosmological observations and searches for the nature of dark matter have now been underway for a number of years. However, dark matter direct detection experiments have so far failed to find any conclusive evidence for the nature of these elusive particles. One of the leading candidates of dark matter are weakly interacting massive particles (WIMPs). The search for these, while so far inconclusive, have however assumed that the WIMP mass is of the order of hundreds of GeV/c^2. However, if the mass of such WIMPs is in fact much lighter (or order GeV/c^2 or less), then the energy deposited by such particles in a detection system (typically large chambers of liquid xenon) is in the keV range, below the range of current experimental thresholds. This could provide an explanation as to why no evidence has yet emerged for WIMPs.

The detection of dark matter particles takes place through elastic dark matter-nucleus scattering. This process results in detection signatures via ionization (as the recoiling atom collides with its surrounding atoms), scintillation, or the production of heat in the detector. During the elastic dark matter-nucleus scattering, it is normally assumed that the atomic electrons immediately follow the motion of the nucleus. In reality it takes time for the electrons to catch up with the nucleus; a process that can result in ionization or excitation of the atomic electrons. In the nuclear physics literature this is termed the Migdal effect [1, 2, 3, 4, 5, 6] and is also a variant of the "sudden approximation". This has recently been discussed in detail [7, 8] where analysis has been done that shows that the Migdal effect may significantly enhance the direct detection sensitivity to lighter (sub-GeV) dark matter candidates. A number of previous studies have been made that explore the

A convenient proxy for the scattering of WIMPs by nuclei can be found in the elastic scattering of neutrons from nuclei. Neutrons, as neutral particles, have no Coulomb interaction with the nuclei or atomic electrons, which allows a reasonable analogy to hypothetical scattering of WIMPS from nuclei. Some recent work has been done in examining the ionization of Helium atoms that can result from such a process [9] building on earlier work [1, 10]. Other studies [11] explored the unique role (compared to photon or charged-particle scattering) that neutron scattering plays in investigating electronic correlation in small atoms. Because the neutron does not directly couple to the electrons, the sudden removal of the nucleus (from neutron elastic scattering) allows the atomic electrons to evolve due to only their mutual interactions, potentially resulting in break up patterns that are quite different from those expected in photon or electron ionization events. Subsequent studies [12, 13, 14] have examined excitations of light atoms by (elastic and inelastic) neutron scattering, including how electronic excitations are influenced by nuclear reactions.

In this paper we examine the neutron scattering from helium atoms, based on our previous work using a time-dependent close-coupling method [15, 16]. This work is a first step in exploring the Migdal effect for scattering from heavier atoms of relevance to dark matter searches. We examine significantly higher impact energies than in our previous work [16] and in addition present ionized electron angular distributions. This latter quantity provides useful information that can narrow the search range of future experimental searches for ionization events. Strongly anisotropic electron ejection would also provide a strong signature for future low-mass dark matter searches. The extension to higher neutron impact energies has uncovered some interesting physics that we discuss in this paper.

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

2. Theory

2.1. Neutron-Alpha Particle Collisions

Neutron-alpha particle cross sections are presented in Table 1 from tabulated values for head-on collisions [17]. These data are produced by taking the angular differential cross section for elastic scattering from alpha particles at an incident angle of zero degrees and multiplying by 4π (see [16] for details). These data are from the 'ENDF' (evaluated nuclear data format) compilations, which are derived from critically evaluated experimental and theoretical (often R-matrix) results, and are presented in the center-of-mass frame. In Figure 1 we present the *total* elastic cross section for neutron scattering from helium over a wide energy range. The difference in magnitude between the figure 1 data (total cross sections) and the data in Table 1 (from angular differential cross sections) is due to the anisotropy of the angular differential elastic scattering cross sections. The neutron-alpha particle collision resonance around 1120 keV is evident and arises from the $p_{3/2}$ nuclear state of the composite ^{5}He system (another $p_{1/2}$ resonant state lies at an energy of several MeV). This resonance has been extensively studied in the nuclear physics literature (eg [18, 19]) in exploration of few-body nuclear systems. Comprehensive R-matrix analyses of nuclear experimental data have been made [20], which has resulted in the ENDF data tabulations that we use here. The increase in cross section at very low energies is due to the inclusion of thermal broadening (to room temperature) effects on the incident neutron beam.

2.2. Neutron-Helium Atom Collisions

Neutron-helium atom cross sections for single and double ionization are calculated using the time-dependent close-coupling (TDCC) method [15, 16]. The close-coupled equations are given by:

$$i\frac{\partial P_{l_1 l_2}^{LM}(r_1, r_2, t)}{\partial t} = \sum_{i=1,2} (T_{l_i}(r_i)) P_{l_1 l_2}^{LM}(r_1, r_2, t)$$

$$+\sum_{l_1',l_2'} V^L_{l_1l_2,l_1'l_2'}(r_1,r_2)P^{LM}_{l_1'l_2'}(r_1,r_2,t)\ , \tag{1}$$

where $T_l(r)$ contains one-body kinetic and nuclear operators and is given by

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

and $V_{l_1l_2,l_1'l_2'}(r_1,r_2)$ are two-body interaction operators between the atomic electrons defined as

$$\begin{aligned} V^L_{l_1l_2,l_1'l_2'}(r_1,r_2) &= (-1)^{L+l_2+l_2'}\sqrt{(2l_1+1)(2l_1'+1)(2l_2+1)(2l_2'+1)} \\ &\times \sum_\lambda \frac{(r_1,r_2)^\lambda_<}{(r_1,r_2)^{\lambda+1}_>}\begin{pmatrix} l_1 & \lambda & l_1' \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_2 & \lambda & l_2' \\ 0 & 0 & 0\end{pmatrix} \\ &\times \begin{Bmatrix} L & l_2' & l_1' \\ \lambda & l_1 & l_2 \end{Bmatrix}\ . \end{aligned} \tag{3}$$

In equation (1), $P^{LM}_{l_1l_2}(r_1,r_2,t)$ is the time-dependent radial wave function for the two electrons that results from the expansion in spherical coordinates of the full time-dependent wavefunction [16]. The initial condition is given by:

$$\begin{aligned} P^{LM}_{l_1l_2}(r_1,r_2,t=0) &= \sum_{l_1',l_2'} \bar{P}^{L_0M_0}_{l_1'l_2'}(r_1,r_2) \\ &\times < (l_1,l_2)LM|e^{-iv(z_1+z_2)}|(l_1',l_2')L_0M_0 >\ , \end{aligned} \tag{4}$$

where the ground state wavefunctions, $\bar{P}^{L_0M_0}_{l_1'l_2'}(r_1,r_2)$, are obtained by relaxation of the close-coupled equations in imaginary time and v is the speed of the nucleus (alpha particle) moving off in the z direction after the neutron collision. The interaction of the neutron with the atom is entirely contained within this boundary condition, which is another way of expressing the sudden approximation. Migdal [?] and subsequent works use effectively the same approximation in their studies.

The total single ionization cross section for He is given by:

$$\begin{aligned} \sigma_{single}(n_1l_1,E_n) &= 2\sigma_{n\alpha}(E_n) \\ &\times \sum_L\sum_{l_2}\int_0^\infty dk_2|\hat{P}^L_{single}(n_1l_1,k_2l_2)|^2\ , \end{aligned} \tag{5}$$

where $\sigma_{n\alpha}(E_n)$ are the neutron-alpha particle cross sections and $\hat{P}^L_{single}(n_1l_1,k_2l_2)$ are single ionization probability amplitudes found by projecting $P^{LM}_{l_1l_2}(r_1,r_2,t\to\infty)$ from Eq.(1) onto products of single particle states, $P_{n_1l_1}(r_1)P_{k_2l_2}(r_2)$. The factor of two in equation 3 arises from the indistinguishability of the two electrons. Here, $P_{nl}(r)$ are radial functions for a bound nl state, and $P_{kl}(r)$ are radial functions for continuum states with orbital angular momentum l and linear momentum k. The bound states are obtained by diagonalization of the one-electron Hamiltonian and the continuum orbitals are obtained by solving the radial Schrödinger equation [16]. The angle differential cross section for the single ionization of He may also be expressed in terms of the products of neutron-alpha particle cross sections and single ionization probability amplitudes.

The total double ionization cross section for He is given by:

$$\sigma_{double}(E_n) = \sigma_{n\alpha}(E_n) \times \sum_L \sum_{l_1,l_2} \int_0^\infty dk_1 \int_0^\infty dk_2 |\hat{P}^L_{double}(k_1 l_1, k_2 l_2)|^2 \ , \qquad (6)$$

where $\hat{P}^L_{double}(k_1 l_1, k_2 l_2)$ are double ionization probability amplitudes found by projecting $P^{LM}_{l_1 l_2}(r_1, r_2, t \to \infty)$ from Eq.(1) onto products of single particle states, $P_{k_1 l_1}(r_1) P_{k_2 l_2}(r_2)$. The angle differential cross section for the double ionization of He may also be expressed in terms of the products of neutron-alpha particle cross sections and double ionization probability amplitudes.

3. Results

We solved the time-dependent close-coupled equations using a 720 × 720 point radial lattice with a mesh spacing of $\Delta r_1 = \Delta r_2 = 0.20$ a.u. partitioned over 5184 cores on a parallel computer. Relaxation of the TDCC equations in imaginary time used 4 coupled channels while propagation of the TDCC equations in real time used 16 coupled channels. Spot checks on the convergence of the resulting cross sections were made by varying radial meshes and the energy grid for the continuum states used in the projections in Eqs. 3 and 4. These checks confirm that our cross sections appear well converged.

Angle differential cross sections for the single ionization of He are presented in Figure 2 for a fixed ejected electron momentum of 1.0 a.u. At these energies (and at other energies, not shown), the electron is predominantly ejected at angles around 180^o, that is, back along the incident neutron direction and in a direction opposite to that of the recoiling nucleus, which is to be expected from momentum conservation. The change in magnitude of the angular distributions reflect two factors. The first is the rapid increase in the single ionization cross section from 500 kE to around 1000 keV, after which the cross section slowly decreases (see Table 2). The increase in the total cross section is reflected in the much larger angular differential cross section at 1000 keV (figure 2b). For angular distributions at higher energies (figure 2c and 2d), the angular cross sections are smaller at this fixed electron momenta. Ionization resulting in an electron with 1 a.u. is now less probable than ionization resulting in electrons with larger momentum values. These quite highly anisotropic angular distributions will help constrain the required range of detection of these ejected electrons in future neutron scattering experiments.

For double ionization of helium by neutron-impact, angular differential cross sections may be characterized by the energy sharing between the two ionized electrons as well as their escape angles with respect to the z-axis defined by the incoming neutron direction. Thus the cross section units are cm^2 per (electron) momentum squared and per solid angle squared. Here we only focus on the equal energy sharing break-up as a function of electron angle and impact energy. In figure 3 we present angle differential cross sections for a zero degree fixed ejection angle of one electron and for four incident neutron energies as indicated. In this example, the momenta of the two ionized electrons are set equal at 1.0 a.u. (which is near the cross section maximum at 500 keV incident neutron energy). We find that the electrons are ejected back-to-back, 180^o apart, which is consistent with their mutual Coulomb repulsion after the sudden removal of the nucleus. The magnitude of the differential cross sections peaks at an incident neutron energy of 1000 keV, and then decreases rather quickly for this example where the ejected electron momenta are fixed. This is again mostly because the peak of the energy differential cross section moves to higher electron energies as the incident neutron energy is increased.

In Figure 4 we show the angular differential cross sections for double ionization at a fixed incident neutron energy of 1000 keV and for various fixed ejection angles of one of the outgoing electrons. We find that, as the fixed angle of electron 1 is increased, the cross section decreases and more structure is visible in the angular distributions. This structure reflects the coupling between the two outgoing electrons that is described by the spherical harmonic coupling found in the angular differential cross section expression [16]. We note that the dominant ejection mechanism of back-to-back emission is consistent with the findings of the earlier study of Berakdar [11], who examined ionization induced by neutrons at much lower impact energies. Our cross sections are also of a similar magnitude to those obtained by Berakdar.

Total cross sections for the neutron-impact single and double ionization of He are presented in Table 2. Our calculations of the single and double ionization of He by neutron impact appear to track the nuclear resonance that occurs for impact energies around 1120 keV. The single ionization cross sections peak at 1000 keV, whereas the double ionization cross sections peak at slightly higher energies (near 1250 keV). Moreover, we find that, unexpectedly, our double ionization cross sections become larger than our single ionization cross sections at around 1250 keV. We find that, at incident neutron energies above 1500 keV, the double ionization cross section is almost twice that of the single ionization cross section. This is the opposite of other multiple ionization processes, such as by photon or electron impact, where normally the double ionization is a few percent of the single ionization cross section.

In this case the enhancement of the double ionization cross section appears to arise from a consequence of the Migdal effect. That is, at higher neutron impact energies the Helium nucleus moves off with considerable speed. The electrons take some time to 'catch up' with the recoiling nucleus, and it appears that one electron catching up with the atom is less probable than neither electrons catching up, which results in a double ionization cross section that is larger than the single ionization cross section.

This may be further understood by considering the relative velocities of the particles, and by remembering that recombination of the electrons with the alpha particle will be most probable when the velocities of the electrons and recoiling alpha particle are similar. At low neutron-impact energies (eg 250 keV), the alpha particle recoil velocity ($= 0.4 v_{neutron}$) [16] is around 1.26 atomic units. For an equivalent electron velocity, the electron energy should be around 22 eV. This is comfortably within the 79 eV of energy available to the two helium electrons after the nucleus suddenly 'disappears', and there is even sufficient available energy for both electrons to match the alpha particle velocity and possibly recombine with the nucleus. However, at a neutron-impact energy of 1000 keV, the electron energy that is required to match the recoiling alpha-particle velocity is around 87 eV, which is larger than 79 eV. This makes single ionization more probable, and double ionization highly probable, since it is unlikely that either electron will be able to match the velocity of the recoiling alpha particle and recombine. Therefore, at neutron impact energies that result in a fast alpha particle recoil, the helium electrons may never be able to catch up with the alpha particle, which makes double ionization a much more probable process compared to lower neutron impact energies. This somewhat unexpected finding implies that multiple ionization processes should also be accounted for in dark matter studies, unlike recent work that only included single ionization [7].

4. Summary

In conclusion, we have carried out time-dependent close-coupling calculations for the neutron-impact ionization of the He atom. Our extension of previous work [16] to higher energies has explored the effect of the neutron-alpha particle collision resonance on the single and double ionization cross sections of Helium. In particular, at energies around and above the resonance position, the double ionization cross sections become larger than the single ionization cross sections.

We note that this work is just the first of many steps that will be needed to provide comprehensive theoretical support to ongoing searches for dark matter interactions with atoms. Subsequent work will include studies of the energy and angular distributions of ejected electrons from dark matter-relevant experiments (Ge and Xe), from both valence and inner shells. Some of this work may require relativistic treatments of the ionization process.

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Table 1. Neutron-Alpha Particle Cross Sections obtained from the ENDF database [17]. (1.0 b = 1.0 × 10^{-24} cm^2)

Energy (keV)	Cross Section (b)
250	0.172
500	0.452
750	4.339
1000	13.245
1250	16.424
1500	14.263
1750	11.846
2000	10.137

Table 2. Neutron-Helium Atom Cross Sections (1.0 b = 1.0 × 10^{-24} cm^2)

Energy (keV)	Single Ionization Cross Section (b)	Double Ionization Cross Section (b)
250	0.088	0.005
500	0.254	0.047
750	2.001	0.797
1000	4.618	3.159
1250	4.223	4.408
1500	2.699	3.993
1750	1.662	3.316
2000	1.067	2.766

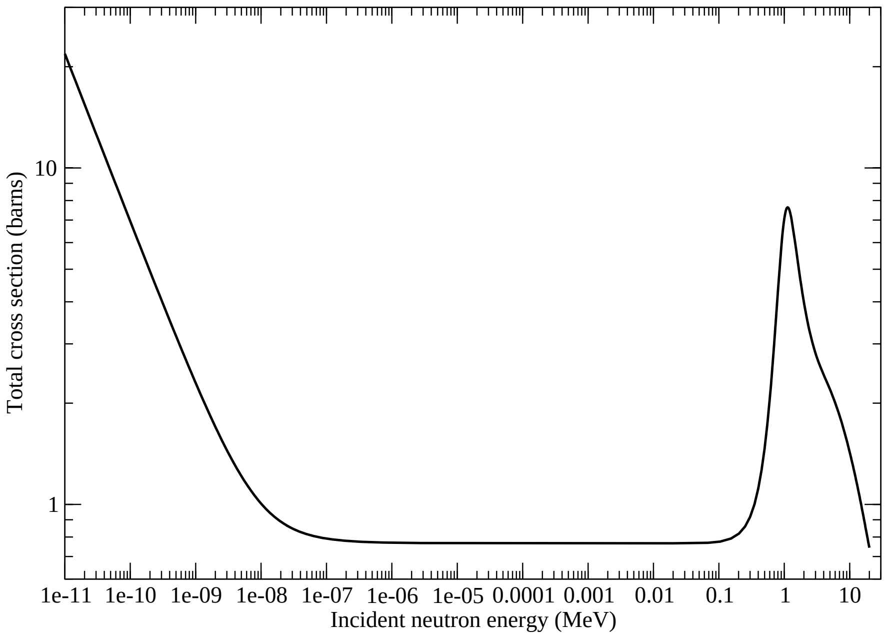

Figure 1. Total cross sections for elastic scattering of neutrons from helium, as obtained from the ENDF data compilation [17, 20].

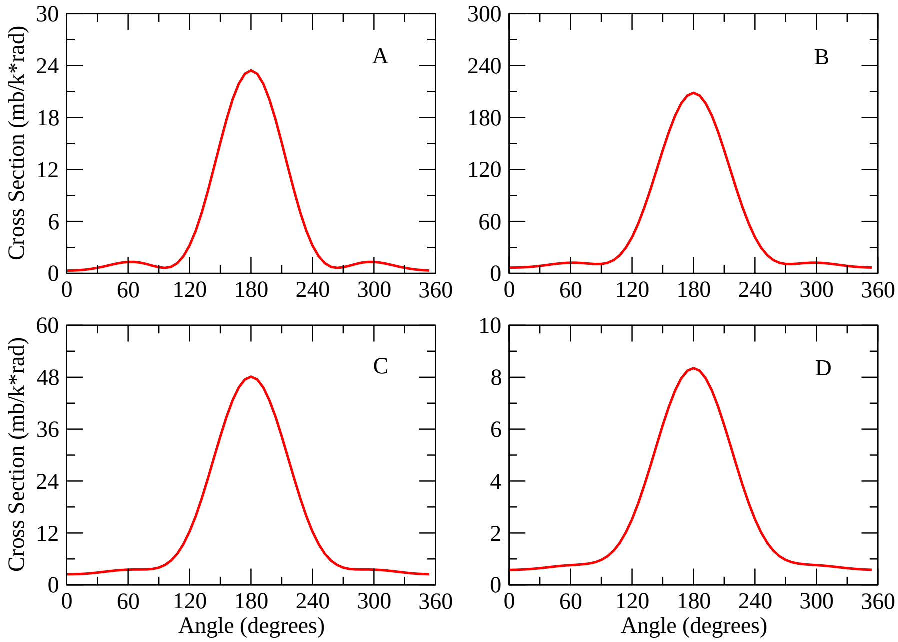

Figure 2. Neutron single ionization of He, Differential cross section with $k = 1.0$ and $\phi = 0$, A. 500 keV, B. 1000 keV, C. 1500 keV, D. 2000 keV, (1.0 mb = 1.0×10^{-27} cm^2, k = momentum in au, rad = solid angle in radians).

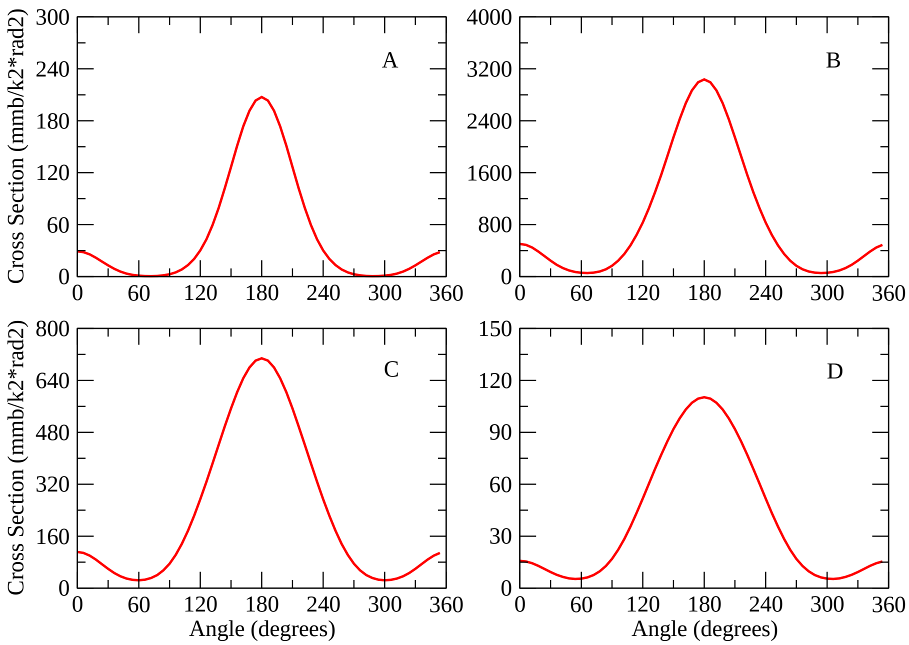

Figure 3. Neutron double ionization of He, Differential cross section with $k_1 = k_2 = 1.0$ and $\theta_1 = \phi_1 = \phi_2 = 0$, A. 500 keV, B. 1000 keV, C. 1500 keV, D. 2000 keV, (1.0 mmb $= 1.0 \times 10^{-30}$ cm^2, k2 = momentum in au squared, rad2 = solid angle in radians squared).

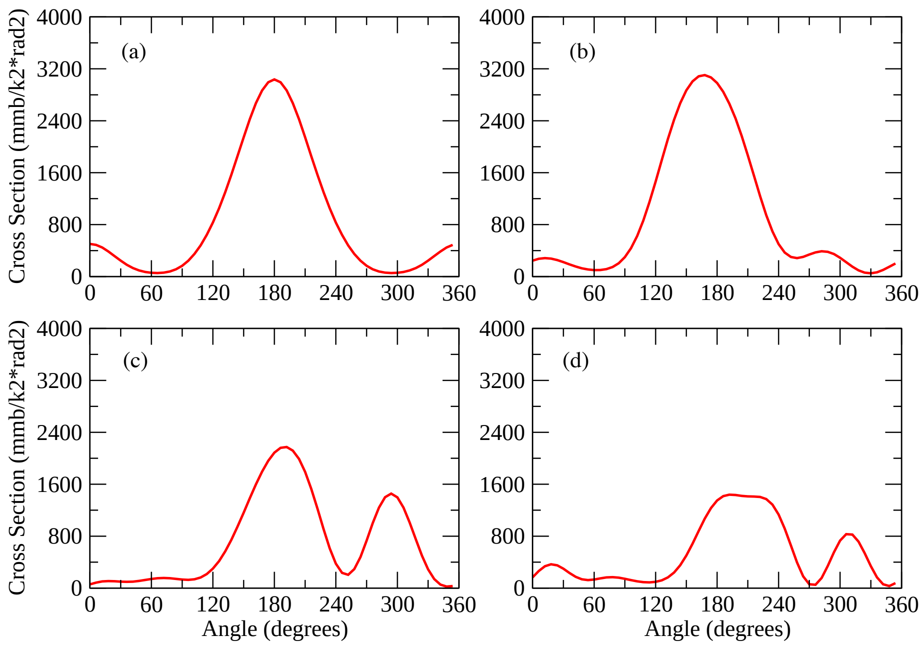

Figure 4. Same as figure 3, except for a fixed neutron impact energy of 1000 keV and for various fixed angles of electron 1: (a) $\theta_1 = 0^o$; (b) $\theta_1 = 30^o$; (c) $\theta_1 = 60^o$; and (d) $\theta_1 = 90^o$; (1.0 mmb = 1.0×10^{-30} cm^2, k2 = momentum in au squared, rad2 = solid angle in radians squared).