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Neutron Ionization of Germanium

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ABSTRACT: Neutron-impact single and double ionization cross sections of the Ge atom are calculated. Cross sections for the single and double ionization of the 4p and 4s subshells are found for neutron incident energies of 1.0 MeV, 2.0 MeV, 3.0 MeV and 4.0 MeV

1. INTRODUCTION

Non-perturbative methods have been used to calculate the neutron-impact ionization of Helium. Both the Exterior Complex Scaling (ECS) method[1] and the Time-Dependent Close-Coupling (TDCC) method[2] were found to yield cross sections for the single and double ionization of the He atom that were in good agreement over an energy range from 0.0 to 150.0 keV. Recently the TDCC calculations have been extended to calculate cross sections for the single and double ionization of the He atom up to energies of 2000.0 keV[3].

The study of the neutron 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.

In this paper we use the TDCC method to examine the ionization of the Ge atom. Cross sections for the single and double ionization of the 4p and 4s subshells are found for neutron incident energies from 1.0 MeV to 4.0 MeV.

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 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-Germanium Nuclear Collisions

Neutron-Germanium ($Z = 32, A = 72$) nuclear cross sections are presented in Table 1 from tabulated values for head-on collisions[4]. The cross sections in Table 1 are obtained by multiplying the head-on collision cross sections at 0.0 degrees by 4π.

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 m_t is the target nuclear mass. For Ge atoms:

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

2.2. Neutron-Germanium Atomic Collisions

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

$$i\frac{\partial P_{l_1 l_2}^{LM}(r_1, r_2, t)}{\partial t} = (T_{l_1}(r_1) + T_{l_2}(r_2))P_{l_1 l_2}^{LM}(r_1, r_2, t) + \sum_{l_1', l_2'} V_{l_1 l_2, l_1' l_2'}^{L}(r_1, r_2) P_{l_1' l_2'}^{LM}(r_1, r_2, t) \ , \tag{3}$$

where $T_{l_i}(r_i)$ is the one-body interaction operator and $V_{l_1 l_2, l_1' l_2'}^{L}(r_1, r_2)$ is the two-body interaction operator. For Ge the one-body interaction operator is given by:

$$T_l(r) = -\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{2r^2} - \frac{32}{r} + V_l^{HX}(r) \ , \tag{4}$$

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

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

$$\sigma_{single}(n_1 l_1, E_n) = \sigma_{nGe}(E_n) \times 2 \sum_L \sum_{l_2} \int_0^\infty dk_2 |\hat{P}_{single}^{L}(n_1 l_1, k_2 l_2)|^2 \ , \tag{5}$$

where $\sigma_{nGe}(E_n)$ are the neutron-Ge nuclear cross sections and $\hat{P}_{single}^{L}(n_1 l_1, k_2 l_2)$ 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 for Ge is given by:

$$\sigma_{double}(E_n) = \sigma_{nGe}(E_n) \times \sum_L \sum_{l_1, l_2} \int_0^\infty dk_1 \int_0^\infty dk_2 |\hat{P}_{double}^{L}(k_1 l_1, k_2 l_2)|^2 \ , \tag{6}$$

where $\hat{P}_{double}^{L}(k_1 l_1, k_2 l_2)$ 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

Following a Hartree-Fock calculation[5] for the $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$ configuration of Ge^{2+}, a complete set of bound $P_{nl}(r)$ and continuum $P_{kl}(r)$ orbitals for Ge^+ were calculated by solving the radial Schrodinger equation. For each l a local exchange potential parameter is adjusted so that the single particle energies for the active outer subshells match the experimental binding energies[6], where available.

3.1. Ionization of the $4p^2$ subshell

We employ a 480×480 point radial lattice with a uniform mesh spacing of $\Delta r_1 = \Delta r_2 = 0.20$. The 5s orbital has a binding energy of -8.18 eV, the 4p orbital has a binding energy of -15.92 eV, the 4d orbital has a binding energy of -

6.68 eV, and the 4f orbital has a binding energy of -3.50 eV. Bound orbitals are generated for l = 0-6 with the l = 0-2 being pseudo-orbitals. The use of pseudo-orbitals prevents the unphysical excitation of the 1s, 2s, 2p, 3s, 3p, 3d, and 4s filled subshells. Continuum orbitals are also generated for l = 0-6. For each l we used 200 continuum orbitals with $\Delta k = 0.02$, that is up to k = 4.0. Atomic cross sections are presented in Table 2. The double ionization cross sections from Eq.(6) are generally much smaller than the single ionization cross sections from Eq.(5).

3.2. Ionization of the $4s^2$ subshell

Again we employ a 480 × 480 point radial lattice with a uniform mesh spacing of $\Delta r_1 = \Delta r_2 = 0.20$. The 4s orbital has a binding energy of -23.78 eV, while the 4p, 4d, and 4f orbitals have the same energies as before. Bound and continuum orbitals were generated for l = 0-6 with l = 0-2 bound pseudo-orbitals. Atomic cross sections are presented in Table 3. The single and double ionization cross sections for the $4s^2$ subshell are much smaller than the cross sections for the $4p^2$ subshell.

4. SUMMARY

In this paper we presented calculations for the neutron-impact single and double ionization of the 4p and 4s subshells of Ge at incident energies between 1.0 MeV and 4.0 MeV using a TDCC method. The ratio of double to single ionization cross sections at 4.0 MeV was found to be 0.0158 for the 4p subshell and 0.0028 for the 4s subshell.

In the future we plan to carry out more TDCC calculations for the neutron ionization of atoms. In particular the existing codes could be used for the neutron ionization of the outer subshells of the C and F atoms.

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[6] [https:/physics.nist.gov/PhysRefData /Handbook/Tables]

Table 1. Neutron + Ge Nuclear Cross Sections (1.0 b = 1.0 × 10^{-24} 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 2. Neutron + Ge Atomic Cross Sections (1.0 b = 1.0 × 10^{-24} cm^2)

Energy	4p Single Ionization Cross Section	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 3. Neutron + Ge Atomic Cross Sections (1.0 b = 1.0 × 10^{-24} cm^2)

Energy	4s Single Ionization Cross Section	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