Abstract

WALKER, CARRIE L. Neutron Capture Measurements on $^{97}\text{Mo}$ with the DANCE Array. (Under the direction of Gary Mitchell and Undraa Agvaanluvsan.)

Neutron capture is a process that is crucial to understanding nucleosynthesis, reactors, and nuclear weapons. Precise knowledge of neutron capture cross-sections and level densities is necessary in order to model these high-flux environments. High-confidence spin and parity assignments for neutron resonances are of critical importance to this end. For nuclei in the $A=100$ mass region, the p-wave neutron strength function is at a maximum, and the s-wave strength function is at a minimum, producing up to six possible $J^\pi$ combinations. Parity determination becomes important to assigning spins in this mass region, and the large number of spin groups adds complexity to the problem. In this work, spins and parities for $^{97}\text{Mo}$ resonances are assigned, and best fit models for photon strength function and level density are determined. The neutron capture-cross section for $^{97}\text{Mo}$ is also determined, as are resonance parameters for neutron energies ranging from 16 eV to 2 keV.
Neutron Capture Measurements on $^{97}$Mo with the DANCE Array

by
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A dissertation submitted to the Graduate Faculty of North Carolina State University in partial fulfillment of the requirements for the Degree of Doctor of Philosophy

Physics

Raleigh, North Carolina

2013

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Biography

I come from the small college town of Oxford, Mississippi. I attended primary and secondary school in the Oxford School District, where I discovered early on a love for mathematics and, later, physics. In 2002 I graduated from high school second in my class and entered my first year as a physics major at the University of Southern Mississippi. While at USM I enrolled in the Honors College and completed my honors thesis under the direction of Dr. Alina Gearba. I also completed two undergraduate internships at the National Institute of Standards and Technology studying ultracold atomic physics under Dr. Trey Porto, Dr. Paul Lett, and Dr. Jennifer Strabley. In 2006, I moved to Raleigh, North Carolina to begin my graduate studies at North Carolina State University. It was there that I met Dr. Gary Mitchell and decided to join his research group. I’ve been conducting nuclear physics research ever since, crossing the country a few times and finally settling down in Los Alamos, New Mexico.
Acknowledgements

First, I want to say thanks to all the other DANCE experimentalists who welcomed me into the group and gave me a place to learn. John Ullmann and Aaron Couture – you guys have been immensely helpful to me every step of the way. Thank you, Milan Krticka, for all your assistance with DICEBOX modeling. Your talents in this field are unparalleled, and I deeply appreciated the input and expertise you’ve offered.

A very special thanks to Bayar, who, over the course of several years, has been a constant guide and occasional sounding board in this long process. I believe that only google has fielded more questions from me than you!

Another special thank you to Undraa, who took me under her wing and really went above and beyond to show me new opportunities and encourage my curiosity. I have always admired and been inspired by the passion for what you do and your ability to communicate it so enthusiastically to others.

I also want to thank those people who have inspired and supported my education since it’s early days. Thanks, Mr. Reidy, for being the coolest stinking science teacher ever! Your knowledge, enthusiasm and candor lit up those long, boring days at OHS. Thank you, Dr. Maung, Dr. Mead, and Dr. Whitehead for guiding and pushing me in my study of physics at USM. You guys really never failed me, and I can’t begin to tell you how useful all your instruction has been! Dr. Gearba: thank you for taking time to introduce me to research. I made mistakes of all kinds, but you encouraged me to keep going. That meant a lot to me. I’d also like to express my deep gratitude to Dr. Hannelore Giles and the late Dr. William Giles, who supported my undergraduate education through their generous contributions to the USM Presidential Scholarship program.

On a very personal note, I’d like to thank all my special loved ones. My parents, who have always offered their unconditional love. Mary Alice, Lindsey, Nancy, Megan, Brittney, Paula, Kaycee, Georgina, for all your emotional support. Thanks, Toby and Sierra, for lifting my spirits in the worst of times. And especially Bryan, my best friend, my better half – thanks for letting me lean on you. I love you all!

Most of all, I owe a great debt of gratitude to my advisor and mentor Dr. Gary Mitchell. You took a chance on me and generously supported me for seven long years. I appreciate all the time, effort, and patience that was no doubt expended in serving as my mentor. I cannot easily put into words how much this opportunity has meant to me or how much I’ve appreciated your kindness and, at times, your candor. Also, your advice was never wrong.
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Chapter 1

Introduction

The modeling of nuclear reactions for energy and defense applications requires knowledge of nuclear cross sections, some of which are difficult to measure experimentally. These must be calculated using theoretical models, such as those implementing Hauser-Feshbach theory. Both nuclear level densities and photon strength functions are key components of calculated cross sections for nuclear reactions, and they must be known for a broad range of isotopes and nuclear temperatures.

The calculation of nuclear level densities relies in part on high-confidence spin and parity assignments for neutron resonances. Spin determination for many nuclei can be problematic, particularly for those in the mass range of $A = 100$. The centrifugal potential barrier typically suppresses the formation of resonances with angular momentum higher than $\ell = 0$. However, for nuclei in this mass region the p-wave neutron strength function is at a maximum, and the s-wave strength function is at a minimum. As a result, the expected number of p-wave resonances is roughly equal to the number of s-wave resonances. There are then six possible $J^\pi$ combinations to consider: s-wave resonances can have two different spin values, and p-wave resonances up to four spin values. Given this complication, determining the parity of resonances is also particularly important. The spins and parities of many documented resonances in this mass region are unknown, and current nuclear data libraries often disagree in cases where assignments do exist. Thus there is a need for spin and parity assignment methods that improve upon existing results.

After neutron capture, an excited nucleus commonly decays to its ground state by sequentially emitting several $\gamma$ rays. Parity and angular momentum must be conserved for each transition, and the emitted radiation is primarily E1, M1, or E2, in accordance with Weisskopf estimates. The spin and parity of the capture state influences the cascade pattern, specifically the “multiplicity” of the cascade, or the number of transitions emitted to reach the ground state. The multiplicity of $\gamma$ rays for a nuclear cascade can then provide information as to the spin of the resonance. The Detector for Advanced Neutron Capture Experiments (DANCE) is well-
suited for measuring multiplicity distributions and for assigning resonance spins. DANCE is a highly segmented 4π γ-ray calorimeter array located at the Los Alamos Neutron Science Center (LANSCE), which provides a white beam of spallation neutrons for experiments. At DANCE the full Q-value of the reaction is detected with high efficiency, while detailed γ-ray multiplicity information is preserved, as well as individual γ-ray energy and time-of-flight information.

Distinguishing s-wave resonances from p-wave resonances historically has proven to be a difficult task. Resonances whose strengths fall between the expected values for s- and p-waves are particularly hard to assign. This ambiguity in parity assignments is dealt with using simulations of γ decay with the Monte Carlo code DICEBOX. Spectra from γ decay are simulated using details from a combination of known nuclear levels and levels which are artificially generated from level density (LD) and photon strength function (PSF) models. The γ-ray spectra from two-step cascades in particular can give strong indications of the parity of the resonance.

Once the parities of resonances have been determined, a statistical approach is employed to analyze γ-ray multiplicity distributions for spin assignments. For each resonance, the normalized experimental yields for each multiplicity constitute an N-dimensional vector, where N is the total number of multiplicities considered. In this multi-dimensional “multiplicity space,” the vectors fall into localized clusters, one per spin group. Using the well-known method of pattern recognition, probability density functions (PDFs) are extracted to make spin assignments. This statistical approach offers many advantages over previous methods. This method offers improved sensitivity over those using only average multiplicities by utilizing all of the multiplicity distribution information. It even offers advantages over some newer methods by eliminating the need to rely on a prototype resonance to determine an ideal multiplicity distribution for each spin group. This feature allows for variations in distributions due to both Porter-Thomas fluctuations and experimental error. The explicit use of a PDF also provides quantification of the certainty of assignments.

Experimental data from $^{97}$Mo is examined, where six $J^\pi$ combinations for resonances are possible. The task of separating p-wave spin groups pushes the limits of the computational capability of this method, but given large enough sample sizes, high-confidence spin assignments can be extracted for roughly half of the resonances. For the rest of the resonances, two possible spin values can be assigned. In addition, LD and PSF model parameters have been determined. Experimentally obtained γ-ray spectra have a complex dependence on both the LD and the PSFs. Recovering these parameters from experiment is not straightforward. Several combinations of both the LD and the PSFs are explored until optimum parameters from best fit models are obtained. Additional resonance parameters such as $\Gamma_\gamma$ and $\Gamma_n$ are also extracted from experimental data using the R-Matrix code SAMMY.
Chapter 2

Theory

2.1 Compound Nuclear Reactions

The physical theory describing nuclear reactions varies with the type and energy of the particles involved. In general, reactions can be categorized as either direct or compound. In direct reactions, the incident neutron passes through nucleus for a short time, only long enough to interact with one or a few nucleons. In the case of a compound reaction, the impinging particle thermalizes with the other nucleons of the target, creating a compound nucleus in an excited state. The compound nucleus has no “memory” of how it was formed; thus the mode of its formation and the mode of its decay are independent. This assumption is referred to as the Bohr hypothesis. Interaction times for compound reactions are much longer than those of direct reactions.

The excitation energy of the compound nucleus is equal to the neutron separation energy of the newly formed nucleus plus the kinetic energy of the incoming neutron. The compound nucleus may then decay by means of multiple channels available to it. In the absence of particle emission or fission, the nucleus transitions to an intermediate state by emitting a $\gamma$ ray. In this way multiple $\gamma$ rays may be emitted before the nucleus reaches its ground state. This series of $\gamma$ rays emitted is sometimes referred to as the $\gamma$-ray cascade.

2.2 R-Matrix Framework

R-Matrix theory is a convenient framework for dealing with many nuclear reactions. The assumptions underlying R-Matrix theory are as follows:

1. Nonrelativistic quantum mechanics are valid for the system, i.e., $H\Psi = E\Psi$, where the Hamiltonian defined in all space is the sum of the kinetic and potential energies of the system.
2. All processes in which more than two product nuclei are formed are ignored.

3. All processes of creation or destruction are ignored (most importantly, the creation or destruction of photons.)

4. Any two nuclei can be separated by some finite distance $a_c$ beyond which neither nucleus experiences any polarizing potential field from the other.

The collision matrix $U$ is defined as the amplitude of the outgoing waves in channel $c'$ that results from the unit-sized flux of collision in channel $c$. The channel notation $c$ specifies all the particles in the channel, including all quantum numbers describing them. The cross section $\sigma_{cc'}$ is then proportional to $|U_{c'c}|^2$. The $U$ matrix is both unitary and symmetric,

$$U^\dagger U = 1$$  \hspace{1cm} (2.1)

$$U_{p,q} = U_{-q,-p} = U_{q,p}$$  \hspace{1cm} (2.2)

following conservation of probability and time-reversal symmetry.

The matrix $U$ depends on energy $E$. “External” interactions, or those in the regions of incoming or outgoing channels, are represented by the diagonal matrices $L$ and $\Omega$. “Internal” interactions, or those occurring inside the compound nucleus, are represented by the non-diagonal matrix $R$. The division between these two regions is denoted by the nuclear radius $a_c$. This division is justified because the nuclear radius is reasonably well defined due to the short range of nuclear forces. The choice of $a_c$ imposes boundary conditions on the nuclear wave functions, giving rise to resonances in the reaction cross section.

The $R$-matrix is given by the equation

$$R_{cc'} = \sum_\lambda \gamma_{\lambda,c'} \gamma_{\lambda,c} \frac{E_{\lambda}}{(E_{\lambda} - E)}$$  \hspace{1cm} (2.3)

where $\lambda$ denotes a compound nuclear state or energy level. $\gamma_{\lambda}$ is the reduced width amplitude. $\gamma_{l,\lambda}^2$ is referred to as the reduced width of the energy level $E_{\lambda}$. Neither $\gamma_{\lambda}$ nor $E_{\lambda}$ depend on the energy of the incoming or outgoing channels.

$$\gamma_{l,\lambda}^2 = \hbar^2/(2mR)[u_{l,\lambda}(R)]^2$$  \hspace{1cm} (2.4)

2.2.1 Resonance Reactions

The $R$-matrix is made of contributions summed from all the levels of the compound nucleus. For low energy reactions and well-isolated resonances, one can assume that the reaction proceeds through only a single nuclear state. Then the cross section of the reaction channel is given by
the Breit-Wigner formula

\[ \sigma_{cc'}(E) = \frac{\pi}{k_a^2} \frac{\Gamma_{c\lambda} \Gamma_{c'\lambda}}{((E - E_\lambda)^2 + 1/4\Gamma_\lambda^2)}, \]  

(2.5)

where \( E \) is the incident energy, \( \Gamma_{c,\lambda} \) and \( \Gamma_{c',\lambda} \) are partial widths of the resonance in the entrance and exit channels, and \( \Gamma_{\lambda} \) is the total width, which is equal to the sum of the partial widths over all channels:

\[ \Gamma_{\lambda} = \sum_{c=1}^{N} \Gamma_{c,\lambda}, \]  

(2.6)

If the level width \( \Gamma \) is larger than the level spacing \( D \) of the nucleus, then the levels will overlap strongly. The R-matrix formalism is thus especially convenient when investigating neutron capture within energy regions containing well-isolated resonances.

### 2.3 Statistical Models of Nuclear Reactions

#### 2.3.1 Hauser Feshbach Theory

When examining aspects of reactions that are not limited to well-isolated resonances, an approach using transmission coefficients is convenient. Hauser-Feshbach theory provides this kind of formulation for reactions that involve contributions from a large number of compound nuclear states. Assuming that the Bohr assumption is still valid, the cross section for a reaction channel can be written as a product of its formation (or, fusion) cross-section and the probability that it will decay into the exit channel b

\[ \sigma_{ab} = \sigma_a P_b. \]  

(2.7)

Assuming time-reversal invariance of the system, then the reaction cross section will satisfy the following relation

\[ k_a^2 \sigma_{ab} = k_b^2 \sigma_{ba}, \]  

(2.8)

where \( \sigma_{ba} \) is the cross section of the inverse reaction. This principle is often referred to as the principle of detailed balance. By introducing the transmission coefficient

\[ T_a = 1 - |U_{aa}|^2, \]  

(2.9)

then the compound reaction cross section in the spinless case may be written as

\[ \sigma_{ab}^{HF} = \frac{\pi}{k_a^2} (2l + 1) \frac{T_a T_b}{\sum_{\gamma} T_{\gamma}}, \]  

(2.10)

However, to generalize to particles with non-zero spin, a statistical weighting factor must
be applied to account for the probability of the channel having a total spin of \( s \) given its constituents. The generalized cross section becomes

\[
\sigma_{ab}^{HF} = \frac{\pi}{k_a^2} \sum_{J, \pi} \frac{(2J + 1)}{(2I + 1)(2i + 1)} T_a T_b \sum_{\gamma} T_\gamma, \tag{2.11}
\]

where \( I \) is the spin of the target nucleus, \( i \) is the spin of the projectile, and \( J \) is total angular momentum sum of \( i+I+\ell \). When concerned with \((n, \gamma)\) reactions, the transmission coefficients are typically treated as the product of two components, the photon strength function \( f^{XL}(E_\gamma) \) and the level density \( \rho(E, J) \).

### 2.4 Level Density

The level density of a nucleus, and in this case of the compound nucleus, is defined as the number of energy levels within a given interval of energy. Theoretically, the level density of the nucleus could be calculated if all the eigenvalues of its Hamiltonian were known. However, this is only possible for the simplest of nuclear models. In practice, nuclear level densities are determined experimentally. At low excitation energies, the energy levels of the nucleus are spaced at intervals much larger than the widths of the states themselves. As excitation energy increases, the number of levels increases, and eventually the nuclear levels are no longer well separated. This region is referred to as the continuum region, and the level density function

\[
\rho(E) = \frac{dN(E)}{dE} \tag{2.12}
\]

can be described using various models, where \( N(E) \) is the cumulative number of levels below an excitation energy \( E \).

#### 2.4.1 Constant Temperature Model

One such model is the Constant Temperature Formula. In this model the nucleus is treated as a Fermi gas with a fixed temperature and chemical potential. In terms of the particle number \( A \) and system energy \( E \), the level density takes the form

\[
\rho(E, J) = \frac{f(J)}{T} e^{(E-E_o)/T}, \tag{2.13}
\]

where \( T \) is the nuclear temperature and \( E_o \) is the energy backshift. \( f(J) \) is a statistical spin distribution factor that denotes the probability that a randomly chosen energy level has spin \( J \)

\[
f(E, J) = \frac{(2J + 1)}{(2\sigma_c^2)} e^{-\left(J+\frac{1}{2}\right)^2/2\sigma_c^2} \tag{2.14}
\]
where $\sigma_c$ is the spin cutoff parameter. Based on empirical evidence, $\sigma_c$ has the form

$$\sigma_c = 0.98A^{0.29},$$

(2.15)

where $A$ is the mass number of the nucleus.

### 2.4.2 Back-Shifted Fermi Gas Model

The constant temperature formula may be augmented by considering the fact that fermions tend to form pairs. This pairing energy can be included by introducing a shift $E_1$ in the nuclear excitation energy. This model is referred to as the Back-Shifted Fermi Gas (BSFG) and alters the spin cutoff parameter in the following way

$$\sigma_c^2 = 0.0888A^{2/3}\sqrt{a(E - E_1)},$$

(2.16)

where $a$ and $E_1$ are adjustable parameters that are fit using experimental level densities found at low excitation energies for that nucleus.

Von Egidy [1] suggested simplifying the spin cutoff parameter to

$$\sigma_c^2 = 0.391A^{0.675}(E - Pd')^{0.312}.$$ (2.17)

### 2.5 Photon Strength Functions

The other component of the transmission coefficient is the photon strength function, sometimes referred to as the radiative strength function. The photon strength function (PSF) is related to the average partial radiation width from an initial state $i$ to a final state $f$

$$\langle \Gamma_{\gamma i f}^{XL} \rangle = \frac{f_{XL}(E_i)E_{2L+1}^2}{\rho(E_i, J_i, \pi_i)},$$

(2.18)

where $XL$ denotes the multipolarity of the radiated photon. Transition probabilities decrease rapidly with increasing $L$, and magnetic transitions are also less likely than electric ones. The result is that $E1$, $M1$, and $E2$ transitions contribute most to any process. In general, the lowest multipolarity allowed by electromagnetic selection rules (ones that conserve angular momentum and parity) will be most likely to occur. Hence the form of the $E1$ PSF is the most important to consider.
2.5.1 Single Particle Model

The simplest model for the E1 PSF is the single particle model. This model does not depend on energy

\[ f_{E1}^{SP} = C \frac{A^{2/3}}{D_s}, \tag{2.19} \]

where \( C = 6.8 \times 10^{-8} \text{ MeV}^{-2} \) and \( D_s \) is the spacing of \( \ell = 0 \) single particle states.

2.5.2 Brink-Axel Model

A more realistic model incorporates the existence of the giant electric dipole resonance (GEDR) observed in \((\gamma,n)\) experiments. The GEDR can be understood as being caused by the collective dipole vibration of proton and neutron fluids within the nucleus. Brink hypothesized that the nature of the resonance was independent of excitation energy. Consequently, any photon strength function would not be a function of excitation energy, only of the energy of the transition. Assuming this hypothesis holds true, the principle of detailed balance for \((\gamma,n)\) and \((n,\gamma)\) reactions allows the PSF for the GEDR to be written

\[ f_{E1}^{(\gamma)} = \frac{1}{3(\pi \hbar c)^2} \frac{\sigma_0 E_G \Gamma_G^2}{(E_G^2 - E_G^2)^2 + E_G^2 \Gamma_G^2}, \tag{2.20} \]

where \( \sigma_0 \) is the peak cross section of the GEDR, \( E_G \) is the peak position of the GEDR, and \( \Gamma_G \) is its full width at half maximum. This model is referred to as either the Brink-Axel or the standard Lorentzian model (SLO). It begins to fail at energies near the neutron binding energy and also at low energies (1 - 2 MeV.)

2.5.3 Kadmenskij, Markushev and Furman Model

Another PSF model was proposed by Kadmenskij, Markushev and Furman (KMF) which is based on the theory of Fermi liquids (i.e., strongly interacting fermions.) The PSF is given by

\[ f_{E1}^{KMF}(E_\gamma, T) = \frac{1}{3(\pi \hbar c)^2} (0.7) \frac{\sigma_0 E_G \Gamma_G \Gamma(E_\gamma, T)}{(E_\gamma^2 - E_G^2)^2}. \tag{2.21} \]

Unlike the SLO model, the KMF model is temperature dependent; the strength function depends not only on the energy of the \( \gamma \) ray but also the excitation energy of the nucleus. This model performs well at the low energy tail of the GEDR, but it diverges as \( E_\gamma \to E_G \).
2.5.4 Generalized Lorentzian Model

Introduced by Kopecky and Chrien [2], the generalized Lorentzian (GLO) model modifies the KMF model by removing the divergence as $E_{\gamma} \rightarrow E_{G}$.

$$f_{GLO}^{E_1}(E_{\gamma}, T) = \frac{1}{3(\pi\hbar c)^2} (0.7) \sigma_0 \Gamma_G \left[ \frac{E_G \Gamma(E_{\gamma}, T)}{(E_{\gamma} - E_G^2)^2 + E_G^2 \Gamma^2(E_{\gamma}, T)} + (0.7) \frac{4\pi^2 T^2 \Gamma_G}{E_G^2} \right]. \quad (2.22)$$
Chapter 3

Experimental Techniques and Data Processing

3.1 The LANSCE Facility and DANCE

The neutron capture experiments described in this work were performed at the Los Alamos Neutron Science Center (LANSCE) using the Detector for Advanced Neutron Capture Exper-
iments (DANCE.) The center houses a linear accelerator which produces both positive and negative hydrogen ions and accelerates them to energies of up to 800 MeV. A proton storage ring (PSR) strips the ions and bunches them into 250 ns-wide pulses before they are injected into the Mark-III neutron spallation target at a rate of 20 Hz. The spallation target, located in the Lujan Center, is made of two cylinders of natural tungsten surrounded by light water and liquid hydrogen moderators. Each proton impinging on the target produces up to 17 neutrons. Beryllium reflectors push the neutron energy flux further into the thermal region. Neutrons then travel radially outward down various flight paths in the Lujan Center to be used for experiments (see Figure 3.1.)

Figure 3.2: Layout of flight path 14 and DANCE.

DANCE is located on flight path 14 (see Figure 3.2.) The flight path length for neutrons is approximately 20.3 m. Flight times of neutrons through the aluminum beam pipe range from hundreds of ns to 14 ms. Collimators are installed on FP14 to reduce the beam size to approximately 70 mm in diameter. The neutron flux at FP14 varies with accelerator operations and the performance of the spallation target. The typical flux distribution at DANCE is shown in Figure 3.3.

DANCE itself is a nearly $4\pi$ $\gamma$-ray calorimeter (see Figure 3.4.) The detector array comprises 160 BaF$_2$ scintillator crystals for $\gamma$-ray detection, each crystal subtending an equal solid angle. Each crystal is 15 cm long and 734 cm$^3$ in volume. Holes in the sphere allow for the entry and exit of the beam pipe. Targets are inserted via the beam pipe into the center of the array and kept under vacuum (0.05 torr) for the duration of data collection. Surrounding the beam pipe is a 6 cm-thick shell of $^6$LiH which serves to absorb scattered neutrons with minimal attenuation of $\gamma$ rays.

The high $\gamma$ detection efficiency of BaF$_2$ and the large solid angle coverage ensure that essentially all $\gamma$ rays from a nuclear cascade are detected. The total efficiency of DANCE for typical cascades of 3 or 4 photons is 95%. The high segmentation of the array allows for a
Figure 3.3: Neutron flux (neutrons/cm\(^2\)/eV/T\(_o\)) at the DANCE detector.

reliable measurement of the \(\gamma\)-ray multiplicity of the cascade. Scintillation signals from BaF\(_2\) contain a fast and a slow component, providing information on both event timing and the total energy deposited. The energy resolution of BaF\(_2\) is less than that of other scintillators but is sufficient to distinguish individual \(\gamma\) rays and measure the summed energy of each cascade.

Figure 3.4: A cross-sectional view of DANCE.
3.2 Data Acquisition

Each crystal’s light output is collected by its own PMT and split into two digitizer channels. The digitizers are triggered by a $T_o$ coming from the PSR beam burst plus a delay. Each channel records event information from the crystal over a set timing window. Together the channels typically cover 500 $\mu$s of looking time, corresponding to neutron energies of 8.5 eV to 2 MeV. The digitizers are capable of sampling at 500 MHz with 8-bit resolution and have 128 kb of fast memory. Since full utilization of the sampling rate would lead to data rates exceeding hundreds of TB per day, only fundamental parameters of the waveforms are extracted and written from each beam burst (see Figure 3.5). A constant fraction discriminator is used to identify events in a crystal. The following quantities are then recorded for each crystal event: a 100 ns-wide integral of the background baseline before the event; 32 points at the maximum sampling rate covering the leading edge of the event (the fast component); five 200 ns-wide integrals of the slow component, giving total energy deposition information; and two time stamps, one relative to a master clock and one relative to the beam pulse trigger $T_o$.

![Figure 3.5: A waveform and its extracted parameters.](image)

It takes about 40 ms to read out the digitizers, process the waveforms and write the compressed event information to a network RAID. The digitizers are rearmed in time for the next beam pulse, which comes every 50 ms. A time line of acquisition for each beam spill is shown in Figure 3.6.

This configuration for acquiring data is referred to as the double-continuous mode. Other
schemes for data acquisition have been utilized at DANCE and have been described elsewhere. The double continuous mode was the only mode implemented for the experiments discussed in this work.

### 3.3 Data Reconstruction

During offline analysis, physics events from each beam spill are reconstructed from the compressed data. Time stamps from each crystal signal within a narrow coincidence window (50 ns) are identified as one physics event. γ-ray cascades alone are not responsible for all physics events; α radiation originating in the crystals themselves is a significant source of background. Since radium is a chemical homologue of barium, there are traces of it within the BaF$_2$. Several isotopes of radium are α emitters. α particle events are distinguishable from γ-ray events by examining the relative amount of energy deposited in the fast component and slow component integrals of the scintillation signal. α particles deposit a greater fraction of their energy in the slow component of the signal than γ rays do. Also, the α-particles are emitted with discrete energies, while the γ rays are emitted with a continuous distribution of energies (see Figure 3.7). Thus a well-chosen gate on the ratio of the two components removes α particle events from the experimental data set.

Once only γ-ray events are left, the time stamp of the event relative to the trigger $T_0$ corresponds to the time-of-flight of the incident neutron. The energy of the neutron is calculated using the estimated flight path length and later is fine-tuned by fitting the time-of-flight spectrum to existing resonance data.

Many crystals fire during one physics event. However, the number of crystals fired may far exceed the number of γ rays emitted by the nuclear cascade. One γ ray may deposit its energy
in multiple adjacent crystals via Compton scattering. Thus the notion of cluster multiplicity is introduced. When multiple adjacent crystals fire within the same physics event, the energy deposited in the cluster is attributed to one γ ray. The cluster multiplicity, not crystal multiplicity, then serves as a more accurate measure of the γ-ray multiplicity of the cascade.

Energy calibrations of the crystals were made by using knowledge of the natural α radioactivity within the crystals. The α particles emitted originate from the $^{226}\text{Ra}$ and $^{228}\text{Ra}$ decay chains and have well-known, discrete energies. The energy peaks measured from the α particles were fit with a sum of five Gaussians. The resulting position of each gaussian’s center corresponds to known energies. The correlation of the known energies to the signal integrals are fit with a simple linear relation using these points.

$$E(x) = a + b \times x$$  \hspace{1cm} (3.1)

These constants were generated for each crystal on a run-by-run basis. A sample of these α fits is provided in Figure 3.8.

Because each PMT channel has a slightly different cable length, time stamps from all the

Figure 3.7: A contour plot of fast versus slow component integrals of signals. Integral units are arbitrary. Events inside the red gates are α particles.
digitizer channels are not perfectly aligned in time when data is recorded. Time stamps from each channel typically differ by less than 20 ns. In order to set a more narrow coincidence window and further reduce backgrounds, it is necessary to perform time calibrations for all the channels. Time stamps from all γ-ray cascade events are collected within a run, and the average time stamp was calculated. The deviation of each channel’s average from an arbitrarily chosen reference channel was calculated, and then applied as a corrective offset. The offsets for each channel are plotted in Figure 3.9 and illustrates how the channel timings are relatively stable over the course of the experiment.

### 3.4 Background Subtraction

The high total efficiency of the DANCE calorimeter allows selection of events with summed energies near the Q-value of the desired reaction. The Q-value of the $^{97}$Mo(n,γ) reaction is 8.642 MeV. The target used for capture measurements is a self-supporting foil of molybdenum enriched to 94.190% in $^{97}$Mo. The isotopic composition of the target is shown in Table 3.1.

Those isotopes with significantly lower Q-values than that of $^{97}$Mo will not have large contributions in the data as long as the summed energy threshold is set above those Q-values. The only isotope that presents a problem in the analysis is $^{95}$Mo, whose Q-value is only 512 keV above that of $^{97}$Mo. Due to the limited efficiency and energy resolution of DANCE, captures on
Figure 3.9: Time card deviations over the duration of experiment for multiple crystals. Channel offsets in ns are plotted versus run number.

Table 3.1: Molybdenum Target: Isotopic Composition

<table>
<thead>
<tr>
<th>A</th>
<th>Composition %</th>
<th>Q-value (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>92</td>
<td>0.216</td>
<td>8.070</td>
</tr>
<tr>
<td>94</td>
<td>0.190</td>
<td>7.369</td>
</tr>
<tr>
<td>95</td>
<td>0.470</td>
<td>9.154</td>
</tr>
<tr>
<td>96</td>
<td>1.250</td>
<td>6.821</td>
</tr>
<tr>
<td>97</td>
<td>94.190</td>
<td>8.642</td>
</tr>
<tr>
<td>98</td>
<td>3.370</td>
<td>5.925</td>
</tr>
<tr>
<td>100</td>
<td>0.307</td>
<td>5.398</td>
</tr>
</tbody>
</table>

\(^{95}\)Mo cannot be separated by a Q-value gate alone. While \(^{95}\)Mo makes up only a small fraction of the target mass, its thermal cross section is approximately six times higher than that of \(^{97}\)Mo. Nonetheless, contributions from \(^{95}\)Mo should be largely negligible, except near strong \(^{95}\)Mo resonances. The strongest resonances from \(^{95}\)Mo are indeed visible in the capture data, but only at energies far from the resonances of interest. By applying a summed-energy gate of 8.20 to 9.20 MeV, signal-to-noise is improved by a factor of 10 (see Figure 3.10).

The next largest source of background results from neutrons scattered into the detector and
Captured by barium. These events have multiple Q-value signatures corresponding to the various isotopes of barium present. The wide range of Q-values assures that scattering background is present regardless of where any summed-energy cut is placed.

Because the $\gamma$ rays from scattered neutrons originate within the crystals themselves, these events are highly localized within the detector, i.e., they have low cluster multiplicity. This is evident by examining the shape of Esum spectra for events of different multiplicities. As multiplicity increases, the portion of events above the 8.642 MeV Q-value decreases, so that by multiplicity three they are no longer a significant source of background. Because most real capture events have average multiplicities of 3 or 4, typically only contributions from multiplicities three and higher are considered in the analysis (see Figure 3.11). $\gamma$-ray spectra from multiplicity two events are still useful for determining parities and resonance spins, as will be discussed in the next chapter.

Typically the contribution from scattering is estimated by comparing data from the target in question to data from a target with a high ratio of scattering to capture. In this experiment, a target of $^{56}$Fe was used. Very few events result from capture on iron, leaving only events due to scattered neutrons capturing in the crystals. This provides both summed energy and $\gamma$-ray energy spectra while accurately reproducing the smooth behavior of the scattering cross section over neutron energies of interest. By normalizing the $^{56}$Fe data to the number of capture events with summed energies higher than the reaction Q-value, one can subtract the estimated
scattering background. However, given the relatively high $^{97}$Mo(n,γ) Q-value and the limited energy resolution of our system, there are few scattering events left to normalize to. Thus we suspect this method of subtraction may be unreliable for this case. The results of this method on the summed-energy spectrum are shown in Figure 3.12 and Figure 3.13.

In response, a second method of subtraction was pursued. By choosing convenient binning by neutron energy, one can estimate that the background from scattering is approximately constant over relevant neutron energies. A constant subtraction can then be applied to the data from each neutron energy bin. The value of the constant was estimated independently for each multiplicity, up to multiplicity five. The results of the background subtraction for multiplicity two are shown in Figure 3.14.
Figure 3.12: Multiplicity two summed energy spectra (MeV) from before (blue) and after (black) scattering subtraction. The iron data are shown in red.
Figure 3.13: Multiplicity three summed energy spectra (MeV) from before (blue) and after (black) scattering subtraction. Iron data shown in red.
Figure 3.14: Counts per neutron energy bin before (black) and after (blue) scattering background subtraction using binwise estimation.
Chapter 4

Spin and Parity Assignments

4.1 Previous methods

Determining the spins of resonances for odd-A nuclei can be problematic, as an impinging neutron with orbital angular momentum $\ell=0$ can form states of two different spin values. Those with $\ell=1$ (or, p-wave resonances) can form up to four different spin states. Several methods for assigning spins have been utilized in the recent past. Methods to which DANCE lends its strengths are ones that utilize multiplicity information. Because parity and angular momentum must be conserved, and lower order electric and magnetic transitions are highly favored, capture states of different spins and parities exhibit different cascade patterns. By examining the multiplicity distribution of events within a resonance, one may deduce the spin.

It is useful to define multiplicity yields for the purpose of explaining these methods. The total experimental yield can be written as a function of energy and broken down by multiplicity

$$Y(E_n) = \sum_{m=M_{min}}^{M_{max}} Y_m(E_n), \quad (4.1)$$

where $Y_m(E_n)$ is the yield of multiplicity $m$ at neutron energy $E_n$, and $M_{min}$ and $M_{max}$ are the lowest and highest multiplicities considered, respectively. For data acquired at DANCE, typically $M_{min} = 3$ and $M_{max} = 7$. For these purposes, any noted summation over multiplicities implies these limits unless stated otherwise.

4.1.1 Average Multiplicity

One simple method of assigning spins compares the average multiplicity of well-resolved resonances. The average multiplicity of a resonance is defined as
\[ \langle M \rangle = \sum_{m} m \int_{E_{\text{min}}}^{E_{\text{max}}} y_{m}(E), \]  

(4.2)

where \(E_{\text{min}}\) and \(E_{\text{max}}\) are the lower and upper bin edges (respectively) of the resonance, and \(y_{m}\) are normalized yields

\[ y_{m} = \frac{Y_{m}}{\sum_{m} Y_{m}}. \]  

(4.3)

When considering only s-wave capture, there are at most two spins that can be formed in the capture state of the compound nucleus. In the case of \(^{97}\text{Mo}\), the average multiplicities from many well-resolved, isolated resonances are plotted in Figure 4.1.

![Average Multiplicity of s-wave Resonances](image)

Figure 4.1: Average multiplicity of s-wave resonances.

Two groups are clearly visible; those with higher average multiplicity correspond to the higher spin group, requiring on average more steps to reach the ground state of the product nucleus. Those with lower average multiplicities correspond to the lower spin group.

This method fails, however, when resonances are weak or not well-resolved. For example, two unresolved resonances may each belong to a different spin group, and the average multiplicity will fall somewhere between the two spin groups. Most importantly, many nuclei have a smaller separation between the average multiplicities.
4.1.2 Oak Ridge Method

Another method was introduced by Koehler [3] which is based on the assumption that resonances of the same spin and parity will have the same multiplicity distribution. Two “prototype” resonances are selected, ones that are well isolated and whose spins are already known. The functions $Z_i^{(J)}(E)$ are introduced

$$Z_1^{(1)}(E) = \sum_m Y_m^{(1)}(E) - N_1 \sum_m Y_m^{(1)}(E) = 0$$  \hspace{1cm} (4.4)$$

$$Z_2^{(2)}(E) = \sum_m Y_m^{(2)}(E) - N_2 \sum_m Y_m^{(2)}(E) = 0,$$  \hspace{1cm} (4.5)

where $N_1$ and $N_2$ are normalization constants, and the subscripts (1) and (2) each denote a different spin group. Effectively, these prototypical multiplicity distributions are subtracted from the experimental distributions at each neutron energy, so that the residual yield function $Z_i$ peaks only at energies of spin $i$ resonances. The normalization constants $N_i$ are calculated to satisfy the equations above. The $Z_i$ functions then each act as spin filters when applied to the experimental data.

This method’s effectiveness is also limited in the case of overlapping resonances, where both spins can yield non-zero residuals. The main drawback of this method is that it relies on the use of a prototype resonance to model all other resonances of that spin. The presence of Porter-Thomas fluctuations and experimental errors implies that multiplicity distributions for a spin group will vary from resonance to resonance.

4.1.3 Prague Method

An alternate method improves upon the Oak Ridge method by taking into account statistical uncertainty in the multiplicity distribution of resonances [4]. The method still relies on the choice of well-resolved prototype resonances and the assumption that all resonances of a given spin will have the same multiplicity distribution. The normalized experimental yields $y_m$ at an isolated resonance at neutron energy $E_n$ can be decomposed in the following way

$$y_m(E_n) = q^+(E_n)\mu^+_m + q^-(E_n)\mu^-_m + \delta y_m(E_n),$$  \hspace{1cm} (4.6)$$

where $q^+$ and $q^-$ are normalized capture yields of spin value $I+1/2$ and $I-1/2$, respectively, and $\mu^+_m$ and $\mu^-_m$ are the probabilities for observing multiplicity $m$ with the same spin values, and $\delta y_m(E_n)$ is the value of random perturbations due to counting statistics uncertainties. Thus the sets of $\{\mu^\pm_m\}$ represent the prototypical multiplicity distributions. Normalization is set by
\[
\sum_m \mu_m^\pm = 1. \tag{4.7}
\]

It is assumed that the expectation value of \(\delta y_m(E_n)\) is

\[
E[\delta y_m(E_n)] = 0 \tag{4.8}
\]

and the variance of \(\delta y_m(E_n)\) is

\[
E[\delta y_m^2(E_n)] = \sigma^2_m(E_n). \tag{4.9}
\]

The quantities \(\nu_m^+\) and \(\nu_m^-\) are constructed so that the following conditions are satisfied:

\[
\sum_m \nu_m^+ \mu_m^- = \sum_m \nu_m^- \mu_m^+ = 0 \tag{4.10}
\]

and

\[
\sum_m (\nu_m^\pm)^2 = 1. \tag{4.11}
\]

The goal of this method is to find the optimum sets of \(\{\nu^\pm\}\) for each \(E_n\) that lead to conditional minima of the estimates of the variances of \(\{q^\pm\}\). A Monte Carlo based trial and error approach is implemented, and further details can be found in the original literature [4].

A simpler version of the method simple utilizes the method of least squares, with the added assumption that the variances \(\sigma^2_m\) are known a priori. The drawback of this simplified approach is that it fails for cases of low counting statistics. The full method is far superior in this case, and succeeds in assigning weaker resonances and even close resonance doublets.

This method is an improvement over the Oak Ridge method as it does not rely on the ad hoc choice of energy independent spin identifiers \(\nu^\pm\); they are determined separately for each neutron energy. However, this method still requires that \(\mu^+\) and \(\mu^-\) do not vary among resonances of the same spin and ignores the reality of statistical fluctuations from resonance to resonance.

### 4.2 Method of Pattern Recognition

A method of spin assignment using pattern recognition was developed in order to overcome some of these limitations. This method offers the advantage of not relying on a prototype resonance to yield multiplicity distribution information. Instead it considers all the neutron resonances at once to estimate the maximum likelihood value of the multiplicity distribution. All multiplicity information is used, allowing a multi-dimensional treatment of the problem,
rather than reducing the experimental data to a single average. This method maximizes on sensitivity to all the experimental data. In addition, the method determines a probability density function, which minimizes classification error and assigns a numerical degree of certainty to the spin assignment.

Consider the previous example using average multiplicities. While the s-wave resonances may be clearly separated, the average multiplicities of p-wave resonances of $^{97}$Mo, as shown in Figure 4.2, do not separate into well-defined groups.

![Figure 4.2: Average multiplicity of p-wave resonances.](image)

When considering resonances of only two spin groups, an histogram of the average multiplicities can be reasonably fitted with the functions of two overlapping Gaussians, as is shown in Figure 4.3. The region between the two peaks represents space where data points from either spin group are likely to exist. In this region, our spin assignments would be unsure. By utilizing all variables available, we can maximize the distance between the centers of the two spin group distributions, and thus maximize the certainty in our assignments.

### 4.2.1 Simple case: two spin groups

For the case of s-wave capture on $^{97}$Mo, two spin groups will exist ($2^+$ and $3^+$.) The normalized multiplicity yields may be written as
Figure 4.3: Two overlapping Gaussian distributions.

\[
y(E) = \begin{bmatrix} y_1(E) \\ y_2(E) \\ \vdots \\ y_{\text{max}}(E) \end{bmatrix} = \alpha_1(E) \begin{bmatrix} \omega_1^1(E) \\ \omega_1^2(E) \\ \vdots \\ \omega_1^{\text{max}}(E) \end{bmatrix} + \alpha_2(E) \begin{bmatrix} \omega_2^1(E) \\ \omega_2^2(E) \\ \vdots \\ \omega_2^{\text{max}}(E) \end{bmatrix},
\] (4.12)

where \( \alpha_1 \) and \( \alpha_2 \) are the weighting factors for the contributions of spin 2 and 3, respectively. Probability normalization then requires that

\[
\alpha_1(E) + \alpha_2(E) = 1,
\] (4.13)

so that for a well-isolated resonance of spin 2, for example, \( \alpha_2 = 1 \) and \( \alpha_3 = 0 \). The experimental data from each neutron energy bin then constitute an \( N \)-dimensional vector in normalized multiplicity space, one dimension for each multiplicity considered. It is helpful to view a 2D slice of those vectors. For example, Figure 4.4 is a scatter plot showing the normalized \( M = 3 \) and \( M = 5 \) yields. Two clusters are clearly visible.

The goal of the optimization routine is to find an axis in this space that maximizes the distance between the two centers of the distributions. This is achieved using a linear discriminant function.
$$h(y) = V^T y(i) + v(o) \begin{cases} < 0 \rightarrow \omega_2 \\ > 0 \rightarrow \omega_1 \end{cases}.$$ (4.14)

A priori probabilities must be assumed; the $2J+1$ level density law provides these values. These probabilities can be fixed throughout the optimization or allowed to vary. This method is described in detail in [5].

4.2.2 Parity Assignments

In nuclei of this mass range, the s-wave strength function is near a minimum, and the p-wave strength function is at a near maximum. Therefore, both s- and p-wave resonances are visible. While s-wave resonances are still typically stronger than p-wave resonances, some strong p-wave resonances are roughly as strong as the weaker s-wave resonances. Thus strength alone cannot determine the parity of a resonance with certainty.

Spin assignments from different evaluated nuclear data libraries are compared. ENDF/B-VII.1, JENDL-4.0, and JEFF-3.1 assign resonance spins based on much of the same experimental data of Shwe [6], Weigmann [7], and Wang [8]. Strong s-wave resonances are easy to identify; the strength of the resonance itself indicates $g \Gamma_n$ is large, and the strength also makes clearly visible the asymmetry that is characteristic of s-wave resonances due to interference.
from resonant and potential scattering. Assignments of s-wave resonances noted in libraries are thus claimed with a higher degree of certainty than most p-wave resonances.

![M=2 Spectra](image)

Figure 4.5: Multiplicity two \( \gamma \)-ray spectra for s- and p-wave resonances.

Resonances whose strengths fall within the range of either s- or p-wave resonances are more difficult to assign. The shape of the resonance offers little information because the difference between the calculated shapes for s- and p-wave resonances is small. Previous studies have relied on a calculation of \( g\Gamma_n \) alone to determine the parity of the resonance [6]. Other methods rely on detecting p-wave resonances with strong E1 transition intensities [9]. In some experiments, p-wave resonances were identified by measuring strong transitions from capture states to low-lying states of positive parity. Given the limitations of these experiments, the number of p-wave resonances assigned in libraries is likely only a lower limit on the actual number of p-wave resonances [10]. According to the \( 2J+1 \) level density law, there should be twice as many p-wave resonances than s-wave resonances in the resonance region. However, it is expected that some p-wave resonances will be weaker than the detection limits of the experiment.

Parity assignments in this work were made by examining the \( M = 2 \) \( \gamma \)-ray spectra for each resonance, when possible. Using the method introduced in [11], resonances were sorted based on their spectral shapes. The assignments are noted in Table 4.1. By convention, \( \ell = 0 \) resonances
are positive parity and \( \ell = 1 \) resonances are negative parity. Many resonances could not be clearly assigned in this manner, and are noted in Table 4.1 with parentheses. Many resonances also show spectral evidence of strongly preferred transitions, indicating a preference for decay through specific nuclear levels. Especially in the case of two-step cascades, these transitions can be used as indicators of the parity of the resonance.

We counted 21 measurable s-wave resonances and 32 p-wave resonances in the data, roughly 50% more p-wave resonances than s-wave resonances. The assignments are in good agreement with parity assignments claimed with certainty in other references. Only resonances with previously tentative parity assignments are in disagreement.

### 4.2.3 Results of s-wave resonances

![Spin Assignment Prototypes](image)

Figure 4.6: Capture yield contribution by spin group for some s-wave resonances.

As the s-wave resonances are relatively easy to assign given average multiplicity alone in this case, the pattern recognition method should handle s-wave resonances without difficulty. That is indeed the case, with clear boundaries and near 100% certainty in all resonances. The contributions to the experimental capture yield from both spin groups are shown in Figure 4.6. The results of s-wave resonances are also in good agreement with previous assignments, giving confidence to the method. Of the 21 s-wave resonances seen in the data, 10 were assigned spin...
2\textsuperscript{+} and 11 were assigned spin 3\textsuperscript{+}. These values are roughly as expected from the 2J+1 level density law.

### 4.2.4 Generalization to p-wave case

In a nucleus such as $^{97}$Mo, p-wave resonances must be considered in addition to s-wave resonances. In this case there are four resulting $J^\pi$ combinations: (1\textsuperscript{−}, 2\textsuperscript{−}, 3\textsuperscript{−}, 4\textsuperscript{−}). If pattern recognition is to be helpful in this case, it must distinguish between four spin groups, as seen in Figure 4.7.

Multiplicity distributions for p-wave resonances overlap considerably. With the added difficulty that most p-wave resonances are much weaker than s-wave resonances (and have lower statistics) determining p-wave resonance spins is a considerably more difficult challenge.

![Figure 4.7: Multiplicity 5 versus multiplicity 3 distributions for p-wave resonances.](image)

### 4.2.5 Results of p-wave resonances

The results from analysis of p-wave resonances are dependent on the \textit{a priori} probability distribution chosen; thus the solutions only represent local minima, rather than global minima. Given the assumed distributions based on the 2J+1 level density law, the solutions converge
after 10 to 12 iterations. Tentative assignments were made for 10 p-wave resonances, and 22 were made with 90% certainty or greater. Of the 32 p-wave resonances, 2 were assigned as 1−, 5 as 2−, 11 as 3−, and 14 as 4−. While definite spin assignments were not achieved for all p-wave resonances, most resonances with sufficient statistics could be assigned two possible spin values. In Table 4.1, for resonances assigned spin with less than 90% certainty, the second most likely spin value is indicated in parentheses. DANCE data was also analyzed by collaborators using the Prague method. Results using the Prague method are in good agreement with those from this work, and are also shown in Table 4.1.

Table 4.1: Spins, Parities of Neutron Resonances

<table>
<thead>
<tr>
<th>En (eV)</th>
<th>Jπ</th>
<th>% Certainty</th>
<th>Jπ</th>
<th>Jπ</th>
<th>Jπ</th>
<th>Jπ</th>
<th>comments</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>This Work</td>
<td>ENDF/</td>
<td>JENDL-4.0/</td>
<td>JEFF-3.1</td>
<td>Prague</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>B-VII.1</td>
<td></td>
<td></td>
<td>Method</td>
<td></td>
</tr>
<tr>
<td>16.2</td>
<td>1−</td>
<td>99.6</td>
<td>NL</td>
<td>(4)−</td>
<td>1−,2−</td>
<td></td>
<td></td>
</tr>
<tr>
<td>55.3</td>
<td>3(2)−</td>
<td>79.6</td>
<td>NL</td>
<td>(3)−</td>
<td>3−,4−</td>
<td></td>
<td></td>
</tr>
<tr>
<td>70.9</td>
<td>2+</td>
<td>100</td>
<td>2+</td>
<td>(2)+</td>
<td>2+</td>
<td></td>
<td></td>
</tr>
<tr>
<td>79.6</td>
<td>3(−)</td>
<td>94.7</td>
<td>(−)</td>
<td>(3)−</td>
<td>(2±,3±)</td>
<td>on tail prev. res.</td>
<td></td>
</tr>
<tr>
<td>109.6</td>
<td>1−</td>
<td>100</td>
<td>(−)</td>
<td>(3)−</td>
<td>1−,2−</td>
<td></td>
<td></td>
</tr>
<tr>
<td>126.9</td>
<td>-</td>
<td>-</td>
<td>(−)</td>
<td>(4)(−)</td>
<td>2−,3−</td>
<td>too weak</td>
<td></td>
</tr>
<tr>
<td>136.3</td>
<td>3+</td>
<td>100</td>
<td>(−)</td>
<td>(3)(−)</td>
<td>3−,4−</td>
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</tr>
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<td>210.0</td>
<td>2−</td>
<td>100</td>
<td>(−)</td>
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Figure 4.8: Capture yield contribution by spin group for some p-wave resonances.
Chapter 5

Neutron Capture Cross-Section and Resonance Parameters

5.1 Cross Section Calculation

The experimentally measured $^97\text{Mo}(n,\gamma)$ cross section can be expressed as the product of the components

$$\sigma_{n,\gamma}(E_n) = \frac{M N_{n,\gamma}(E_n)}{N_A \rho f A_{\text{beam}} \epsilon_{n,\gamma}(E_n) \Phi(E_n)},$$

where $M$ is the atomic mass of $^97\text{Mo}$ (96.906 u), $N_{n,\gamma}(E_n)$ is the number of capture events at neutron energy $E_n$ measured by DANCE, $N_A$ is Avogadro's number ($6.022\times10^{23}$), $A_{\text{beam}}$ is the area of the target illuminated by the beam (0.785 cm$^2$), $\rho$ is the areal density of the molybdenum target (18.7 mg/cm$^2$), $\epsilon_{n,\gamma}(E_n)$ is the total efficiency of DANCE for capturing the event, and $\Phi(E_n)$ is the neutron flux incident on the target for a given $E_n$.

The quantity $N_{n,\gamma}$ is measured by the DANCE array, the neutron flux $\Phi(E_n)$ is calculated using measurements from the neutron beam monitors just downstream from DANCE, and the efficiency $\epsilon_{n,\gamma}$ is calculated using known information.

5.1.1 Neutron Flux

The neutron flux $\Phi(E_n)$ is measured using neutron beam monitors located just past DANCE on flight path 14. Three neutron monitors are installed: a $^6\text{Li}$ silicon detector, a $^3\text{He}$ proportional counter, and a $^{235}\text{U}$ fission fragment chamber. Because the last collimator is located upstream from DANCE on the neutron flight path, the beam continues to diverge before it reaches the monitors, resulting in a lower flux than the flux at the target.
\[ \Phi = \beta \Phi_{\text{mon}}. \]  

The absolute neutron flux at the DANCE target must be determined using additional information. A second target is chosen, one which is geometrically similar to the \(^{97}\text{Mo}\) target and isotopically pure, composed of an isotope whose capture cross-section is well determined. The \(^{197}\text{Au}\) nucleus fits these criterion well. A target of circular dimensions with a 2.0 cm diameter, 0.1 micron thick layer of gold deposited on a thin strip of mylar was used. The mylar makes a suitable backing material in this case because, as an organic molecule, all of its constituents have total cross sections much smaller than that of gold. DANCE data is collected for the Au target in much the same way as it was collected for the Mo target. The looking time window is shifted to slightly longer times in order to see the large Au resonance at 4.9 eV. The cross section at this resonance is very large (27,000 barns) and is known so precisely that it is often used as a standard for flux determination. Counts from all multiplicities are considered in the capture yield; the counts underneath the resonance are fit with a linear function and subtracted as background. The neutron monitor flux is normalized to this single resonance.

![Cross Section of the \(^{197}\text{Au}\) resonance used to normalize the neutron flux.](image)

In order to accurately determine the neutron flux at the target, it is also important to
Figure 5.2: Neutron flux measured at DANCE over the duration of the $^{97}\text{Mo}$ experiment.

calculate the effects of beam attenuation and self-shielding by the target. For a target of uniform thickness and composition, that is larger than the beam spot, and is oriented parallel to the incident beam, the beam attenuation is given by a simple formula

$$
\Phi(E_n) = \Phi_o(E_n) \times e^{-\sigma_{\text{tot}}(E_n)t},
$$  \hspace{1cm} (5.3)

where $\Phi$ and $\Phi_o$ are the final and incident beam fluxes, respectively, $\sigma_{\text{tot}}$ is the total cross-section of the target, and $t$ is the target "thickness" in atoms per barn. For the $^{97}\text{Mo}$ nucleus, $\sigma_{\text{tot}}$ is the sum of the capture and elastic cross-sections, and the thickness is $1.162 \times 10^{-4}$ atoms/barn.

The effect of target self-shielding must also be accounted for. As neutrons pass through the target, some fraction are removed from the beam through either capture or scattering reactions. Thus the entire volume of the target is not illuminated with the same flux, resulting in a lower measured capture yield at the back face of the target than at the front face. For the $^{97}\text{Mo}$ target this reduced yield can be calculated as

$$
y_{n,\gamma}^{\text{obs}}(E_n) = \frac{y_{n,\gamma}^{\text{ideal}}(E_n)}{1 - \frac{\sigma_{n,\gamma}(E_n)}{\sigma_{\text{tot}}(E_n)}(1 - e^{\sigma_{\text{tot}}(E_n)t})}.
$$  \hspace{1cm} (5.4)

The fractional effect of both beam attenuation and target self-shielding over the resonance region are plotted in Figure 5.3. The effects are typically very small except at a few strong resonances, where beam attenuation reaches a 7 percent effect, and self-shielding a 1 percent effect. A correction for both effects is applied to the measured flux and capture yields of the
Figure 5.3: Fractional effect of beam attenuation and target self-shielding as a function of neutron energy.

5.1.2 Detection Efficiency of DANCE

The total efficiency of DANCE can be written as the product of \( \epsilon_o \), the efficiency for detecting the nuclear event and \( \epsilon_{gated} \), the fraction of DANCE events which are included after the application of multiplicity and summed energy gates.

\[
\epsilon_{n,\gamma} = \epsilon_o \epsilon_{gated} \tag{5.5}
\]

\[
\epsilon_{gated} = \frac{\sum_{m=3}^{7} N_{gated}}{N_{ungated}}. \tag{5.6}
\]

The modeling of the detector response for DANCE using GEANT4 has been discussed in great detail in several publications [12], [13]. Sample \( \gamma \)-ray spectra for simulations were generated using the Monte Carlo code DICEBOX, which is described more thoroughly in Chapter 6. The
results of DICEBOX for the $^{97}$Mo nucleus were used as input for the GEANT4 package. The resulting efficiency of DANCE for detecting a single cascade was 97%, and is comparable to values from other DANCE experiments.

The gated efficiency $\epsilon_{\text{gated}}$ was measured to be $66.0(2)\%$ using counts from the strong resonance at 70 eV, where background is low. The total efficiency of DANCE was calculated to be

$$\epsilon_{n,\gamma} = 0.64.$$  \hspace{1cm} (5.7)

5.1.3 Cross Section Results

Utilizing all of the information known concerning the neutron flux, the properties of the target, and the efficiency of DANCE, the neutron capture cross-section for $^{97}$Mo was determined to within 5 percent uncertainty in most regions, and is presented in Figure 5.4. Because the capture cross-section of $^{197}$Au is known very precisely, the $^{97}$Mo measurement may still be called an absolute cross-section.

![Cross Section Determined for $^{97}$Mo](image)

Figure 5.4: Cross section determined for $^{97}$Mo.
5.2 Resonance Parameters

In addition to determining the cross-section in the resolved resonance region for $^{97}$Mo, resonance parameters were determined with the help of the R-matrix code SAMMY [14]. The SAMMY multilevel R-matrix code generates theoretical cross sections using the Reich-Moore approximation to R-matrix theory. SAMMY is also capable of modeling various experimental effects such as target self-shielding or resolution and Doppler broadening associated with time-of-flight measurements. The results of the theoretical models are then compared to experimental data, and model parameters can be fit using Bayes’ method in order to describe the particular set of experimental conditions. Best fit values for resonance parameters such as $\Gamma_n$, $\Gamma_\gamma$, and resonance position $E_n$ are also determined. According to statistical models, values $\Gamma_n$ for resonances of a particular isotope may vary considerably, but $\Gamma_\gamma$ should not. SAMMY can only fit both $\Gamma_\gamma$ and $\Gamma_n$ in the special case of very strong resonances at low energy, where good energy resolution and statistics allow for a shape analysis to be performed. Otherwise, SAMMY calculates the area under a resonance, where

$$A \propto g \frac{\Gamma_\gamma \Gamma_n}{\Gamma_\gamma + \Gamma_n}, \quad (5.8)$$

where $g$ is the spin statistical factor. For most resonances in $^{97}$Mo, $\Gamma_\gamma \gg \Gamma_n$, so $A \propto g \Gamma_n$. In these cases, SAMMY can only reliably determine $\Gamma_n$. A few strong, low energy resonances may allow for determination of both widths.

The resulting fit of SAMMY for the $^{97}$Mo experiment is shown in Figure 5.5. The best fit values for resonance parameters are summarized in Table 5.1. Initial values of $\Gamma_\gamma$ and $\Gamma_n$ for each resonance were taken from the JENDL-4.0 library. A few resonances were strong enough to allow for a determination of $\Gamma_\gamma$ as well as $\Gamma_n$. Best-fit values for $\Gamma_\gamma$ are shown in bold; others listed remain unchanged from JENDL-4.0 values. All values of $\Gamma_\gamma$ were fit by SAMMY. Neutron energies listed in Table 5.1 are also the results of fitting each resonance position individually.

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Table 5.1: Resonance Parameters for $^{97}$Mo as fit by SAMMY
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<th>$\Gamma_n$ (meV)</th>
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<td>$\Gamma_\gamma$ (meV)</td>
<td>$\Gamma_n$ (meV)</td>
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Figure 5.5: Experimental cross-section fit using SAMMY.
Chapter 6

Photon Strength Function and Level Density Parameters

6.1 Simulation of $\gamma$-ray Cascades

6.1.1 DICEBOX Code

Extracting level density (LD) and photon strength function (PSF) parameters from experimental spectra is not a straightforward task; multiple parameters must be fit simultaneously, taking into account the complex nature of their interaction with each other. An iterative approach is adopted. Decays from the capture state are simulated using artificially generated level schemes. The subsequent detector response is also simulated, and the resulting spectra are compared with experiment. The parameterizations of PSF and LD models are varied in order to find the model that provides the best fit.

First the level scheme of the product nucleus must be reproduced using a combination of experimentally known levels and artificially generated ones. One defines a critical excitation energy $E_{\text{crit}}$ below which levels of the compound nucleus are completely known, as are their widths, spins and parities. Above $E_{\text{crit}}$, where the spacing of nuclear levels is no longer large compared to the level widths, the quasicontinuum of levels is better described by a level density function. This function is both spin and parity dependent. Using the Monte Carlo code DICEBOX, levels below $E_{\text{crit}}$ are taken as input and levels from $E_{\text{crit}}$ up to the capture energy of the compound nucleus are generated according to a level density formula.

In addition to information on level energies and quantum numbers, the partial radiation widths, branching ratios, multipole mixture coefficients, and internal conversion coefficients must either be known a priori or generated artificially in order to simulate the $\gamma$ decay. Values for transitions below $E_{\text{crit}}$ are taken from experiment, and those above $E_{\text{crit}}$ are generated as a
random discretization of the PSF formula such that the expectation value of $\Gamma_{if}^{(XL)}$, the partial radiation width, is the center of a $\chi^2$ distribution

$$
\langle \Gamma_{if}^{(XL)} \rangle = \frac{y_{XL}^2 f_{XL}(E_f) E_{\gamma}^{(2L+1)}}{\rho(E_i)},
$$

(6.1)

where $(XL)$ denotes the multipolarity of the transition (e.g., E1 or M2) and the subscripts $if$ specify the initial and final states $i$ and $f$, respectively. It is assumed that any pair of partial radiation widths $\Gamma_{if}^{(XL)}$ is statistically uncorrelated.

A priori information on the nuclear levels below $E_{crit}$ together with the artificially generated level scheme and its properties make up one nuclear “realization,” a sample scheme of what the compound nucleus in question might look like. Once the nuclear realization has been constructed, the decay to the ground state is simulated as a Markov chain. At each step, a random number between 0 and 1 is generated. This random number determines which channel the decay proceeds through (see Figure 6.1). This step is repeated at each nuclear level until the ground state is reached, completing the cascade. At each step, all selection rules governing the decay process are fully observed.

Figure 6.1: Level scheme of the nuclear realization. Random number generators are used to govern selection of each decay channel in the Markov Chain.
Tens of thousand of cascades are simulated in order to converge on a stationary distribution for the realization. Typically, ten or twenty realizations is sufficient to produce a complete picture for a given set of LD and PSF parameters.

6.1.2 GEANT4 Simulations

Next the artificially generated cascades are used as input into the modeling of the DANCE array with the GEANT4 toolkit. The module developed in GEANT4 describes all pieces of the DANCE array, including all 160 BaF$_2$ crystals, the PVC foils and aluminum holders surrounding them, and the $^6$LiH shield. The GEANT4 toolkit allows one to simulate the response of the DANCE array using Monte Carlo methods, and agreement of these simulations with experiment has been well-documented [12].

6.2 Previous Calculations

Data on the $^{98}$Mo compound nucleus was recently collected at the Forschungszentrum Dresden-Rossendorf by Rusev et al. [15] using nuclear resonance fluorescence (NRF) experiments. Properties of the Giant Electric Dipole Resonance (GEDR) were parameterized.

Recent data was also published from experiments using the ($^3$He,$\alpha\gamma$) and ($^3$He,$^3$He$'\gamma$) reactions at the Oslo Cyclotron Laboratory. The sequential extraction technique, also known as the Oslo method [16], was used to simultaneously extract PSF and LD information. Notably, Oslo reported a low-energy (below 3 MeV) enhancement of the PSF for all Mo isotopes between A = 93 and A = 98 [17], [18].

6.3 Photon Strength Function for $^{98}$Mo

In the work of Rusev et al. [15], a triple Lorentzian (TLO) model was used to describe the E1 PSF. The peaks of each Lorentzian were calculated to be 14.38, 15.85, and 17.70 MeV. The parameterization with a TLO model yields an E1 PSF shape that is very similar to that of Dietrich and Berman [19] save for a renormalization factor (see Figure 6.2). This discrepancy might be resolved by the suggestion of the renormalization of Saclay photoabsorption data[20].

However, reproduction of DANCE spectra is very difficult using models based on the Rossendorf data. The Rossendorf data shows a “bump” near $E_\gamma$ = 6 MeV for multiplicities 3 and 4 combined with a “valley” near $E_\gamma$ = 3 - 4 MeV. The DANCE data show a different shape: a bump in spectra near $E_\gamma$ = 4 and 3 MeV in multiplicities 3 and 4, respectively. Any TLO simulation that reasonably reproduces the lack of a valley around $E_\gamma$ = 3 - 4 MeV must compensate with a small strength at lower $E_\gamma$, which then leads to multiplicity distributions.
that are unrealistically low compared with the DANCE data. It appears that there is little hope for agreement with the Rossendorf data.

In an attempt to resolve the issue of the proposed low-energy enhancement found by Oslo, additional models that reasonably reproduce the Oslo data were tested as well. These are all temperature-independent models. Models with any significant low-energy enhancement have trouble reproducing multiplicity distributions for both negative- and positive-parity resonances. However, all simulations with temperature-independent models have great difficulty reproducing the bump near $E_{\text{sum}} = 4.7$ for multiplicity two in $2^+$ resonances.

A SLO model of E1 was also tested, but was ultimately unsuccessful in reproducing the experimental data. Simulations using an SLO model resulted in multiplicity distributions significantly lower than those measured in the experiment.

The models used to successfully describe $^{96}$Mo by both Krticka [21] and Sheets [22] were also used as a starting point for calculations for the $^{98}$Mo nucleus. For the E1 PSF, the generalized Lorentzian (GLO) model was used, and the M1 PSF was described by a single-particle (SP) model with a spin-flip (SF) term added. Some sample spectra are shown in Figure 6.3 through Figure 6.6.
Figure 6.3: \( E_\gamma \) spectra from two nuclear realizations using the E1(GLO) and M1(SP+SF) PSF model for a \( 2^+ \) resonance. Multiplicities 1 through 7 are shown; the last histogram is summed over all multiplicities.
Figure 6.4: $E_{\text{sum}}$ spectra from two nuclear realizations using the E1(GLO) and M1(SP+SF) PSF model for a $2^+$ resonance. Multiplicities 1 through 7 are shown; the last histogram is summed over all multiplicities.
Figure 6.5: $E_\gamma$ spectra from two nuclear realizations using the E1(GLO) and M1(SP+SF) PSF model for a $2^-$ resonance. Multiplicities 1 through 7 are shown; the last histogram is summed over all multiplicities.
This model does quite well in reproducing experimental spectra. It is able at least to in part reproduce the bump in $E_{\text{sum}} = 4.5 - 5.0$ MeV for multiplicity two in $2^+$ resonances, while other simulations were unable to do so. Interestingly, the simulated spectra exhibited significant variation from one realization to the next. At energies above 4 MeV, it exactly reproduces data from Oslo as well (see Figure 6.7.) At low energies, the gray band visible in the GLO model exists as a consequence of the temperature dependence of the PSF. Because the Oslo data for $^{98}$Mo seem to exhibit only a small low-energy enhancement, there is good agreement with this model below 4 MeV. Thus, the combination of the GLO (E1) and SP+SF (M1) appears to be a good fit to all but the Rossendorf data. Best-fit parameters of the photon strength function model are listed in Table 6.1.
Figure 6.7: Data from Oslo, Rossendorf and Saclay ("$^{98}\text{Mo}$", "$^{98}\text{Mo renormalized}$") shown with parametrization from GLO, SLO, and Oslo models. The proposed GLO model agrees well with reasonably well with all but the Rossendorf data.

Table 6.1: Parameterization of the photon strength function using the (E1)GLO + (M1)(SP+SF) model.

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<th>Value</th>
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<tr>
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<tr>
<td>M1</td>
<td>$f^{M1}$</td>
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</tr>
<tr>
<td>M1</td>
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<tr>
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6.4 Level Density

Some disagreement exists concerning nuclear level densities of $^{98}\text{Mo}$. RIPL2 [23] gives an average level spacing for $\ell = 0$ ($D_o$) of 75(20) eV while Mughabghab [24] gives a $D_o$ of 46.5(58) eV.
Level density parameterization given by Von Egidy used RIPL2 values.

Both a constant temperature (CT) and a back-shifted Fermi gas (BSFG) model were tested. Better agreement was found using the BSFG model than with CT, at least for resonances of positive parity. Negative-parity resonances seem to fall somewhere between the two models, but this may be complicated by the ambiguity in spin assignments for p-wave resonances. Best-fit parameters of the level density model are listed in Table 6.2.

Table 6.2: Parameterization of the level density function using the BSFG model.

<table>
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<tr>
<td>$E_1$</td>
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</table>
Figure 6.8: Comparison of experimental and simulated $E_\gamma$ spectra for $J^p = 2^+$. The BSFG (gray area) and CT (black lines) models are used. Multiplicities 1 through 7 are shown; the last histogram is summed over all multiplicities.
Figure 6.9: Comparison of experimental and simulated $E_\gamma$ spectra for $J^\pi = 3^+$. The BSFG (gray area) and CT (black lines) models are used. Multiplicities 1 through 7 are shown; the last histogram is summed over all multiplicities.
Figure 6.10: Comparison of experimental and simulated $E_\gamma$ spectra for $J^\pi = 2^-$. The BSFG (gray area) and CT (black lines) models are used. Multiplicities 1 through 7 are shown; the last histogram is summed over all multiplicities.
Chapter 7

Conclusions

Neutron capture experiments on $^{97}$Mo were successfully performed using the DANCE array. Physics events were reconstructed from raw data, providing capture yields, multiplicity distributions, summed energy and $\gamma$-ray spectra over the entire resonance region for this nucleus.

Spins were assigned to 53 resonances, where for $^{97}$Mo six $J^\pi$ combinations are possible. Assignments for the 21 s-wave resonances were made with high confidence, and roughly two-thirds of the p-wave resonances received high-confidence assignments. The remaining p-wave resonances were assigned two possible spin values.

Large fluctuations among resonances of the same spin were readily visible and complicated the matter of assigning parity using multiplicity two spectra. However, DICEBOX simulations were generally able to reproduce these large fluctuations. Multiple models of photon strength function and level density were tested. The E1 photon strength function was best fit with a generalized Lorentzian model, while the M1 strength function was well-characterized using a combination of single-particle and spin-flip terms. Experimental data were consistent with a level density formula corresponding to a back-shifted Fermi gas model.

The neutron capture cross-section in this region was determined over the entire resonance region and was in good agreement with data libraries. Additionally, resonance parameters such as $\Gamma_\gamma$ and $\Gamma_n$ and the best fit for resonance neutron energies were also obtained using the R-Matrix code SAMMY.
References

