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EFFECT OF MULTIPLE SPIN SPECIES ON SPHERICAL SHELL NEUTRON TRANSMISSION ANALYSIS

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16. Abstract

A series of Monte Carlo calculations have been performed in order to evaluate the effect of separated against merged spin statistics on the analysis of spherical shell neutron transmission experiments for gold. It is shown that the use of separated spin statistics consistently results in larger average capture cross sections of gold at 24 keV. This effect is explained by stronger windows in the total cross section caused by the interference between potential and J_+ resonances and by J_+ and J_- resonance overlap allowed by the use of separated spin statistics.

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EFFECT OF MULTIPLE SPIN SPECIES ON SPHERICAL

SHELL NEUTRON TRANSMISSION ANALYSIS

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SUMMARY

A series of Monte Carlo calculations have been performed to evaluate the effect of separated spin statistics on the analysis of spherical shell neutron transmission experiments for gold. Both separated spin statistics, J-state identified, and merged spin statistics, J-states averaged, have been used to generate pseudo resonance cross section sets.

It is found that the merged spin analysis of gold consistently underestimates the capture cross section. This effect is explained by stronger windows in the total cross section caused by the interference between potential and J_+ resonances and by J_+ and J_- resonance overlap allowed by the use of separated spin statistics.

Using the latest published separated spin statistics, the value of the average capture cross section for gold at 24 keV is 710±25 millibarns.

INTRODUCTION

The absolute neutron capture cross section of gold in the keV region is of great interest to measurers and to evaluators (refs. 1 and 2). If uncertainties were less than about 3 percent, the gold cross section could serve as a convenient secondary standard for the measurement of other isotopic capture cross sections. Most of the capture measurements for gold below 200 keV rely on normalization to activation cross sections at 30 keV and to sphere transmission results (ref. 3) using Sb-Be sources of mono-energetic photoneutrons at 24 keV.

Sphere transmission experiments have been analyzed by Monte Carlo methods (refs. 4 to 6) using resolved region statistical resonance data to account for unresolved resonance structure and multiple scattering at 24 keV. Recent analyses of the same experiments (ref. 3) have reported a value of 725±28 millibarns (refs. 5 and 6) using

measured s-wave parameters for each of two compound spin states and values of 650±35 (ref. 7) and 660±28 millibarns (refs. 5 and 6) using the merged spin state s-wave statistics. It is argued in reference 7 that the approximately equal s-wave strength functions found for gold in recent data (refs. 8 and 9) justifies the treatment of the statistical resonances at 24 keV on a merged spin basis. In the present study of the gold-sphere transmission experiments, it is shown that the use of merged spin statistics always underestimates the average capture cross section compared with results obtained using separated spin statistics.

The use of separated spin statistics for gold is necessary to simulate accurately the statistical distribution of highly scattering resonances and the strong cross section windows resulting from the interference of the resonance scattering with potential scattering for each spin state. Furthermore, the use of two independent statistical sets of levels for each spin state permits overlapping of levels and therefore results in resonance combination and effective suppression of some levels. The use of merged statistics introduces a forced level-level effective repulsion, through the single specie Wigner level spacing distribution, which can not exist for gold. The correct interference and overlapping effects are generated only when separated spin state levels are employed.

SPHERE TRANSMISSION ANALYSIS

For nuclei with nuclear spin I, not equal to zero, there exist two different species of s-wave ($1 = 0$) resonances. The spin of those resonances with the neutron spin parallel to the nuclear spin are denoted by $J_+ = I + 1/2$, likewise for the antiparallel states $J_- = I - 1/2$. Thus when it is possible to assign J-values to a significant number of experimentally resolved resonances of a particular monotope, spin dependent strength functions may be determined. The explicit treatment of the two different J-states with their appropriate spin factor g and individual statistical distributions is referred to as the separated spin statistics analysis.

On the other hand, one can combine the separated spin data, as if there were no spin dependence, assign an average s-wave strength function with $g = 0.50$ ($I \neq 0$) and generate a single set of statistical resonances. The treatment of a nonzero spin nucleus with an average value of $g = 0.500$, a single specie Wigner level spacing distribution, and the Porter-Thomas distribution of scattering widths is referred to as the merged spin statistics analysis.

The merged spin analysis uses an estimate of S_0, the merged s-wave strength function, and $\overline{D}_0$, the observed average level spacing. For analysis of the sphere transmission experiments, these parameters are used in a Monte Carlo neutron multiple scattering program, which samples from the distribution of Porter and Thomas for

scattering widths and samples from a single-specie Wigner level spacing distribution to compute resonance cross sections. The potential scattering cross section and the average p-wave capture cross section are varied until agreement between the Monte Carlo calculated transmission and the experimentally measured transmission is obtained while conserving the known measured value of the average total cross section. This merged spin technique is in principle correct only for nuclei with $I = 0$, where there is one level spacing distribution for the s-wave J-state (of course, for $I = 0$, $g = 1.0$).

Since gold has a nuclear spin of $I = 3/2$, the $J = 1$ levels are assumed to have a Wigner single-specie level spacing distribution, which is uncorrelated in position with respect to the $J = 2$ levels that are also assumed to have a Wigner single-specie distribution. If the $(2J + 1)$ level spacing density applies, $3/8$ of the levels should have $J = 1$, $g = 3/8$ and the remaining $5/8$ levels should have $J = 2$, $g = 5/8$. In the present study separated spin statistics analyses have been performed for two different sets of spacing densities: $\overline{D}_{J=2} = \overline{D}_{J=1}$ and $2.0\,\overline{D}_{J=2} = \overline{D}_{J=1}$. Using one of these sets of spacing densities and its associated strength functions for the analysis of the sphere transmission experiments, these parameters are used in a Monte Carlo neutron multiple scattering program, which samples from both spin states to compute realistic resonance cross sections. Again the potential scattering cross section and the average p-wave capture cross section are varied until agreement between the Monte Carlo calculated transmission and the experimentally measured transmission is obtained while conserving the measured value of the average total cross section.

CROSS SECTION DATA

Julien et al. (ref. 8) and Alves et al. (ref. 9) of Saclay have measured the spin-dependent statistical parameters of gold over the energy range from 0 to 2 keV. Early results (ref. 8) for the energy range from 0 to about 1 keV favored average level spacings related in the following manner: $\overline{D}_{J=1} = 2.2\,\overline{D}_{J=2}$. Later analysis (ref. 9) of the data from 0 to about 2 keV has favored $\overline{D}_{J=1} = 1.7\,\overline{D}_{J=2}$ which is quite close to the $(2J + 1)$ prediction.

Using the data of references 8 and 9, spin dependent continuous cross sections were generated by the method of stochastic simulation for gold about 24 keV. Because the average energy of the Sb-Be photoneutrons have been recently measured as 26.0 ± 1.3 keV (ref. 10) and as 22.8 ± 0.7 keV (ref. 11), the analyses in the present report have been performed at a nominal neutron energy of 24 keV. The method is discussed in references 5 and 6. Briefly, the values of Γ_n (J = 1) and Γ_n (J = 2) are sampled from the individual Porter-Thomas distributions; also values of the corresponding level spacings are sampled from the Wigner distributions characterized by the observed average values

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of $D_{J=1}$ and $D_{J=2}$. After sampling a sufficient number of resonance parameters, a Doppler broadening Breit-Wigner code is used to provide a continuous set of cross sections for the Monte Carlo multiple scattering calculations.

Using the simulated set of s-wave cross sections several constant values of the p-wave cross section and the potential cross section are assumed so as to arrive at values that satisfy the measured sphere transmission and the independently measured average total cross section. The resultant average s-wave and p-wave capture cross sections are then obtained.

GOLD SPHERE TRANSMISSION ANALYSES

The gold spherical shells analyzed were the gold sphere neutron transmission experiments of Schmitt and Cook (ref. 3). The resonance statistical data are compatible with the s-wave resonance parameters selected by Froehner (ref. 7). Several sets of calculations have been performed in order to evaluate the effect of the use of merged spin statistics as opposed to separated spin statistics. The details of the cross-section generation used in the present report are shown in the appendix.

Analyses were made using two different sets of values for the separated spin statistics. It is noted that the average merged value of the s-wave strength function was held constant for all analyses in this study. If the merged spin analysis is a valid technique, the results of each of the two separated spin analyses should be equal to the merged spin analysis. The total cross section of gold at 24 keV, 13.7±0.3 barns, has been conserved for each sphere analysis.

RESULTS

The results of a merged spin and two different separated spin analyses for the average capture cross section at 24-keV neutron energy are shown in table I. The results of a previous study using separated spin statistics and merged spin statistics with a stratified sampling technique are shown at the bottom of the table for comparison (refs. 5 and 6). The merged spin results are in every case smaller than the separated spin results for the average capture cross section. A separated spin analysis with $S_{0_-} = S_{0_+}$ gives a 4.6 percent greater result than the merged spin analysis for the average capture cross section. If $2S_{0_-} = S_{0_+}$ the separated spin analysis gives a result 7.6 percent greater than the merged analysis. This difference, illustrated in figure 1, is due to the stronger interference terms associated with the $g = 0.625$ resonances, providing transmission "windows" in the total cross section. Thus more local trans-

TABLE I. - RESULTS OF SEPARATED AND MERGED SPIN ANALYSES

[Average total cross section, 13.7±0.3 b; radiative width, Γ_γ, 0.125 eV.]

Source of data	Type of cross section	Strength functions			Average level spacings, eV			Potential cross section, σ_{pot}, b	Average capture cross section, $\bar{\sigma}_c$, mb
		Merged, S_0	Separated		Merged, D_0	Separated			
			S_{0_-}	S_{0_+}		D_-	D_+		
Present study	Separated	1.95×10^{-4}	1.950×10^{-4}	1.950×10^{-4}	16.0	32.0	32.0	8.3±0.3	706±28
	Separated	1.95	1.30	2.604	16.0	48.0	24.0	7.9±0.3	726±28
	Merged	1.95	----------	----------	16.0	----	----	8.1±0.3	675±28
Stratified sampling (ref. 5)	Separated	1.93×10^{-4}	1.364×10^{-4}	2.501×10^{-4}	15.5	44.0	24.0	7.8±0.3	725±30
	Merged	1.93	----------	----------	15.5	----	----	8.5±0.3	660±30

(a) Representative portion of a merged spin cross section set (one "window") σ_{pot} = 7.5 barns S_0 = 1.95x10^{-4} resonance energies indicated by arrows pointed up.

(b) Representative portion of a separated spin cross section set (seven "windows") σ_{pot} = 7.5 barns S_0 = 1.95x10^{-4} resonance energies and spins indicated by up arrows and signs respectively.
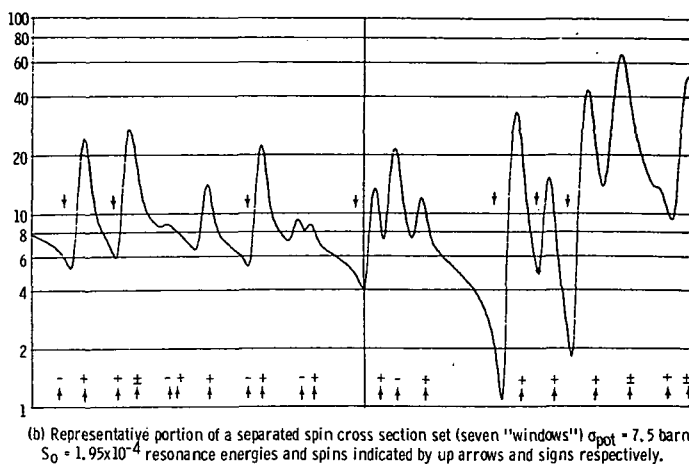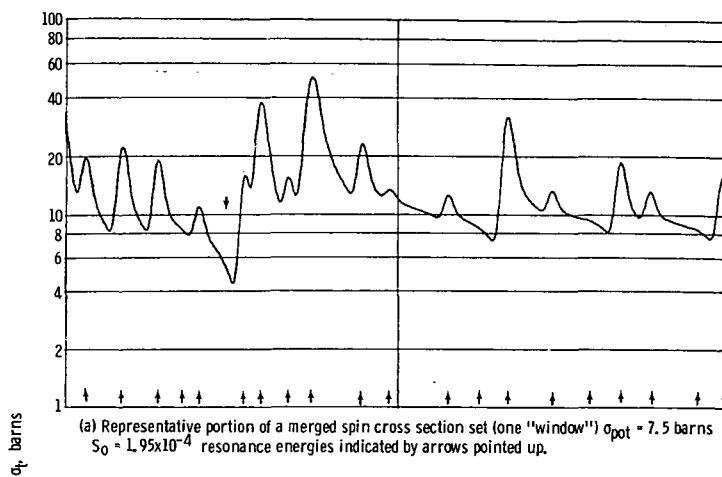
Figure 1. - Representative merged spin cross section sets and separated spin cross section sets (portions of the total cross section less than 6.0 barns have been indicated by arrows pointed down and are considered neutron transmission "windows"). Resonance parameters obtained from the computer code Daisy (no stratified sampling).

missions occur than in the $g = 0.500$ cases, and a larger value of $\bar{\sigma}_c$ is required to realize analytically the value of the experimental transmission. In fact, the value of the average capture cross section seems to be sensitive to the $J = 2$ level density and rather less sensitive to the $J = 1$ level density for the separated spin analyses.

The separated spin analyses have been performed for two quite different values of S_{0_-} and S_{0_+}, and, if the average value of S_0 (merged) is not greatly changed by further experiment, one may obtain separated spin analysis results in the range of $S_{0_+} = S_{0_-}$ to $S_{0_+} = 2S_{0_-}$ by linear interpolation of the present results. Using the statistical data of Alves et al. (ref. 9), $S_{0_+} = 1.1 S_{0_-}$ one obtains $\bar{\sigma}_c = 710 \pm 25$ millibarns. If the low-energy-range spin statistics of Julien et al. (ref. 8), $S_{0_-} = 1.7 S_{0_+}$, are used, $\bar{\sigma}_c = 720 \pm 25$ millibarns.

Characteristics of Resonances Generated by Separated and Merged Spin Statistics

The total cross sections at 24 keV generated for the Monte Carlo multiple scattering analysis of the gold-sphere transmission experiments are significantly different when separated spin statistics rather than merged spin statistics are used. Examination of representative samples for generated sets of total cross sections reveals the existence of deeper cross section windows for the separated spin data; these are caused by the stronger interference of the resonance scattering with the potential scattering for the $J = 2$ levels with neutron widths chosen from the Porter-Thomas distribution. These interference effects are shown in figure 1 where total cross sections are occasionally reduced to less than 2 barns and frequently to less than 6 barns when the separated spin statistics are used. On the other hand, a representative portion of the total cross sections generated using merged spin statistics indicates an occasional interference window less than 5 barns but most interference effects yield cross sections near 8 barns.

· The effect of a reduced scattering cross section is to increase the average capture cross section for a given value of sphere transmission (ref. 12). It is shown that this is indeed the effect obtained wherein the average capture cross section for gold is about 8 percent larger when the separated spin statistics are used rather than the merged spin statistics.

Another effect observed from the statistically generated sets of total cross sections shown in figure 1(b) is the effective suppression of levels when the separated spin statistics are applied. Since the levels in one spin state are uncorrelated with levels in the other spin state, superposition of levels occasionally occurs so as to effectively suppress levels, or create doublets. On the other hand, when the merged spin statistics are used, all levels are correlated and a level-level repulsion is imposed. The use of

separated spin statistics is then to allow pairs of levels to overlap and thereby to concentrate resonance capture in fewer apparent levels. The effect of concentration of capture area in fewer levels on the average capture cross section of a sphere transmission was studied in reference 4 where it was always found to increase the average capture cross section.

It is for the two forgoing reasons that the use of separated spin statistics provides larger average capture cross sections than the use of merged spin statistics.

Value of the Potential Cross Section

The results of the separated spin Monte Carlo analysis for gold indicate a potential cross section σ_{pot} of 8.3±0.3 barns. This value is substantially lower than the 9.5 barns used in reference 7. There is other evidence to substantiate the value of the potential cross section presently evaluated. The value of R', the potential scattering radius, as given by the Monte Carlo analysis may be compared with the average radial density distribution for the ^{197}Au nucleus as determined by electron scattering (ref. 13). The normalized density $\rho(r)/\rho(0)$ is found to be approximately zero at a radius of 8.11×10^{-13} centimeter; with σ_{pot} given by $4\pi(R')^2$, this implies a value of σ_{pot} of 8.2 barns. Therefore, there is good agreement between the Monte Carlo estimate for σ_{pot} and the value inferred from the nuclear density distribution as ascertained by electron scattering experiments. This is in substantial agreement with the recent work reported in references 14 and 15, which suggests only a very small difference between the neutron radius and the proton radius of nuclei.

The total average scattering cross section $\overline{\sigma}_s$ as determined by Monte Carlo is 13.0±0.3 barns as compared with the measurement of Langsdorf et al. (ref. 16) of 12.80±0.20 barns. This indicates agreement between the separated spin Monte Carlo analysis and an independently measured value of $\overline{\sigma}_s$.

CONCLUSIONS

For a material such as gold, with $I \neq 0$, and two different values of g, a merged spin Monte Carlo analysis of sphere transmission experiments consistently underestimates the value of the average capture cross section. Using the latest published separated spin statistics, the value of the average capture cross section for gold at 24 keV is 710±25 millibarns.

A separated spin analysis is more accurate for gold because it uses the correct values of g and does not force level-level repulsion, and the consequent effective sup-

pression of capture, through the use of the single specie Wigner distribution. However, the separated spin analysis is dependent on a set of experimentally determined separated spin strength functions. As accurate values of separated spin strength functions become available, the Monte Carlo analysis of spherical shell neutron transmission may be applied with precision to the analysis of other sphere transmission experiments.

It may be conjectured that, for monotopes with large I such that $g_+ \cong g_- \cong 0.500$, the merged spin analysis may be sufficient. But in these cases one should perform analyses similar to those above in order to justify the particular merged result.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, February 28, 1972,
112-02.

APPENDIX - PROGRAM DAISY

A series of Monte Carlo calculations have been performed to evaluate the difference between the average capture cross section arrived at from a merged spin calculation and the more accurate separated spin analysis of some spherical shell transmission experiments at 24 keV.

It was suggested (ref. 7) that the stratified sampling technique used in references 5 and 6 may have been inadequate and may be the cause of the differences in the respective analyses. Therefore, the computer program DAISY (ref. 17) has been used to generate the resonance parameters for the present analyses. A short description of DAISY is given herein.

The program DAISY is given the average level spacing for a resonance chain (for a particular spin state) and the average reduced scattering width. It then generates many pseudoresonance chains (up to 9999 chains of up to 5000 resonances) with level spacings chosen from Wigner's level spacing distribution and scattering widths chosen from the distribution of Porter and Thomas. The code then rejects, at a preselected probability level, those chains whose averages are beyond the limits associated with this level. This allows one to select a probability level, say 95 percent, and to reject a chain if it does not approximate the average level spacing better than 95 percent of such chains. This process limits the allowable variation in the average cross sections computed from such chains. The code then chooses, from these well approximating chains, that chain whose individual parameters best fit the theoretical distribution functions. Either the Kolmogorov-Smirnoff or chi-square tests for goodness of fit are used for such a selection of the "best" chain (ref. 17). Thus, the chain finally chosen by the program DAISY shall have the correct average values, and the distribution of the chain's individual parameters will most closely resemble their theoretical distribution functions. The s-wave average dilute resonance cross sections generated herein have been checked against analytic average cross sections obtained using the technique of Lane and Lynn (ref. 18) and were found to agree to three significant figures. Thus in the present analyses there is no question of the adequacy of the technique of stratified sampling.

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