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by Donald Bogart
Lewis Research Center
Cleveland, Ohio

TECHNICAL PAPER proposed for presentation at Conference on Nuclear Data - Microscopic Cross Sections and Other Data Basic for Reactors sponsored by the International Atomic Energy Agency
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CLEVELAND, OHIO, UNITED STATES OF AMERICA

REVISED ABSTRACT

Sphere transmission experiments for measuring average capture cross sections $\bar{\sigma}_C$ in the unresolved resonance region have been interpreted in the past by an analysis adapted from that of Bethe, which assumes capture and scattering cross sections to be energy independent in the keV region. Because of the resonant nature of these cross sections, relatively large resonance self-protection corrections have been applied to these results.

Monte Carlo calculations that account directly for energy-dependent cross sections and multiple-scattering processes in the sphere experiments have provided significantly larger values of $\bar{\sigma}_C$ as a result of including effects of resonance scattering. The consequences of this are particularly important for Au, for which interpretation of the same experiments provides a value of $\bar{\sigma}_C$ at 24 keV of 635±50 mb by Monte Carlo analysis compared with 532±60 mb by Bethe analysis with a resonance self-protection correction. This difference can be attributed to the incorrect inclusion of an average resonance scattering cross section in using the Bethe analysis.

The problem in applying the Bethe method when microscopic cross sections are energy dependent may be reduced to the determination of an effective scattering cross section. By comparing values of average capture cross sections obtained from the Monte Carlo analyses with values obtained from the Bethe analyses for Ag, Sb, I, and Au, a suitable criterion was obtained. The use of the potential scattering cross section as the effective scattering cross section in the Bethe analysis was shown to provide results that were in reasonable agreement with the Monte Carlo results without the necessity for applying resonance self-protection corrections.

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1. INTRODUCTION

The sphere transmission method has been used with Sb-Be neutron sources to measure absolute values of average capture cross sections at 24±2 keV for many elements by SCHMITT and COOK [1], and BELANOVA, et al. [2]. Average capture cross sections are obtained from the values of transmission by a method described by BETHE, et al. [3]. This calculational method accounts for the neutron multiple scattering processes prior to capture or escape from the sphere. However, a major limitation of the method is that the cross sections are considered to be independent of neutron energy. At 24 keV, even for medium-weight and some heavy nuclei of interest, the average spacings of resonances far exceed average Doppler-broadened neutron widths so that resonances retain their characteristic shape, and cross sections vary considerably with energy. For these nuclei, the average spacing of resonances is ~10 eV so that hundreds of levels are encompassed in the 4 keV spread of Sb-Be source neutrons. It is, therefore, necessary to take into account the effects of neutron resonances in interpreting the sphere transmission experiments.

In the Monte Carlo analysis, described by BOGART and SEMLER [4], the resonance cross sections enter directly into the problem as primary input data in addition to the assumed values of potential scattering cross sections. In this way, values of sphere transmission as a function of assumed cross sections are obtained. The calculations yield values of average p-wave capture and potential scattering cross sections that preserve published values of total cross sections and that satisfy the experimental values of sphere transmission.

It is shown that the use of the Bethe method as applied in the past [1,2,5] without the use of resonance self-protection corrections provides values of average capture section that underestimate significantly the values obtained by Monte Carlo analyses of the same sphere transmission experiments. The application of resonance self-protection corrections [1,5] to the results obtained by the Bethe analysis considerably improves agreement with the Monte Carlo results for Ag, Sb, and I, but not for Au.

Both the Monte Carlo calculations and the Bethe method with resonance self-protection corrections require a priori knowledge of average s-wave resonance parameters as input data. For many isotopes, accurate statistical data are not available. In addition, the direct Monte Carlo analysis is laborious and perhaps is not a working method for general interpretation of sphere transmission experiments. Therefore, a method of interpretation of sphere transmission experiments that uses the Bethe analysis but avoids the necessity for applying resonance self-protection corrections is desirable. By comparing values of average capture cross section obtained from the Monte Carlo analyses with values from the Bethe analyses for Ag, Sb, I and Au, a suitable criterion is presented.

2. MONTE CARLO ANALYSIS

Sphere transmission experiments have been analyzed by a Monte Carlo method [4] that employs resonance cross sections that are based on published s-wave statistical data. Spherical shell dimensions and transmission data for spheres of Ag, Sb, I, and Au that have been analyzed [1,2] and the average s-wave resonance parameters at 24 keV that have been obtained from published statistics from slow-neutron spectroscopy studies are presented in Table I. Cross sections based on these parameters are employed in the Monte Carlo analysis and are generated from the Porter-Thomas distribution of reduced neutron widths as represented by 10 Doppler-broadened Breit-Wigner resonances and from the Wigner distribution of level spacings as represented by 10 values; each value is the average of a decile of the respective normalized populations. The scattering and capture cross sections for each resonance are represented by 200 energy values at 1/2 eV intervals. The general operation of the Monte Carlo program is described in reference [4]. An isotropic point source of neutrons is assumed to be centrally located in the shell. For each shell 100,000 case histories are followed either to capture or to transmission. The average energy a neutron may lose in an elastic collision is from 1 to 2 percent of its energy; at 24 keV, this energy loss is very much greater than the average level spacing. Therefore, a collided neutron encounters energy intervals with equal probability. The reaction cross sections for an energy interval are generated as the sum of the contributions of the scattering and capture cross sections of two adjacent noninteracting Wigner-spaced Doppler-broadened resonances chosen at random.

The conditions that are satisfied simultaneously by the Monte Carlo analyses are the experimental values of average total cross section $\bar{\sigma}_T$ and transmission T. The constituent parts of $\bar{\sigma}_T$ are the s-wave and p-wave capture cross sections $\bar{\sigma}_{C_s}$ and $\bar{\sigma}_{C_p}$, the s-wave resonance scattering component $\bar{\sigma}_{S_s}$, and the potential scattering cross section σ_{pot}. In the Monte Carlo calculations the p-wave scattering component is assumed to be small and the p-wave capture cross section is considered to be energy independent and is approximated by an average value. The s-wave resonance parameters used are averages over all isotopes of elemental samples; a spin weight factor g of 1/2 was used.

Some limitations of the Bethe method of sphere analysis were explored by BOGART and SEMLER [4] in performing several idealized sphere transmission problems by the Monte Carlo method. Illustrative calculations were made for Au and I shells using several arbitrary repetitive step scattering and capture cross sections superimposed on the potential scattering. The spacings and magnitudes of the steps were such that the same average value of capture cross section was provided as that used for a nucleus possessing constant scattering and capture cross sections. It was found that all values of $\bar{\sigma}_C$ that satisfy a given value of sphere transmission and that consider the resonance nature of the cross sections as represented by the steps, are larger than the values of $\bar{\sigma}_C$ for energy independent cross sections. These step values of $\bar{\sigma}_C$ are particularly increased by resonance scattering. In the same way, the present Monte Carlo calculations that account directly for energy dependent cross sections and multiple scattering processes in the sphere experiments have provided significantly larger values of $\bar{\sigma}_C$ as a result of including the effects of resonance scattering, which are particularly important for Au. Interpretation of Au transmission experiments provides a value of $\bar{\sigma}_C$ at 24 keV of 635 ± 50 mb by Monte Carlo analysis[1] compared with 532 ± 60 mb reported by SCHMITT [5] which includes a resonance self-protection correction; a value of $\bar{\sigma}_C$ for Au of 660 ± 60 mb by Monte Carlo is to be compared with a value of 570 ± 30 mb by BELANOVA [2].

The results of the sphere transmission experiment analyses by Monte Carlo and a comparison of results at 24 keV by Bethe and Monte Carlo analyses are presented in Table II. The internally consistent values of $\bar{\sigma}_{C_s}$, $\bar{\sigma}_{C_p}$, $\bar{\sigma}_C$, $\bar{\sigma}_{S_s}$ and σ_{pot} obtained by the Monte Carlo analyses that satisfy the experimental transmissions and reported values of $\bar{\sigma}_T$ are also listed in Table II. The effects of an estimated 10-percent uncertainty in Γ_γ and the measured uncertainties in Γ_n and D are evaluated by separate calculations and are combined to provide the listed uncertainties in $\bar{\sigma}_{C_s}$ and $\bar{\sigma}_{S_s}$. The uncertainties in $\bar{\sigma}_{C_p}$ result from the uncertainties in in the measured values of shell transmission T. Although the values of $\bar{\sigma}_{C_s}$ and $\bar{\sigma}_{C_p}$ are found individually to have the listed uncertainties, their sums $\bar{\sigma}_C$ have been found to vary slowly with relatively larger changes in σ_{pot} and $\bar{\sigma}_T$ because of partial compensation in satisfying experimental transmissions. Therefore, the precision of the Monte Carlo value of $\bar{\sigma}_C$ is not believed to be the sum of the uncertainties in $\bar{\sigma}_{C_s}$ and $\bar{\sigma}_{C_p}$ but has been taken to be of the same order of magnitude as

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[1] A biasing error in the coding of those Monte Carlo problems of reference [4] that employed the Wigner distribution of level spacings, forced convergence on erroneously high values of s-wave capture and scattering cross sections for Au and I. As a result, the inferred values of p-wave capture that satisfied observed values of sphere transmission for these nuclei were too low. This coding error has been corrected, and the results presented herein have been corrected for this computational error.

The Bethe method has been used to compute the values of σ_C that satisfy the experimental values of transmission for several shells for a range of scattering cross section σ_S. Because the Monte Carlo code employed herein is readily capable of reproducing the Bethe calculations for energy independent cross sections, several Monte Carlo calculations were also made as a check. The two methods were found generally to agree quite accurately. Inasmuch as there are many combinations of constant scattering cross section σ_S and constant capture cross section σ_C that satisfy a given value of transmission for a shell, the locus of such values has been determined.

The locus curves have been calculated for shells that were measured by SCHMITT [1], namely Ag, Sb, I, and Au-2. The curves are presented in Fig. 1. In each case reduction of σ_S results in an increase in σ_C.

The problem in applying the Bethe method when microscopic cross sections vary with energy can be reduced to the determination of an effective scattering cross section $\sigma_{S_{eff}}$. In the past, the measured average total cross section $\bar{\sigma}_T$ at 24 keV has been used to estimate $\sigma_{S_{eff}}$:

$$\sigma_{S_{eff}} = \bar{\sigma}_T - \bar{\sigma}_C \qquad (1)$$

Since $\bar{\sigma}_C$ is generally much smaller than $\bar{\sigma}_T$, a single iteration results in a good value for $\sigma_{S_{eff}}$. However, since $\bar{\sigma}_T$ consists of the sum of σ_{pot}, $\bar{\sigma}_S$, and $\bar{\sigma}_C$, relation (1) is equivalent to using

$$\sigma_{S_{eff}} = \sigma_{pot} + \bar{\sigma}_S$$

in the Bethe analysis.

The question arises as to what the effective value of energy-independent scattering cross section is that provides a value of $\bar{\sigma}_C$ that is in reasonable agreement with the results of the present Monte Carlo analysis. Indicated in Fig. 1 are the values of σ_C for values of $\sigma_{S_{eff}}$ that correspond to $\sigma_T - \sigma_C$ and to σ_{pot}. The Monte Carlo values of $\bar{\sigma}_C$ are shown to correspond closely to the values obtained by using $\bar{\sigma}_{pot}$ as the effective scattering cross section. Values of $\bar{\sigma}_C$ reported by Schmitt that have been corrected for resonance self-protection are also shown. These corrected values increase the values of $\bar{\sigma}_C$ so as to agree reasonably well with Monte Carlo values for Ag, Sb, and I. They disagree, however, for Au. Therefore, it appears that the method of Bethe may be used to interpret sphere transmission experiments; it can provide a good approximation to the average capture cross section at 24 keV, if the potential scattering cross section is known with reasonable precision and is used as the effective scattering cross section.

An analogy to the present finding that a complex multiple scattering resonance capture problem may be treated by simply ignoring the resonance scattering contributions of absorptive nuclei is to be found in the methods evolved to handle the problem of the calculation of heterogeneous effective resonance integrals for absorbers possessing wide resoances (see DRESNER [7]). Dresner discusses the essential expression for the escape probability from spatially uniform volume sources in lumps of the resonance absorber, for which the width of the resonance in lethargy units greatly exceeds the average lethargy increment per collision. He notes that the escape probability can be expressed accurately over a large range of scattering probability per collision in the lump by a relation that ignores resonance scattering completely.

It would appear that for nuclei having large s-wave strength functions and small average level spacings such as Au, average s-wave resonance scattering contributions are large. These s-wave scattering cross sections coincide in energy with capture cross sections with the result that probability of capture is reduced and the probability of scattering is increased. Therefore, inclusion of the average resonance scattering cross section in estimating the value of $\sigma_{S_{eff}}$ that is to be used in the Bethe method is incorrect. It was shown by BOGART and SEMLER [4] that the s-wave levels with the larger neutron widths in the Porter-Thomas distribution account for the larger share of the resonance capture integral; for example, 50 percent of the resonance capture integral is contributed by about 20 percent of the levels with the larger neutron widths. Therefore, a first order representation of the cross sections that are effective for capture at 24 keV consists of the potential scattering cross section with the superposition of cross sections for relatively widely spaced resonances possessing the larger neutron widths.

4. CONCLUSIONS

A method of interpretation of sphere transmission measurements that uses the Bethe analysis but avoids the necessity for applying resonance self-protection corrections is suggested. By comparing values of average capture cross sections obtained from Monte Carlo analyses with values obtained from the Bethe analyses for Ag, Sb, I, and Au, a suitable criterion for estimating the value of the effective scattering cross section to be used in a Bethe analysis was obtained. The use of the potential scattering cross section as the effective scattering cross section in the Bethe analysis provides results that are in reasonable agreement with the Monte Carlo results without the necessity of applying resonance self-protection corrections.

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TABLE I. - SPHERICAL-SHELL TRANSMISSION DATA AT 24 keV AND

AVERAGE s-WAVE PARAMETERS USED IN MONTE CARLO ANALYSES

Spherical-shell transmission						s-wave parameters				
Shell	Reference	Inner sphere radius (cm)	Outer sphere radius (cm)	Atom density (atom/cm^3)	Transmission	Strength function, S_0	Average observed level spacing, $\bar{D}_{obs}$ (eV)	Average neutron width, $\bar{\Gamma}_n$ (eV)	Average radiation width, $\bar{\Gamma}_\gamma$ (eV)	Reference
Ag	[1,5][a]	4.30	7.46	0.0581×10^{-24}	0.694±0.004	$0.46 \pm 0.06 \times 10^{-4}$	9.4±0.8	0.265	0.150	[8]
Ag	[2][a]	2.05	3.05	.0581	.9222±0.0025	.46±0.06	9.4±0.8	.265	.150	[8]
Ag	[2][a]	2.05	5.05	.0581	.7277±0.0045	.46±0.06	9.4±0.8	.265	.150	[8]
Ag	[2][b]	2.05	5.05	.0581	.7146±0.0050	.46±0.06	9.4±0.8	.265	.150	[8]
Sb	[1,5][a]	2.54	7.62	.0328	.873±0.005	.32±0.03	8.0±0.5	.160	.125	(c)
I	[1,5][a]	4.96	11.21	.01227	.923±0.006	.62±0.09	13.5±0.5	.260	.107	[8]
Au-1	[1,5][a]	5.93	7.62	.0587	.876±0.005	1.50±0.20	16.8±0.5	.780	.170	[9]
Au-2	[1,5][a]	5.08	7.62	.0587	.800±0.004	1.50±0.20	16.8±0.5	.780	.170	[9]
Au	[2][a]	2.05	3.55	.0587	.8955±0.0023	1.50±0.20	16.8±0.5	.780	.170	[9]
Au	[2][b]	2.05	3.55	.0587	.8887±0.0027	1.50±0.20	16.8±0.5	.780	.170	[9]

[a]Transmission determined by long counter.

[b]Transmission determined by water bath.

[c]Private communication from J. B. Garg, Columbia University.

TABLE II. - RESULTS OF SPHERE TRANSMISSION EXPERIMENT ANALYSES BY MONTE CARLO;

COMPARISON OF RESULTS AT 24 keV BY BETHE AND BY MONTE CARLO ANALYSES

Shell	Reference	Average cross sections from Monte Carlo analysis						σ_{pot}[b] (b)	Average capture cross section, $\bar{\sigma}_C$		
									Bethe (mb)		Present Monte Carlo (mb)
		$\bar{\sigma}_{C_S}$ (b)	$\bar{\sigma}_{C_p}$ (b)	$\bar{\sigma}_C$ (b)	$\bar{\sigma}_{S_S}$ (b)	σ_{pot} (b)	$\bar{\sigma}_T$[a] (b)		Uncorrected for resonance self-protection[c] [1,2,5]	Corrected for resonance self-protection [1,5]	
Ag	[1,5]	0.600±0.060	0.480±0.050	1.080±0.060	1.65±0.3	5.2±0.3	7.9±0.3	6.0±0.5	958±45	1127±80	1080±60
Ag	[2]	0.600±0.060	.360±0.040	.960±0.070	1.65±0.3	5.2±0.3	7.9±0.3	6.0±0.5	960±60	-------	960±70
Ag	[2]	0.600±0.060	.470±0.050	1.070±0.070	1.65±0.3	5.2±0.3	7.9±0.3	6.0±0.5	975±66	-------	1070±70
Ag	[2]	.600±0.060	.540±0.050	1.140±0.070	1.65±0.3	5.2±0.3	7.9±0.3	6.0±0.5	1095±55	-------	1140±70
Sb	[1,5]	.325±0.040	.235±0.025	.560±0.040	1.35±0.2	5.4±0.2	6.0±0.2	4.2±0.5	509±27	578±45	560±40
I	[1,5]	.340±0.040	.455±0.050	.795±0.050	1.46±0.3	4.4±0.4	6.6±0.3	4.8±0.6	653±70	768±90	795±50
Au-1	[1,5]	.485±0.050	.135±0.025	.620±0.050	3.18±0.4	9.9±0.4	13.7±0.3	10.8±0.6	495±52	532±60	620±60
Au-2	[1,5]	.485±0.050	.150±0.015	.635±0.050	3.18±0.4	9.9±0.4	13.7±0.3	10.8±0.6	480±83	518±90	635±50
Au	[2]	.485±0.050	.155±0.030	.640±0.060	3.18±0.4	9.9±0.4	13.7±0.3	10.8±0.6	560±28	-------	640±60
Au	[2]	.485±0.050	.195±0.040	.680±0.060	3.18±0.4	9.9±0.4	13.7±0.3	10.8±0.6	590±30	-------	680±60

[a]Values of $\bar{\sigma}_T$ privately obtained from E. G. Bilpuch, Duke University.

[b]Values of σ_{pot} obtained from effective nuclear radii of Seth et al. [6].

[c]Values have been corrected from Sb - Be spectrum averages to 24 keV values.

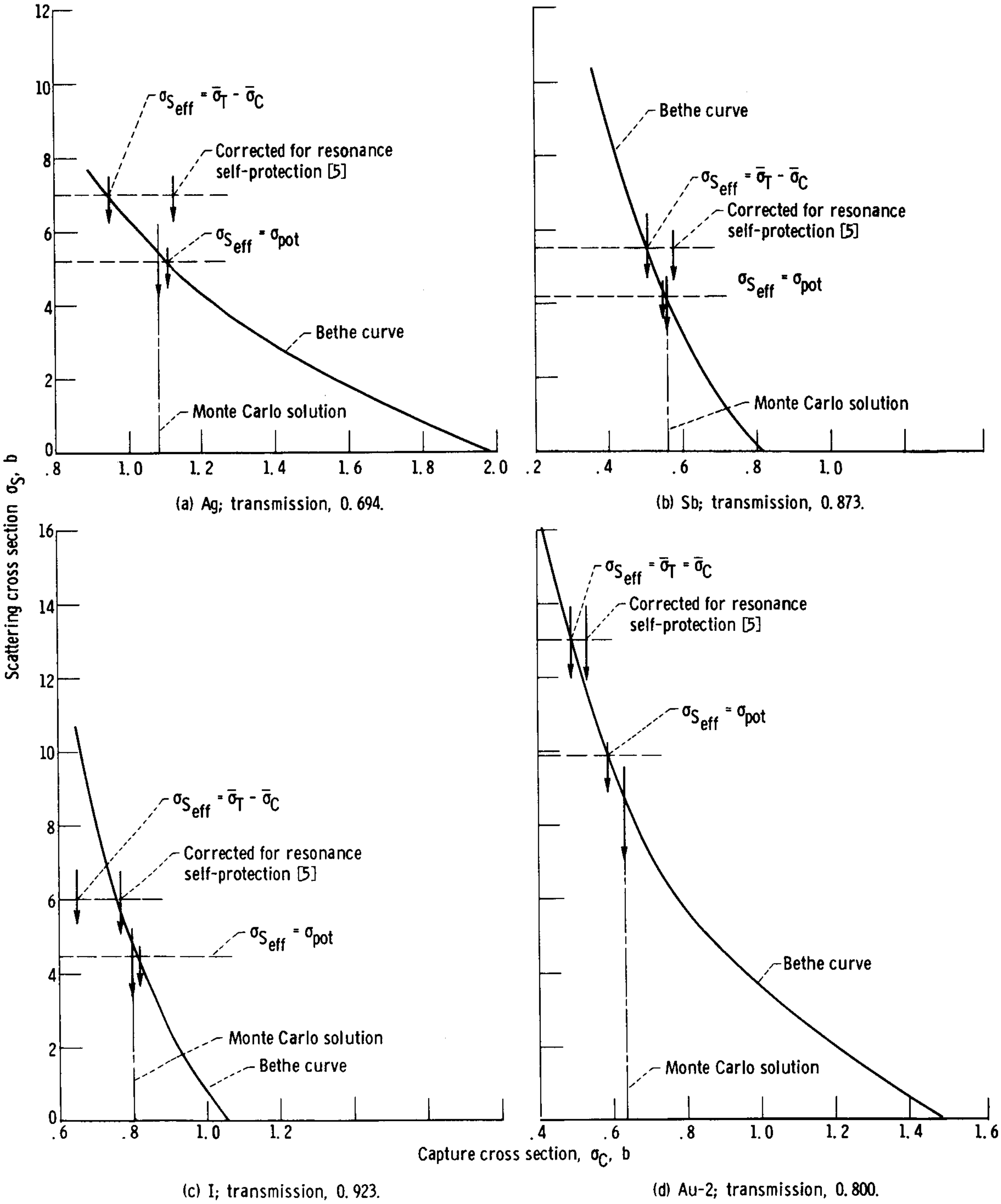

Figure 1. - Loci of Bethe solutions for Ag, Sb, I, and Au-2 shells (SCHMITT [1, 5]).

The Bethe method has been used to compute the values of σ_C that satisfy the experimental values of transmission for several shells for a range of scattering cross section σ_S. Because the Monte Carlo code employed herein is readily capable of reproducing the Bethe calculations for energy independent cross sections, several Monte Carlo calculations were also made as a check. The two methods were found generally to agree quite accurately. Inasmuch as there are many combinations of constant scattering cross section σ_S and constant capture cross section σ_C that satisfy a given value of transmission for a shell, the locus of such values has been determined.

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Au-2	[1,5][a]	5.08	7.62	.0587	.800±0.004	1.50±0.20	16.8±0.5	.780	.170	[9]
Au	[2][a]	2.05	3.55	.0587	.8955±0.0023	1.50±0.20	16.8±0.5	.780	.170	[9]
Au	[2][b]	2.05	3.55	.0587	.8887±0.0027	1.50±0.20	16.8±0.5	.780	.170	[9]

[a]Transmission determined by long counter.

[b]Transmission determined by water bath.

[c]Private communication from J. B. Garg, Columbia University.

TABLE II. - RESULTS OF SPHERE TRANSMISSION EXPERIMENT ANALYSES BY MONTE CARLO;

COMPARISON OF RESULTS AT 24 keV BY BETHE AND BY MONTE CARLO ANALYSES

Shell	Reference	Average cross sections from Monte Carlo analysis						σ_{pot}[b] (b)	Average capture cross section, $\bar{\sigma}_C$		
									Bethe (mb)		Present Monte Carlo (mb)
		$\bar{\sigma}_{C_S}$ (b)	$\bar{\sigma}_{C_p}$ (b)	$\bar{\sigma}_C$ (b)	$\bar{\sigma}_{S_S}$ (b)	σ_{pot} (b)	$\bar{\sigma}_T$[a] (b)		Uncorrected for resonance self-protection[c] [1,2,5]	Corrected for resonance self-protection [1,5]	
Ag	[1,5]	0.600±0.060	0.480±0.050	1.080±0.060	1.65±0.3	5.2±0.3	7.9±0.3	6.0±0.5	958±45	1127±80	1080±60
Ag	[2]	0.600±0.060	.360±0.040	.960±0.070	1.65±0.3	5.2±0.3	7.9±0.3	6.0±0.5	960±60	-------	960±70
Ag	[2]	0.600±0.060	.470±0.050	1.070±0.070	1.65±0.3	5.2±0.3	7.9±0.3	6.0±0.5	975±66	-------	1070±70
Ag	[2]	.600±0.060	.540±0.050	1.140±0.070	1.65±0.3	5.2±0.3	7.9±0.3	6.0±0.5	1095±55	-------	1140±70
Sb	[1,5]	.325±0.040	.235±0.025	.560±0.040	1.35±0.2	5.4±0.2	6.0±0.2	4.2±0.5	509±27	578±45	560±40
I	[1,5]	.340±0.040	.455±0.050	.795±0.050	1,46±0.3	4.4±0.4	6.6±0.3	4.8±0.6	653±70	768±90	795±50
Au-1	[1,5]	.485±0.050	.135±0.025	.620±0.050	3.18±0.4	9.9±0.4	13.7±0.3	10.8±0.6	495±52	532±60	620±60
Au-2	[1,5]	.485±0.050	.150±0.015	.635±0.050	3.18±0.4	9.9±0.4	13.7±0.3	10.8±0.6	480±83	518±90	635±50
Au	[2]	.485±0.050	.155±0.030	.640±0.060	3.18±0.4	9.9±0.4	13.7±0.3	10.8±0.6	560±28	-------	640±60
Au	[2]	.485±0.050	.195±0.040	.680±0.060	3.18±0.4	9.9±0.4	13.7±0.3	10.8±0.6	590±30	-------	680±60

[a]Values of $\bar{\sigma}_T$ privately obtained from E. G. Bilpuch, Duke University.

[b]Values of σ_{pot} obtained from effective nuclear radii of Seth et al. [6].

[c]Values have been corrected from Sb - Be spectrum averages to 24 keV values.

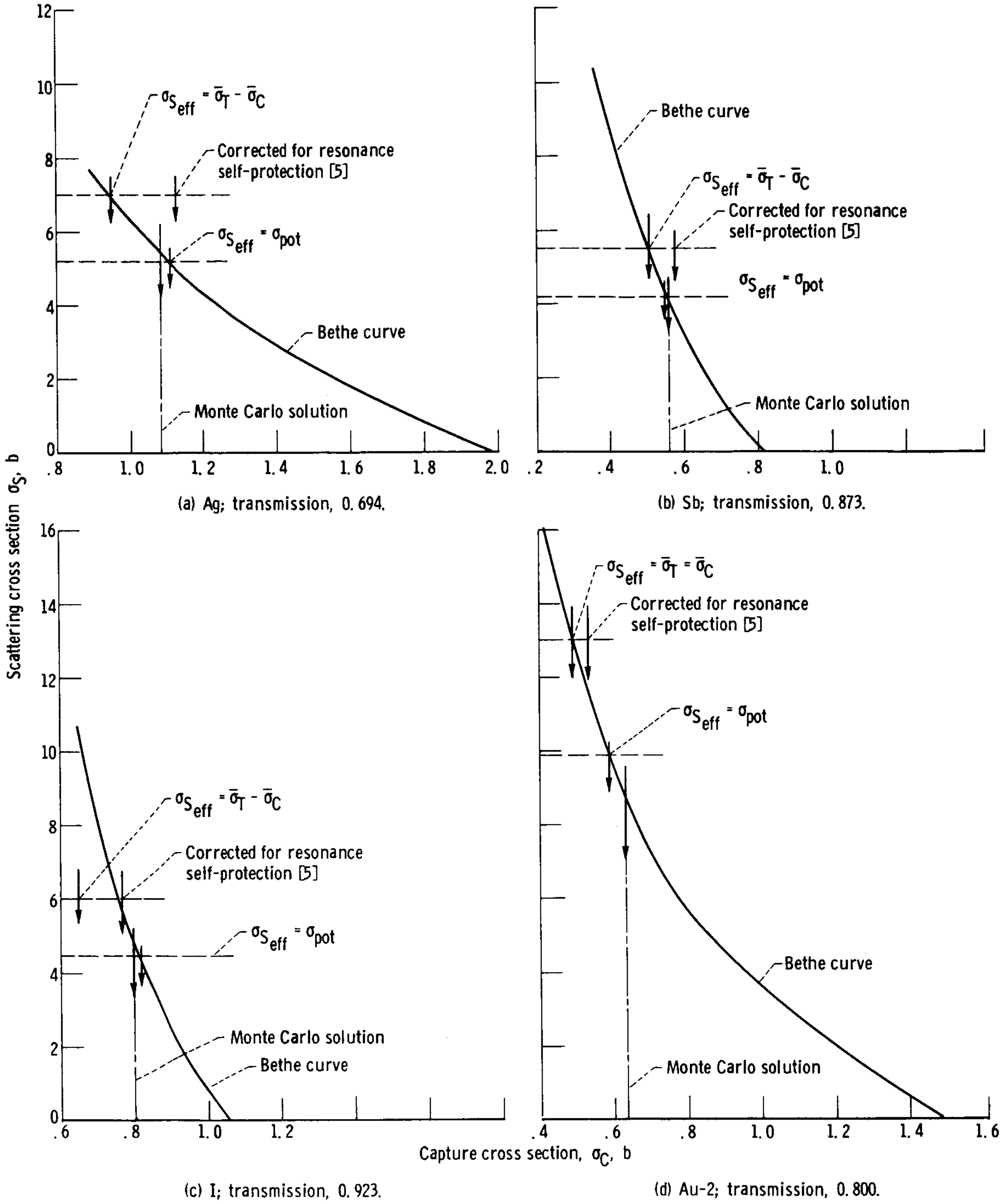

Figure 1. - Loci of Bethe solutions for Ag, Sb, I, and Au-2 shells (SCHMITT [1, 5]).