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Minimizing the statistical error of resonance parameters and cross-sections derived from transmission measurements

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Abstract

Total neutron cross-sections are usually measured by a transmission experiment. In this experiment the transmission through a sample is measured by taking the ratio of the background corrected counts measured with and without the sample in the beam. This procedure can be optimized to reduce the statistical error in the measured cross-section. The objective is to find the optimal sample thickness and time split between the open beam, sample and background measurements. An optimization procedure for constant cross-section measurement is derived and extended to the area under the total cross-section curve of an isolated resonance. The minimization of the statistical error in the measured area also minimizes the statistical error in the inferred neutron width. Comparison of the analytical expression developed in this paper and resonance parameters obtained from the SAMMY (Updated users's guide for SAMMY: Multilevel R-Matrix fits to neutron data using Bays' equation, version m2, ORNTL/TM/-9179/R4) code is shown. The comparison was done with both simulated data and data from transmission experiments that were previously done at RPI. It is shown that the analytical expression can be used as a design tool for optimizing transmission experiments. This will consequently result in more accurate measurements of resonance parameters and can shorten the time required to reach a given accuracy. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

Transmission measurements are one of the simplest experiments that can be done to obtain total neutron cross-sections and resonance parameters. The measurement is done by placing a sample in a well-collimated neutron beam and measuring the number of neutrons passing through the sample with a neutron detector. The background count rate is also measured and the transmission is calculated as the ratio of the background corrected count rate measured with and without the sample. The total cross-section can be a smooth function or contain resonances at specific neutron energies. The transmission is normally measured as a function of the neutron time of flight. The transmission T at time of flight

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channel i is given by

$$T = \frac{r_s - kr_b}{r_o - r_b} \quad (1)$$

where r_s and r_o are the count rates in time-of-flight channel i for the sample and open beam respectively. The background count rate with no sample in the beam in time of flight channel i is denoted by r_b and k denotes a normalization factor that corrects for the attenuation of the background when the sample is in the beam. Background measurements are the most complicated procedure in a transmission measurement and involve measurements of the time dependent and independent background count rates, the details of such measurements can be found elsewhere [1,2]. In our previous measurements [2] it was found that the assumption that k is energy independent gives very good results [2]. The relation between the transmission and the samples cross-section is given by

$$T = \exp(-N\sigma_t(E)) \quad (2)$$

where N is the sample number density (units of atoms/b) and $\sigma_t(E)$ is the microscopic total cross-section (units of barns) of the sample at energy E that corresponds to time-of-flight channel i.

When conducting an experiment to determine the total cross-section from the measured transmission, it is desirable to reduce the statistical error in the measured cross-section. Rose and Shapiro [3] derived the optimum conditions for an experiment with a constant cross-section. For an experiment that is done in a fixed measurement time they derived the optimal time split between the open, sample and background measurements and also the optimal sample thickness. In this work we extend the treatment to find the optimum experimental conditions for an experiment where the objective is to minimize the statistical error in the measured resonance parameters. In this case we fit a resonance in the measured transmission with a computer code such as SAMMY [4] or REFIT [5] to obtain resonance parameters. Our goal is to find the optimal experimental parameters that would yield the lowest possible error in the fitted resonance parameters.

2. Optimizing energy independent total cross-section

First we will derive the optimal solution of the constant cross-section case. This assumes that the transmission is calculated using Eq. (1). The derivation of the optimal solution is similar to the work of Rose and Shapiro [3]. The current work uses the expression for the transmission given by Eq. (1), which is used in the RPI data reduction codes. The results of this derivation are required in order to extend the treatment to cross-section resonances. The cross-section at some neutron energy is obtained from Eq. (2):

$$\sigma = -\frac{1}{N}\ln(T). \quad (3)$$

We can use error propagation to evaluate the error in the total cross-section σ due to the statistical error in the measured transmission (we neglect errors in the sample thickness). The square of the fractional error in the cross-section is calculated to be:

$$\left(\frac{\Delta\sigma}{\sigma}\right)^2 = \left(\frac{\partial\sigma}{\partial T}\frac{\Delta T}{\sigma}\right)^2 \quad (4)$$

where $\Delta\sigma$ and ΔT represent the statistical error in the cross-section and transmission, respectively. The derivative of the cross-section with respect to the transmission (evaluated from Eq. (3)) can be inserted to the above equation to get

$$\left(\frac{\Delta\sigma}{\sigma}\right)^2 = \left(-\frac{1}{NT}\frac{\Delta T}{\sigma}\right)^2 = \left(\frac{1}{N\sigma}\right)^2\left(\frac{\Delta T}{T}\right)^2. \quad (5)$$

This equation indicates that in order to minimize the fractional error in the cross-section, the fractional error in the measured transmission has to be also minimized. The fractional error in the transmission is calculated using the fact that the statistical errors in the count rate measurements with the open beam, sample and the background measurements are independent. Propagating the errors in the counting rates of Eq. (1), the fractional error in the transmission is then given by

$$\left(\frac{\Delta T}{T}\right)^2 = \frac{1}{T^2}\left[\left(\frac{\partial T}{\partial r_s}\Delta r_s\right)^2 + \left(\frac{\partial T}{\partial r_o}\Delta r_o\right)^2 + \left(\frac{\partial T}{\partial r_b}\Delta r_b\right)^2\right]. \quad (6)$$

Evaluating this expression with the partial derivates of Eq. (1) yields:

$$\left(\frac{\Delta T}{T}\right)^2 = \frac{1}{(r_s - kr_b)^2}\Delta r_s^2 + \frac{1}{(r_o - r_b)^2}\Delta r_o^2 + \frac{(r_s - kr_o)^2}{(r_o - r_b)^2 (r_s - kr_b)^2}\Delta r_b^2. \quad (7)$$

The statistical error in the counting rate of the sample (r_s) and open beam (r_o) measurements are related to the measurement time t_s and t_o respectively,

$$\Delta r_s^2 = \frac{r_s}{t_s}, \ \Delta r_o^2 = \frac{r_o}{t_o}. \quad (8)$$

The statistical error in the background is normally derived from a separate measurement such as the one-notch two-notch method [1]. The basic assumption is that similar to the open and sample measurements, the squared counting error in the background will also be inversely proportional to the measurement time t_b

$$\Delta r_b^2 = \frac{\varepsilon^2 r_b}{t_b}. \quad (9)$$

A constant ε^2 ($\varepsilon^2 > 1$) was added in order to allow treatment of counting errors that are larger due to the background measurement method or the manipulation of the data. One example where we might want to change ε^2 is when the background counting rate is fitted to a smooth function and the error in the background is derived from the covariance of this fit [2].

Substituting Eqs. (8) and (9) in Eq. (7) and after some manipulation one can obtain.

$$\left(\frac{\Delta T}{T}\right)^2 = \frac{1}{(r_o - r_b)^2}\left[\frac{1}{T^2}\frac{r_s}{t_s} + \frac{r_o}{t_o} + \left(1 - \frac{k}{T}\right)^2 \frac{\varepsilon^2 r_b}{t_b}\right]. \quad (10)$$

The background-to-signal ratio of the system m can be defined as the ratio of the background count rate to the net open sample count rate

$$m = \frac{r_b}{r_o - r_b}. \quad (11)$$

The counting time for each measurement can be written as fractions of the total counting time:

$$t_s = \alpha_s t, \quad t_o = \alpha_o t, \quad t_b = \alpha_b t. \quad (12)$$

Inserting Eqs. (11) and (12) in Eq. (10), the expression for the squared fractional statistical error in the transmission becomes:

$$\left(\frac{\Delta T}{T}\right)^2 = \frac{m+1}{r_o t} \times \left(\frac{e^{2x}(km + e^{-x})}{\alpha_s} + \frac{m+1}{\alpha_o} + \frac{(1 - ke^x)^2 \varepsilon^2 m}{\alpha_b}\right) \quad (13)$$

where $x = N\sigma_t$ is the optical thickness of the sample. It is important to note that the fractional error in the transmission will be minimized for infinitely thin sample ($T = 1$) where the statistical error in the counting rate is minimized. This is of course not a useful result. However, the actual quantity that is of interest is the total cross-section, which has a unique minimum with respect to the sample thickness and time split.

Inserting Eq. (13) back to Eq. (5) an expression for the square of the fractional statistical error in the cross-section can be obtained

$$\left(\frac{\Delta\sigma}{\sigma}\right)^2 = \frac{m+1}{r_o t x^2} \times \left(\frac{e^{2x}km + e^x}{\alpha_s} + \frac{m+1}{\alpha_o} + \frac{(1 - ke^x)^2 \varepsilon^2 m}{\alpha_b}\right). \quad (14)$$

This expression can be rewritten as

$$\left(\frac{\Delta\sigma}{\sigma}\right)^2 = \frac{m+1}{r_o t x^2}\left(\frac{f_s^2}{\alpha_s} + \frac{f_o^2}{\alpha_o} + \frac{f_b^2}{\alpha_b}\right) \quad (15)$$

where:

$$f_s^2 = e^{2x}km + e^x$$
$$f_o^2 = m + 1$$
$$f_b^2 = (1 - ke^x)^2 \varepsilon^2 m.$$

Assuming a fixed counting time t, this expression can be minimized with respect to α_s, α_o and α_b, keeping in mind the restriction $\alpha_s + \alpha_o + \alpha_b = 1$. The values of α_s, α_o and α_b, for an optimum time split are:

$$\alpha_s = \frac{f_s}{f_o + f_s + f_b}, \quad \alpha_o = \frac{f_o}{f_o + f_s + f_b},$$
$$\alpha_b = \frac{f_b}{f_o + f_s + f_b}.$$

Substituting these values back to Eq. (15) yields an expression for $(\Delta\sigma/\sigma)^2$ where the time split between the open, sample and background measurements is optimized.

$$\left(\frac{\Delta\sigma}{\sigma}\right)^2_{opt} = \frac{m+1}{r_o t x^2}(f_s + f_o + f_b)^2$$
$$= \frac{m+1}{t r_o x^2}((km e^{2x} + e^x)^{1/2} + (m+1)^{1/2} + (1 - k e^x)\varepsilon m^{1/2})^2. \quad (16)$$

Eq. (16) can be numerically minimized to find the optimal sample thickness x assuming fixed counting time t. The results of such optimization are shown in Fig. 1. The calculations were done for the case of $k = 1$ and $\varepsilon^2 = 1$. Comparing the results with those of Rose and Shapiro [3], for high values of m there is a small discrepancy. This was traced to an error in one of the derivatives used to obtain Eq. (8) in the Rose and Shapiro paper. This difference is small and does not effect the main conclusions of their paper.

This result gives some guidance for selecting samples for a transmission experiment; Fig. 1 indicates that even for cases where the background dominates (large m), the transmission should not exceed 0.37. For the case of a small background-to-signal ratio, the transmission should not be lower than 0.08. Results of a calculation of the variation of the optimal time split evaluated at the optimal thickness for different values of m are plotted in Fig. 2. The open beam time fraction α_0 is almost independent of m and has a value of about 20% of the experiment time. When the background-to-signal ratio m changes, there is a trade off between the time spent on the sample and the time spent on the background measurement. When the background is large the time needed for the background measurement will increase at the expense of the time spent on the sample. In the worst condition when the background dominates, only about 30% of the time should be allocated to the background measurement.

The change in the statistical error of the cross-section as a function of the sample's transmission is plotted in Fig. 3. The results are shown normalized to the fractional error of the optimal sample and time split. The point where the curve is tangent to the $y = 1$ axis corresponds to the optimal thickness. As the background-to-signal ratio m increases the optimal transmission is

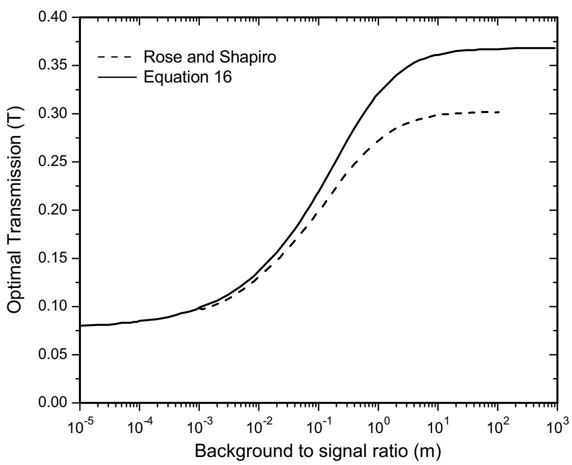

Fig. 1. Optimal transmission calculated as a function of the background-to-signal ratio m.

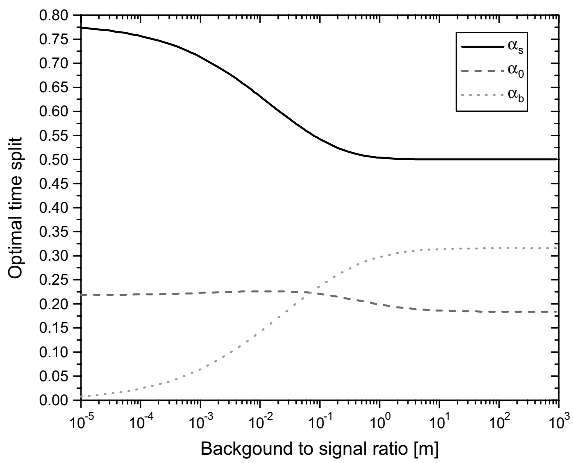

Fig. 2. Calculation of the optimal time splits $\alpha_s, \alpha_o, \alpha_b$ at the optimal thickness as a function of the background-to-signal ratio.

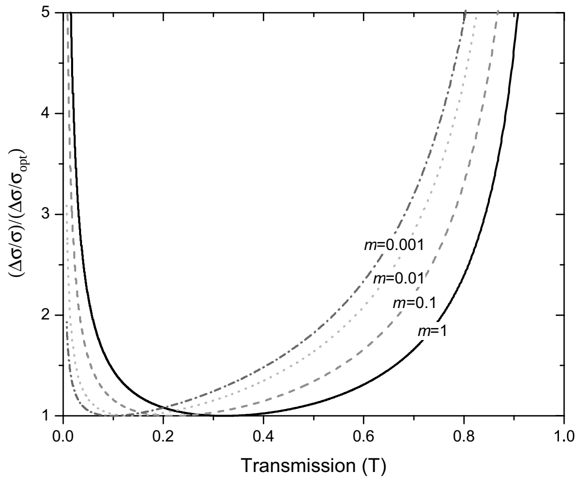

Fig. 3. Calculation of the fractional statistical error in the cross-section as a function of the sample's transmission. The data are normalized to the fractional statistical error of an optimal sample measured with an optimal time split.

larger, which indicates that a thinner sample should be used. This is reasonable since a measurement of larger transmission yields higher count rates for the sample measurement and is thus less sensitive to the background. When the transmission deviates from the optimal value, the statistical error in the measured cross-section will increase. The fractional error increases very fast as the sample becomes thicker and the transmission becomes closer to zero.

These results can be used to design experiments that involve a constant cross-section which may be good for light elements. However, in many cases the cross-section varies as a function of the neutron energy and exhibits resonances at specific neutron energies. We will now consider the case of an isolated resonance.

3. Optimizing resonance parameters measurements

Transmission measurement using a white-spectrum neutron source and the time-of-flight method is the simplest method to obtain the variation of the total cross-section as a function of the neutron energy. The measured transmission can be analyzed with a computer code such as SAMMY [4] or REFIT [5] to obtain the resonance parameters that represent the data. These resonance parameters are used to represent the data in cross-section libraries such as ENDF/B-VI. It is therefore desirable to extend our previous analysis and find the optimal experimental conditions that will yield the lowest possible statistical error in the derived resonance parameters with the restriction of a fixed experiment time.

One method to find the optimal thickness is to simulate a transmission measurement as a function of energy for various sample thicknesses, fit the transmission with a code like SAMMY and obtain resonance parameters. The minimum error can be found for a certain time split of the open, sample and background measurement. This procedure is very tedious and does not easily lend itself to optimizing both the time split and sample thickness for a given resonance. However it will be used to verify some of the results derived in this paper. We can extend the optimization results previously obtained for a constant cross-section measurement to measurements that include a resonance in the cross-section.

Consider an isolated s-wave (angular momentum $l = 0$) resonance at energy E_0, the total cross-section can be expressed using the Breit–Wigner formula [6],

$$\sigma_t(E) = \sigma_0\sqrt{\frac{E_0}{E}}\frac{\Gamma^2}{4(E-E_0)^2+\Gamma^2} \times \left[1+\frac{4(E-E_0)R}{\Gamma \quad \bar{\lambda}}\right] + \sigma_{pot} \tag{17}$$

where Γ is the total width ($\Gamma = \Gamma_n(E_0) + \sum_x \Gamma_x$), $\bar{\lambda}$ is the reduced neutron wavelength, R is the nuclear radius and σ_0 is the peak of the non-Doppler broadened cross-section given by

$$\sigma_0 = 4\pi\bar{\lambda}_0^2 g\frac{\Gamma_n(E_0)}{\Gamma} \tag{18}$$

where g is a statistical factor determined by the spin of the nucleus, $\bar{\lambda}_0$ is the reduced neutron wavelength at the resonance energy and Γ_n is the neutron width. Integrating the cross-section with respect to energy, the area under the resonance is given by [6]

$$A = \int_0^\infty (\sigma_t(E) - \sigma_{pot})\,dE \approx \frac{1}{2}\pi\sigma_0\Gamma. \quad (19)$$

Thus combining Eqs. (18) and (19) we can rewrite the area under the resonance:

$$A = 2\pi^2\lambda_0^2 g\Gamma_n(E_0). \quad (20)$$

This result for the area under the resonance is valid even when considering Doppler broadening [6]. This expression for the resonance area implies that when the neutron width is determined from the resonance area A, minimizing the statistical error of the area under the resonance will consequently minimize the error in the neutron width.

The resonance area can be calculated from the transmission measurement by converting the transmission data to cross-sections and integrating over the entire resonance energy range. This can be approximated by

$$A \approx \sum_{i\in \mathrm{res}} \sigma_i \mathrm{d}E_i \quad (21)$$

where σ_i is the total cross-section at channel i, which corresponds to neutron energy E_i where $\mathrm{d}E_i$ is the channel width in energy units. This expression neglects the potential scattering, which is usually small relative to the resonance.

The procedure of converting the measured transmission to cross-section and calculating the area under a resonance should yield the same area regardless of the sample thickness. However this will not work for samples where the transmission is blacked out for many channels or for high transmission where the data are dominated by large statistical fluctuations.

The statistical error in the cross-section $\Delta\sigma_i$ can be propagated to a statistical error in the area under the resonance.

$$\Delta A^2 = \sum_{i\in \mathrm{res}} \Delta\sigma_i^2 \Delta E_i^2 = \sum_{i\in \mathrm{res}} \left(\frac{\Delta\sigma_i}{\sigma_i}\right)^2 \sigma_i^2 \Delta E_i^2. \quad (22)$$

Using Eq. (14) and making the approximation that m and r_o are constant over the resonance energy range, the squared error in the resonance area is given by

$$\Delta A^2 = \frac{m+1}{tr_o N^2} \sum_{i\in \mathrm{res}} \left(\frac{e^{2N\sigma(E_i)}km + e^{N\sigma(E_i)}}{\alpha_s} + \frac{m+1}{\alpha_o} + \frac{(1-ke^{N\sigma(E_i)})^2\varepsilon^2 m}{\alpha_b} \right) \Delta E_i^2. \quad (23)$$

Eq. (23) can be minimized using a procedure similar to that done for optimizing the constant cross-section case. The equation can be rewritten by defining some constants as:

$$\Delta A^2 = \frac{m+1}{tr_o N^2} \left(\frac{C_s^2}{\alpha_s} + \frac{C_o^2}{\alpha_o} + \frac{C_b^2}{\alpha_b} \right) \quad (24)$$

where

$$C_s^2 = \sum_{i\in \mathrm{res}} (e^{2N\sigma(E_i)}km + e^{N\sigma(E_i)})\Delta E_i^2,$$

$$C_o^2 = \sum_{i\in \mathrm{res}} (m+1)\Delta E_i^2,$$

$$C_b^2 = \sum_{i\in \mathrm{res}} (1-ke^{N\sigma(E_i)})^2\varepsilon^2 m \Delta E_i^2.$$

Minimizing this equation with the constraint that $\alpha_s + \alpha_o + \alpha_b = 1$ yields the solution:

$$\alpha_s = \frac{C_s}{C_o + C_s + C_b}, \quad \alpha_o = \frac{C_o}{C_o + C_s + C_b}, \quad \alpha_b = \frac{C_b}{C_o + C_s + C_b}.$$

Inserting these values in Eq. (24) yields the solution

$$\Delta A^2 = \frac{m+1}{tr_o N^2}(C_s + C_o + C_b)^2 \quad (25)$$

or

$$\Delta A^2 = \frac{m+1}{tr_o N^2} \left[\left(\sum_{i\in E} (e^{2N\sigma(E_i)}km + e^{N\sigma(E_i)})\Delta E_i^2 \right)^{1/2} + \left(\sum_{i\in \mathrm{res}} (m+1)\Delta E_i^2 \right)^{1/2} + \left(\sum_{i\in \mathrm{res}} (1-ke^{N\sigma(E_i)})^2\varepsilon^2 m\Delta E_i^2 \right)^{1/2} \right]^2. \quad (26)$$

This equation can be numerically minimized with respect to N to get the optimal sample thickness

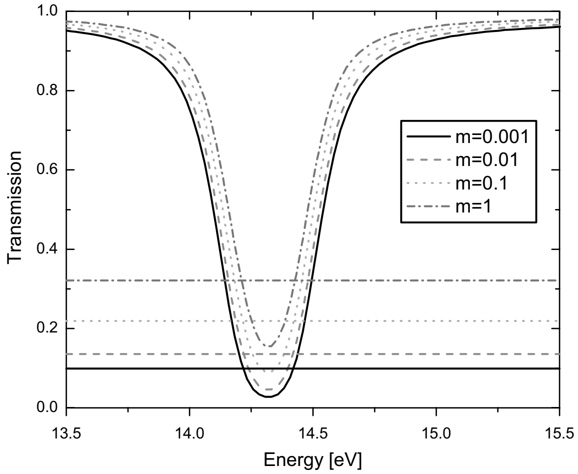

Fig. 4. Plot of the optimal transmissions calculated for the 14.34 eV resonance in Tm, also shown lines representing the optimum transmission for the case of a fixed cross-section.

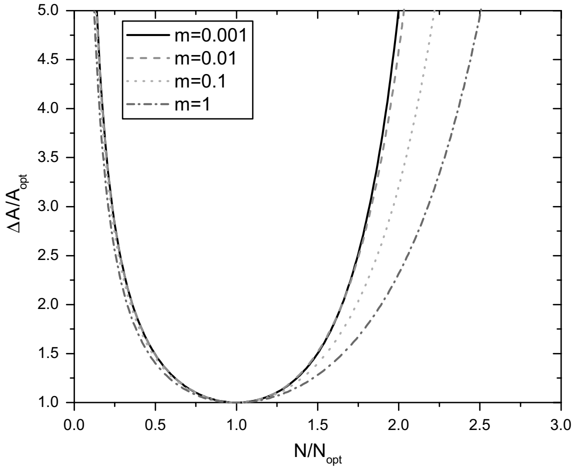

Fig. 5. Variation of the statistical error in the area under the resonance as a function of the sample thickness for various background-to-signal ratios. Calculated for the 3.9 eV resonance in Tm.

for the optimal time split. To demonstrate such calculations, analysis was done for the 14.32 eV resonance in Tm over the energy range 13.5–15.5 eV. The optimal thickness and time split were calculated for several values of m. The transmission calculated at the optimal thickness for several values of m, are shown in Fig. 4. Lines showing the optimal transmissions for constant cross-section measurements are also plotted. These calculations indicate that for the case of a resonance, the minimum transmission at the resonance peak is much lower than the optimal transmission when the cross-section is constant. The ratio of the optimal transmission for a constant cross-section to the optimal transmission at the resonance peak decreases as m increases. The ratio for this case is about 3.54 for $m = 0.001$ and 2.06 for $m = 1$. The transmission at the resonance energy is 0.028 for a background-to-signal ratio $m = 0.001$ and 0.156 for $m = 1$. This result is somewhat surprising and indicates that in order to minimize the statistical error a rather thick sample is needed.

Fig. 5 shows a comparison of the variations in the statistical error in the resonance area as a function of the sample thickness for various background-to-signal values. This calculation indicated that the "penalty" for deviating from the optimal thickness is more severe when the background-to-signal ratio is small. For example, when $m = 0.01$ using a sample with half the optimal thickness will result in an error about 1.4 times larger than the optimal error. In order to achieve the same statistical error of the optimal thickness, a running time that is about 2 times longer is required.

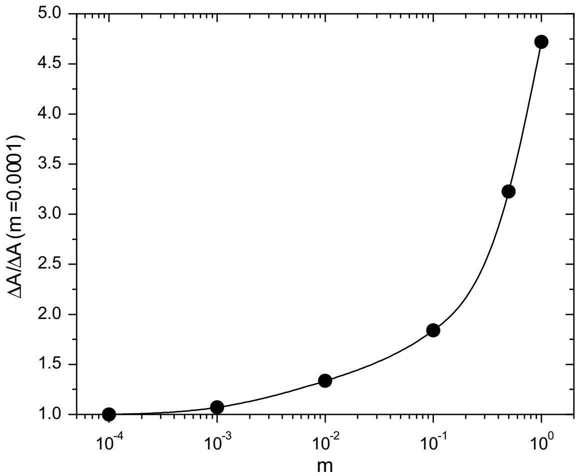

Fig. 6. Variation of the statistical error of the resonance area as a function of the background-to-signal ratio for the 14.32 eV resonance in Tm.

A plot of the normalized statistical error in the resonance area for the optimal time split and sample thickness as a function of the background-to-signal ratio m is shown in Fig. 6. The largest error reduction occurs when m changes from 0.01 to 1. A relatively smaller gain in the fractional error of the resonance area is obtained for values of $m<0.01$.

4. Experimental verification

In order to verify the results, analysis of Tm data that were previously published [7] was used. First, we examine Eq. (14) for the case of a constant cross-section. The fractional error in the cross-section is a function of the optical thickness of the sample x ($x = N\sigma$). The wing of a resonance provides an excellent continuous variation of x as a function of the neutron energy. The measured transmission can be converted to cross-section using the relation given in Eq. (2). The statistical error in the cross-section is then given by

$$\frac{\Delta\sigma}{\sigma} = \frac{-1}{\ln(T)}\frac{\Delta T}{T}. \tag{27}$$

A sample with thickness of 0.0066484 atoms/b was used for this comparison. The time split in the experiment was: $\alpha_s = 0.34$, $\alpha_o = 0.24$, $\alpha_b = 0.42$.

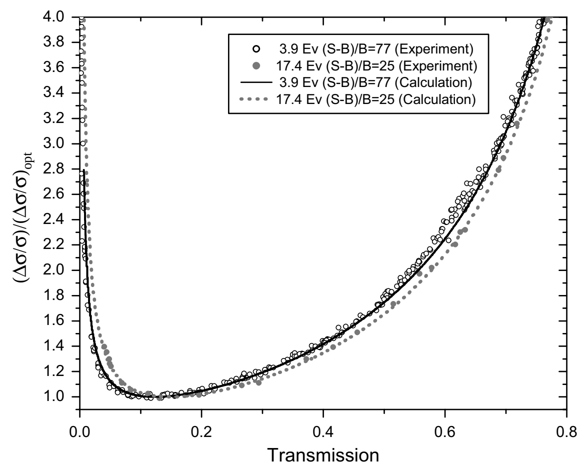

Fig. 7. Comparison of the measured and calculated fractional errors in the cross-section as a function of the sample's transmission.

The background normalization constant for this sample was $k = 0.7$ and ε^2 was set equal to one. Fig. 7 shows the measured and calculated fractional errors in the cross-section normalized to the optimum value. The calculations are shown for the 3.9 eV resonance with $m = 1/77$ and 17.4 eV resonance with $m = 1/25$. These background-to-signal ratios were taken from our previous measurement of the signal to background for the RPI Enhanced-Thermal-Target [2].

The agreement between the measured and calculated errors is very good. This is not surprising since the experimental error was calculated from the measurements in a manner similar to that described by Eqs. (1)–(14). The process of calculating the experimental error involves additional steps such as normalizing runs to the beam monitors and a more complicated treatment of the background [2]. As expected, the resonance at the higher energy where the background-to-signal ratio has a smaller value reaches a minimum error for a thinner sample (higher transmission). The fact that ε^2 was set equal 1 and the agreement between the theory and experiment is good indicates that the error in the background scales with time in a very similar way as the open and sample measurements. This type of comparison also serves as a confirmation of the quality of our previous error analysis.

The optimization procedure described previously in Eq. (26) was done only for the cross-section area under the resonance. Eq. (20) indicates that if the statistical error in the area under the cross-section is minimized this subsequently minimizes the error in the derived neutron width. In order to demonstrate that this is valid, resonance parameters have to be obtained from transmission data. This can be done by using the fitting code SAMMY [4].

Since SAMMY is a shape fitting code it does not determine the neutron width directly from the resonance area but rather from the shape of the measured transmission. The theoretically calculated transmission is fitted to the measured transmission data. Nevertheless if the statistical errors are propagated properly through the code it is expected that the statistical error in the neutron width will still be proportional to the statistical error in the area under the resonance cross-section since Eq. (20) still holds true.

A simulation program was written to generate transmission data for several sample thicknesses. The program simulates a transmission measurement and the associated statistical error as a function of the neutron energy. The program samples the counts for the open, sample and background measurements from a Gaussian distribution. The simulation can use any value of the background-to-signal ratio m and any time split. The sampled counts are calculated from an open sample count rate typical of our observed count rate. The statistical error in the transmission is calculated based on the statistical error of the sampled counts. A Doppler broadened cross-section was used to calculate the transmission through the sample. The simulation does not include the instrumental resolution of our experiment.

The comparison was done for the 3.9 eV resonance in Tm. The radiation width for this resonance [7] is $\Gamma_\gamma = 102.4$ meV and the neutron width is $\Gamma_n = 7.38$ meV. The optimal sample thickness and time split were calculated using Eq. (26) for background-to-signal value of $m = 1/77$ ($k=1, \varepsilon^2 = 1$). The optimal values found are $N = 1.45 \times 10^{-4}$ [atom/b], $\alpha_o = 0.365$, $\alpha_s = 0.479$, $\alpha_b = 0.157$. A simulation of the transmission of this resonance was calculated for 5 samples with thickness ranging from 0.00005 to 0.0002 atoms/b while still keeping the optimal time split. The simulated data were fitted by the SAMMY code by letting the code vary the resonance energy and the radiation and neutron widths. The simulated data and the fits of three representing sample thicknesses are shown in Fig. 8.

According to Eq. (20) the statistical error in the neutron width should correlate to the statistical error of the resonance area under the cross-section. Fig. 9 shows a comparison of these two errors. The error in the resonance area was calculated using Eq. (26). Both errors were normalized to the lowest value obtained (which also occurs close or at the optimal thickness). The minimum in both cases occurs for the same optimum thickness. However the minimum curve is much flatter for the error in the neutron width. For thinner samples the normalized error calculated for the resonance area overestimates the normalized error obtained from the neutron width. The deviations are attributed to the fact that SAMMY obtains the neutron widths by fitting the shape of the resonance and the fit is weighted by the statistical error in the transmission. This gives more importance to the shape of the resonance wings where the error is smaller than in the transmission valley.

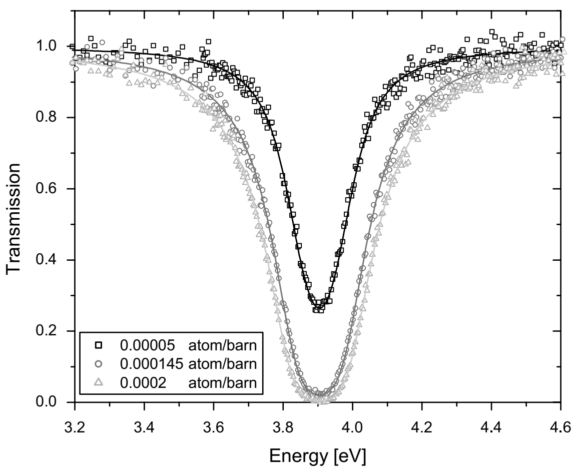

Fig. 8. SAMMY fit to simulated data for the thickest, optimal and thin sample thicknesses.

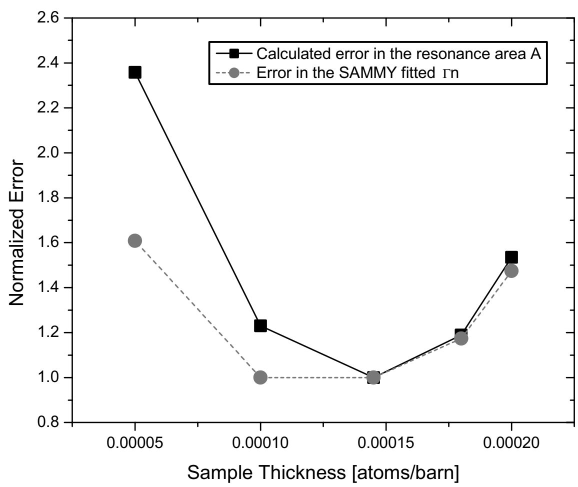

Fig. 9. Comparison of the calculated fractional statistical error in the resonance area and the fractional error in the fitted neutron width for the 3.9 eV resonance in Tm.

As seen from Fig. 9, optimizing the resonance area is very effective in reducing the statistical error in the obtained resonance parameters for a given run time. Since the error in the transmission scales with the square root of the time the benefit of running with optimum thickness could amount to large saving in measurement time for the same statistical error in the fitted neutron width.

To further confirm the minimization procedure a comparison to experimental [2] data was performed. The resonances at 14.32 and 17.44 eV in Tm were used for this comparison; the resonances were fitted with the SAMMY code. The experimental and fitted data for the 17.44 eV resonance are plotted in Fig. 10.

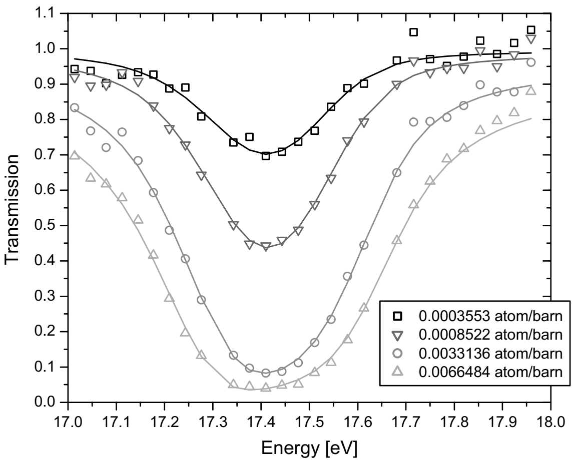

Fig. 10. Experimental and SAMMY fitted results for the 17.44 eV resonance in Tm.

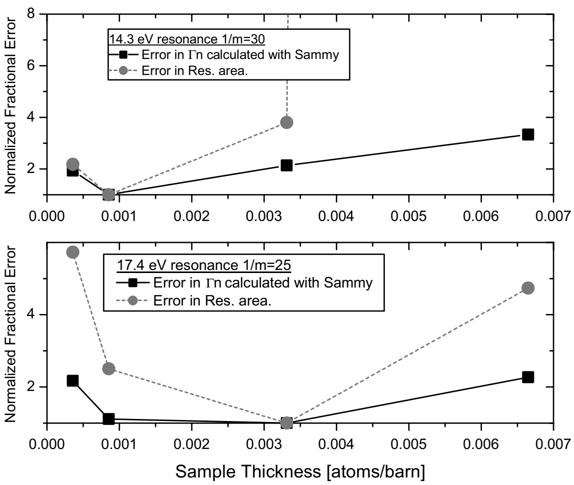

Fig. 11. Normalized error in the resonance area calculated from Eq. (26) compared with the normalized error in the neutron width obtained by SAMMY.

The error in the inferred neutron width was normalized to the minimum valve and plotted for both resonances in Fig. 11. The time split and the background-to-signal ratios of the experiment were used in order to calculate the statistical error in the resonance area under the cross-section curve. The experimental data were taken with a different measurement time for each sample and the calculations of the error in the resonance area were normalized accordingly. The calculated values were then minimized to the sample that gave the smallest error.

For the 14.32 eV resonance with background-to-signal ratio of $m = 1/30$, the minimum error is obtained at sample 2 with thickness $N = 0.0008552$ atoms/b. As we previously obtained with the simulation, the errors obtained with the analytical expression change much faster with the sample thickness. However the minimum error in the analytical calculation and the SAMMY fit occurs at the same sample thickness. The error in the neutron width obtained from the experimentally measured samples indicates that changes of a factor of two in thickness relative to optimal thickness yield about a factor of two larger errors in the fitted neutron width. Thus optimizing the experiments has direct impact on the obtained parameters and can help reduce the error for a fixed measurement time experiment.

Similar results were obtained with the 17.44 eV resonance. As expected for a smaller background-to-signal ratio of about $m = 1/25$ the optimal thickness is larger. Again the minima valley is much shallower for the error in the neutron width but the location of the minimum agrees with the analytical calculations.

5. Summary and conclusions

Optimization of transmission measurements can reduce the statistical error in the measured cross-section. The optimization procedure assumes that a transmission experiment is comprised of the three measurements; an open beam, a sample in the beam and a background measurement. The optimization procedure finds the optimal sample thickness and the time split between the three measurements that will minimize the statistical error in the cross-section.

In case of a resonance, it was demonstrated that minimization of the statistical error in the measured area under the cross-section will in turn reduce the statistical error in the inferred neutron width. Calculations of the statistical error in the area under the cross-section curve of a resonance were compared with the statistical errors in the inferred neutron width. Simulated and experimental data were fitted using the SAMMY code. The error obtained from the code was compared with the error calculated for the area under the cross-section curve of the same resonance. For a certain condition of the time split the statistical error calculated for the resonance area or obtained from the neutron width exhibits a minimum in the same location. However the statistical error in the neutron width has a shallower valley and is less sensitive to changes in the sample thickness compared to the analytical calculations. This is attributed to the fact that the SAMMY code is a shape fitting code. Thus the parameters are obtained from the resonance shape in transmission and not the resonance area under the cross-section curve. Nevertheless dependence of the area under the cross-section curve on the neutron is still preserved and results in the correct prediction of the optimal experimental conditions.

The methods described here can serve as a design tool for future experiments. Optimizing transmission experiments will result in more accurate resonance parameters and reduction of the measurement time. For transmission measurements that are done in order to resolve a specific resonance, only one sample with the optimal thickness measured with the optimal time split is required.

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