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A SUGGESTION FOR SPECIFICATION OF THE NEUTRON ENERGY SCALE IN MEASUREMENTS, ANALYSES AND EVALUATIONS OF DIFFERENTIAL REACTION CROSS-SECTION DATA

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ABSTRACT

Neutron energy distributions (spectra) in differential neutron cross section measurements are represented conventionally by giving the energies (not well defined) and full widths at half maximum of the spectra. In most modern experiments, it is possible for investigators to provide a much more thorough representation of neutron spectra. However, reporting such information would entail more numerical detail than appears practical to document. Therefore, it is suggested that such spectra be represented in publications and files of experimental data by providing the following four moments of each distribution: mean value (energy), standard deviation (resolution), skewness (asymmetry), and kurtosis (sharpness). Implementation of such a standard for data reporting would offer evaluators a much more complete and rational basis for comparing reported values and performing evaluations than previously possible. Some examples are provided to illustrate the concepts.

1. Introduction

Differential neutron measurements are performed in order to acquire knowledge of the energy and/or angular dependence of important physical parameters (e.g., cross sections). However, energy differential measurements are never truly monoenergetic, and no measurement exercise is ever complete due to limitations of time and technique. Thus, all differential measurements - even those with very high resolution - are somewhat inadequate and require profound assumptions about the physical processes to reach conclusions about those fundamental quantities involved. Also, basic information is lost or distorted by the effects of finite resolution. Finally, interpretation of data from experiments can be thwarted by arbitrary and/or inadequate specification of neutron spectra involved in the measurements. The objectives of this paper are to discuss these issues, make some suggestions for improvement in the current ways of handling the problem, and provoke constructive thought.

2. Energy Scale Effects

A differential measurement aims to provide a value q for a physical quantity Q, corresponding to parameters $\underline{p}$, i.e., $q = Q(\underline{p})$. Examples

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are $s = \sigma(E)$ or $y = d\sigma(E,\theta)/d\Omega$. Errors, biases or general confusion over the definition of the energy scale for a measurement can impact severely on the interpretation of such differential information. To understand this, consider $\sigma(E)$ to be the "true" differential cross section. Let E_m be a measured, specified or assumed energy, while E_0 is its true (but unknown) equivalent value. Then, there is a systematic error, $\Delta\sigma = \sigma(E_0)-\sigma(E_m)$, in our knowledge of σ near E_0 due to energy scale uncertainty. It can be significant for rapidly changing σ.

3. Loss of Information

If $\sigma(E)$ is the true cross section, then its measurement will lead, inevitably, to the result $\sigma'(E) = \int R(E,\epsilon)\sigma(\epsilon)d\epsilon$, where $\int R(E,\epsilon)d\epsilon = 1$ for all E (in the discussions of this paper, integration extends from 0 to ∞). The process of converting σ to σ' is irreversible, in a practical sense, even if measurements of σ' are made for many closely spaced values of E, and $R(E,\epsilon)$, the resolution function, is well known. We must accept as inevitable that information about $\sigma(E)$ is irretrievably lost by the measurement process. However, interpretation of σ' as representative of σ becomes more meaningful if we follow consistent procedures for specifying $R(E,\epsilon)$. In particular, the measured results $\sigma'(E)$ will then be free of biases and distortions so that physical principles can be used with some reliability to infer the nature of σ from the measured values of σ'. Figs. 1 and 2 show how the resolution function distorts basic information. For example, it is seen that finite resolution leads to cross sections that are too large near threshold. This can have a profound effect on C/E comparisons with integral data. Nuclear model results are often preferable to real data near threshold unless the measurements are of very high resolution.

4. Characterization of Differential Neutron Spectra

Modern experimental methodology, aided by computer analysis, allows for characterizing the neutron spectra from differential measurements with considerable accuracy and detail[1-8]. It is impractical to record all this detail in computer data files for posterity, so a consistent system for identifying and recording key spectrum parameters is needed. Contemporary practice generally offers ad hoc and inadequate characterization, e.g., differential energy ⇒ peak neutron yield, and resolution ⇒ full width at half maximum. <u>It is suggested that differential neutron spectra be treated as probability distributions and that well defined low-order moments from statistics be used to characterize these distributions for practical purposes</u>. As an example, consider Fig. 3 which is derived from printout of a data analysis code used to determine neutron activation cross sections as measured against a fission standard. The neutron energy spectrum shown corresponds to the activation sample in this experiment.

5. Moments of Localized Neutron Distributions

Let us assume that the shape of the neutron energy distribution is defined by p(E) and that it is normalized, i.e., $\int p(\epsilon)d\epsilon = 1$. For

convenience, the following change of notation is made: $p(\epsilon) \Leftrightarrow R(E,\epsilon)$ for a particular E. Neutron energy for a differential measurement can be equated to the distribution mean value, $E = \int \epsilon p(\epsilon) d\epsilon$. The neutron energy resolution can be associated with the distribution standard deviation, $\sigma = [\int (\epsilon - E)^2 p(\epsilon) d\epsilon]^{1/2}$. Note that in this context, σ ought not be confused with a cross section. As an example, consider the distribution $p(\epsilon) = \exp[-(\epsilon - E)^2/(2\sigma^2)]/(2\pi\sigma^2)^{1/2}$, i.e., the normal or Gaussian distribution with mean value E and standard deviation σ. Then, FWHM $\approx 2.35\ \sigma$. Deviations of the spectrum relative to a Gaussian can be examined by considering two additional distribution moments: skewness, $a_3 = \mu_3/\sigma^3$, where $\mu_3 = \int (\epsilon - E)^3 p(\epsilon) d\epsilon$, and kurtosis, $a_4 = \mu_4/\sigma^4$, where $\mu_4 = \int (\epsilon - E)^4 p(\epsilon) d\epsilon$. The skewness is zero for a distribution which is symmetric about the mean value, while it is negative for one with a tail sloping to the left and positive for one sloping to the right. For a Gaussian distribution, the kurtosis equals 3. If $a_4 < 3$, the distribution has drops off more rapidly to zero on the wings than a Gaussian, while $a_4 > 3$ signifies a distribution which drops off more slowly than a Gaussian[9]. These four quantities embody the principle features of a localized distribution function. Therefore, it is suggested that a reasonable characterization of the spectrum associated with a differential measurement can be recorded for posterity by preserving E, σ, a_3 and a_4. This approach does not suggest a major new commitment of effort or data storage space since all that is required is a consistent determination of E and σ, plus two additional parameters beyond what is conventionally expected from an experimenter.

6. A Suggested Standard for Data Reporting and Filing

Consideration needs to be given to a means for implementing this suggestion in the reporting of experimental data submitted for publication in the literature or storage in archival files. The issue should be debated but, for simplicity, let us assume energy differential cross section data, such as a reaction cross section, are to be presented. An experimenter could attend to detailed characterization of all his measurement spectra and then calculate E, σ, a_3 and a_4, as defined earlier, for each data point. The experimenter would then report for each experimental data point: σ_{meas}, E, σ, a_3 and a_4, where σ_{meas} is the measured differential cross section. These five values could be introduced into computer files for each data point, along with any descriptive information of a conventional nature, as available.

7. To What Extent Can We be Successful in Reconstructing a Differential Spectrum Given only Four Parameters?

It is clear that generally we could not do an outstanding job because the conversion process, $p(\epsilon) \Rightarrow E$, σ, a_3 and a_4, certainly entails loss of information. In fact, it is not suggested here that provision of four parameters is a substitute for knowledge of the complete distribution. However, a user of reported data would be in a far better position to evaluate the significance of the information if he knew exactly how the energy scale were determined and how broad the spectrum used was in terms of its standard deviation, which is well

defined. Furthermore, he would benefit by knowing whether or not the spectrum used was skewed and if it dropped to zero in the wings more quickly or more slowly than a Gaussian. Nevertheless, it is interesting to examine just what can be done with four parameters, and the following discussion is offered in this spirit. The approach presented here is to represent $p(\epsilon)$ by a 4th-order polynomial expansion. There are a couple of possibilities which come to mind. The first is to use a simple Taylor series, namely, $p(\epsilon) \approx \Sigma_{k=0,4}\, p^k(E)(\epsilon-E)^k$, where $p^k(E)$ is the kth-order derivative of p at $\epsilon = E$. This approach is conceptually rigorous, but not particularly useful because the parameters, $p^k(E)$, are not easily related to the moments we have chosen to consider. The second approach is to consider an empirical expansion which does directly involve E, σ, a_3 and a_4, namely, $p(\epsilon) \approx p(E)\{1 + \Sigma_{k=1,4}\, c_k[(\epsilon-E)^k/(k!\sigma^k)]\}$. The coefficients, c_k, are defined as follows (with indicated justification): $c_1 = 0$ (simplicity and it works for a Gaussian), $c_2 = -1$ (it works for a Gaussian), $c_3 = a_3$ (a reasonable guess), and $c_4 \approx 0.6a_4$ (it works for a Gaussian). The results for a Gaussian are shown in Fig. 4, where various values of $A = c_4/a_4$ are considered. With this empirical expansion, fairly good results were obtained for both a Gaussian and a spectrum obtained from analysis of an actual neutron activation experiment[10]. In this measurement, for several spectra corresponding to the D(d,n)He-3 source reaction, the empirical polynomial expansion provides a pretty good shape representation of $p(\epsilon)$ over the approximate energy range $E-1.5\sigma < \epsilon < E+1.5\sigma$ (e.g., see Fig. 5). However, the spectra calculated from the empirical expansion are found to be shifted to lower energies relative to the true $p(\epsilon)$, by an amount ΔE that is dependent very roughly in linear fashion on a_3 (see Fig. 6). Even though the agreement is not very good for energy deviations ϵ of more than 1.5σ to 2σ (see Figs. 4 and 5), and one must account for the energy shift when the spectrum is skewed, it is encouraging that the approach does provide the user with a much better understanding of the spectrum shape than deduced from knowing only the mean energy and standard deviation alone.

8. Summary

The approach suggested in this paper capitalizes on the ability which experimentalists now possess to characterize differential neutron energy spectra quite reliably and in considerable detail. Representation of these spectra by four low-order distribution moments offers a statistically rigorous way to define energy and resolution, and also provides useful information on higher-order spectrum features, i.e., skewing and rapidity of the drop off to zero. Given these four parameters, it is possible to reconstruct spectral shapes in qualitative fashion in the vicinity of the mean energy, provided that allowance is made for a small shift in energy which roughly depends linearly on a_3.

9. References

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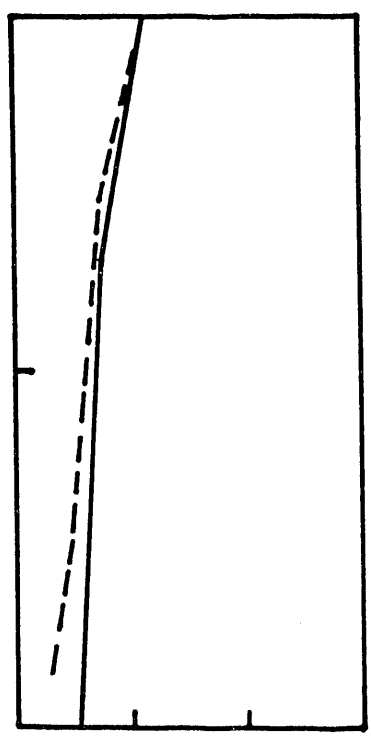


Fig. 1: Effect of finite resolution on threshold data Original (___), Broadened (_ _ _). Vertical scale is logarithmic.

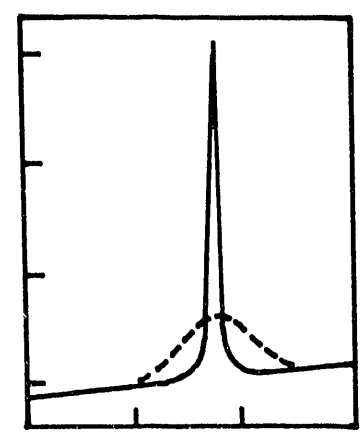


Fig. 2: Effect of finite resolution on resonance data Original (___), Broadened (_ _ _).

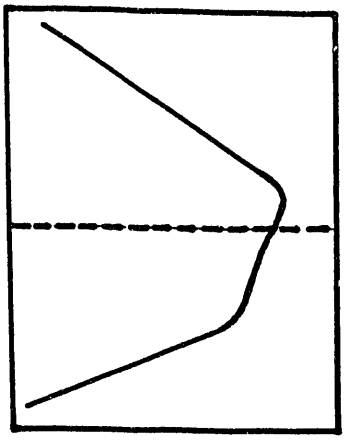


Fig. 3: Calculated neutron energy spectrum for a fast neutron activation experiment (dashed horizontal line marks mean value of the energy).

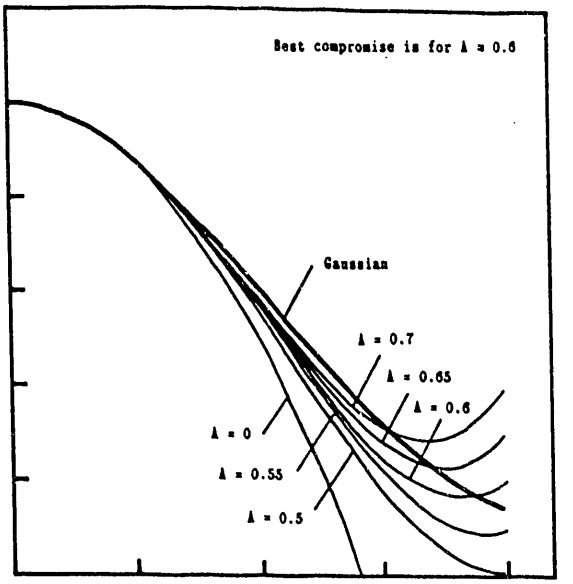


Fig. 4: Comparison of a Gaussian spectrum shape with an empirical polynomial expansion for $c_4 = A a_4$ and various values of A (see text).

Fig. 5: Various representations of an experimental "monoenergetic" neutron energy spectrum.

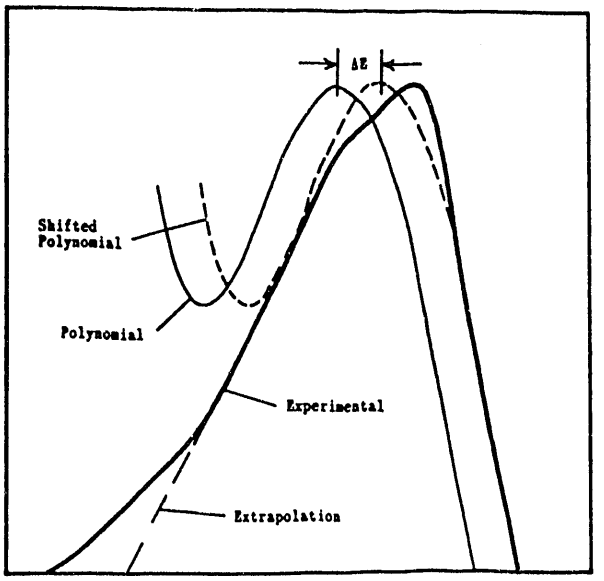
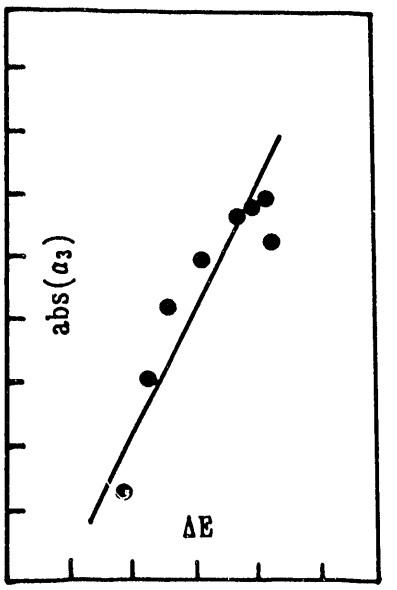


Fig. 6: Energy shift versus skewness as required for polynomial spectra to agree with their experimental counterparts.



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