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Thoughts on Uncertainties in the Moments Formalism of the Statistical Theory of Fission Chains

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Abstract

A LANL paper says it provides an uncertainty analysis of subcritical benchmark measurements using the Hage-Cifarelli moment's formalism. The goal of the LANL work is to provide uncertainties in the leakage and total multiplication values for use in subcritical benchmark measurements. Data of the bare BeRP ball taken September 17-20 2012 as part of experiment IER-161 for the Department of Energy Nuclear Criticality Safety Program are used as an example to determine the measured uncertainties in leakage and total multiplication. The contribution of each parameter to the total uncertainty is then examined.

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1 INTRODUCTION

A problematic feature of the LANL paper titled *Uncertainty Analysis of Subcritical Benchmark Experiments Using the Hage-Cifarelli Formalism* is noted in the section "Uncertainties in the Singles and Doubles Counting Rates" at the bottom of page 1:

> "This work will concentrate on using the singles and doubles rates to solve for neutron multiplication and spontaneous fission rate. The estimation of these rates is performed by fitting the Feynman Y parameter, or Y_2, as a function of gate-width. Typically chi-squared minimization is the method used for fitting the Feynman Y as a function of amplitude and neutron diffusion lifetime. However, the reduced chi-squared used during this fitting is typically not equal to one. This means the data used for the fit does not follow a normal distribution and hence many of the uncertainty evaluation methods won't work."

Two paragraphs later, in the second paragraph on page 2, one of the above issues is expanded on:

> "In the examples presented in this paper, the minimum reduced chi-squared values for the fits were on the order of 0.01 or less."

Under fairly general conditions with the method of least-squares in the large sample limit, the χ^2 function takes on a Gaussian shape. The importance of the Gaussian distribution stems from the central limit theorem which states that the sum of n independent continuous random variables becomes a Gaussian random variable in the limit of large n. The central limit theorem holds regardless of the distribution functions of individual variables. This is the formal justification for treating measurement errors as Gaussian random variables because the total error is nearly always the sum of of a large number of small contributions.

Finding values of the diffusion lifetime λ^{-1} and the asymptote $R_{2\mathrm{F}}$ that minimize χ^2 can be nontrivial because of the nonlinear nature of the fit. One reliable method is to use the Nelder-Mead nonlinear optimization method. The relationship between the true values and confidence regions for λ^{-1} and $R_{2\mathrm{F}}$ is nonetheless almost certainly not an ellipse as would be the case for a linear two-parameter fit.

Another issue is that the number of degrees of freedom n_{DOF} is not well defined for any time interval construction where T is chosen in such a way that neutrons used for one value of T get reused for another.

The simplest interpretation for values of $\chi^2/n_{\mathrm{DOF}} \lll 1$ (i.e. "reduced chi-squared" much less than 1) is that the uncertainties on Y_2 for a given time interval T are badly overestimated or, more likely, the covariance matrix between different time intervals is incorrect.

Another open question is the size of the quantile Q_γ that corresponds to a particular confidence interval (e.g. one standard deviation) when the covariance

matrix between the different time intervals T is not diagonal (i.e. neutrons have been reused across different time gates).

Furthermore, if the "data used for the fit does not follow a normal distribution," then the Neyman construction for confidence intervals should be used. Another issue arises in the construction and interpretation of confidence intervals when a parameter can only take on values in a restricted range. As an important example, consider the case where the mean of a Gaussian distributed variable is constrained on physical grounds to be non-negative. In such cases, one method has been suggested by Feldman and Cousins and applies an ordering principle to the usual Neyman construction.

2 REVIEW

The jth combinatorial moment $\mathcal{M}_j(T)$ of the multiplicity distribution $b_n(T)$ is just the jth factorial moment of $b_n(T)$ divided by $j!$, or more simply

$$\mathcal{M}_j(T) = \sum_{n=j}^{\infty} \left(\begin{array}{c} n \\ j \end{array} \right) b_n(T) \tag{1}$$

Furthermore, we define the following constants:

$$\overline{\nu_\mu} = \sum_{\nu=\mu}^{\infty} \left(\begin{array}{c} \nu \\ \mu \end{array} \right) C_\nu \tag{2}$$

which are the combinatorial moments of the neutron multiplicity distribution for induced fission, and

$$\overline{\nu_{\mathrm{S}\mu}} = \sum_{\nu=\mu}^{\infty} \left(\begin{array}{c} \nu \\ \mu \end{array} \right) C_{\mathrm{S}\nu} \tag{3}$$

which are the combinatorial moments of the neutron multiplicity distribution for spontaneous fission.

As a practical matter, the combinatorial moments $\mathcal{M}_j(T)$ of the multiplicity distributions $b_n(T)$ are easy to compute. The quantities $Y_j(T)$ can be expressed in terms of $\mathcal{M}_j$ as

$$Y_1(T) = \mathcal{M}_1(T) \tag{4}$$

$$Y_2(T) = \mathcal{M}_2(T) - \frac{[\mathcal{M}_1(T)]^2}{2!} \tag{5}$$

$$\begin{aligned} Y_3(T) &= \mathcal{M}_3(T) - Y_2(T)\mathcal{M}_1(T) - \frac{[\mathcal{M}_1(T)]^3}{3!} \\ &= \mathcal{M}_3(T) - \mathcal{M}_2(T)\mathcal{M}_1(T) + \frac{[\mathcal{M}_1(T)]^3}{3} \end{aligned} \tag{6}$$

It is also well known that

$$Y_1(T) = R_1 T \tag{7}$$

$$Y_2(T) = R_2 \left(T - \frac{1 - e^{-\lambda T}}{\lambda} \right) \tag{8}$$

$$Y_3(T) = R_3 \left(T - \frac{3 - 4e^{-\lambda T} + e^{-2\lambda T}}{2\lambda} \right) \tag{9}$$

By summing the contributions from fission chains initiated by both induced and spontaneous fission, it is well known that

$$R_j = \epsilon^j \begin{cases} F_{\mathrm{I}} M_{\mathrm{e}} + F_{\mathrm{S}} M_{\mathrm{e}} \overline{\nu_{\mathrm{S1}}} & j = 1 \\ F_{\mathrm{I}} M_{\mathrm{e}}^2 \dfrac{M_{\mathrm{e}} - 1}{\overline{\nu} - 1} \overline{\nu_2} & \\ \quad + F_{\mathrm{S}} M_{\mathrm{e}}^2 \left[\overline{\nu_{\mathrm{S2}}} + \dfrac{M_{\mathrm{e}} - 1}{\overline{\nu} - 1} \overline{\nu_{\mathrm{S1}}}\ \overline{\nu_2} \right] & j = 2 \\ F_{\mathrm{I}} M_{\mathrm{e}}^3 \dfrac{M_{\mathrm{e}} - 1}{\overline{\nu} - 1} \left[\overline{\nu_3} + 2 \dfrac{M_{\mathrm{e}} - 1}{\overline{\nu} - 1} \overline{\nu_2}^2 \right] & \\ \quad + F_{\mathrm{S}} M_{\mathrm{e}}^3 \left[\overline{\nu_{\mathrm{S3}}} + \dfrac{M_{\mathrm{e}} - 1}{\overline{\nu} - 1} \left(\overline{\nu_{\mathrm{S1}}}\ \overline{\nu_3} + 2 \overline{\nu_{\mathrm{S2}}}\ \overline{\nu_2} \right) \right. & \\ \quad\quad \left. + 2 \left(\dfrac{M_{\mathrm{e}} - 1}{\overline{\nu} - 1} \right)^2 \overline{\nu_{\mathrm{S1}}}\ \overline{\nu_2}^2 \right] & j = 3 \end{cases} \tag{10}$$

It is convenient to define the following:

$$Y_{2\mathrm{F}}(T) = \frac{Y_2(T)}{Y_1(T)} \tag{11}$$

$$R_{2\mathrm{F}} = \frac{R_2}{R_1} \tag{12}$$

$$Y_{3\mathrm{F}}(T) = \frac{Y_3(T)}{Y_1(T)} \tag{13}$$

$$R_{3\mathrm{F}} = \frac{R_3}{R_1} \tag{14}$$

Applying Eqs. 7, 8 and 9, the quantities normally used in the analysis are found to be

$$Y_{2\mathrm{F}}(T) = R_{2\mathrm{F}} \left(1 - \frac{1 - e^{-\lambda T}}{\lambda T} \right) \tag{15}$$

$$Y_{3\mathrm{F}}(T) = R_{3\mathrm{F}} \left(1 - \frac{3 - 4e^{-\lambda T} + e^{-2\lambda T}}{2\lambda T} \right) \tag{16}$$

or, as expressed in terms of the combinatorial moments of the count distributions,

$$Y_{2\mathrm{F}}(T) = \frac{\mathcal{M}_2(T)}{[\mathcal{M}_1(T)]} - \frac{[\mathcal{M}_1(T)]}{2!} \tag{17}$$

$$Y_{3\mathrm{F}}(T) = \frac{\mathcal{M}_3(T)}{[\mathcal{M}_1(T)]} - \mathcal{M}_2(T) + \frac{[\mathcal{M}_1(T)]^2}{3} \tag{18}$$

It is worth noting that

$$\lim_{\lambda T \to 0} Y_{2\mathrm{F}} = 0 \tag{19}$$

$$\lim_{\lambda T \to 0} Y_{3\mathrm{F}} = 0 \tag{20}$$

$$\lim_{\lambda T \to \infty} Y_{2\mathrm{F}} = R_{2\mathrm{F}} \tag{21}$$

$$\lim_{\lambda T \to \infty} Y_{3\mathrm{F}} = R_{3\mathrm{F}} \tag{22}$$

3 ERROR PROPAGATION

Let N be the number of time intervals of duration T which are examined, and let $B_n(T)$ be the number of those time intervals in which n neutrons were detected. So in other words, suppose that during the first time interval, six neutrons were counted; B_6 would be incremented by one. During the next time interval, say eight neutrons were counted; B_8 would be incremented by one, and so on for all N time intervals. In this way, the count distribution $B_n(T)$ is built up. The multiplicity distribution $b_n(T) \approx B_n(T)/N$ is just the probability of counting n neutrons during a time interval of duration T, assuming $N \ggg 1$. The total number of neutrons counted n_{Total} during all N time intervals is

$$n_{\mathrm{Total}} = \sum_{n=0}^{\infty} n B_n \tag{23}$$

The count distribution $B_n(T)$ is fundamentally a multinomial distribution: For a given time interval of duration T, there are N independent observations with B_0 cases of zero neutrons counted, B_1 cases of one neutron counted, B_2 cases of two neutrons counted, and so on up to some $B_{n_{\max}}$ cases of $n_{\max}$ neutrons counted. The total number of time intervals N is a fixed number however with

$$N = \sum_{n=0}^{n_{\max}} B_n \tag{24}$$

The numbers for any two $B_n(T)$ are negatively correlated; if there are a greater-than-average number of time intervals where a particular number n of neutrons were counted, then the probability is increased that there are a fewer-than-average number of time intervals where a different number m ($m \neq n$) of neutrons have been counted. In general, the covariance matrix for a multinomial distribution is

$$V_{mn} = \begin{cases} -N b_m b_n & m \neq n \\ N b_n \left(1 - b_n\right) & m = n \end{cases} \tag{25}$$

where, again, $b_n \approx B_n/N$. This can easily be written in terms of the count distributions as

$$V_{mn} = \begin{cases} -\dfrac{B_m B_n}{N} & m \neq n \\ B_n\left(1 - \dfrac{B_n}{N}\right) & m = n \end{cases} \tag{26}$$

Define the row vectors

$$\mathbf{D_{2F}} = \frac{\partial Y_{2F}}{\partial B_n} \tag{27}$$

$$\mathbf{D_{3F}} = \frac{\partial Y_{3F}}{\partial B_n} \tag{28}$$

where it can easily be shown that the elements of the row vectors are

$$\frac{\partial Y_{2F}}{\partial B_n} = \binom{n}{2} \frac{1}{N\mathcal{M}_1(T)} - \frac{nY_{2F}}{N\mathcal{M}_1(T)} - \frac{n}{N} \tag{29}$$

$$\frac{\partial Y_{3F}}{\partial B_n} = \binom{n}{3} \frac{1}{N\mathcal{M}_1(T)} - \binom{n}{2} \frac{1}{N} + \frac{n\mathcal{M}_1(T)}{2N} - \frac{nY_{2F}}{N} - \frac{nY_{3F}}{N\mathcal{M}_1(T)} \tag{30}$$

The variance on Y_{2F} and Y_{3F} for a given T would then be calculated in the usual way as

$$\sigma^2_{Y_{2F}} = \mathbf{D_{2F}}\, V\, \mathbf{D}^T_{\mathbf{2F}} \tag{31}$$

$$\sigma^2_{Y_{3F}} = \mathbf{D_{3F}}\, V\, \mathbf{D}^T_{\mathbf{3F}} \tag{32}$$

where the superscript T in these two equations denotes transpose.

Values for λ and R_{2F} are determined by minimizing the quantity

$$\chi^2 = \mathbf{E_{2F}}^T\, W^{-1}\, \mathbf{E_{2F}} \tag{33}$$

where W_{ij} is the covariance between time gates T_i and T_j and where the error vector

$$\mathbf{E_{2F}} = \frac{\mathcal{M}_2(T_i)}{\mathcal{M}_1(T_i)} - \frac{\mathcal{M}_1(T_i)}{2!} - R_{2F}\left(1 - \frac{1 - e^{-\lambda T_i}}{\lambda T_i}\right) \tag{34}$$

is constructed from Eqs. 17 and 15 and is understood to be a column vector corresponding to different values for T_i.

The quantity R_{3F} and a redundant value for λ are similarly determined by minimizing the quantity

$$\chi^2 = \mathbf{E_{3F}}^T\, W^{-1}\, \mathbf{E_{3F}} \tag{35}$$

where

$$\mathbf{E_{3F}} = \frac{\mathcal{M}_3(T_i)}{\mathcal{M}_1(T_i)} - \mathcal{M}_2(T_i) + \frac{\left[\mathcal{M}_1(T_i)\right]^2}{3} - R_{3\mathrm{F}}\left(1 - \frac{3 - 4e^{-\lambda T_i} + e^{-2\lambda T_i}}{2\lambda T_i}\right) \tag{36}$$

The covariance matrix W depends on the structure of the time gates. W depends on how the different values of T are chosen: if the same neutron counts are used to populate count distributions with different values of T, W will not be diagonal. In particular, if any of the neutrons are reused in multiple time gates (different values of T), then W can become very complex.

Because the χ^2-fit can trace its lineage to the method of maximum likelihood,

$$\chi^2\left(\hat{\theta} + \sigma_\theta\right) = \chi^2\left(\hat{\theta}\right) + Q_\gamma \tag{37}$$

where $\hat{\theta} = (\widehat{R_{2\mathrm{F}}}, \widehat{\lambda})$ is the vector of values that minimizes χ^2 (e.g. Eq. 33) and Q_γ is the quantile which defines the confidence region.

$$\chi^2_{1\sigma} = \mathbf{E_{2F}}^T W^{-1} \mathbf{E_{2F}} - \left[\chi^2\left(\widehat{R_{2\mathrm{F}}}, \widehat{\lambda}\right) + Q_\gamma\right] \tag{38}$$

to determine $R'_{2\mathrm{F}}$ and λ'. The statistical errors on $R_{2\mathrm{F}}$ and λ were then computed as

$$\sigma_{R_{2\mathrm{F}}} = \left|R'_{2\mathrm{F}} - \widehat{R_{2\mathrm{F}}}\right| \tag{39}$$

$$\sigma_\lambda = \left|\lambda' - \widehat{\lambda}\right| \tag{40}$$

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