JOURNAL OF COMPUTATIONAL PHYSICS 13, 338–347 (1973)

A Method for Reducing Bremsstrahlung-Produced Photoneutron Spectra to Partial (γ, n) Cross Sections*

S. J. MECCA

Department of Physics, Providence College, Providence, Rhode Island 02918

AND

P. F. YERGIN

Department of Physics, Rensselaer Polytechnic Institute, Troy, New York 12181

Received March 28, 1973

A new procedure is presented for reducing a series of bremsstrahlung-produced photoneutron spectra to partial (γ, n) cross sections to various possible states of the residual nucleus. The essentially new features of the method consist of the minor one of using linear interpolation to bridge gaps across regions where the cross sections cannot be calculated uniquely from the data, and the major one of requiring that the final computed partial cross section curves exhaust the entire yield spectra, not just the parts near the "tip" region which are usually used. The initially computed (and interpolated) "exact" cross sections are used to establish branching ratios to the various final states, which are held fixed in a fitting or normalization procedure. The method has the advantage that it permits reasonably good estimates of cross sections without requiring the large amount of data-taking the more conventional analysis would require, and it makes full use of the whole extent of the spectrum curves measured. The method is illustrated, and tested to a limited degree, by assuming cross sections for a fictitious nucleus Hy^4. Suggestions for improvements of the method are also presented. The general procedure may be useful in analysis of data from experiments other than photoneutron reactions, especially those where the effective resolution is as unfavorable as it is where the bremsstrahlung photon spectrum is the controlling factor.

1. INTRODUCTION

While it is often true that one is content to leave raw data, which is recorded as a function of a continuous (independent) variable, "as is" with respect to this variable, it frequently arises that the information of interest has been concealed or "smeared out" by the conditions of the experimental arrangement, which effectively give rise to a "resolution function." If one knows this function accurately

* Work supported in part by NSF.

over the whole range of the variable, it may be possible to extract this information, particularly if the data is of sufficient precision and occur at closely spaced values of the independent variable. A common example of this "unfolding" process is the extraction of multiple resonances from data of finite resolution in atomic or nuclear spectroscopy. In these cases, the "resolution function" is usually a reasonably tractable one, especially in having the property that it falls off fairly rapidly and continuously from the central value of the independent variable. A somewhat more complex analysis of the problem has been studied by Cook [1] and Penfold and Leiss [2]. This is the unfolding of data taken as a series of photonuclear total yield values, for a "closely" spaced set of bremsstrahlung end-point energies, to obtain a set of values for the photonuclear cross section. The point that causes trouble here is that the bremsstrahlung spectrum is not localized to a narrow photon energy region, and in fact rises monotonically from the highest energy (end-point) towards lower energies. The early photon difference analysis method of Penfold and Leiss [2] gives a straightforward method of solution in this case, but is plagued by the strong correlations of nearby points in the result, so that statistical fluctuations of the input data make large apparently systematic swings in the final results. While the "practiced eye" can discount these appropriately, the method of Cook [1] has the advantage that it eliminates all "swings" except such as can be statistically justified by the data. In brief, their method consists of choosing an arbitrary cross section curve which is then used to construct an artificial set of yield points. These artificial points are compared with the actual data, and the assumed cross section is considered to be acceptable if the chi-quare per degree of freedom is approximately equal to unity. The cross section is adopted by exploiting the analytic aspects of the problem.

Our interest has been in using data taken in photonuclear experiments to produce *partial* (γ, n) cross sections (i.e., to different states of the residual nucleus) as a function of photon energy, as contrasted to the total cross sections obtained by Cook [1] and others [2] from total yield data. For this purpose one measures the photoneutron energy spectra from nuclei, for a number of bremsstrahlung end-point energies. The more detailed data thus obtained permits analysis into more detailed results, i.e., into partial cross sections. It is true, however, that the energy resolution of the spectra is finite, and, more importantly, the end-point (electron energy) steps are finite, and in some cases rather wide, even compared to the spacings of the residual nucleus energy levels.

The customary procedure has been to take "small" steps in electron energy (i.e., steps comparable in size to the energy difference between the ground and first excited states, at any rate). Then the "tip" of the photoneutron spectrum, from the maximum energy down to E_1 less than this (where E_1 is the energy of the first excited state of the residual nucleus) must be entirely produced by photoneutrons which leave the residual nucleus in its ground state. Analysis of this part of the

spectrum into a ground state cross section is essentially trivial. Given enough spectra, taken at end-points E_1 apart, one can obtain an essentially continuous curve of ground-state cross section versus photon energy. This can then be used to construct the values of ground state yields of all energies, for the spectrum at each electron energy. Subtracting these ground state yields from the data leaves a set of spectra produced by excited state transitions only. Iteration of the above process, now for the first excited state, will produce a cross section curve for transitions to the first excited state. However, since in general the separation of the first and second excited states will be less than E_1, the cross section curve may have gaps in it and, unless one bridges these with arbitrary (if plausible) interpolations, one cannot repeat the process again to obtain second-excited state cross sections, and so on. In principle, one could have taken sufficiently small steps in the electron energies originally to permit any degree of "unfolding" one wished. In practice, the required expenditure of time and money, and the rapid decrease in spacing of nuclear energy levels as the energy increases, make this procedure unfeasible for more than the first few states, and in some cases not even the first excited state can be separated in a clearly unambiguous fashion.

Our method of attack on the problem bears a generic resemblance to that of Cook, described above for the total cross section analysis of yield data, in that it makes "reasonable" assumptions about the energy dependence of the cross sections to eliminate all but one of an infinite number of possible solutions. It goes further, however, in that it makes use of redundant data. This, as will be seen, enables one to obtain "plausible" partial cross section values in cases where the simpler analysis just described would give no results at all.

The assumptions, computational details, results with hypothetical test data, and suggestions for improvement are presented in the sections that follow.

2. Computational Details

The equation relating the measured neutron spectrum to the partial (and in our case differential) cross sections is

$$Y(E_n, \chi_j) = n \sum_{i=1}^{NS} \phi(E_\gamma \chi_j) \frac{d\sigma(E_\gamma)}{d\Omega}\Big)_i K_i, \tag{1}$$

where E_n, E_γ, and χ_j are neutron, photon, and electron energies, respectively, Y is the measured number of neutrons per unit energy, per electron, per unit solid angle corrected of course for detector efficiency, ϕ is the bremsstrahlung flux on the sample per electron, n is the number of sample nuclei in the photon beam, and $(d\sigma/d\Omega)_i$ is the differential cross section to the ith state of the residual nucleus

($i = 1$ is the ground state). NS is the number of final states being accounted for. K_i is a kinematic factor relating photon and neutron energy. Its presence arises from the inclusion of nuclear recoil effects.

Our problem is then to take data which consists of several neutron spectra, Y, each rather closely spaced (i.e., of "high" resolution) in E_n, but with the spacing in χ_j relatively large, and invert the above equation to obtain values of $d\sigma_i/d\Omega$ as a function of E_γ for as many values of i as possible or as may be of interest. While we will discuss here only the application of the method to a fictitious nucleus Hy^A, we remark that with increasing "crudeness" one can apply it to relatively complex cases, if one is willing to lump the possible residual-nucleus states into rather broad bands of energies, and then treat each such band as though it were a single state. What one learns from this latter situation is not precisely which states are populated in the residual nucleus, but rather what general ranges of energies are excited. This is often of considerable value in understanding the reaction mechanism.

For the nucleus Hy^{A-1} we assume a very simple energy level structure (Fig. 1),

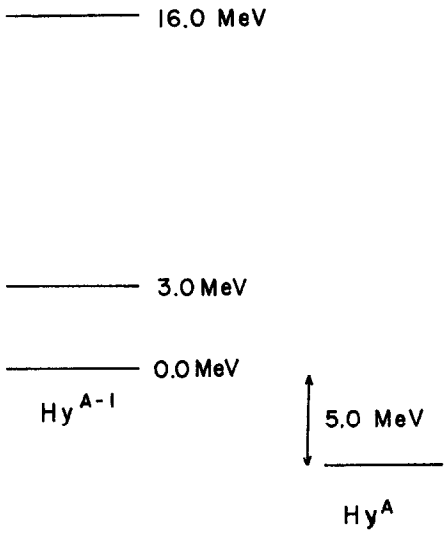

FIG. 1. Energy level scheme for a hypothetical nucleus, Hy^{A-1}.

(which has been made up to resemble that of Li^5) and partial cross sections to the three possible states as shown in Fig. 3. These (solid lines) latter exhibit "typical" giant dipole resonance behavior in the 20-MeV photon energy range, with some structure included to test the method, and they also exhibit fairly typical behavior in the higher energy regions, where the cross sections decrease rapidly, reaching

values as low as one microbarn per steradian. We assume that neutron spectra are measured for electron (bremsstrahlung end-point) energies of 80, 65, 50, 35, and 20 MeV, and that at all energies the neutron spectra have energy resolution much narrower than the smallest residual energy level separation, which is 3 MeV. We can now construct by computer the "true" neutron spectra, since all the factors on the right of Eq. (1) are assumed known. From these "true" spectra, we will now try to reconstruct the cross sections of Fig. 3 as accurately as possible.

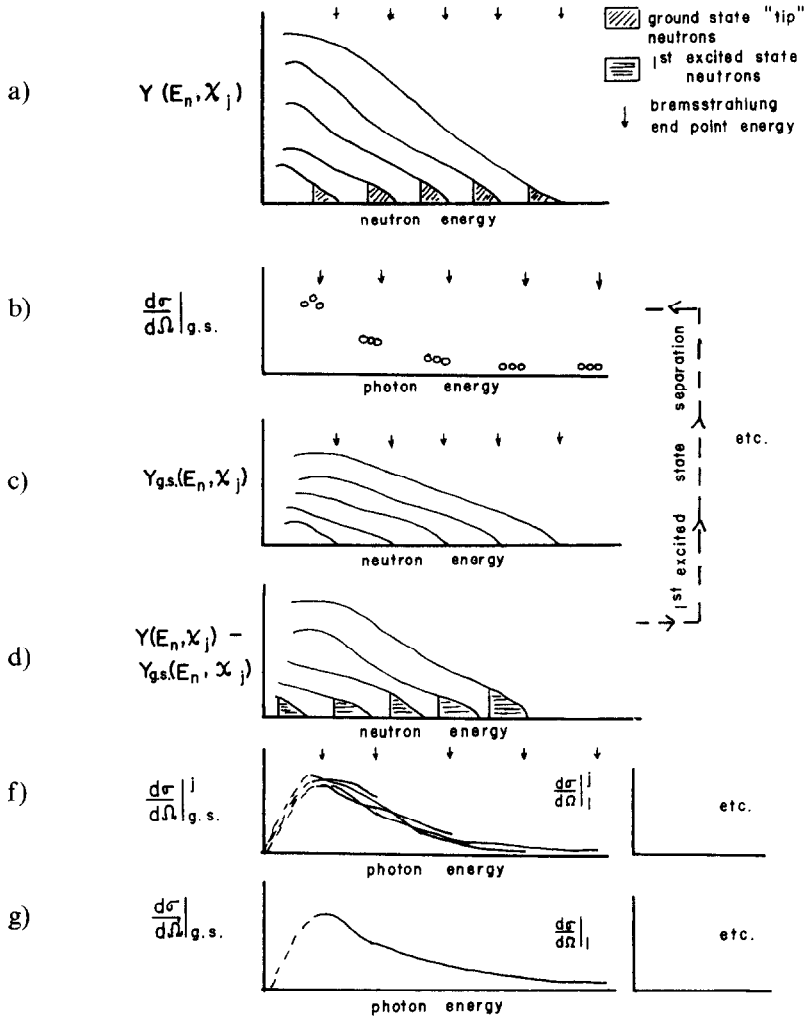

FIG. 2. Schematic of computational analysis using five sets of yield data.

Figure 2 schematizes the method we have developed. In part (a) the shaded regions under the yield curves represent neutrons which must come from ground-state transitions. From these we directly calculate ground state cross sections, producing the sets of points in part (b). We can do this because in this case the right side of Eq. (1) has only one term in the sum, so it can be solved exactly. We cannot proceed any further on an "exact" basis, however, because of the gaps between the sets of points in Fig. 2(b). Therefore, we make an assumption of "minimum astonishment," and simply interpolate linearly across the gaps (including the one between the zero-cross section value at the reaction threshold and the lowest-energy set of points in Fig. 2(b)). This gives us a tentative complete partial cross section curve for the ground state. We use this with Eq. (1), with only the first term in the sum, to compute $Y_{g.s.}$ curves for each value of χ_j , where Y_i is the neutron yield from transitions to the ith energy level of the residual nucleus. These curves are shown in Fig. 2(c). We then subtract $Y_{g.s.}$ from Y, to obtain the next excited state yield curves of Fig. 2(d). Next, the entire procedure is iterated, now using the energy of the first excited state instead of the ground state energy, and the separation of the first and second excited states instead of that of the ground and first excited states. In principle, we can iterate any number of times, to obtain cross section curves for "all" excited states. In practice, a total of three states is likely to be the most the data will support without complete loss of precision as a result of repeated subtractions and/or as a result of rapid decrease of energy level separations.

At this point what we have done is no more than to make arbitrary smooth (actually linear) interpolations across gaps in the cross section curves produced by entirely "standard" procedures. The next step is to observe that in every case the cross sections have been computed using only the neutrons which occur near the upper energy tip of each spectrum (including the subtacted spectra, as in Fig. 2(d)). These are of necessity few in number because they arise from photons near the tip of the bremsstrahlung spectrum, which are always few in number. Referring now back to Fig. 2(a), where the original "measured" spectra are shown, we observe that for neutrons of energy near the middle of the energy range covered in the figure, we have in fact three or four separate spectra. The one produced by the photons from bremsstrahlung of electrons of the highest energy is the highest curve and has a large counting rate in this energy region. The motivation behind the present method is to use the information contained in these extended high precision regions to produce improvements in the *tentative* partial cross sections.

In the spirit of the above remarks, we proceed to adjust the tentative cross sections so that they reflect as well as possible the exhaustion of all the measured yield data. To preserve some semblance of the "reality" involved in the tentative cross sections, we must adopt some limits on how we will let the cross sections vary from the first tentative ones. We have chosen to adopt the restriction that the

branching ratios to the various residual nucleus states will be maintained the same as those obtained in the tentative cross sections. The branching ratios as a function of photon energy, $B_N(E_\gamma)$, and as a function of neutron energy, $B_N(E_n, \chi_j)$, are given respectively by

$$B_N(E_\gamma) = \frac{d\sigma/d\Omega)_N (E_\gamma)}{\sum_{i=1}^{NS} d\sigma/d\Omega)_i (E_\gamma)}$$

and

$$B_N(E_n, \chi_j) = \frac{Y_N(E_n, \chi_j)}{\sum_{i=1}^{NS} Y_i(E_n, \chi_j)},$$

where N refers to the final state in question and NS is the total number of final states being considered. $Y_N(E_n, \chi_j)$ is the yield to the Nth final state.

It is important to note that the numerators and denominators in the branching ratios are computed from the unique "tip" regions and linear interpolations between these regions. It is to be noted, too, then, that the sum of the computed partial yields at this point is not necessarily equal to the total measured yield. That is,

$$Y(E_n, \chi_j) \neq \sum_{i=1}^{NS} Y_i(E_n, \chi_j).$$

The branching ratios are now used with the total measured yields to recompute cross sections over extended regions which bridge and supplement the "exact" point results (Fig. 2(e)). In this process the whole yield at any energy is exhausted.

$$\left.\frac{d\sigma}{d\Omega}\right)_N^j = \frac{Y_N(E_n, \chi_j)}{\sum_{i=1}^{NS} Y_i(E_n, \chi_j)} \frac{Y(E_n, \chi_j)}{\phi(E_\gamma, \chi_j)} \frac{1}{n \cdot K_N}.$$

This adjustment can be looked on as a normalization of the total measured yield to the total computed yield producing self consistent partial cross sections. Thus, we obtain for *each* partial cross section a family of curves, one for each yield curve, as in Fig. 2(e). We then average these together for each residual state to obtain a final "best" partial cross section, as in Fig. 2(f). In the averaging, the various values are weighted according to the statistics of the yield data from which they are obtained.

3. Results and Discussion

Figure 3 shows the result of this process on Hy^A. The dots are the deduced cross section values. We see that the correspondence with the true cross section values,

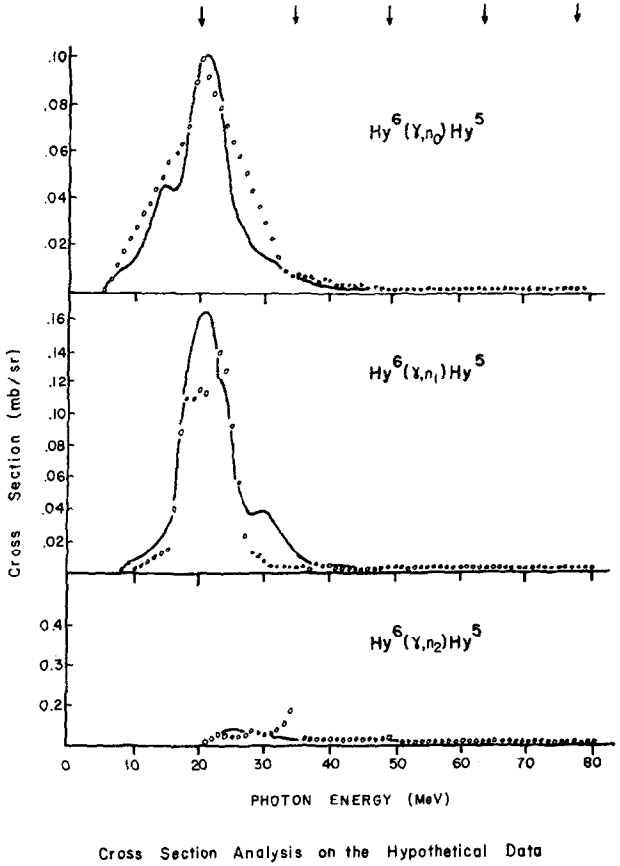

FIG. 3. Results on hypothetical data for a 3-final-state partial cross section analysis. The solid curves are the exact cross sections used to generate the hypothetical data points. The dots are the results using the present analysis.

the solid curves, is reasonably good where the cross section varies fairly rapidly and nonmonotonically, and is very good where it varies slowly and monotonically. Our choice of specifications for the computer experiment has, in fact, produced two features. One is that we took one yield curve with its end-point exactly at the peak of the giant resonance part of the cross section curve. This has the good result that the giant resonance is reasonably well reconstructed. In a real experiment (where the giant resonance was known from other experiments) where the lowest end-point energy E_L was above the giant resonance, the results near and below E_L were totally unreliable. The other feature of note is that despite our rather drastic choice of 15 MeV between yield end-point energies, the results are as good as

they are. There is a small but significant point apparent in Fig. 3. Just below 35 MeV the partial cross section to the second excited state makes an abrupt excursion. This is a typical result where the distance between endpoint energies is so large that the assumption that one cannot interpolate linearly between the gaps in the "exact" cross sections will show the excursion, and it is possible that several may. It is certain that when the procedure cannot reconstruct the correct cross sections, even approximately, this *will* be signaled by such abrupt excursions. It is also plausible that lack of such excursions indicates lack of significant structure in the cross section curves. (We have not explored the question of whether further efforts might be made to recover improved cross sections by making explicit use of the occurrence of these abrupt excursions.) The validity of any questionable structure or "excursions" in the final cross sections can be checked by examining the appropriate neutron energy regions of the measured yields for peaks or breaks. Finally, there is an interesting appearance of structure apparent on the low energy edge of the ground state cross section results. (While the points look linear in the figure, there is a slight deviation from the initial linear interpolation made between the 20 MeV region and threshold.) This structure coincides with that in the true cross section. This information as well as the other cross section results could not have been extracted from the data using the previous simple "exact" techniques.

To summarize then, what we have presented is a computational method for extracting partial photoneutron cross section information from data where the continuous bremsstrahlung spectrum conceals such yield information. The method has the advantage of utilizing the whole energy extent of the yield spectra not just the unique tip regions. It permits reasonable estimates of the partial cross sections without the large amount of data taking the more conventional analysis would require.

The computing time required is not small, but is reasonable, considering the effort ordinarily invested in obtaining the raw data in the first place. Typical run time for analysis of the kind illustrated here (three final states, five different yield curves) was about 6 min using Fortran IV-G on an IBM 360/50.

In conclusion, we suggest two modest further steps which might serve to improve the final cross section estimates. One would be to smooth the branching ratio curves before using them in the adjusting process. We actually used the independent values at each energy point, and the only smoothing effect arose naturally from the fact that in some regions the tentative cross curves consisted of linear interpolations. The other improvement would be to take the "final" cross sections which, since they are the result of averaging curves obtained from the various fits to the various yield curves, do not necessarily correspond to the same branching ratios as were used up to this point, and calculate new branching ratios, and then iterate the fitting process again.

Finally, it should be noted that the experimental aspects of the problem, which

have not been explored here, contribute to the computational difficulties of the problem by introducing uncertainties in the input information, viz., the neutron yield data and the energy dependence of the incident bremsstrahlung. While there are reliable theoretical results for the latter, experimental conditions, e.g., the momentum spread of the electrons, affect the detailed shape of the spectrum particularly in the end-point or tip region which is so critical in the unfolding procedure. No analytical or numerical methods for treating errors are detailed in this paper. To obtain some estimate for these effects, however, one can allow the input data to swing through their uncertainties and note the effect on the partial cross section results. If the data near the tips of the yields have 10% statistics, such a procedure performed under conditions similar to those in the hypothetical case presented earlier produces a comparable (about 10%) uncertainty in the ground state partial cross section and successively greater uncertainties in the excited state results. This procedure is time consuming computationally and has not been performed in an exhaustive or systematic fashion. It is hoped that simplified methods of treating error propagation will be developed for this method.

ACKNOWLEDGMENTS

The use of the computer facilities at Rensselaer Polytechnic Institute is gratefully acknowledged. The discussions with the Nuclear Physics group at RPI and with Dr. Joseph Robertshaw at Providence College were most helpful and are kindly acknowledged.

REFERENCES

1. B. C. COOK, *Nucl. Instr. Methods* **24** (1963), 256.
2. A. S. PENFOLD AND J. E. LEISS, *Phys. Rev.* **114** (1959), 1332.