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LEAST STRUCTURE SOLUTION OF PHOTONUCLEAR YIELD FUNCTIONS*

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A new method for the solution of experimental photonuclear yield functions for cross sections is presented. The method gives the "smoothest" set of cross sections as a function of photon energy consistent with the experimental yield. For this reason the term "least structure analysis" is used to describe the method of analysis. Cross sections derived by least structure analysis of trial yield functions are presented. The resulting cross sections are compared to the assumed cross sections used to derive the trial yield function.

This comparison fully justifies the use of least structure analysis at all energies including energies higher than the giant resonance energy where other methods have failed to give physically acceptable solutions. Errors and resolution functions corresponding to the least structure solution of the trial yields are also given.

1. Introduction

When high energy electrons strike atoms in a target, X-rays are produced. When high energy X-rays strike nuclei in a sample, photonuclear reactions may occur. Typical photonuclear reactions would be the (γ, n), (γ, p) or the (γ, pn) processes. For a quantitative study of such processes, the intensity of the X-rays incident on the sample must be monitored. The ratio of the number of nuclear disintegrations of a given type in the sample to the monitor response is the photonuclear yield Y. Y depends upon the kinetic energy T_0 of the electrons incident upon the X-ray target; i.e. Y is a function of T_0. This function, which can be experimentally determined, is called the photonuclear yield function. Typical units of $Y(T_0)$ would be the number of nuclear disintegrations of a given type per mole of sample atoms per erg of X-ray dose.

Unfortunately a spectrum of photon energies is produced when high energy electrons strike matter. This spectrum is known as the bremsstrahlung spectrum. Thus photonuclear disintegrations produced by bremsstrahlung X-rays are induced by photons of many energies. For this reason, $Y(T_0)$ is of little direct physical significance. However, $Y(T_0)$ is related to the photonuclear cross section σ as a function of photon energy k. $\sigma(k)$ has been determined for many photonuclear reactions by the analysis of yield functions $Y(T_0)$. Photonuclear cross sections for most elements are found to be large for k in the energy region from 15 to 25 MeV. Thus, this region of photon energies has been called the "giant resonance" energy region.

However, unless $Y(T_0)$ has been measured with extreme precision, the cross section $\sigma(k)$ derived from the experimentally measured $Y(T_0)$ oscillates drastically as a function of photon energy k unless a smoothing procedure is adopted. The tendency for oscillations in $\sigma(k)$ is especially pronounced at high energy k. For this reason (among other reasons) photonuclear cross sections are, as yet, little known above the giant resonance region. A new method for the analysis of photonuclear yield functions $Y(T_0)$ for cross sections $\sigma(k)$ has been developed and is reported here. For reasons which will become apparent from later sections of this paper, the method is named "least structure solution of photonuclear yield functions" or, more briefly "least structure". Basically least structure is a systematic smoothing technique. The method is applicable at all photon energies k, but is particularly useful for k above the giant resonance region. Solutions of test yield functions are presented in a later section and the interpretation of these solutions is discussed. The distortion in $\sigma(k)$ is calculated for the test yield functions and is found to be nominal. Moreover,

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least structure analysis of yield functions measured with only moderate precision (1% or better) give useful solutions of $\sigma(k)$ for all k.

2. Photonuclear Yield Functions

The photonuclear yield $Y(T_0)$ at electron energy T_0 is related to the photonuclear cross section $\sigma(k)$ by the photonuclear yield equation:

$$Y(T_0) = A \int_{E_{th}}^{T_0} \mathrm{d}k\sigma(k)N_{Exp}(k, T_0) , \qquad (1)$$

where E_{th} is the threshold energy for the reaction studied, $N_{exp}(k, T_0)\,\mathrm{d}k$ is the number of photons between energy k and energy $k + \mathrm{d}k$ striking the sample per unit monitor response. A is the constant of proportionality representing such factors as the number of atoms in the sample and perhaps other factors relating to the exact conditions of the experiment. In eq. (1), $N_{exp}(k, T_0)$ is the actual spectrum of photons striking the sample for the conditions of the experiment and not the spectrum $N(k, T_0)$ for an electron of energy T_0 striking a single nucleus of the target, the bremsstrahlung spectrum. The bremsstrahlung spectrum $N(k, T_0)$ is distorted by absorption of photons in the target, in any material between the target and the sample, and in the sample itself. The electrons striking the target may have an initial energy spread, and energy losses in the target itself will further distort $N(k, T_0)$. Moreover, $N_{exp}(k, T_0)$ is normalized to a unit monitor response while $N(k, T_0)$ is usually normalized per incident electron and per target atom. The monitor itself can be of any type with a known response $M(k)$ for X-rays as a function of photon energy k. That is, the photonuclear yield equation (1) is dependent upon the particular conditions of the experiment. Penfold and Leiss[1]) discuss a function $y(T_0)$, "the reduced yield function", which may be obtained from the experimental yield $Y(T_0)$ in an unequivocal fashion. $y(T_0)$ is related to the "reduced cross section" $s(k)$ by a universal photonuclear yield equation.

$$y(T_0) = \int_{E_{th}}^{T_0} \mathrm{d}ks(k)N(k, T_0) \approx \int_{E_{th}}^{T_0} \mathrm{d}k\sigma(k)N(k, T_0), \qquad (1a)$$

where $s(k)$ is related to $\sigma(k)$ and in most cases can be taken as equal to $\sigma(k)$ to good approximation. (For this reason the symbol $s(k)$ will not be used further in this paper.) Eq. (1a) is now independent of the exact nature of the experimental arrangement. Note also that the constant A in eq. (1) has been incorporated into the definition of reduced yield.

In this paper all experimental yield functions are assumed to be transformed into reduced form. Since this paper deals only with the mathematical problems associated with the solution of eq. (1a) and not with the problem of measurement of valid photonuclear yield functions, we assume that all experimental yields can be transformed into the reduced form without error. This, of course, implies that the monitor response function $M(k)$ is known exactly as well as other experimental factors distorting the spectra. With reasonable care valid reduced yield functions can be obtained from experimental data[2]).

2.1. NATURE OF THE SPECTRUM

The bremsstrahlung function $N(k, T_0)$ appearing in eq. (1) has been extensively studied both experimentally and theoretically[3]). However, to date, its exact form is known imperfectly, especially for values of $k \approx T_0$, the so-called spectrum tip. In this paper $N(k, T_0)$ will be taken as the integrated over-angle Schiff spectrum[3]), an approximation to $N(k, T_0)$ which has been used extensively in the past for the solution of photonuclear yield functions. Distortions in $\sigma(k)$ due to the use of an approximate spectrum will not be discussed for reasons given previously. These distortions have been considered by others in the literature[1]) and are thought to be minor.

In practice $y(T_0)$ is measured only at a finite number n of energies T_{0i}; usually at energies T_{0i} spaced in equal intervals ΔT_0 starting from the threshold energy E_{th}. Thus the ith energy T_{0i} is related to the threshold energy E_{th} by

$$T_{0i} = E_{th} + i\,\Delta T_0 , \quad i = 1, 2, \ldots, n . \qquad (2)$$

[1]) A. S. Penfold and J. E. Leiss, Phys. Rev. **114** (1959) 1332.
[2]) D. W Anderson, A. J. Bureau, B. C. Cook, J. E. Griffin, J. R. McGonnell and K. Nybö (submitted to Phys. Rev. Letters)
[3]) H. W. Koch and J. W. Motz, Rev. Mod. Phys. **31** (1959) 920.

Similarly the ith yield point y_i can be defined as $y_i = y(T_{0i})$.

2.2. SOLUTION OF THE PHOTONUCLEAR YIELD EQUATION

Many authors have presented methods for the solution of the photonuclear yield equation (1a). All such methods can be divided into two categories: (1) solution of the integral equation (1a) directly or (2) solution of a set of linear equations which approximate the integral equation.

The photonuclear yield equation (1a) is a Volterra equation of the first kind with kernel $N(k, T_0)$. Several authors[4]) have given solutions, but all use approximations to the bremsstrahlung spectrum $N(k, T_0)$. The approximations are in general rather poor for k near the tip of the spectrum ($k \approx T_0$). Moreover, the yield $y(T_0)$ is not known as a continuous function of T_0, a condition implicit in the solution of the integral equation, but rather it is known only at a finite set of energies T_{0i}. For these reasons the solution of eq. (1a) in this paper is based on method 2.

2. The Volterra integral equation can be replaced by a set of linear equations if $N(k, T_{0i})$ is approximated in the following way. In each interval of photon energy, $k_j - \Delta T_0$ to k_j, the spectrum $N(k, T_{0i})$ is replaced by a constant N'_{ij}. N'_{ij} depends upon the electron energy T_{0i} and the photon energy k_j. The value of N'_{ij} is chosen such that

$$N'_{ij}\Delta T_0 = \int_{k_j - \Delta T_0}^{k_j} \mathrm{d}k N(k, T_{0i}) \,, \quad \text{i.e.,}$$

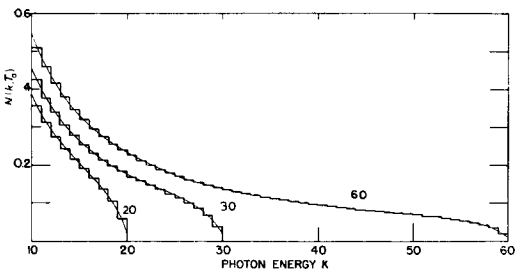


Fig. 1. The Schiff integrated-over-angle bremsstrahlung spectrum $N(k, T_0)$. The continuous spectrum $N(k, T_0)$, as well as the "step wise" approximation to $N(k, T_0)$, N'_{ij}, are given for T_0 of 20, 30 and 60 MeV and for k from 10 to 60 MeV. An energy interval ΔT_0 of 1 MeV is assumed.

each interval of the approximate spectrum has the same number of photons as the true spectrum $N(k, T_0)$. The bremsstrahlung spectrum $N(k, T_0)$ and this "step-wise" approximation to the spectrum is shown in fig. 1. Penfold and Leiss[5]) have discussed conditions on $\sigma(k)$ for which this approximation to $N(k, T_0)$ is valid and estimate the distortions in σ introduced by these approximations.

In the "stepwise" approximation eq. (1a) becomes

$$\begin{aligned} y(T_{0i}) \equiv y_i &= \sum_{j=1}^{i} \int_{k_j - \Delta T_0}^{k_j} \mathrm{d}k N'_{ij}\sigma(k) \\ &= \sum_{j=1}^{i} (N'_{ij}\Delta T_0) \left[\frac{1}{\Delta T_0} \int_{k_j - \Delta T_0}^{k_j} \sigma(k)\right] \qquad (3) \\ &= \sum_{j=1}^{i} N_{ij}\sigma_j \quad i = 1,2, \ldots, n \,, \end{aligned}$$

where

$$\sigma_j = \frac{1}{\Delta T_0} \int_{kj - \Delta T_0}^{kj} \sigma(k)\mathrm{d}k$$

is the average value of $\sigma(k)$ in the interval of photon energy between $k_j - \Delta T_0$ and k_j, and $N_{ij} = N'_{ij}\Delta T_0$ is the number of photons in the bremsstrahlung spectrum in the same photon energy interval with electron energy T_{0i}. In matrix notation eq. (3) becomes

$$\vec{y} = \mathsf{N} \cdot \vec{\sigma} \qquad (3a)$$

where $\vec{\sigma}$ is a column matrix with n rows with elements σ_j, $\vec{y}$ is a column matrix with n rows with elements y_i, N is an nth order square matrix with elements $N_{ij}(N_{ij} = 0$ if $j > i)$ called the bremsstrahlung matrix. Eq. (3a) has the a solution

$$\vec{\sigma} = \mathsf{N}^{-1} \cdot \vec{y} \,. \qquad (3b)$$

The matrix N^{-1} has been tabulated for many electron energies up to 1 GeV for various energy intervals ΔT_0 for the Schiff spectrum[5]). Equation (3) or its equivalent form, eq. (3a), are the basic equations

[4]) L. V. Spencer, Phys. Rev. **87** (1952) 196;
R. Malvano, A. Molinari and M. Omini, Supplemento Nuovo Cimento XXIII, (1962) 253.

[5]) A. S. Penfold and J. E. Leiss, "Analysis of Photo Cross Sections", Physics Research Laboratory, Univ. of Ill., Champaign, Ill., May 1958 (unpublished).

used in this paper. Unfortunately the solutions, eq. (3b), oscillate violently as a function of photon energy at energies above the giant resonance energy if the yields are known to moderate precision. For this reason these solutions are unacceptable physically. Thus smoothing of some nature must be used.

2.3. THE INTERPRETATION OF SOLUTIONS AS TRANSFORMED YIELDS

In order to understand the validity of least structure, it is useful to consider the solution of eq. (3a) from another viewpoint. The yield $\vec{y}$ is obtained from the cross section $\vec{\sigma}$ by the application of the operator N to $\vec{\sigma}$. If an arbitrary (operator) matrix O acts on each side of eq. (3a), one obtains

$$\vec{y}^* = O\cdot\vec{y} = O\cdot N\cdot\vec{\sigma} = N^*\cdot\vec{\sigma}, \tag{4}$$

where $\vec{y}^*$ is the result of applying the operator $O\cdot N = N^*$, the transformed spectrum N^*, to $\vec{\sigma}$. That is, the transformed yield $\vec{y}^*$ is related to $\vec{\sigma}$ through N^* just as $\vec{y}$ is related to $\vec{\sigma}$ through N. Experimentally this implies that if one could obtain in the laboratory a spectrum $N^*(k, T_0)$ which could be approximated by the matrix N^*, using this spectrum one would measure a yield $\vec{y}^*$. A solution $\vec{\sigma}$ is obtained by setting $O = N^{-1}$ such that $N^* = O\cdot N = N^{-1}\cdot N = I$, the unit matrix, i.e. $\vec{y}^* = \vec{\sigma}$. From this viewpoint N^{-1} is the operator which transforms y into another yield $\vec{y}^*$ which is equal to the average cross section $\vec{\sigma}$. However other transformed spectra N^* than the unit matrix I may have simple physical interpretation. For example, $\vec{y}^* = N^*\cdot\vec{\sigma}$ could represent the average of $\vec{\sigma}$ over several energy intervals ΔT_0. From this viewpoint, the solution of eq. (3a) is no longer unique; in fact an infinite number of physically acceptable solutions to eq. (3a) are possible.

2.4. MOTIVATION OF LEAST STRUCTURE

The least structure solution of eq. (3) was motivated from the following considerations:

1. All smoothing should be applied to $\sigma(k)$ and not to $y(T_0)$. If the smoothing were applied directly to the experimental curve $y(T_0)$, small distortions in y may be reflected as large non-significant deviations in σ.

2. Since the functional form of $\sigma(k)$ is unknown, no assumptions about the functional form of $\sigma(k)$ may be made. Thus all curve fitting procedures, such as least squared adjustment of parameters, are inappropriate.

3. Completely numerical methods should be employed. If French curves are used for smoothing, no objective assignment can be made to the errors to be associated with each solution. The solution is then subjective; another observer analyzing the same data may give a differing solution.

4. The amount of smoothing to be employed should be non-arbitrary and determined only by the quality of the input data. That is, such questions as whether one should use a three, five, or seven point formula for smoothing must be answered a priori from the input data only.

5. One must be able to estimate the distortions introduced by smoothing unequivocally. These distortions must be small enough so that the smoothed solutions may be identified as the cross section or have another simple physically significant interpretation.

3. Least Structure

For the present, consider the solutions of eq. (3a) from viewpoint one. Since there are n inhomogeneous linear equations in n unknowns, there are n unique solutions to these equations in a strict mathematical sense. However, the yields y_i are experimentally determined so that they are subject to errors, Δy_i; i.e. $y_i = \bar{y}_i + \Delta y_i$ where $\bar{y}_i$ would be the "true" yield with no error. $\bar{y}_i$ is related to the true cross section $\bar{\sigma}_j$ by

$$\bar{y}_i = \sum^{i} N_{ij}\bar{\sigma}_j \qquad i = 1, 2, \ldots n. \tag{5}$$

Thus any set of σ_j's can be considered to be an acceptable solution to the physical problem if $\sum_j N_{ij}\sigma_j \approx y_i$; i.e., a solution is acceptable if the calculated yield, $\bar{\bar{y}}_i = \sum N_{ij}\sigma_j$, is close to the experimental yield y_i at each energy T_{0i}.

This loose usage of "close" must be made precise

before a mathematical analysis can be stated. Consider for the moment that the true cross section $\bar{\sigma}(k)$ were known; then the true yield $\bar{y}(T_0)$ derived from $\bar{\sigma}$ would also be known. In statistical theory the statistical variable χ^2 where

$$\chi^2 = \sum_{i=1}^{n} \frac{(y_i - \bar{y}_i)^2}{(\nabla y_i)^2} \tag{6}$$

is frequently defined. ∇y_i is the standard deviation in y_i. The distribution function for χ^2 is given in many standard texts in statistics. The most probable value of χ^2 is $n - 2$, its average value is n and its variance is $2n$. χ^2 distribution tables are readily accessible. Note the main properties of χ^2 are independent of the knowledge of the true cross section and depend only on the number of points in the photonuclear yield y_i and the standard deviations ∇y_i.

3.1. DEFINITION OF $\bar{\chi}^2$

Now define a function $\bar{\chi}^2$ closely related to χ^2 of statistics; namely

$$\bar{\chi}^2 = \sum_{i=1}^{n} \frac{(\bar{\bar{y}}_i - y_i)^2}{(\nabla y_i)^2} = \sum_{i=1}^{n} \frac{(\Sigma N_{ij}\sigma_j - y_i)^2}{(\nabla y_i)^2}, \tag{7}$$

where σ_j is any set of n numbers. That is $\bar{\chi}^2$ is a function of σ_j, $j = 1, 2, \ldots, n$. Note that $\bar{\chi}^2$ is related to χ^2 in the same way as likelihood is related to probability. A set of σ_j's will be considered an acceptable solution to eq. (a) if

$$\bar{\chi}^2(\sigma_j) \leqslant n. \tag{8}$$

Such solutions σ_j are said "to satisfy the photonuclear yield equation in a $\bar{\chi}^2$ sense" or are said to be "acceptable solutions to the physical problem." Solutions of eq. (3a) are acceptable solutions to the physical problem in this sense as $\bar{\chi}^2$ is zero in this case. However there are now an infinite set of solutions, σ_j, all acceptable. Thus a solution is said to be "close" if the $\bar{\chi}^2$ corresponding to this solution is less than n, the number of data points. The standard deviation ∇y_i in the experimental yields, y_i, can be estimated from the counting statistics or, preferably, by the reproducibility of the yields at the same electron energy.

3.2. THE STRUCTURE FUNCTION S

We will attempts to select from this infinite manifold of physical solutions the "smoothest" set of solutions. For this purpose an auxiliary function $S(\sigma_j)$ called "the structure function" will be defined. Within certain wide limits, the exact definition of $S(\sigma_j)$ is arbitrary. Several definitions of $S(\sigma_j)$ have been extensively explored, namely:

$$S_1(\sigma_j) = \sum_{j=1}^{n-1} (\sigma_{j+1} - \sigma_j)^2 \tag{9a}$$

and

$$S_2(\sigma_j) = \sum_{j=2}^{n-1} (\sigma_{j+1} - 2\sigma_j + \sigma_{j-1})^2. \tag{9b}$$

Note no functional form for the cross section σ_j as a function of photon energy k_j is assumed; in these definitions σ_j are arbitrary numbers. The least structure solution to the bremsstrahlung yield function (3a) is now defined as that set of σ_j which minimizes the structure function (eq. 9) with the restriction that $\bar{\chi}^2 = n$. The solution with $\bar{\chi}^2 = n$ is called the solution with optimum smoothing, or more briefly the solution; solutions with $\bar{\chi}^2 < n$ are said to be undersmoothed and solutions with $\bar{\chi}^2 > n$ are said to be oversmoothed.

The form of the structure function $S(\sigma_j)$ while arbitrary, is motivated by the following intuitive considerations. Without restrictions imposed by the experimental data, the least structure function $S(\sigma_j)$ should have value zero. Solutions of $S(\sigma_j) = 0$ should satisfy our intuitive concepts of a very smooth function or a structureless function. (A solution σ_j with many hills and valleys should have a large value of the structure function $S(\sigma_j)$.) The solution of $S_1(\sigma_j) = 0$ and $S_2(\sigma_j)$ are shown in fig. 2. The first is a constant independent of k_j while the second solution corresponding to $S_2 = 0$ is a linear function of k_j. Both solutions are intuitively acceptable as a function with no structure.

However if an experimental yield curve is known, the least structure solution will not be in general a straight line but may have more structure, as all acceptable solutions are constrained to satisfy the photonuclear yield equation in a $\bar{\chi}^2$ sense. From an operational standpoint, the least structure solution is quite desirable, as speaking loosely, it is the most conservative solution to the yield equations (3a).

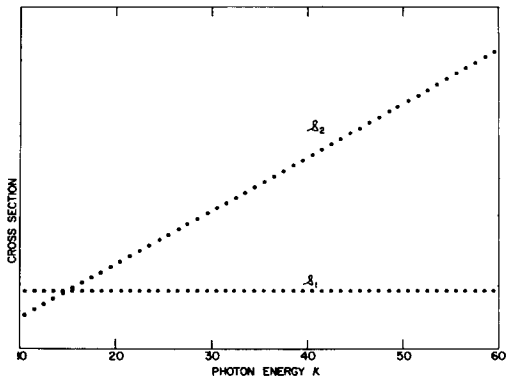


Fig. 2. Least structure solutions without restraints. Solution of $S_1(\sigma_j) = 0$ and $S_2(\sigma_j) = 0$ are given corresponding to no knowledge of the yield function. The solution σ_j corresponding to $S_1(\sigma_j) = 0$ is labeled S_1 and similarly for S_2. The magnitude of the S_1 solution is arbitrary while the slope and intercept at the threshold energy of a line through the S_2 solution are both arbitrary.

This corresponds closely to the way in which data are normally presented. If a peak or valley seen in an experimentally determined curve is statistically improbable, no claim is ordinarily made that the effect is real. Thus a peak found in a cross section derived from a photonuclear yield function without smoothing should be considered spurious if another physically acceptable solution can be found in which the peak disappears. This, of course, does not imply the peak is or is not valid in nature; only that more precise data would be required to answer the question.

3.3. THE LEAST STRUCTURE SOLUTION AS A VARIATION PROBLEM

The mathematical procedure for finding the solution σ_j which minimizes $S(\sigma_j)$ with the additional restraint that $\bar{\chi}^2(\sigma_j) = n = \text{const.}$ is a well known problem in the calculus of variations. $S(\sigma_j)$ can be considered as a Lagrangian with dynamical variables σ_j. The variables σ_j are constrained to lie on a surface $\bar{\chi}^2 = \text{const.}$ Using standard methods of variational calculus, the problem can be written as

$$\lambda \delta S(\sigma_j) + \delta \bar{\chi}^2(\sigma_j) = 0\,, \qquad (10)$$

where λ is a Lagrangian multiplier introduced in the conventional way. In eq. (10), the variations are to be taken with respect to the σ_j's. After some algebraic manipulations eq. (10) can be placed in the following simple form:

$$(N + \lambda\,(\tilde{N})^{-1} \cdot (W)^{-1} \cdot S) \cdot \vec{\sigma} = \vec{y}, \qquad (11a)$$

where N is the bremsstrahlung matrix,

$(\tilde{N})^{-1}$ is the inverse of the transposed N matrix,

S is a smoothing matrix the exact form of which depends on the form of $S(\sigma_j)$,

$\vec{y}$ is the experimental yield,

$\vec{\sigma}$ is the least structure solution for the cross section,

W is a diagonal matrix with elements $W_{ii} = (1/\nabla y_i)^2$.

An equation similar to (11a) has been used for the numerical solution of integral equations previously[6]). Equation (11a) represents n equations in n unknowns σ_j plus an additional unknown λ; i.e., n nonlinear equations in $n + 1$ unknowns. However (repeated here for convenience as 11b), Eq. (8) must also be satisfied, namely

$$\bar{\chi}^2 = \sum_{i=1}^{n} W_i \left(\sum_{j=1}^{i} (N_{ij}\sigma_j - y_i)^2 \right) = \sum_{i=1}^{n} W_i (\bar{y}_i - y_i)^2 \qquad (11b)$$

where the weighting factors W_i are given by $W_i = (1/\Delta y_2)^2$. In (11b) solutions σ_j with $\bar{\chi}^2 = n$ have optimal smoothing, $\bar{\chi}^2 < n$ are undersmoothed solutions, and $\bar{\chi}^2 > n$ are oversmoothed solutions. S depends upon the exact form of $S(\sigma_j)$, and a technical point about the nature of the variations $\delta\sigma_j$ at the beginning and end points. (In Hamilton's principle of mechanics $\delta t = 0$ at $t = t_{\text{initial}}$ and $t = t_{\text{final}}$; in least structure similar restrictions may be made if desired.) If no restrictions on the variation $\delta\sigma_j$ are made, the smoothing matrix S, corresponding to $S_1(\sigma_j)$ is

$$S_1 = \begin{bmatrix} 1 & -1 & 0 & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\ 1 & -2 & 1 & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & 1 & -2 & 1 & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & 0 & 1 & -2 & 1 & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & 0 & 1 & -2 & 1 & 0 \\ 0 & \cdot & \cdot & \cdot & \cdot & 0 & 1 & -2 & 1 \\ 0 & \cdot & \cdot & \cdot & \cdot & 0 & 0 & -1 & 1 \end{bmatrix}$$

[6]) D. L. Phillips, Journal of the Association for Computing Machinery 9 (1962) 84.

$$S_2 = \begin{bmatrix} 1 & -2 & 1 & 0 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ -2 & 5 & -4 & 1 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ 1 & -4 & 6 & -4 & 1 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & 1 & -4 & 6 & -4 & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & 0 & 1 & -4 & 6 & -4 & 1 & 0 \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot & 0 & 1 & -4 & 6 & -4 & 1 \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 & 1 & -4 & 5 & -2 \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 & 0 & 1 & -2 & 1 \end{bmatrix}$$

Thus each smoothing matrix is a matrix with constant coefficients, independent of σ_j. The values of the coefficients are determined by the functional form of $S(\sigma_j)$. Note S_1 is the second difference operator while S_2 is the fourth difference operator (except for the first and last few rows). That is, $S_1 \cdot \vec{\sigma}$ is the second difference in $\vec{\sigma}$, and a similar interpretation of $S_2 \cdot \vec{\sigma}$ holds.

A computer program in Fortran has been written for an IBM 704 to solve the equations of least structure (eq. 11). In this code λ is chosen arbitrarily as an input parameter and eq. (11a) is solved for fixed λ. The solutions are then substituted into eq. (11b) and a $\bar{\chi}^2$ is computed. This estimate of λ is compared with the input χ^2_{in} and an allowed error in χ^2_{in}, $\nabla\chi^2_{in}$. If the calculated $\bar{\chi}^2$ is within $\chi^2_{in} \pm \Delta\chi^2_{in}$, the solution is considered acceptable; otherwise by an iterative procedure a new λ is selected and new solutions are obtained. The iterations are repeated until eqs. (11a) and (11b) are both satisfied (11b in an approximate fashion).

Once λ has been obtained, the matrix $M = N + \lambda(N)^{-1} \cdot W^{-1} \cdot S$ is determined uniquely as well as $y^* = M^{-1} \cdot y$. The entire correlation matrix $(\mathrm{ERM})_{ij} = \mathrm{av}(\Delta\sigma_i \Delta\sigma_j)$

$$= \sum_{\alpha} M^{-1}_{i\alpha} M^{-1}_{j\alpha} (\nabla y_\alpha)^2 \qquad (13a)$$

as well as the error $\nabla\sigma_j$ in σ_j

$$\nabla\sigma_j = \sqrt{(\overline{ERM})_{jj}} = \sqrt{\sum_{\alpha=1}^{n} (M_{j\alpha} - 1) 2 (\nabla y_\alpha)^2} \qquad (13b)$$

can be calculated. The transformed spectrum N^* (eq. 5)

$$N = N^* = M^{-1} \cdot N$$

is also calculated. The form of N^* as a function of photon energy k justifies an alternative name: call it the resolution function R.

Five smoothing requirements were made ealier. Least structure meets all five:

1. $S(\sigma_j)$ is a function of the σ_j's; not the y_i's.
2. The functional form of σ_j as a function of k_j is not assumed. Instead an arbitrary function of the σ_j's as parameters. $S(\sigma_j)$, is assumed.
3. Explicit forms for the σ_j's are given and also for the associated errors.
4. The condition for stopping is when the solution has optimal smoothing, i.e., $\chi^2 = n$.
5. The distortions can be estimated by explicit calculations of the transformed matrix N^*. For all calculations made to date N^* can be interpreted as a resolution function R averaging $\vec{\sigma}$ over a few energy intervals with an approximate Gaussian function weighting.

4. Use of Trial Yield Function

To test the usefulness of least structure for the analysis of photonuclear yield functions, two artifical cross sections, GRA and GRH, were assumed. GRA is single Gaussians centered at 20 MeV and GRH had two Gaussians, one centered at 20 MeV and the second at 40 MeV. The function form of the assumed cross sections were

$$\sigma(k) = A_1 \exp -\tfrac{1}{2}\left(\frac{k - k_1}{\Gamma_1}\right)^2 + A_2 \exp -\tfrac{1}{2}\left(\frac{k - k_2}{\Gamma_2}\right)^2 \qquad (14)$$

where the constants were assigned the following values:

	GRA	GRH
A_1	1.0	1.0
A_2	0.0	0.20
k_1	20 MeV	20 MeV
k_2	—	40 MeV
Γ_1	2 MeV	2 MeV
Γ_2	—	4 MeV

The cross sections are shown in fig. 3 GRA (Giant Resonance; Absence of Harmonic) is a single "giant resonance" type cross section while GRH (Giant Resonance plus Harmonic) is a gaint resonance plus an upper resonance. Hypothetical yield curves were

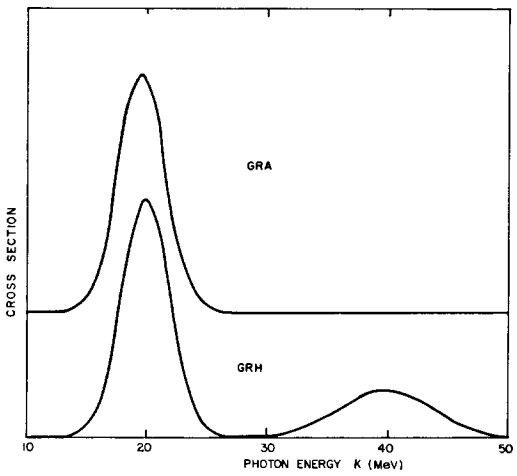


Fig. 3. Test cross sections. Cross section "GRA" (giant resonance with absence of harmonic) simulates $\bar{\sigma}(k)$ with a single resonance at 20 MeV while "GRH" simulates $\bar{\sigma}(k)$ with a giant resonance at 20 MeV and a harmonic at 40 MeV. The integrated cross section of the 40 MeV resonance is 40% of that at 20 MeV.

generated by integration of each assumed cross section weighted by the Shiff bremsstrahlung spectrum (eq. 1). The threshold energy was taken at 10 MeV and a maximum electron energy T_0 of 60 MeV was assumed. The resulting yield function $\bar{y}(T_0)$ is shown for each cross section in fig. 4. Yield curve GRA is generated from cross sections GRA; and similarly for GRH. Simulated experimental yield functions were generated from both $\bar{y}(T_0)$ by assigning errors Δy_i in $\bar{y}_i$ and letting $y_i = \bar{y}_i + \Delta y_i$. The electron energy T_{0i} was taken in intervals of 1 MeV from 11 MeV to 60 MeV; i.e., a yield function measured at 50 energies was assumed. The errors Δy_i assigned at electron energy T_{0i} were selected randomly with a normal error distribution. For each hypothetical yield curve $\bar{y}(T_0)$, ten simulated yields y_i were generated with standard deviations in y_i of 1% of y_i and ten curves were generated for both yields with standard deviations of 0.3%. Thus the percentage accuracy in each yield point y_i was assumed to be a constant independent of energy. (Experimentally activation functions are frequently measured with constant percentage accuracy except at energies near threshold). Since the same random numbers were used to generate the 1% data as the 0.3% data, the error Δy_i assigned for the 0.3% data is 0.3 times the error assigned for the 1% data for corresponding curves at the same

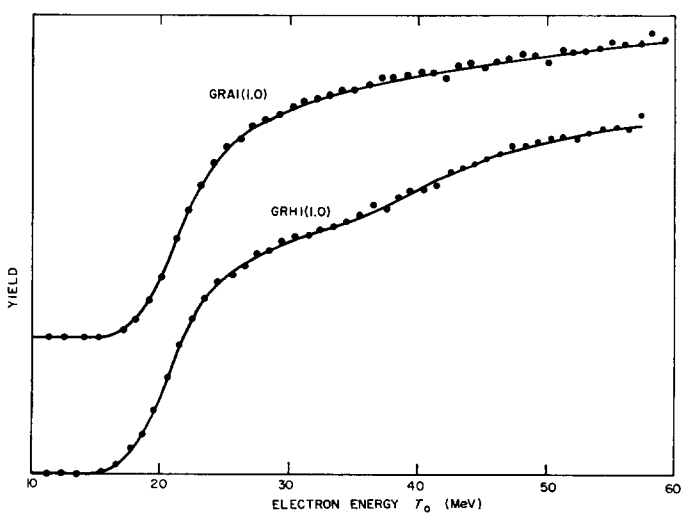


Fig. 4. Yield functions generated from GRA and GRH. The continuous curve is a smooth curve drawn through the yields generated from the assumed cross sections. The points shown represent a test yield function with 1% statistical error. The notation is as follows: GRH 1 yield function generated from cross section GRH and the first set of random numbers used to assign errors at each point; (1.0), percentage error assumed.

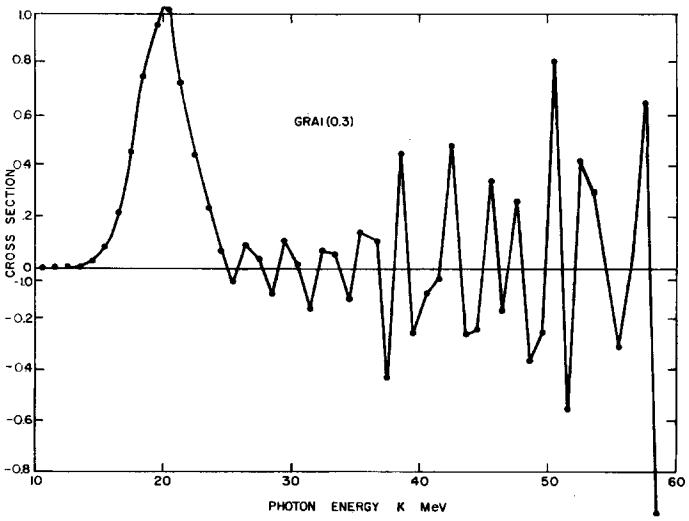
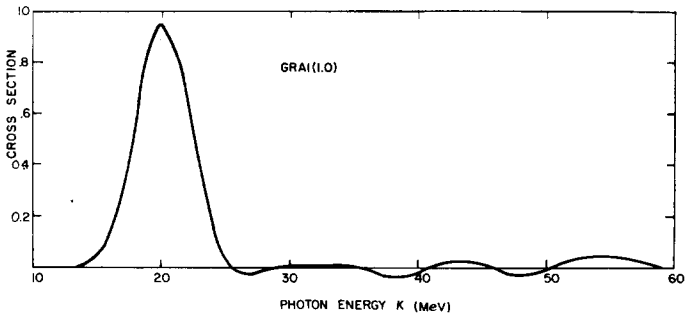
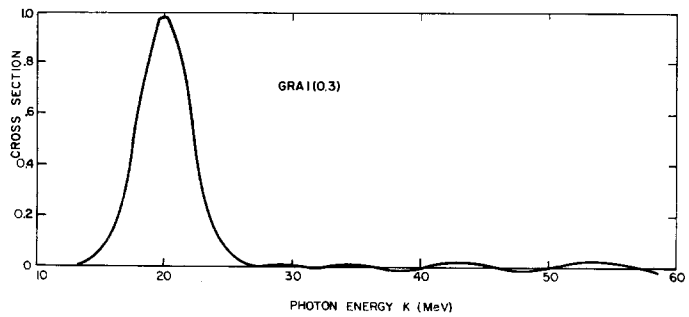


Fig. 5. Solution of GRA 1(0.3) without smoothing.





Figs. 6 and 7. Least structure solutions of GRA 1 for 1% and 0.3% statistical accuracy of the yield function.

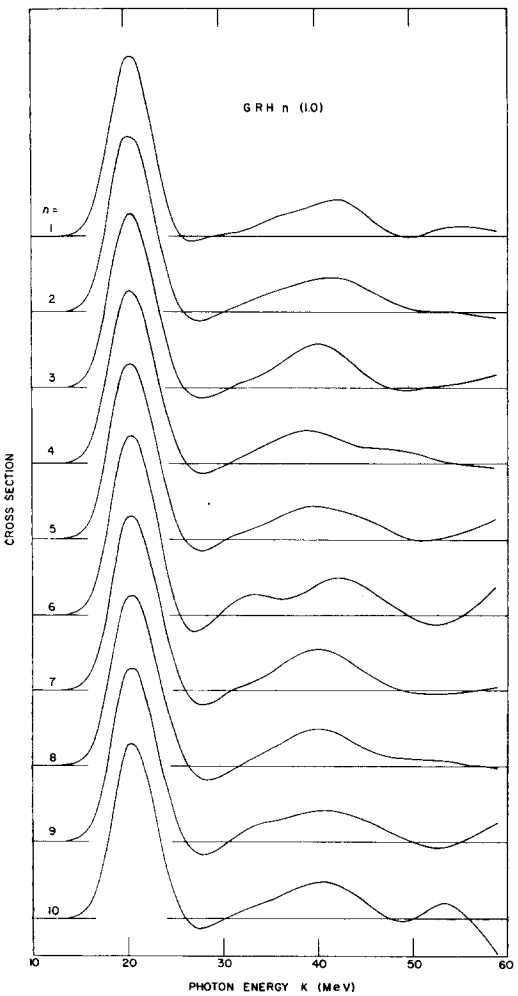


Fig. 8. Least structure solutions of GRH for 1% data. Ten solutions are given corresponding to ten yields functions generated from the test cross section. The residual effects of statistical errors in y_i on the cross section can be estimated from the fluctuation from example to example. The negative cross section near 27 MeV in all solutions is a distortion produced by the method of analysis.

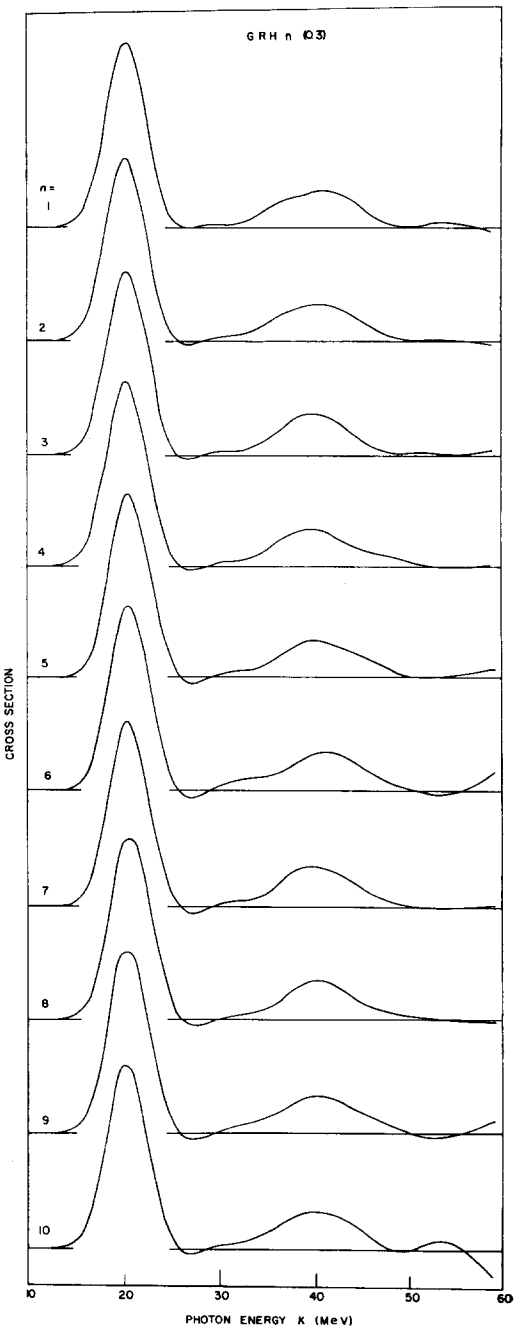


Fig. 9. Least structure solutions of GRH for 0.3% data. Solutions corresponding to those of fig. 8 are given for yield curves with 0.3% accuracy. The solutions are improved over those of fig. 8 but qualitatively the solutions are the same.

energy. Thus cross sections derived from 0.3% yield data can be compared point by point with cross sections derived from 1% data without the additional complications introduced by random fluctuations if independent errors were assumed. The points shown in fig. 4 represent a simulated yield function with 1% error. Note the existence of the 40 MeV resonance in GRH is clearly evident as a change in slope near 40 MeV although 1% errors are assumed. Simulated experimental yield functions y_i and the least structure solutions σ_j are labeled by the cross section assumed, GRA or GRH, by the set of random numbers used to select the errors (1–10), and by the standard deviation of the errors (0.3 or 1.0%). For example GRH 1 (1.0) implies cross section GRH, the first set of random numbers, and 1.0% errors.

A typical solution without smoothing is shown for 0.3% data in fig. 5. No 40 MeV resonance was assumed but the fluctuations in σ_j are too large to make any statements about σ_j above 30 MeV. For 1% data the fluctuations are ten times the giant resonance peak at 20 MeV. Least structure solutions corresponding to yield function GRA 1 for 1% and 0.3% data is shown in figs. 6 and 7, respectively. The least structure solutions σ_j although differing from the underlying "true" cross section in some respects, are quite acceptable. Unless otherwise specified, all least structure solutions illustrated will be for structure functions S_2.

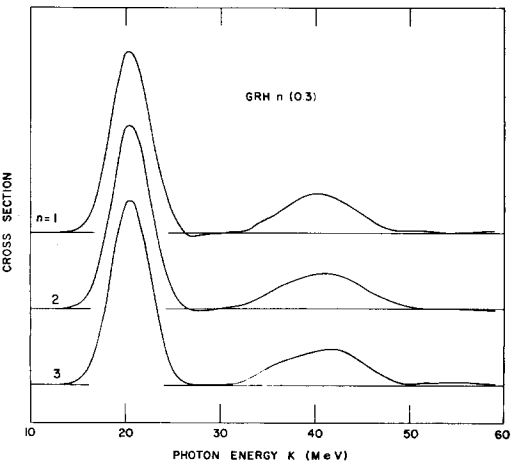
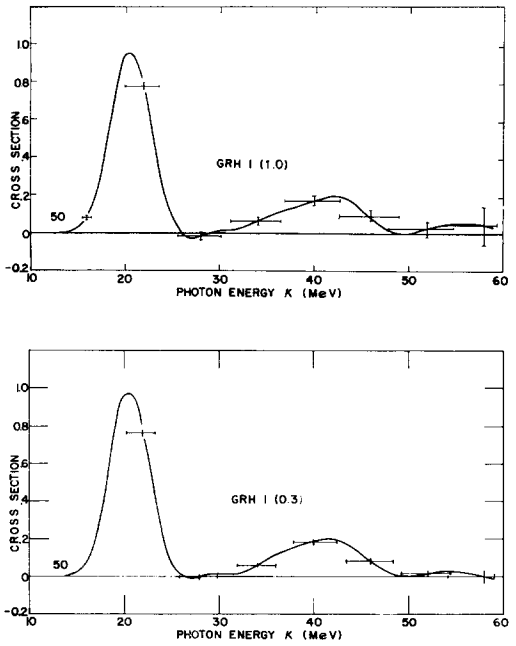


Fig. 12.
Least structure solutions of GRH using a S_1 structure function.

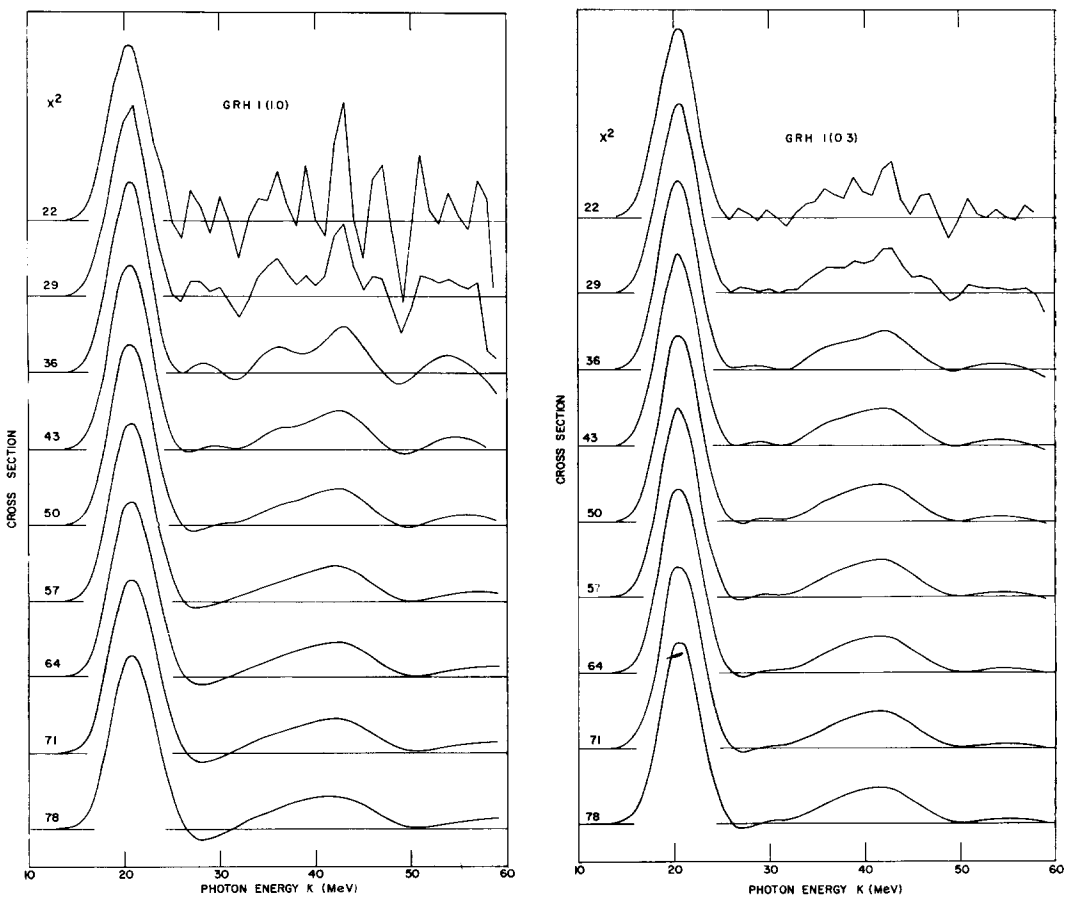


Figs. 10 and 11. Least structure solutions of GRH 1(1.0) and GRH 1(0.3). The statistical errors and resolution are shown at representative energies. The resolution is the full width at half maximum of the resolution function R determined by the least structure analysis.

Least structure solutions for simulated yield functions generated by GRH n (40 MeV resonance) are shown in figs. 8 and 9. Ten solutions, each corresponding to an independent yield function are given. Fig. 8 represents 1% data and fig. 9, 0.3% data. The 20 and 40 MeV peaks in σ_j are clearly evident in all solutions although fluctuations in σ_j due to statistical fluctuation in the yields have not been completely eliminated. Solutions of yield curves GRH 1(1.0) and GRH 1(0.3) are repeated in figs. 10 and 11 with the statistical errors at representative energies (eq. 13b) indicated as well as the energy resolution (full width at half maximum) implicit in least structure. Least structure solutions do not fluctuate as a function of photon energy as the solutions at adjacent energies are correlated. This correlation in σ_j must be recognized for the proper interpretation of the assigned error but does

not invalidate least structure. (Solutions without smoothing are more strongly anticorrelated than the least structure solution is correlated). The complete correlation matrix $(\mathrm{ERM})_{ij}$ (eq. 13a) has been calculated in a few cases but will not be reproduced here. The correlations are found to be large for energy intervals comparable to the resolution. The fluctuations seen in the solutions σ_j shown in figs. 8 and 9 are comparable in magnitude to the errors calculated by eq. (13b).

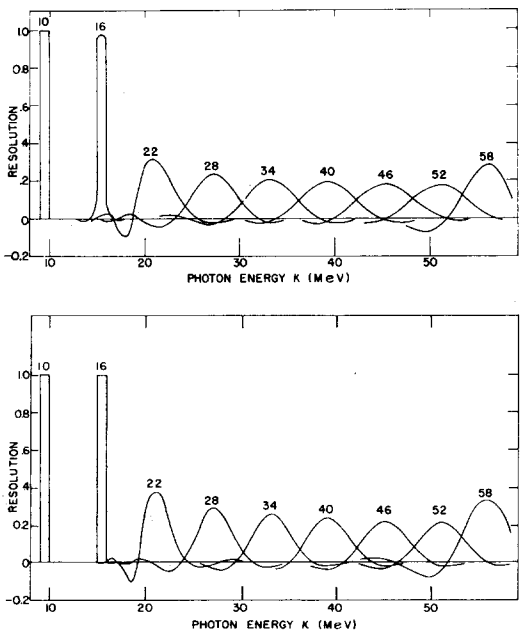
In fig. 12 solutions for GRH (0.3) using a S_1 structure function are presented. The similarity of these solutions to those using S_2 is clear. Thus least structure solutions are gratifyingly independent of the particular arbitrary formulation of least structure used. In figs. 13 and 14 solutions for GRH 1 are shown with $\bar{\chi}^2$ as a parameter for 1% and 0.3% data. Solutions corresponding to $\bar{\chi}^2 < 50$ are undersmoothed solutions and those corresponding to $\bar{\chi}^2 > 50$ are oversmoothed solutions. Again it is found that the nature of the solutions is not strongly dependent upon the smoothing chosen.



Figs. 13 and 14. Effects of smoothing. Solution of GRH 1(1.0) and GRH (0.3) are given with $\bar{\chi}^2$ as a parameter. The solution with $\bar{\chi}^2 = 50$ corresponds to optimum smoothing, solutions with $\bar{\chi}^2 < 50$ are undersmoothed and solution with $\bar{\chi}^2 > 50$ are oversmoothed.

5. Validity and Interpretation of Least Structure Solution

The validity of least structure has been unequivocally justified for cross sections of the type tested in this section by a direct comparison of the least structure solutions to the original solution. An objection might be raised that the solution may be completely invalid for other cross sections. However the transformed spectrum N^*(eq. 5) can be calculated for all least structure solutions without a knowledge of the true σ. In this way distortions in $\sigma(k)$ can be estimated using the experimental data only. In figs. 15 and 16 N^*, calculated for 1% and 0.3% input data, is shown at representative electron energies T_0. Except at the highest energies $N^*(k, T_0)$ is approximately symmetrical about T_0 as a function of k. For $|T_0-k|$ large, N^* is small although one to two oscillations about zero are found. However the term, resolution function R for the more general expression "transformed spectrum" is completely justified in this case. The interpretation of the least structure solutions as cross sections for the test curves is valid as transformed yield (eq. 4) ($\vec{y}^* = N^* \cdot \vec{\sigma}$) can be interpreted as a cross section since N^* has the nature of a resolution function. On the contrary, if N^* were a drastically distorted function of k, least structure would fail. Thus distortions produced by least structure can be estimated from the input data only, without an a priori knowledge of the "true cross section". The calculated errors (eq. 13b) represent standard deviations of the cross section weighted by the resolution function R and not deviations of the least structure solution from the true cross section.



Figs. 15 and 16. Least structure resolution functions. Resolution functions determined using GRH 1, a S_2 structure function, and optimum smoothing. Each curve represents a smooth curve through a row of R. The curves are labeled by the electron energy T_0 in MeV of the yield point to which it corresponds.

6. Conclusion

In conclusion, least structure has been shown to be a useful method for the solution of photonuclear yield functions. Any distortion introduced by the method can be estimated *a posteriori* so that the validity of the solution can be tested. Errors can be assigned to the solution. The method has been used successfully in this laboratory for several experimentally measured yield functions as well as other test functions not described in this paper.

Acknowledgements

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