Conf-9210476--2

An invited paper to be presented at Symposium on Nuclear Data Evaluation Methodology
October 12 - 16, 1992 Brookhaven National Laboratory, Upton, New York, U.S.A.

R-Matrix Parameters in Reactor Applications

ANL/RA/CP--77609

DE93 001679

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* Work supported by the U.S. Department of Energy, Nuclear Energy Programs under Contract W-31-109-ENG-38.

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I. Introduction

The key role of the resonance phenomena in reactor applications manifests through the self-shielding effect. The basic issue involves the application of the microscopic cross sections in the macroscopic reactor lattices consisting of many nuclides that exhibit resonance behavior. To preserve the fidelity of such a effect requires the accurate calculations of the cross sections and the neutron flux in great detail. This clearly not possible without viable resonance data.

The recently released ENDF/B VI resonance data[1] in the resolved range especially reflect the dramatic improvement in two important areas; namely, the significant extension of the resolved resonance ranges accompanied by the availability of the R-matrix parameters of the Reich-Moore type. The improvements all but eliminate the long standing difficulties in conjunction to the use of the Breit-Wigner representation particularly inadequate for the closely spaced resonances and at the same time, removed at least in part the ambiguity of having to extend the unresolved treatment too far into the low energy region where the self-shielding effect is apparently deterministic in nature. The benefit of such a development is not without costs to the users. Aside from the obvious increase in computing time required for the significantly greater number of resonances, the main concern is the compatibility of the Riech-Moore representation to the existing reactor processing codes which, until now, are based on the traditional cross section formalisms.

As described previously[2], one convenient way to alleviate the compatibility problem is to convert these Reich-Moore parameters into the pole and residue parameters whereby the cross sections can be cast into the similar form of the traditional cross section formalisms readily amenable for the ENDF/B format based code systems. The purpose of this paper is to summarize our recent efforts to facilitate implementation of the proposed methods into the production codes at ANL.

II. Brief Review of the Proposed Pole Representation

As reported previously[2], the rigor of the R-matrix cross sections based on the Reich Moore formalism[1] and the traditional feature of Doppler-broadening via the Voigt profile essential to many existing methods in reactor applications can be preserved by the use of either a rigorous pole representation or a simplified alternative based on pole and residue parameters numerically converted from any given set of Reich-Moore parameters[2]. By taking into account all energy dependent quantities in the R-matrix representation, one obtains, via partial fraction, the pole representation with $2(\ell+1)$ simple pole terms in $\sqrt{E}$-domain per resonance for a given ℓ- and J-state. The genuine energy-independent pole and residue parameters can be obtained by

using the WHOPPER-code[2] developed for this purpose. Of the $2(\ell+1)$ poles per resonance, only two exhibit the usual sharp fluctuations that resemble the Breit-Wigner resonances as a function of $\sqrt{E}$ while the remaining 2ℓ poles are characterized by the extremely large half 'width' corresponding to the imaginary part of the pole. Upon Doppler-broadening using the rigorous kernel defined by Solbrig, one has[2]

$$\sigma_x(\sqrt{E},T) = \frac{1}{E}\sum_{\ell}\Re e\left\{\sum_{J}\sum_{\lambda=1}^{N}\sum_{j=1}^{2} R^{(x)}_{\ell,J,\lambda,j}\left[\frac{\sqrt{\pi}}{\Delta_m}W\left[\frac{\sqrt{E}-P^{(j)*}_{\lambda}}{\Delta_m}\right]\right] + q^{(x)}_{\ell}(\sqrt{E})\delta_{\ell}\right\} \quad (1)$$

where $R^{(x)}_{\ell,J,\lambda,j}$, $p^{(j)}_{\lambda}$ and Δ_m are residues (or its product with hard sphere shift factor where appropriate), poles and the Doppler width in $\sqrt{E}$-domain respectively, and the complex probability integral, W(z), is related to the usual Doppler-broadened line shape functions as

$$\sqrt{\pi}\,y\,W(z) = \psi(x,y) + i\,\chi(x,y) \quad (2)$$

The quantity $q^{(x)}_{\ell}(\sqrt{E})$ here represents the superposition of all poles with 'giant width' for a given ℓ not affected by the Doppler effect. One obvious concern from practical point of view is that the evaluation of Eq-1 will undoubtedly require excessive computing cost although it may not be prohibitive. Hence, a simplified version of this approach was developed to provide an alternative more attractive to reactor applications. The procedure is equivalent to the direct extraction of the Humblet-Rosenfeld[3]-type parameters and the associated 'background' term with weak $\sqrt{E}$-dependence explicitly from the converted pole and residue parameters described above. This can be accomplished by regrouping the sum of rational terms into a 'fluctuating' term and a 'smooth' term. The latter consisting of ensemble of pole terms, attributable to the outlying poles and poles with extremely large 'width' defined in Eq-1, can be approximated effectively by a rational function of low order via the non-linear least square fit via the use of the WHOPPER.JUNIOR code[2]. These fitted poles can be viewed as the 'pseudo' poles analogous to resonances assigned to regions outside of the effective resolved energy range. It has been demonstrated[2] that only three 'pseudo' pole terms for each smooth term are required for a given ℓ to provide sufficient accuracy for all major nuclides processed so far.

Upon Doppler-broadening, it leads immediately to the familiar form defined by the traditional formalisms[2]:

$$\sigma_x(E,T) = \frac{1}{E}\sum_{\ell}\Re e\left\{\sum_{J}\sum_{\lambda=1}^{N} 2\sqrt{E}R^{(x)}_{\ell,J,1,\lambda}\frac{\sqrt{\pi}}{\Delta_E}W\left[\frac{E-\epsilon_{\lambda}}{\Delta_E}\right] + \hat{S}^{(x)}_{\ell}(\sqrt{E},T) + \hat{q}^{(x)}_{\ell}(\sqrt{E})\cdot\delta_{\ell}\right\} \quad (3)$$

$$\text{for } \sqrt{E_{\ell}} \le \sqrt{E} \le \sqrt{E_u}$$

where

$$\Delta_E = 2\sqrt{E}\,\Delta_m$$

$$\hat{S}_\ell^{(x)}(\sqrt{E},T) = \sum_{k=1}^{NN} r_k^{(x)} \left[\frac{\sqrt{\pi}}{\Delta_m} W\left[\frac{\sqrt{E}-\alpha_k^*}{\Delta_m}\right]\right] \tag{4}$$

$$\epsilon_\lambda = [p_\lambda^{(1)*}]^2 \tag{5}$$

and $r_k^{(x)}$ and, α_k^* are the fitted residue and pole respectively.

Thus, the only difference between Eq-3 and the traditional formalisms is the presence of the 'background' terms with weak energy and temperature dependence. Its compatibility to all ENDF/B format[1] based codes is quite evident.

II. Cross Section Representations and Self-Shielding Effects

One representative quantity that characterizes the self-shielding effect is the self-shielding factor. With no loss of generality, it suffices to view it as a measure of correlation between the microscopic cross section and neutron flux in energy as well as in space at a given temperature[2]

$$f_x = \frac{\langle \sigma_x \phi \rangle_{E\&\bar{r}}}{\langle \sigma_x \rangle \langle \phi \rangle_{E\&\bar{r}}} = 1 + \frac{COV(\sigma_x,\phi)}{\langle \sigma_x \rangle \langle \phi \rangle_{E\&\bar{r}}} \tag{6}$$

The averages involved can be cast into the form of either the usual Reimann integral or Lebesgue integral. It is quite apparent that a concise description of the cross section as a function of energy and temperature is essential to both the theoretical modeling and the practical computation of this potentially complex problem involving neutron slowing-down and transport in a reactor cell. For the resolved energy of interest here, the degree of correlation is clearly deterministic and multivariant in nature.

All traditional cross section representations[1] prior to the availability of the R-matrix parameters were essentially expressible as the linear combinations of the Breit-Wigner - like terms supplemented by the pointwise smooth data. Aside from the obvious consideration of the inherent advantage of the Doppler-broadening, the overriding consideration to preserve the traditional form in terms of the Voigt profiles[1] is its concise mathematical behavior upon which many fundamental concepts and numerical methods are based. In particular, such a description made possible the coexistence of two fundamental concepts based on the resonance integral approach and continuous energy approach respectively. The former treats the resonance integral for individual resonances separately while the later retains the continuous nature of the flux in energy over the entire resolved range. Various methods based on these concepts differ only in the rigor by which the neutron flux is treated. Thus, by preserving the traditional form, the proposed method is readily amenable to most of the reactor codes in existence with minor modifications.

As long as the resonance cross sections are represented as the linear combination defined by Eq-1 or Eq-3, the W-function alone dictates their behavior as a function of energy and temperature. The analytical characteristics of practical interest can be summarized in Table I. To be consistent with the traditional description of ψ and χ, the variables x and t will henceforth be taken to be $2(E-E_o)/\Gamma$ and $(\Delta/\Gamma)^2$ respectively instead of the generic z.

Table 1: Analytical Behavior of Voigt Profiles of Practical Interest

	ψ (x,t)	χ (x,t)
Lorentzian Limits ($\mid z \mid >>> 1$)	$1/(1+x^2)$	$x/(1+x^2)$
Extreme-Broadening ($t >>> 1$)	$\frac{1}{2}\sqrt{\pi/t}\ \exp(-x^2/4t)$	$(1/\sqrt{t})\ D(x/2\sqrt{t})$ (Dawson integral)
Derivatives: 1st order	$[\chi - x\cdot\psi]/2t$	$[1-\psi-x\chi]/2t$
2nd order	$[1-(1+2t-x^2)\ \psi-2\chi\cdot\psi]/(2t)^2$	$-[x(1-2\psi)+(1+2t-x^2)x]/(2t)^2$

The Lorentzian limits define the short range nature of fluctuations exhibited by these functions. The practical importance will be further addressed in the next section. The explicit knowledge of the derivatives not only provides the analytical insight of how the cross section slope varies as a function of energy but also specifies various extreme points exactly. The latter include the maximum, minimum and points of inflection for each pole term, which are generally difficult to pin-point by means of the brute force approach. For sharply varying function in question, their exact locations will have significant impact on the accuracy of the interpolation of cross sections that follows if the pointwise entry is used. It is worth noting that the points of inflection represent the locations where the temperature derivative vanishes. This stems from the fact that both ψ and χ must satisfy the heat equation of the form

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial f}{\partial t} \qquad (7)$$

They are especially important from the point of view of the Doppler effect calculations.

Numerically, these extreme points for ψ, χ, and $(\psi+a\chi)$ can be determined readily as a function of t. A computer code based on the Newton-Raphson scheme has been developed to compute these extreme points as a function of t (and a where appropriate) using the zero temperature limits as initial guesses. It turns out that these points generally exhibit behavior closely resemble a hyperbola with asymptos identifiable with the expected limits inferred by two limiting cases given in Table I. Fig. 1 illustrates the minimum $\mid X_{min} \mid$ of $(\psi+a\chi)$ as a function of $\sqrt{t}$ for a = 0.20. Two asymptos correspond to $\mid X_{min} \mid = \mid (-1-\sqrt{1+a})/a \mid$ for the zero temperature limit and $\mid X_{min} \mid \approx \cdot 54104\ (2\sqrt{t})$ for the extreme broadening limit reflected by

the Dawson integral respectively. The relationship can be readily characterized by a family of hyperbolas with coefficients as a function of a. Such information can be incorporated into the scheme to construct the pointwise cross sections to be described.

IV. Facilitation of the Proposed Method in Progress

From the practical point of view, the most essential consideration is the potential trade-offs among accuracy, computing cost and computer storage requirement that are suitable to one's objectives and computing tool available. For our purpose here, the discussions will be focused on issues pertinent to the entry of the basis resonance data to the existing deterministic and Monte Carlo codes at ANL. There are only two ways that the basic resonance data can be brought into the reactor applications; namely, the direct entry at run time and the entry with pre-computed pointwise cross sections as a function of energy and temperature. In conjunction to such applications two unique features of the proposed method of particular interest are the prior knowledge of the analytical behavior of the cross sections and the accuracy of the Doppler-broadening which is clearly difficult to match by any finite difference methods implicitly based on the Taylor's expansion without the recourse of using an exceedingly large number of mesh points.

In the following discussion, our efforts to implement the proposed method in the processing codes with two completely different data-entry philosophies will be described.

1. Entry at Run-Time

This type of data entry is obviously attractive for the deterministic approach in which the rigor of the composition and temperature dependence is required. It is particularly important to the code such as the MC^2-2/RABANL in which both resonance integral approach and continuous energy integral transport theory approach coexist.

However, the rigor clearly can not be achieved without the accompanying computing cost and simplifications are obviously required. The points in question is how to enhance the computational efficiencies with acceptable sacrifice in accuracy.

The question of how to manage the numerous number of resonances at run time is nothing new for the MC^2-2/RABANL code[4]. It has been demonstrated how this problem can be alleviated by taking advantage of the ultra-fine group structure of the code essential for fast reactor applications. The basic structure consists of 2000 energy group with the width approximately equal to 1/2 of the maximum energy loss per collision incurred to a neutron by the elastic scattering of the heaviest nuclide of practical interest. The basic logic of the code involves the creation of a base library of 'smooth' cross sections of all nuclides of interest beforehand but the resonance cross sections are computed for each ultra-fine group at run time. Two main cost-saving features already in place prior to the availability of the R-Matrix data are summarized briefly as follows.

(A) Pre-screening procedure

One obvious way to take advantage of the ultra-fine group structure is the use of a pre-screening process while construction the base library, whereby all resonances with the total width much greater than both the ultra-fine group width and the Doppler width corresponding to the highest temperature anticipated will be processed into the 'smooth' library. Many s-wave resonances of structural material apparently will fall into this category. Thus, it helps reduce the needs to compute them at run time.

(B) Treatment of distant resonances

As described earlier, each pole term characterized by the W-function exhibits strong fluctuations only in the energy region near the peak of the resonance. Thus, with exception of a handful of resonances within and close to a given ultra fine group in question, it suffices to evaluate the contributions of the distant levels at the ultra-fine group mesh instead of the hyper-fine meshes required to ensure the adequate treatment of the self-shielding effect.

The viability of these schemes have been successfully demonstrated especially when the continuous energy integral transport option is used[4]. The same techniques are readily amenable to the proposed method[2] based on the Hamblet-Rosenfeld[3] type of parameters. It is worth noting that the contributions of the distant tails of the latter are generally more important than those based on the traditional formalisms according to our experience with the WHOPPER code[2]. Modification and further explorations of the known analytical properties to expedite the calculations are still under way.

(2) Entry As Pre-Computed Pointwise Cross Section

For calculations based on continuous energy Monte Carlo approach, the entry of resonance data at run time is obviously out of question. One must rely on the pre-computed pointwise cross sections as a function of energy and temperature. Although the storage is no longer a prohibitive constraint for the new generation computers, nevertheless, some viable criteria for the mesh spacings are obviously required to ensure the accuracy of the subsequent interpolation at run time.

For the cross section expressed as the linear combination of $\psi(x_i, t_i)$ and $a_i\chi(x_i, t_i)$, it suffices to investigate the problem in two stage: (a) Determine the mesh points adequate to cover any individual term for various values of a_i and t_i within $-\infty \leq x_i \leq \infty$; (b) optimization of the union of the individual sets within the resolved energy boundaries. In the following discussion, various steps pertinent to such a procedure will be described along with some preliminary results.

a) Rational Transformation and Preliminary Grids

One necessary but not sufficient condition for the pointwise cross section and energy pairs generated for each term must preserve the expected average upon numerical integration. It is, therefore, reasonable to conjecture that the preliminary grids required may be taken to be the quadrature points adequate to preserve the rigor of the integration. As described in Ref-5, one of the most efficient way is via the use of the Gauss-Jacobi quadrature.

It is equivalent to carry out a rational transformation of the form

$$f(x)dx = \frac{f(u)}{1-u^2}\,\frac{du}{\sqrt{1-u^2}}\;; \qquad -\infty \le x \le \infty \tag{8}$$

where

$$u^2 = \frac{(Kx)^2}{1+(Kx)^2}\;; \qquad -1 \le u \le 1 \tag{9}$$

and K is a constant dependent only on the Doppler width and total width under consideration. For our purpose here it was found that $K=\frac{1}{5}[\Gamma/(\Delta+\Gamma)]$ is satisfactory for the cases considered.

In terms of the Gauss-Jacobi quadrature a set of mesh points $\{u_i\}$ is specified once the total number of points is given. Extensive investigations indicate that 13 points are sufficient to reproduce the expected value adequately. A set of points $\{E_i\}$ in energy domain corresponding to $\{u_i\}$ can be obtained readily and vice versa. The transformation fully utilizes the Lorentzian behavior of ψ and χ functions, because $\lim_{u\to\pm1}(\psi/(1-u^2)) = \text{const.}$; and $\lim_{u\to\pm1}(\chi/1-u^2) = \text{const.}/\sqrt{1-u^2}$.
Thus, the transformation amounts to optimization of number of points needed to describe each term in question from the perspective of integration.

b) Addition of Points

Although the preliminary grids provide a good start, they are by no means adequate to ensure the accuracy of values to be interpolated at run time. In particular, those extreme points described earlier can play an important role in the interpolation process that follows. Hence, these points are included into the set determined by the quadrature.

The addition of extreme points, however, still does not guarantee the accuracy of the interpolated values especially between points where the gradient changes significantly. To ensure the accuracy of values to be interpolated, the spacing of predetermined meshes obviously must be correlated to their higher order derivatives as defined explicitly by the remainder associated with the interpolation scheme used. The precise knowledge of the derivatives for every preliminary mesh provides the needed criteria. Extensive investigations are under way and some preliminary results will be presented in the later section.

C) Union of Individual Sets and Further Addition or Reduction of Points

The individual $\{u_i\}$ or $\{E_i\}$ sets can be combined to form an union that covers the entire resolved region. Two common scenarios that one encounters are: (1) the ensemble consists of either the well-isolated poles (or resonance where appropriate); or (2) closely-spaced poles. The former may result in an union of disjoint sets while the latter tends to produce the ensemble of strongly overlapping sets. Hence, additions or reduction of points are required accordingly.

The intersections of various sets may be defined at the average of two end points (in energy) of the neighboring sets. These intersecting points define the subset center around a given pole consisting of points that happen to fall into this interval. The table may consist of either $\{\sigma_{xi}\}$ and $\{E_i\}$ pairs or $\{\sigma_{xi}/(1-u_i^2)\}$ and $\{u_i\}$ pairs. If the subsequent interpolation scheme is to be carried out in the u-domain, all energy points within the interval must be converted into the u-mesh points based on the pole in question. For the nuclides with a dominant s-wave sequence (such as ^{238}U), the mesh points generated for the p-wave poles can be included as subsets in the interval defined by the s-wave pole in which they happen to fall.

d) Preliminary Results

An experimental code capable of generating pointwise cross sections using the scheme described above along with plotting and interpolation routines has been developed. Although, many criteria pertinent to addition and reduction of points are still being explored, the preliminary results presented here are believed to be useful to illustrate the general features of the proposed method.

Fig. 3 and Fig. 4 show the U^{238} absorption and scattering cross sections vs energy respectively as obtained by the direct calculations using 'fine' energy meshes and the preliminary grids quadrature points for individual s-wave as well as p-wave poles with the minimum points added. They clearly indicate that the preliminary grid can already provide reasonable resolution for the energy region with many sharp resonances prior to the addition of extra points. The difficulties of pin-pointing the peaks and valleys by the brute force means inspite of the extremely fine points used are quite evident as illustrated by the solid lines. The problem can be alleviated readily by the proposed method when the extreme points are added.

For illustration purposes, some preliminary results were obtained via some ad-hoc conditions in lieu of the finished criteria at this time. One area of particular interest in the optimal choice between interpolation scheme and the number of mesh points required.

Fig. 5 and Fig. 6 show the relative errors of U^{238} absorption cross sections in percent resulting from the interpolation of the pointwise data based on the 4-point and 2-point LaGrange interpolation scheme respectively in the low energy region where the high accuracy is the most difficult to achieve. Since the results were obtained by using the same set of pointwise cross section data, the significant difference in the relative errors is directly attributable to the interpolation scheme. These figures clearly illustrate the difficult choice between the accuracy and computing cost that one must make whenever the entry of the pointwise cross sections is considered. It is believed that the accuracy of the proposed scheme can be significantly improved by removing a handful of peaks and valleys in the relative error via the use of the more viable criteria.

It is worth noting that the inherent errors attributable to the pointwise entry of cross section data are seldom noticeable in the cursory reactor bench-mark calculations based on the average quantities over considerably large energy span due to the error cancellations. Nevertheless, they do provide a point of reference as to the potential limitations of this mode of data entry especially for problems where the localized details are important.

V. Conclusions

The proposed method for converting the R-matrix parameters given by the ENDF/B VI file into pole and residue parameters prior to their deployment in Reactor applications is believed to be of practical importance especially for the code systems at ANL. It can be used effectively in the context of either one of the two modes of data entries commonly adopted. For the methods based on the data entry at run time, the pole representation is readily amenable to the codes in existence with minor modifications. Although no quantitative results are available at this time, the implementation of the method into the MC²2/RABANL code[5] is well under way. For methods that the pointwise entries are more appropriate, the proposed scheme can also be used as a powerful tool in constructing the pointwise cross section libraries. Aside from the rigor in the Doppler broadening of cross sections, it also provides the invaluable analytical insight in the optimization of the mesh structures. The most important feature still under investigation is the correlation between mesh spacing and the rate of change in derivatives between points that obviously determines the accuracy of any interpolation scheme.

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Figure 1. $|X_{min}|$ vs t

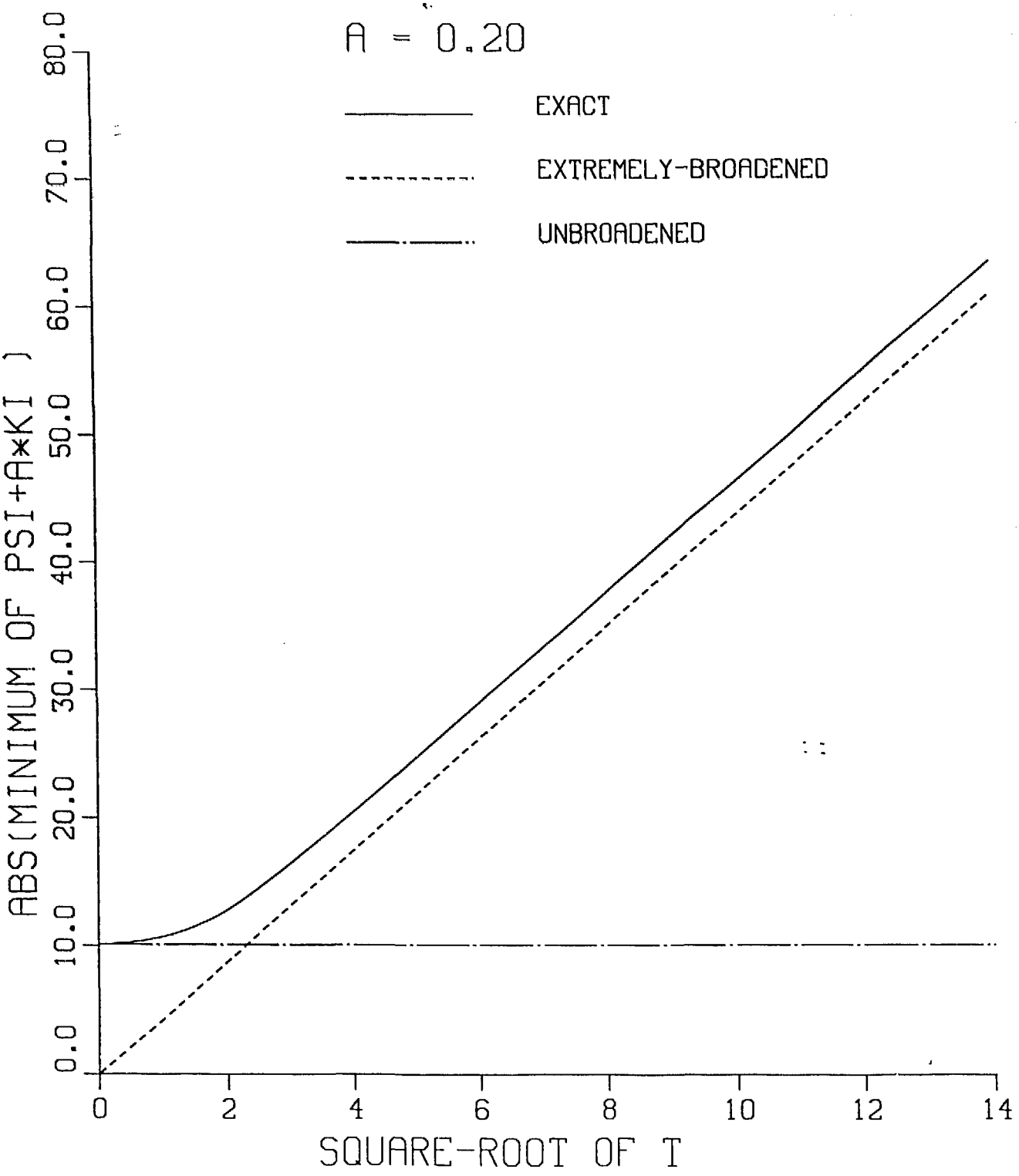

Figure 2. σ_a of ^{238}U vs E

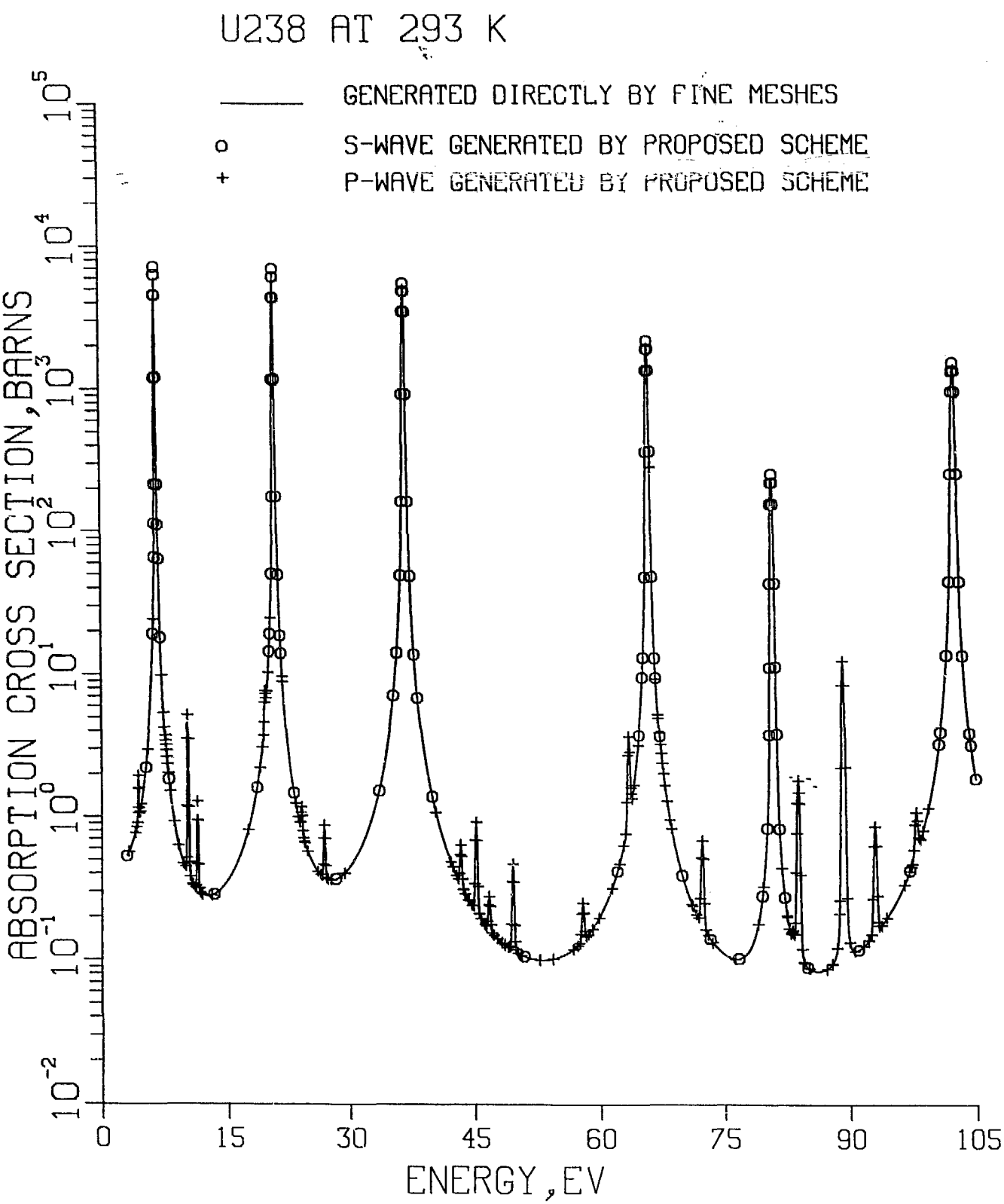

Figure 3. σ_s of ^{238}U vs E

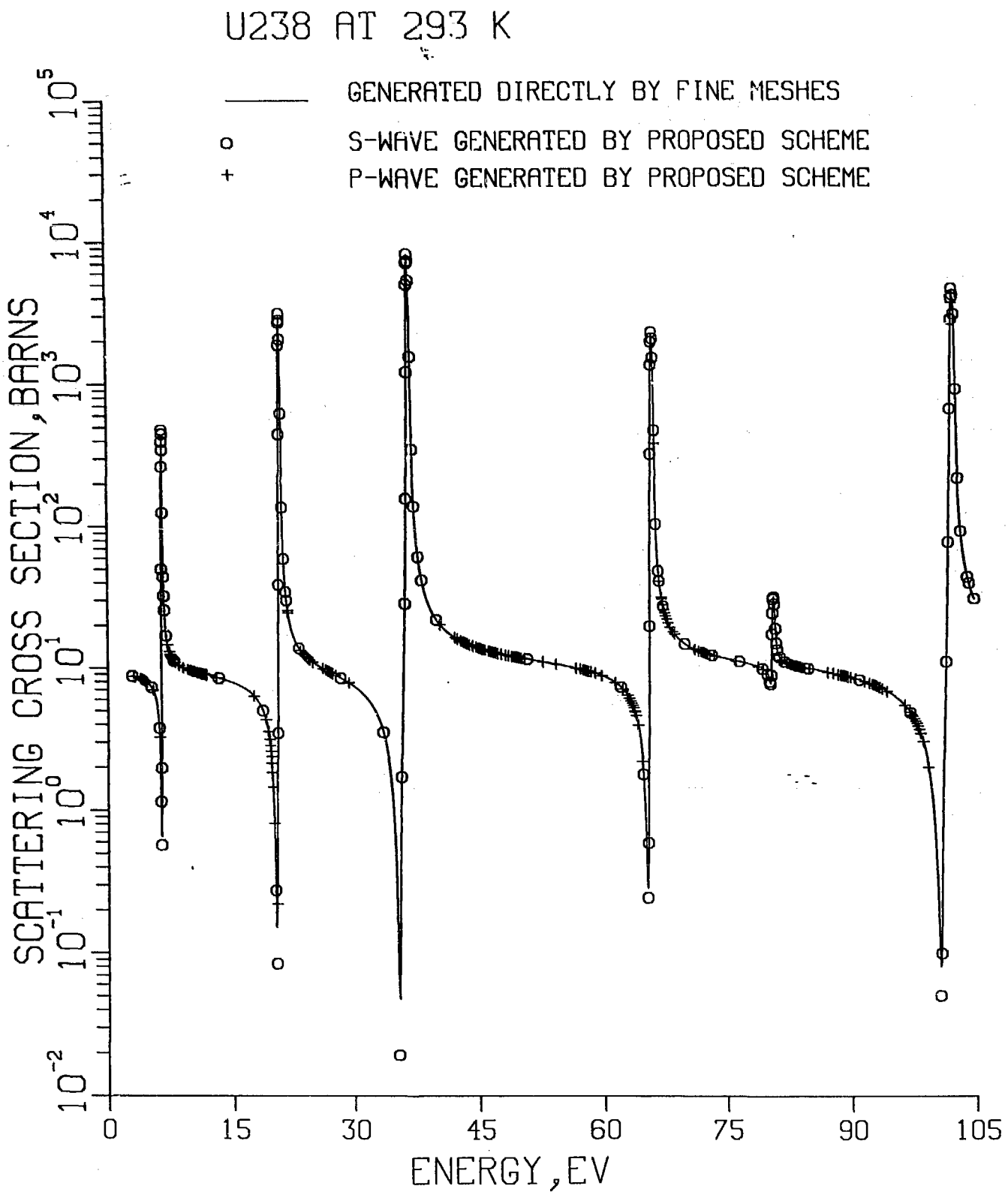

Figure 4. % Error in σ_a (4-point)

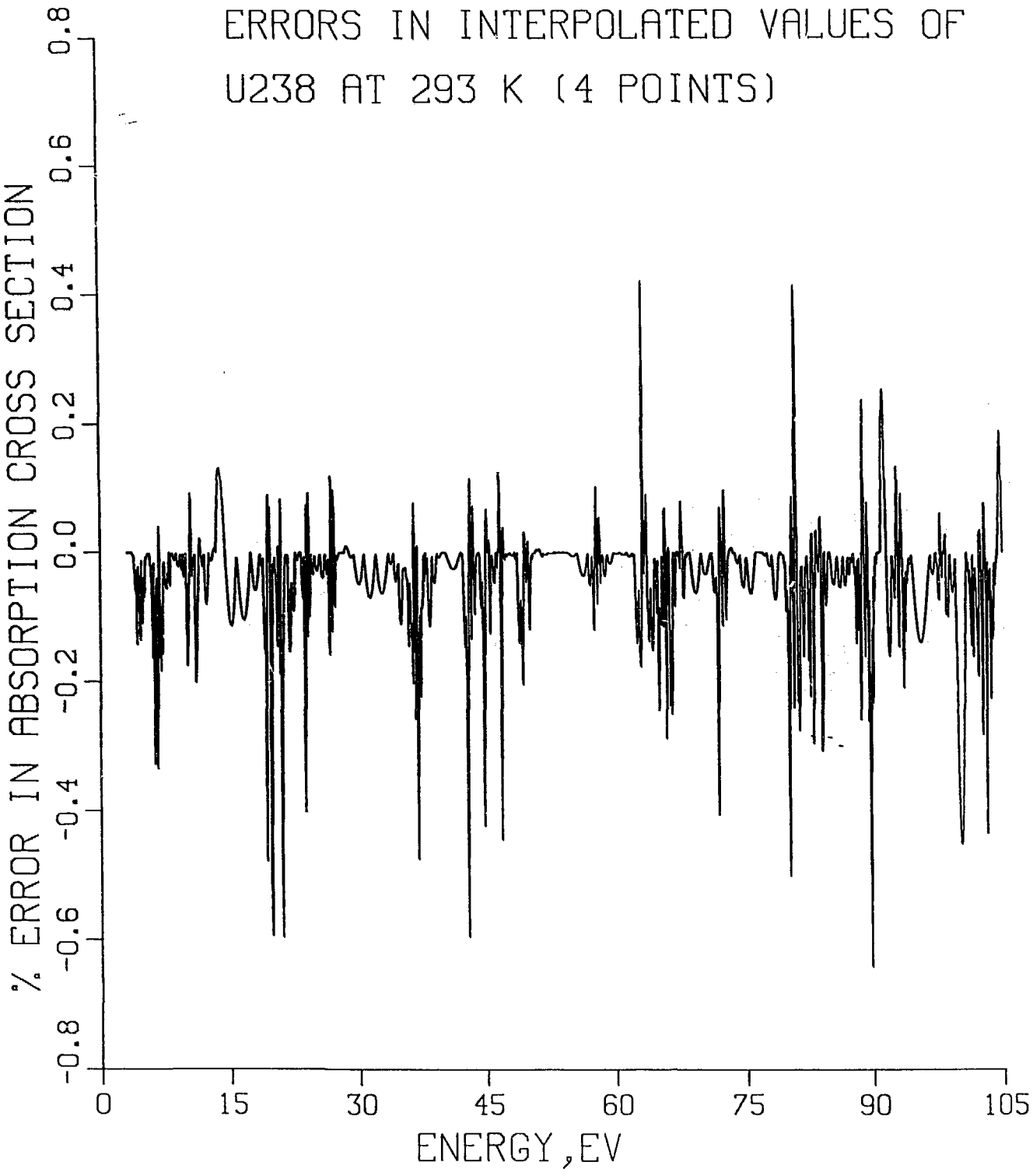

Figure 5. % Error in σ_a (2-point)