

BNL 50004 (C-48)

MASTER

**PROCEEDINGS OF THE NATIONAL TOPICAL MEETING ON
REACTOR PHYSICS IN THE RESONANCE AND THERMAL REGIONS:**

AN ADDENDUM

February 7 to 9, 1966

RELEASED FOR ANNOUNCEMENT
IN NUCLEAR SCIENCE ABSTRACTS



**Sponsored by the San Diego Section
American Nuclear Society**

**BROOKHAVEN NATIONAL LABORATORY
ASSOCIATED UNIVERSITIES, INC.**

under contract with the

UNITED STATES ATOMIC ENERGY COMMISSION

Handwritten notes:
380
11-10-66
356
C-48

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

CONF-660204(Add.)

PROCEEDINGS OF THE NATIONAL TOPICAL MEETING ON REACTOR PHYSICS IN THE RESONANCE AND THERMAL REGIONS:

AN ADDENDUM

CFSTI PRICES

February 7 to 9, 1966

H.C. \$ 3.00; MN 50

65

RELEASED FOR ANNOUNCEMENT
IN NUCLEAR SCIENCE ABSTRACTS

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

Sponsored by the San Diego Section
American Nuclear Society

BROOKHAVEN NATIONAL LABORATORY
UPTON, NEW YORK 11973

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

PRINTED IN USA

PRICE \$3.00

Available from the
Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards
U.S. Department of Commerce
Springfield, Virginia

October 1966

850 copies

PREFACE

An American Nuclear Society National Topical Meeting on Reactor Physics in the Resonance and Thermal Regions was held in San Diego during February 7-9, 1966. Some 26 invited papers and 11 contributed papers were presented at the meeting. The rapporteur system was used to review the contributed papers. In addition, panel discussions were held on the two main topics.

Unfortunately, the discussions were poorly recorded and were therefore omitted from the volumes of the proceedings. Because of the interest of the attendees, the imperfect transcript of the proceedings has nevertheless been edited for publication.

Jack Chernick
Editor

**THIS PAGE
WAS INTENTIONALLY
LEFT BLANK**

Table of Contents

Preface	iii
List of Contributed Papers on Neutron Thermalization	1
Reporter's Remarks on Contributed Papers on Neutron Thermalization	2
Panel Discussion on Neutron Thermalization	9
List of Contributed Papers on Resonance Absorption	15
Reporter's Remarks on Contributed Papers on Resonance Absorption	16
Panel Discussion on Resonance Absorption	33

List of Contributed Papers on Neutron Thermalization

1. Slow Neutron Scattering by Liquids: A Hindered-Translation Model. V. Ardente, Euratom; G. F. Nardelli, Universita degli Stude, Milan; L. Reatto, Associazioni Ricerche Scientifiche, Milan.
2. Calculation of the Space Dependent Thermal Neutron Energy Spectrum in Heterogeneous Assemblies by Flux-Synthesis Methods. H. Hembd, Euratom.
3. Approximation Treatment of Neutron Thermalization in Heterogeneous Systems. P. R. Haubert, N. R. Meyvaert, Belgo Nucleaire, Belgium.
4. Experimental and Theoretical Thermal Fine Structure, Spectral Indices and Relative Conversion Ratios in Boiling Heavy Water Lattices of Slightly Enriched Uranium Oxide Clusters.
A. Jonsson, H. Pekarek, E. Sokolowski, and C. E. Wikdahl, Aktiebolaget Atomenergi, Sweden.
5. Operating Experience with UNC-THERMOPILE, An Advanced Monte Carlo Program for the Evaluation of Thermal Assemblies.
F. R. Nakache, S. Kellman, United Nuclear Corporation.
6. An Energy Dependent Calculation of the Disadvantage Factor.
A. H. Robinson, J. H. Ferziger, Nuclear Engineering Laboratory, Stanford University.
7. Application of a Phenomenological Thermalization Model to Irradiated Lattices. A. Kind and G. Rossi, Euratom.

Reporter's Remarks on Contributed Papers on
Neutron Thermalization

P. Zweifel, Rapporteur

It is virtually a truism to point out how closely the development of reactor physics in the past dozen or so years has been tied to the high-speed digital computer. It is extraordinary to compare the discussion at this conference with those, say, of the first ANS meeting I attended 10 years ago. Today people are discussing calculations techniques and methods which were unheard of in those days - due entirely to the larger, faster machines which have become available.

In the light of this progress, I have tried to consider with some care the classes of problems which reactor physicists are thinking of today, and I have more-or-less arbitrarily come up with three such classes. Before I describe them, let me just mention some of the dangers of the present computer age, and then mention how I think these dangers can be, and are being, avoided.

Clearly, with the computer we can solve problems which were hopeless before. We have thus the danger that we lose physical insight into the nature of the problems (insight which was provided by old-fashioned phenomenological methods like age theory,

four-factor formulas, etc., etc.,). Another real, but not so obvious danger is that we lose understanding of the mathematical nature of the solution of the transport equation. This brings us directly to what I have called Class I problems; essentially exact analytical solutions of highly idealized physical situations. Such problems serve the dual role of giving the physical and mathematical insight that only analytical solutions can and, at the same time, providing test cases against which numerical methods can be tested. Examples of work in this area are the transport theoretical studies of K. M. Case, and all of the work to which it has led, e.g. the paper in this session by Robinson and Ferziger to be described later.

Many of the papers presented at this conference, and in particular, in this session, fall into this category. However, the advent of the computer has created another important field, namely the necessity for producing nuclear data of great accuracy and detail to serve as input for the refined calculations now possible. This I call Class II. There are such papers at this conference - both experimental and theoretical, and I will describe one by an Italian team later in this report.

The third class involves the attempt to obtain solutions on the computer for more or less practical problems. This may be an essentially exact procedure, like THERMOS, or Monte Carlo, which solves any part of a problem exactly, or it may involve a combination of several calculations, in which case, even with our present computers, some parts must involve phenomenology. (Example - two or three dimensional multigroup with group constants obtained from MUFT).

Thus, I have outlined three general categories:

1. Exact solutions of idealized physical situations.
2. Generation of highly refined input data.
3. Practical solutions.

The papers which I have been asked to review today fall into all three classes. Let me begin with paper #1, Slow Neutron Scattering by Liquids: A Hindered-Translation Model by Ardente, Nardelli, and Reatto. This paper clearly falls into Class II. In this model, a liquid is considered to be composed of oscillating atoms which, however, become free to translate whenever their oscillatory energy exceeds a certain value V_0 taken to be the "activation energy" of the liquid. Applying a method originally developed by Wang and Uhlenbeck to account for energy transfer between vibrational and translational modes, these authors are able to derive an expression for the velocity auto-correlation function which we know (cf. Dr. Rahman's talk, for example) can be related to the neutron scattering cross section. They compare with scattering experiments in liquid argon, sodium, and water. While it is not clear that this model gives substantially better agreement than other models in all cases, it has, as the authors point out, the virtue that it has no arbitrary parameters, so that it is a truly physical rather than phenomenological model. (In some cases, particularly argon, agreement is better than with previous calculations.) This type of analysis represents an important attempt towards calculation of accurate cross-sectional data for liquid scattering systems, and is certainly worthy of more comment than the brief remarks I am able to make here.

Let me next skip to paper #6, An Energy Dependent Calculation of the Disadvantage Factor, by Robinson and Ferziger. This paper clearly falls into Class I, an exact calculation of an idealized physical problem. Unfortunately the problem is not sufficiently idealized that an exact solution can be obtained, but a result of very high accuracy is found. Essentially, the authors apply the method of Leonard and Ferziger (based on Case's method of singular eigenfunctions) for solving the energy-dependent transport equation (by expansion into orthogonal eigenfunctions of the energy transfer kernel). Then two approximations must be made:

1. The expansion must be truncated.
2. The resulting equation must be solved numerically.

The first difficulty can be avoided to some extent by truncating successively after n , $n+1$, $n+2$, etc. terms. The second is handled either by reducing the singular integral equation to a Fredholm equation and iterating, or, as Professor Ferziger tells me he finds better, to solve the singular integral equation directly on the computer.

The results are applied to natural U-H₂O systems, and are compared with THERMOS, with reasonable agreement and a saving of two orders of magnitude in computer time. Clearly much more needs to be done in this method, to apply to more practical geometries (cylinders) and to make the agreement with THERMOS even better. Incidentally, THERMOS itself is an essentially exact method which can be used to test approximation schemes, so in this case the attempt is to save computer time in the exact solution.

Next, paper #7, Application of a Phenomenological Thermalization Model to Irradiated Heavy Water Lattices. This paper falls into Class III, as it attempts to combine thermalization in the presence of a large resonance (Pu-239), a procedure which, while again amenable to "exact" numerical solution (THERMOS), in a practical case would run into excessive computing time. So the authors combine numerical integration of the Wilkins equation (as the authors point out other thermalization models may be tested similarly) with a phenomenological treatment of the resonance. Their code, THERMIDOR, shows good agreement with THERMOS, and thus gives hope of practical application to highly complex geometrical systems.

Paper #5, Operating Experience with UNC-THERMOPILE, An Advanced Monte Carlo Program for the Evaluation of Thermal Assemblies, by Nakache and Kellman is another example of Class III and is an attempt to generate practical solutions for complex geometries. Again results are compared with THERMOS for simple cases (note the universal use of THERMOS as a Class I case and Robinson's-Ferziger's attempt to improve on it). This code consists of an almost infinite number of subroutines such as NELICERN, SLODOPOX, EZGEOM, etc. for using all available information. There is no point in my trying to describe a Monte Carlo program here, except to point out that as data improves and good phenomenological models are found for handling portions of the problem, the Monte Carloists are bound to come up with new codes incorporating the latest results. THERMOPILE appears to be much of an evolutionary study in this direction.

Paper #3, Approximate Treatment of Neutron Thermalization in Heterogeneous Systems, by Haubert and Meyvaert. This paper again

falls into Class III, in that it attempts to solve the spatial problem as carefully as possible (by multiple collision methods) so it replaces the thermalization problem by the celebrated Cadillhac approximation. The method is applied to cylindrical cells, but with no numerical results or comparison with experiment reported.

Paper #4, Experimental and Theoretical Thermal Fine Structure, Spectral Indices and Relative Conversion Ratios in Boiling Heavy Water Lattices of Slightly Enriched Uranium Oxide Clusters, by Jonsson, Pekaret, Sokolowski, and Wikdahl, is more of Class I, as it uses 40 thermal groups, again with multiple collision methods for spatial dependence. It does, however, replace the resonance region with one group and puts all fast neutrons into one group, so it is not really "exact", but those parts could be compared with "exact" calculations of those portions of the spectrum. Here the results are compared extensively with experiment - fine structure of absorption in U^{238} - with excellent results. I might comment that multiple collision calculations (as expounded extensively by Grossjean some years ago, seem to be coming back into vogue, a development which I, for one, had not foreseen).

The last paper is #2 - Calculation of the Space Dependent Thermal Neutron Energy Spectrum in Heterogeneous Assemblies by Flux-Synthesis Methods, by Hembd. In this method, the energy-dependent flux is expanded as a linear superposition of energy distributions weighted by spatial amplitudes. Then the transport approximation, for example, can be applied, and the resulting energy equation solved numerically. This I would put into Class I, except that the described calculations have been done

in the diffusion approximation. It would be interesting to see this method combined, for example, with Case's exact treatment of the spatial distributions.

In conclusion, I should say that my division into classes is somewhat arbitrary because so few exact solutions are possible that one tends to combine exact analytical with numerical or phenomenological as the best possibility. Total numerical solutions are still not possible, so that one tends to combine phenomenological with numerical methods, and so forth.

Panel Discussion on Neutron Thermalization

P. Zweifel - University of Michigan
(Chairman)
E. R. Cohen - North American Aviation
Science Center
J. E. Wilkins - General Atomic
H. Honeck - USAEC
R. Beyster - General Atomic

(The following report is not verbatim - only the gist of the comments is presented).

P. Zweifel - Dr. Cohen will make an opening statement.

E. R. Cohen - With respect to the many comments on both Monte Carlo calculations and physical insight, I think physical insight is very helpful in preparing Monte Carlo calculations, but I doubt if much insight can be gained from the output of such a problem. I also believe that as computers get bigger and faster more physical data can be usefully used in Monte Carlo calculations. However, the larger computers may not be as efficient in handling Monte Carlo calculations as is hoped because of input-output speed limitations.

J. Askew(UKAEA) - It may be possible to overlap the computing with input-output routines.

E. Wilkins - There must be a good balance between computing speed and input-output times if we are to realize the full benefit from future machines. The balance is not correct now - computing speed has improved much faster than input-output capability.

H. Honeck - Changing the subject for a moment, I have not seen any breakthroughs in the thermalization field since the 1962 BNL conference. However, the theory and its application to the computation of scattering kernels has advanced considerably since then. We are able to calculate space dependent spectra provided we have the time and money.

It appears that the integral data and single differential data are both valuable in developing and evaluating scattering kernels, but I wonder if the double differential data is similarly useful. To my knowledge, it has never been used. Can anyone comment on that? With respect to the "physical insight" opinions of our panel moderator, it seems to me that one can obtain more insight from the purely numerical study of A. Rahman than from singular integral equations, for example.

D. T. Goldman (National Bureau of Standards) - I have found that double differential data was valuable in developing a polyethylene kernel.

P. Daitch (Rensselaer Polytechnic Institute) - I agree with Honeck that the theory has improved, and that double differential measurements have improved tremendously. This data can be used to discriminate between scattering models, and one can conceive of eventually foregoing cross section measurements, and instead using double differential data to determine the best cross

P. Daitch(RPI) (Cont'd.)

section model and then deriving cross sections from that model. One could also estimate the magnitude of multiple scattering errors by measuring the double differential cross section between energies and angles which should yield the same value for $S(\alpha, \beta)$. Differences in $S(\alpha, \beta)$ would be informative in this regard.

At RPI we use very thin scattering foils and the multiple scattering corrections are small. We are also doing a Monte Carlo analysis of the subject.

J. Young(GA) - In our work we have not used double differential data, except for the excellent work of Schmunk and Brugger on the dispersion relations for beryllium. We also expect to use their results for BeO. If you look at the scattering cross section measured at the same values of α and β , the scattering law varies by as much as a factor of 10.

R. Jarvis (Chalk River) - We have found the double differential data useful in developing kernels in spite of multiple scattering problems.

R. Brugger (Phillips Petroleum) - I believe all of this data is useful. Better spectrum measurements motivated and led to effective mass free gas kernels for water and eventually Nelkin's bound kernel. Recent double differential data has led to the McMurray-Russell kernel, and I trust that further measurements will lead to further improvements.

R. Beyster(GA) - The re-entrant hole problem is an important problem but the experimental studies that we have been able to make on this point indicate that the effect can't be too large.

R. Beyster(GA) (Cont'd.)

I also believe that the double differential data that has already been generated should be carefully studied and analyzed to maximize its usefulness. If multiple scattering corrections are very large, it may be worthwhile to determine how to make the correction reliably before doing too many more measurements, although I realize this may be a minority opinion.

We have had difficulty analyzing our own data at times, and we are publishing the data in great detail so that other people can study it. We try to make measurements which are susceptible to calculation but we aren't always successful.

R. Brugger(Phillips Petroleum) - Re-entrant hole problems don't stop GA from making further measurements, and we don't feel that multiple scattering corrections need stop us from doing useful double differential scattering experiments.

D. T. Goldman(National Bureau of Standards) - I'd like to re-emphasize my feelings about numerical calculations and the errors that creep into them when one changes from differential or integral type equations to difference equations. I personally have always been unhappy about the procedure of averaging cross sections over groups of any width whatsoever, rather than solving equations themselves point by point. I just wish to point out that errors creep in when one wishes to make detailed comparisons with experiment which are very difficult to determine.

P. Zweifel - I take it then that you're in favor of Monte Carlo calculations, since that is one way of getting around the problem of using average group cross sections.

D. T. Goldman - Not necessarily. Group averaged cross sections are sometimes used in Monte Carlo calculations, especially in the epithermal range. Then cross sections, resonance parameters, etc. must be averaged and the answer you get is dependent on just how you took the average. It is possible to do it accurately, but it requires care.

R. Sullivan (Nuclear Utility Services) - I'd like to come back to the question of how much all this is worth. Part of the answer will be given about a month from now in a cross-section meeting in Washington, where one of my co-workers is going to present the results of a parametric study on the effects of uncertainties in nuclear parameters on fuel cycle costs.

P. Zweifel - Perhaps we should adjourn this meeting and all reconvene at that time.

E. Gelbard (Bettis) - I think there has been some misconception about the amount of time involved in running Monte Carlo calculations. If you do a calculation where you throw everything in, it will certainly take a lot of time, but the typical design calculation at Bettis takes 3 to 5 minutes. This is with the Philco-2000. Another generation of machines is coming in the door, and we should be able to realize a speed increase of a factor of 5. So the times involved are not very great.

P. Zweifel - Are you talking about a thermal multi-group calculation?

E. Gelbard - Yes, not about a calculation which couples all energies together. I don't know how much time that will take.

P. Zweifel - That is probably still not feasible for the next generation of computers.

E. Gelbard - I don't think it's unfeasible. I think it would take about 30 minutes of time on the present computer for such a problem.

P. Zweifel - Then in the future, all exact numerical calculations may be done with Monte Carlo.

E. Gelbard - If the machines keep getting faster and faster, by perhaps a factor of 20 over Philco-2000, then the type of problems I'm talking about will be almost trivial.

P. Zweifel - A statement like that doesn't distress me as much as it used to. Now that I have set up my classification, I see that you'll only be able to make progress in Class 3 and not in Classes 1 and 2.

F. Nakache (UNC) - I'd like to say a few words about Monte Carlo codes. First, the amount of time it takes to run a Monte Carlo program depends completely on how big a problem you have set up. Problems of interest to us take perhaps 3-4 minutes on the IMB-7090. Secondly, we have also checked our program results (UNC-THERMOPILE) against lattice experiments with good results and against infinite medium spectra.

Finally, I disagree with the position that you get no physical insight from using a Monte Carlo code. I think it takes great physical insight to run a Monte Carlo calculation intelligently.

P. Zweifel - We could argue at length on this, I guess. I just don't feel that you get much physical insight from the results of the calculation, although I'll admit that writing the program in the first place requires a real understanding of the physical processes.

List of Contributed Papers on Resonance Absorption

1. Resonance Absorption in Heavy Water Lattices - Development Work at Ispra. L. Amyot, F. Beonio-Brocchieri, A. Doeuf, G. Casini, W. De Haan, E. Diana, S. Tassan, Euratom.
2. Some Problems in the Calculation of Resonance Capture in Lattices. J. R. Askew, UKAEA, United Kingdom.
3. Two Level Interference Effects in Neutron Cross Sections. J. D. Garrison, General Atomic Division of General Dynamics Corporation.
4. Measurement of Infinite Dilution Capture Resonance Integrals with Moxon-Rae Detector. L. LeSage and R. Sher, Stanford University, Stanford, California.

Reporter's Remarks on Contributed Papers on
Resonance Absorption

J. Chernick, Rapporteur

The plan of the present meeting is to use the reporter system to review contributed papers. The reporter system has become quite popular at scientific meetings because of time limitations.

There are times when it is even successful. A good example was the Brookhaven Conference on Neutron Thermalization in 1962, where judging by post conference comments, there was general satisfaction with the work of the several reporters. However, the papers of the latter conference were all contributed papers on narrow topics and therefore quite cohesive in content. The papers contributed to the present meeting are much more diverse in character and one would face a more complex task in any attempt to unravel them in depth.

For this reason, I will spend much of my time setting the papers into some historical perspective, make some observations concerning the character of the work and, I hope, leave some time for the audience to ask questions not clarified by the authors' summaries.

There are four contributed papers to the present session. The first of these is a review of work at Ispra in Italy on Orgel type of lattices. The second paper by John Askew of Winfrith is concerned, as was the paper we heard yesterday, by George Tyror, with possible inadequacies in the U-238 resonance absorption data as indicated by analysis of critical experiments. The paper by LeSage and Sher is primarily experimental, while that of Garrison discusses a two-level formulation of resonance structure for the analysis of strong interference effects between adjacent levels.

To understand how these papers fit into the general framework of resonance absorption theory, it is necessary to review some of the history of the subject. As you know, the early work on the resonance absorption of neutrons was completely dominated by the methods developed by the Manhattan Project and in particular by Wigner's pioneering report CP-4. Wigner's formulas were admittedly rough and empirical with constants which were fitted to the nuclear data. Nevertheless, in the immediate post-war era, few dared to tamper seriously with the tested recipes of the Manhattan Project because of the caliber of its physicists and for lack of better data. As late as the first Geneva Conference in 1955, we reported the Manhattan Project value of 240 barns for the dilute resonance integral of uranium along with a current estimate by Jack Harvey of 276 ± 12 barns based on the then known resonances. It was in this paper that we first suggested the use of collision probability methods as a hopeful way of treating resonance absorption in reactor lattices. We were also able to report results of the first Monte Carlo calculations by Richtmyer of resonance capture of neutrons by individual resonance levels of U-238.

Wigner's original study led to a division of resonance integrals into volume and surface terms with by far the chief emphasis on the volume term. In 1955, Wigner pointed out the need to modify this formula - at least the surface term - which was based on the weak assumption that the fuel lump was impenetrable to resonance neutrons entering the lump. The early studies at Brookhaven of resonance capture of low energy U-238 resonances indicated the dominant importance of the low energy resonances and hence the importance of the surface term in the resonance integral formula. At the same time the inadequacy of the conventional narrow resonance approximation became evident and we suggested the equally simple NRIA or wide resonance formulation as it is now sometimes called. That the Russians were also dissatisfied with the standard US formula became apparent when the USSR recipe for resonance integrals was unveiled at the first Geneva Conference. The USSR formulation expressed the surface term as proportional to the square root of the surface to mass ratio of the lump.

The first analytical studies indicating serious inadequacies in both the NR and NRIA formulas for individual levels was carried out by the late K. T. Spinney at Brookhaven in 1955 and 1956, and was presented at the 1956 Brookhaven Conference on Resonance Absorption of Neutrons in Nuclear Reactors.

In spite of Spinney's results, Wigner's formulations continued to influence prominent workers in the field until early 1958. By then, the results of Vernon and myself at Atomic International had convinced many workers of the need at least to distinguish between the NR and NRIA resonances on the basis of

what Wigner called the practical width of the resonance. It became clear also that the Russian formula for resonance integrals was to be preferred, a preference also indicated by Hellstrand's experiments. There was a suggestion at the time by Dick Cohen for a compromise resonance integral formula that was first used by Vernon and later blossomed into the Goldstein-Cohen-Brooks intermediate resonance or IR approximation which was discussed this morning by Goldstein. The sponsorship of these serious deviations from Wigner's original methods by Nordheim beginning early in 1958 did much to convince people of both the soundness of these methods and of their usefulness for quantitative calculations.

The calculations that Vernon and I had carried out at Atomic International had not aimed for high accuracy. Thus, we had to admit the uncertainty of our estimate of the p-wave contribution to resonance capture, the lack of accurate knowledge of the high energy contribution in reactor lattices, and we corrected for Doppler broadening by applying a rough equivalence principle to older calculations by Dresner. This latter defect was shortly remedied by Nordheim and his co-workers, by Vernon, and others.

The statistics of resonance parameters is also important to quantitative estimates of resonance absorptions in the unresolved resonance range. Dancoff was the first to concern himself with the statistics of U-238 resonance parameters and in 1949 Wigner pointed out their importance for estimates of α for fissionable nuclides at intermediate energies. In the early 50's these questions were pursued by Sophie Oleksa and by Don Hughes at Brookhaven. Oleksa's work attracted the attention of the late Charles Porter and led to the derivation of the Porter-Thomas

distribution of neutron widths which now plays such a key role in the theory of statistical fluctuations of resonance parameters. The recent book by Porter on fluctuation theory indicates the wide diversification of this field.

Garrison, a couple of years ago, carried out a comprehensive review of the implications of this work to neutron cross sections. We have had reports at this conference from Moore and Schmidt, which represent further advances in this direction. A contributed paper by John Garrison which we shall discuss later probes in deeper waters along this same path.

Since 1958, the most important advances in the field have been in the improvement of the quantitative methods. I shall not go into these methods in any detail, since they were reviewed for the last Geneva Conference. In brief, they consist of improvements in the accuracy of collision probability methods, in numerical methods of solving the slowing down integral equation, in faster Monte Carlo methods, and in the improvement of integral experiments.

Under the narrow resonance approximation for the moderator, our collision probability method for lattices yields a single integral equation in energy to be solved. Nordheim and his co-workers at General Atomic have developed a numerical method, ZUT, to solve this equation which is adequate for many lattices and is in widespread use in the United States. The codes ZUT, and ARES II, the latter based on the intermediate resonance formulation, will be discussed later in connection with a paper from Euratom. Similar, accurate US codes exist for other energy ranges, for example, Dr. Herbert Rief's (Euratom) Monte Carlo code (MOCA) for high energy neutrons and Henry Honeck's code

THERMOS for low energy neutrons. By combining these codes, it is possible to achieve rapid and accurate analyses of lattice experiments as Hellens and Honeck have shown in the case of water lattice experiments and Honeck and Crandell have shown in the case of single rod lattices in heavy water. Several of these codes have recently been combined into a single code called HAMMER by John Suich of Savannah River Laboratories and by Henry Honeck, now with the AEC. The methods developed abroad for the same purpose are on a par with US methods if perhaps slower and less automated. Since high speed computing machines are not as prevalent abroad, ingenuity and patient analytical calculations have taken the place of machine time consuming numerical methods and Monte Carlo calculations which are more prevalent in the United States.

A remarkable development in the past several years has been the growth in power of collision probability methods for reactor physics calculations. While such methods were used in a limited way during the Manhattan Project they were never generally popular in the United States. We first utilized them at Brookhaven in the early 50's to obtain fast fission factors in water lattices and then to solve such problems as the Peierl's equation for slab lattices and finally to attack the problem of resonance absorption of neutrons in general reactor lattices. Our reasons at the time were the same as those still existing in Europe and in Asia today, the lack of easy access to high speed computers. Although such computers are, with time, becoming more and more readily available we expect an even greater diversification of the use of collision probability methods in the future. It has been stated here that one can never do calculations for clustered lattices by such methods but it is

dangerous to make such a statement because people who don't know any better are going to go ahead and do it anyway.

With these introductory remarks we can pass now to the consideration of the contributed papers. The paper by the team from Euratom, Ispra, reports work on clustered rod, organic cooled, heavy water moderated lattices. The reported work includes measurements at Ispra of resonance integrals on single rods of uranium monocarbide and on clusters of metal and carbide rods. While the analysis of some of these experiments is incomplete, good agreement with calculations is reported. Now, if you recall, Dr. Hellstrand pointed out some disagreement in the experimental numbers that he has obtained with those given in this paper. Perhaps we can get to this question later.

The calculations for ORGEL type lattices are based on the multi-region code, apparently developed locally, called SKAOL. Resonance integrals are based on equivalence theorems with constants obtained from Nordheim's ZUT and TUZ codes.

Dancoff coefficients for clustered fuel rods are found by use of a code called SHOCK which is apparently based on approximate collision probability methods but has been checked out against a more exact code by Amyot and Benoist. Since neutron capture in the 1 ev resonance in Pu-240 is important to fuel burnout studies of power reactors, the effect of conventional approximations such as flat flux, the NR approximation in the moderator and the neglect of thermal motion of the moderator, have been studied by use of a multigroup S_n code for ORGEL lattices. Comparison with the ZUT, TUZ, and ARES II codes show that errors in latter codes of about 10% in estimates of resonance capture can accrue under these approximations in cases of

interest. However, before condemning these codes it is fair to point out that they were being used in an area for which they were really not applicable. At least in the United States, I think most people would normally use a thermalization code: THERMOS, GATHER, etc., for this purpose with initial energy above the resonance at 1 ev. Comparisons of various numerical methods of dealing with such low energy resonances, I should also like to point out, were also given at a session of the 1965 winter meeting of the American Nuclear Society in Washington, D.C. The reference is Reactor Calculations, Session I, Transactions of the ANS, Vol. 8, Number 2.

For some time George Tyror of the UK has felt that there was something wrong with the standard U-238 resonance parameters based on his analyses of graphite moderated lattices. Askew now adds fuel to the controversy by reporting extensive series of calculations for other lattices. Again, a quite adequate complex amalgam of UK codes called WIMS is used for the calculations. An idiosyncrasy of WIMS is that it tends to somewhat overestimate Dancoff factors. In contrast to most US codes, however, there are collision probability options for clusters of rods, finite cylinders and other odd geometries as well as single rod lattices. Since the discussion of this paper will probably prove lively, judging by a preview which I attended at Brookhaven, and judging by the remarks following Tyror's paper, I will restrain myself from further comments. As the author points out himself, his estimate of the p-wave contribution is larger than most US estimates. He also uses an epithermal value of α of 0.67 above half a volt, whereas the weight of the evidence from integral experiments indicates a value closer to 0.5. It appeared to me, at the 1965 ANS meeting at Gatlinburg, that

advocates of the value obtained by integral measurement had all the better of the argument. This impression is only reinforced by the talks given us by both Brooks and Feiner. Askew's calculations are based on the present U-238 resonance data and are, like Tyror's calculations, in agreement with Hellstrand's measurements. However, they disagree with the calculations of Hellens, Honeck and Sehgal at Brookhaven which tend to give good agreement with experimental bucklings for water lattices. One of Askew's points is a discrepancy in cadmium ratio which was also observed by Sehgal, but the scatter in experimental data is large and the extent of the discrepancy seems to require further experimentation.

The calculations reported by Askew appear to be comprehensive and well documented. There remains then a clear contradiction between present US and UK calculations of water lattices but the difference is principally attributable to differences in estimates of the epithermal value of α in U-235. For graphite lattices, however, the problem is not so easily traced while again this needs verification by independent calculations and pertinent experiments.

For some time I have wondered when experimentalists would try to make accurate measurements of resonance integrals of other absorbers besides uranium and thorium. The paper by LeSage and Sher reports measurements of dilute resonance integrals for a number of absorbers of particular interest to reactors. These include cobalt, niobium, molybdenum, silver, indium, hafnium, tantalum and several other elements. In some cases, for example palladium and platinum, the previously known data were of very poor quality. In some cases the standard error of the determination has been improved as in the case of rhodium where a value

of 1075 ± 50 b is attained against previous values of 1200 ± 100 b. The value obtained for niobium of 18.5 ± 3 barns considerably exceeds the values and the claimed accuracy of earlier determinations. The method employed was detection of capture gamma rays with a Moxon-Rae counter. Counts were taken for a sample exposed to a beam geometry with and without a cadmium filter in the beam. Resonance integrals were calculated from the cadmium ratio or by using only the cadmium filter count and assuming linearity of the counter with respect to gamma ray energy. In general, the agreement is very good. The lower limit for the measurement of resonance integrals by this technique is near the value of 18.5 barns which they obtained for niobium. Resonance self-shielding factors seemed in some cases to be considerable, being 0.44 for indium foils and varying from 0.7 to 0.9 over the range of silver and hafnium foils.

Finally, the paper by Garrison discusses the Kapur-Peierls (KP) formalism for nuclear reactions. This parallel approach to R-matrix theory apparently first used by Adler and Adler, was felt to be particularly convenient in the study of strong interference effects between resonance levels. The study is limited to a two level approximation in order to reduce the complications.

One of Garrison's findings is that under intermediate interference conditions, the KP resonance parameter distributions are apparently not the same as those of R-matrix parameters but in fact turn out to be a function of the average width to spacing ratio. (The results, of course, for large ratios of width to spacing are admittedly invalidated by their limitation to the two level formulation). Since Porter and Thomas' original work, the explanation of missed levels has always been a problem. From Michaudon's work it appears that 20% of the total levels are

not observed in U-235. Garrison indicates that his work is sufficient to explain the missing levels although it appears that at Saclay they have also been able to explain the missing 20% of the levels without the issue of interference between levels, so it is not a unique explanation. The cross section shape predicted by the two level KP formulation is examined in detail for the case of a pure scatterer and for certain fissile cases under strong interference. It is noted that weak levels can have an important distorting effect on strong levels.

Further details on the actual shapes of the resonances from the two level formulation are given in the summary.

This is as much as I feel competent to comment upon these papers. For the rest, I'm going to ask the authors to answer questions here, from the platform, and I'd like to use the prerogative of Rapporteur to ask the first question.

I'd like to call first on Dr. Askew. Could he indicate what he feels needs to be done to resolve the discrepancies that they have found both with US calculations and the whole group of experiments that they have done in England.

J. Askew - Of course, one of the difficulties that we have had in convincing ourselves, let alone other people, that these discrepancies we have found in U-238 resonance are real and not just a result of errors in our calculations, has been the inability to show some plausible hypotheses as to what was the cause of these discrepancies.

It may be that there is just one clue which I think we may have now. The clue in which the natural uranium lattices tended to give us not dissimilar errors in reactivity estimation. We looked at this as well as reaction rate methods, and when we come

J. Askew (Cont'd.)

to repeat these calculations with better data for U-235 it does seem that our discrepancy is going to be greatest on the massive metal rod systems as compared to the oxide systems. Now, in fact, from buckling evidence, the natural uranium - graphite lattices do need something like a 15% change in epithermal capture as opposed to numbers like 6 to 10% for some of the oxide clusters which were referred to yesterday. This is the only lead we have on this at the moment. It does seem conceivable that if this is true that the discrepancy lies mainly in some part of the resonance calculation where the cross sections are not heavily shielded. The unshielded contribution which is constant makes a bigger contribution to the total resonance integral of say, 10 barns for the one inch metal rods, as opposed to 20 or 30 barns for some oxide lattices. Because the discrepancy seems particularly big in these massive metal rods and because we are absolutely convinced that we can see it, one of the things we are proposing to do is some conversion ratio measurements upon a system, at low energy, with large metal rods. If we can see in this case at least 15%, we really should be able to see a major difference, we should both be convinced of the fact and also we shall have some idea if the problem is in the unresolved region or conceivably due to the shape of resonances out on the wings or in between resonances where direct differential measurements are perhaps least accurate. There is one other possibility. Perhaps there is something uncertain in the cross section in between resonances.

Q - Have you estimated the effects of p-wave resonances?

J. Askew - Yes, we do have a contribution from p-wave resonances. It does seem consistent with the latest measurements.

J. Chernick - I should like to ask Dr. LeSage and Sher what can be done to improve the accuracy of present detection systems for the measurement of resonance integrals. Obviously, now that we are calculating them so well, one demands more and more of the experimentalists and we don't want 20 or 30% errors anymore. So, can you tell us what hope there is to reduce the minimum measurable resonance integral from say 18.5 barns to get even smaller values? What hope is there for improvements in accuracy?

L. LeSage - The thing that limited us really in our accuracy - we quoted 10 barns but maybe 18 is more realistic - is the constant background that we got - since we were taking the incident beam directly from the reactor even with considerable shielding.

It may be that we can cut the background by a factor of two, but there is not too much further one can go in this direction.

J. Chernick - I should like to ask Dr. Garrison to amplify the discussion of the meaning of the non-agreement of the statistics resulting from the R-matrix and KP formulation of resonance theory. Perhaps he could amplify on that when he comes to the microphone.

J. Garrison - Perhaps I should make a few introductory remarks. I started this study in order to understand what is happening in the interference between two levels. People have investigated the cross sections of U-233, U-235 and Pu-239, but this is a weak interference condition for the most part. I wanted to study interference in a more general way. It turns out that J. E. Lynn who is at Harwell is also making a study of this type which duplicates what I am doing in some ways.

J. Garrison (Cont'd.)

In looking for some sort of framework to hang this study on, one looks at the formalisms which are available to start making these calculations. There is the R-matrix theory, the Kapur-Peierls theory, and the Rosenfeld-Humblet formulation for the nuclear reactions. You can make calculations with all of these. The problem is what do you use for parameters for making these calculations. The basis on which I started was motivated by seeing the work that was done by Adler and Adler at Illinois. It seemed that having a relationship between - or being able to present - the same cross section in two different ways by using both the R-matrix theory and the Kapur-Peierls theory is a good way of seeing what was going on. There is a transformation which can take you from one formalism to the other. This allows you to look at the same cross section in terms of two different sets of parameters.

Now the work which was done by Wigner, Porter and Thomas and others gives information as to what to expect for the distribution of the resonance parameters of nuclei. This has been considered mostly for widely spaced resonances. However, if you try to explain the distributions in terms of R-matrix theory, there is no reason why these distributions should not be the same for narrow spacings when the widths of the resonances are of the order of the spacings. In assuming this you have some way of knowing what sort of values of the parameters you should put into the R-matrix theory when the resonances are close together. That is, if you say the distributions are the same when the resonances are close together as when they are far apart, you know how to pick the R-matrix parameters for interfering levels to study their interference. The transformation which takes you

J. Garrison (Cont'd.)

from the R-matrix theory to the Kapur-Peierls theory allows you to say what the Kapur-Peierls parameters are if you specify the R-matrix parameters. Since these are functional relationships between the R-matrix and Kapur-Peierls parameters, if you say you know the distributions of the R-matrix parameters are the same as for widely spaced resonances, then this automatically says what distribution you will have for the Kapur-Peierls parameters. It further says that there will be a correlation between these Kapur-Peierls parameters which is quite complicated.

In some ways the R-matrix theory is the preferred point of view since it gives a very explicit energy dependence in cross section; all the energy dependence is showing. However, when you get these resonances close together, even in the two level case, then you can look at the formulas of the cross sections and not be able to say in any way what the cross section is going to look like because it is so complicated. However, by coupling this with the Kapur-Peierls formulation you are able to say a little bit better what the shape of the cross section is going to be. Several things come out of this. One fact is that when we bring two levels together, in the intermediate region the shape is complicated, but for very strong interference where the separation is quite small compared to the width of the resonances, then both these resonances assume Breit-Wigner shapes and parameters again. The viewpoint that you should take is that the R-matrix parameters be considered the parameters which say what shape these resonances, their strength and so on, would have when the resonances are far apart. Then you proceed to bring the resonances together keeping the R-matrix parameters the same and see what happens to the shape. Of course, the Kapur-Peierls parameters will change when you bring the resonances together, but when you do this process you find that

J. Garrison (Cont'd.)

Kapur-Peierls indicates that the cross section will be two Breit-Wigner shapes when the resonances are very close together.

J. Chernick - Any questions or comments.

G. Bell (Los Alamos) - I would like to inquire whether in the study of the interference between two levels you have looked at how, on the average, alpha would be changed by the effect of interference, where by alpha for two levels I mean the ratio of the integral under the capture cross section to the integral under the fission cross section.

J. Garrison - Yes, I can say a little bit about that. In the Kapur-Peierls formulation the cross sections are represented by the sum of two resonance terms which look like Breit-Wigner shape terms, plus an interference term for each resonance. You can use this to get the areas under the resonances just as they are obtained for isolated single Breit-Wigner resonances. You can compare the area which you get under the cross section when they are interfering with the area which these resonances would have when they are far apart. When you do this, for all possible cases, when the fission is large compared to capture and capture large compared to scattering, under the assumption that interference is equally likely plus or minus, you find the capture cross section is enhanced relative to the fission cross section. I do not know what will happen when capture is large compared to fission.

G. Bell - Good, we find this in studies we have made too.

J. Garrison - The same thing happens for scattering. It is enhanced relative to fission.

M. S. Moore(Phillips) - I have my own ideas as to why this might be so, but I would like to hear your comments, as to why capture will be enhanced relative to fission.

J. Garrison - I don't have any simple answer. It comes out this way. It is a nonlinear effect. I do not know how to explain it.

Panel Discussion on Resonance Absorption

J. Chernick - Brookhaven National
(Chairman) Laboratory
L. Nordheim - General Atomic
J. J. Schmidt - Karlsruhe
E. Hellstrand - Sweden
P. F. Gast - Argonne National
Laboratory

J. Chernick - I shall ask each of the panel members to make a statement of about five minutes, and then we will entertain questions from the floor. First, I'll call on Dr. Lothar Nordheim.

L. Nordheim - In my personal involvement in the subject of resonance absorption, I soon became convinced that this topic needed mechanization and machine computations. There are just too many resonances, and simplifications such as rationalized collision probabilities, and un-Dopplered line shapes introduce considerable errors. After all, the slowing down equations can be easily integrated numerically for arbitrary cross sections obviating the necessity for special procedures such as the narrow (NR) or wide (IM) resonance approximations.

When I worked on this program some years ago, I tried to include all effects that seemed to be relevant, and good agreement with experiment was achieved as discussed here by Hellstrand. Nevertheless, even at that time I remained fully conscious about the limitations and shortcomings. The main limitations were the neglect of interferences between close resonances, the treatment of the moderator in the NR approximation and the calculation of

L. Nordheim(Cont'd.)

escape or collision probabilities on the basis of a flat flux in each region. Now the first two of these are easily remedied. It is easy to superpose different resonances. For the moderator flux, one can write down a separate integral equation and solve it simultaneously with the one for the absorber. Such a code exists and is presently in use (GAROL, GA-6632 by L. A. Stevens and N. K. Smith). It is much more difficult to get away from the flat flux approximation since this involves the full complexity of a space-energy problem. However, this effect is important only for rather thick absorbers. Adler has mentioned here that he has now developed a numerical method, and if it is needed one can always fall back on Monte Carlo calculations. So in general, the situation is quite satisfactory for thermal reactors.

Fast reactors, however, pose quite different problems. A large amount of effort and ingenuity has been spent on these problems during the last years. Looking at these efforts I have come to a perhaps startling and heretic conclusion:

"In practical reactor calculations for large reactors, do not waste your time on the Doppler coefficient for the unresolved resonances in the fissile isotopes."

The reasons are as follows:

1. Experimentally no clear cut effect of significant magnitude has been detected. In the recent Argonne experiments, the first one which showed an indication of a real effect, it was small and of the same order as thermal expansion effects. In real fast assemblies containing predominantly fissile isotopes only small upper limits have been obtained, while in assemblies more representative of practical designs with a ratio of fertile

L. Nordheim (Cont'd.)

to fissile nuclei of order ≥ 5 , the effect from the fertile isotopes alone is in reasonable agreement with experiment.

2. The sign of the Doppler coefficient is theoretically still in doubt. Of course fission and absorption will both increase with temperature, but the balance is precarious. This is well illustrated by some recent calculations (Kelber and Kier, Trans. ANS 8.2, 469(1965)) in which possible "ladders" are constructed from assumed statistical distribution of resonance parameters. Different ladders of which only one would correspond to reality provided the statistics which were used were correct, give somewhat different results. The important result is that the variance in the Doppler coefficient is larger than the effect itself. Thus, there is not much point in calculating it.

There are some additional remarks. From the discussions by Moore and Schmidt at this conference there is now mounting evidence of two different series of resonances in the fissile isotopes corresponding to the two different spin states. This is most pronounced for Pu-239. The resonances with $J=0$ have a large fission width and are thus wide and little affected by Doppler broadening, while the resonances with $J=1$ have a small fission width, give thus mostly absorption and are more sensitive to the Doppler effect. Thus it seems that with this more realistic distribution of parameters, the Doppler coefficient of reactivity will be smaller, or even negative, as compared to calculations based on the usual assumption of some average distribution.

The second remark pertains to the interference between resonances belonging to different sequences or isotopes. When

L. Nordheim (Cont'd.)

Codd and Collins brought this effect to general attention two years ago it was thought to be of considerable importance. Since then it has been shown by various authors (Froelich, Ott, Nicholson, Greebler) that it largely drops out if one uses proper flux weighted average cross sections such as:

$$\tilde{\Sigma}_x = \frac{\langle \frac{\Sigma_x}{\Sigma_t} \rangle}{\langle \frac{1}{\Sigma_t} \rangle} .$$

It seems now that applications of procedures based on this definition, and for regimes where the resonances can still be considered as discrete with s-waves alone will give adequate results for large fast reactors. The greatest source of error will be in the calculation of the fraction contained in the low energy part of the flux spectrum itself. I believe at the present stage the situation can hardly be improved by the rather doubtful treatment of higher energies and higher l-values. It remains, however, a challenge to improve our knowledge of the resonance structure of the fissile nuclei and its incorporation in a meaningful theory.

J. Chernick - I'd like next to call on Dr. Schmidt.

J. J. Schmidt - Thank you very much. I think that Dr. Nordheim has already said much of what I would like to say. I might underline with respect to Doppler coefficients that if there isn't any real positive Doppler coefficient in the plutonium resonances, this is probably due to s-wave resonances at lower energies and

J. J. Schmidt (Cont'd.)

not to p-wave resonances. For p-wave fission, I think the knowledge is still much less than for s-wave resonances.

I personally suspect the fission resonances in U-235 to raise many more questions than the fission resonances in plutonium-239. Especially important are the probable correlations between capture and fission half-widths.

I have a feeling that the large variance in the capture widths observed in the single level analysis of resonance experiments on U-235 is due to differences in interpretations. The number of capture channels used is 20 or 30 instead of the expected number of 100, or so.

I think it was Lynn who pointed out that the capture widths might be very much more narrowly distributed.

Another important topic is that of spin states. Any realistic estimate of the fission widths of different spin and parity states is still impossible.

It would be very useful to have more good spectroscopy in the range 0.5 and 2 mev beyond the ground state to get a better feeling for the location of bound states and their properties.

J. Chernick - Thank you very much Dr. Schmidt. I'd like next to call on Dr. Hellstrand.

E. Hellstrand - I said most of what I wanted to say last Monday, but I will make a few random comments. The first one concerns the discrepancy between calculations and measurements on resonance absorption which our English friends have discussed. I guess, at least for graphite lattices, one would obtain at least some improvement by using the intermediate resonance approach which Dr. Goldstein talked about today. But in the other

E. Hellstrand(Cont'd.)

direction, the average values which I gave last Monday for the resonance integral are somewhat larger than those used by our English colleagues. These effects are small, however, especially for uranium metal.

A second point concerns the thorium resonance integrals. I showed in my earlier talk a limited number of experimental results, and it was pointed out to me later that some recent work has been done on this subject at NRTS. I showed a curve of the adjoint flux which had been calculated for those experiments, but resonance integrals for ThO_2 and UO_2 have also been measured. There were mostly for S/M values larger than those I talked about earlier, but there is some overlap and in that region the agreement is good between the new values and the ones I showed on the slides. Concerning the discrepancy between the calculations and measurements of the thorium resonance integral, there is some uncertainty in the calculated values, especially between 3 kev and 12 kev.

The third point concerns the energy cutoff. A value of 0.65 ev has been recommended by the European-American Nuclear Data Committee, and Dr. Feiner quoted integral values consistent with 0.5 ev. I think it would be nice to fix on one number.

Finally, for the future, I don't see much point in repeating 1/E resonance absorption measurements. At low temperatures, at least, we should concentrate on measuring such things as conversion ratios, for example. As for the temperature dependence, I think recent results from KAPL are very interesting where they have shown the adequacy of a simple formula which has the resonance integral as linearly proportional to the square root of the

E. Hellstrand (Cont'd.)

temperature. They have made measurements to 1800°K and higher. Further work of this type as well as work on non-uniform temperature distributions would be worthwhile, I think.

J. Chernick - Thank you. Finally, I'd like to call on Dr. Gast.

P. Gast - In following Dr. Nordheim, I find most of the things I wanted to say have already been said. I agree with him that it is possible to do very accurate resonance integral calculations, limited mostly by the uncertainty in the nuclear data.

This is not the solution to some people's problems, however. In the business of trying to design reactors, it is usually not feasible to do detailed resonance calculations. For survey calculations, a good approximate method is needed for obtaining resonance integrals. In this area, we've also made significant progress, exemplified by the intermediate resonance method. Why it is not too good in some cases is not yet fully understood, but it might be due to any one of a number of things. But there are some situations where one might expect on theoretical grounds that such an approximation might occasionally go astray. Such a situation is one where there is a lot of scattering in the resonance. You recall from Dr. Goldstein's talk this morning that his method essentially assumes a trial function for the flux which has a flux depression symmetric with respect to energy in the resonance and is flat in space. In most cases, after one iteration the flux depression will shift a little downstream. But actually in scattering resonances one has a rather violent fluctuation in flux as shown in some of Adler's slides yesterday, and flux peaks can occur. There may be room for improvement in this area - perhaps by using a more complex trial function. Actually, it may

P. Gast (Cont'd.)

make little difference in the calculated integrals for a single isolated resonance, but in overlap situations, it could make a big difference.

I have only one other thing to say - a speculative suggestion. If the adjoint is normalized in a certain way, then it tends asymptotically to the value $(1-p)$ on the high energy side of the resonance. So one might toy with the idea of calculating resonance escape (or non-escape) by calculating the adjoint instead of the resonance integral. At first glance, this may not appear to be a good idea since the equations are not much simpler. But the source term for the adjoint is just the absorption cross section, and in a heterogeneous lattice this gives a flat source in the absorber region. So maybe the adjoint doesn't vary as violently as the collision density, and one might be able to carry out the calculation by assuming a delta function in energy as the source and then integrating these solutions over the entire resonance to infer a value for $(1-p)$.

However, I'm encouraged by Adler's calculation, described yesterday, which showed the collision density to be pretty smooth through some of these resonances and, hence, maybe one can still get away with a simple assumption for the adjoint trial function.

J. Chernick - Thank you very much. Are there any questions of any of our speakers?

H. Goldstein - I'd like to make a few comments on what Dr. Gast said. The I.R. program was developed to primarily calculate resonance integrals, whether you use a variational method or a successive approximation method.

H. Goldstein (Cont'd.)

If you are interested in the flux shape, it pays to use a second or third order function of the flux depending on the accuracy you want. The second iterate does reflect the characteristics of the scattering resonance that you referred to. If one wants to make use of this second order flux in a variational principle as a trial function, there is no formal difficulty in doing this. Of course the variational results can get quite complicated and that is, perhaps, why people are using the iterative approach.

To return to the asymptotic value of unity rather than $(1-p)$ in the I.R. formalism, I don't think that this is important with respect to resonance integral calculations because it's weighted by the absorption cross section. If you're interested in the flux shape, however, this could probably be improved upon.

M. Dyos (GA) - You can extend the I.R. method to a third iteration which can be obtained in closed form. The Placzek oscillation below the resonance energy is shown very markedly in this third iterate, for a predominantly scattering resonance. The conditions for this Placzek oscillation to exist can be established from the second iteration, i.e. by how much a resonance has to be predominantly scattering.

J. Garrison (GA) - I'd like to comment on Dr. Schmidt's remarks. I've already said that the fluctuations in the radiation widths might arise from the way in which the data is analyzed. In the two-resonance calculations that I've done, I've always held the R-matrix radiation width constant. If the resonances are moved together, the Kapur-Peierls radiation widths change. So if you analyze the resonances in any other way than using R-matrix theory in which Γ_γ is constant, then you'd find fluctuations. Further, a lot of these resonances look like one instead

J. Garrison (Cont'd.)

of two or more when they are interfering and this could lead to difficulties in determining the correct radiation widths.

G. Tyror (UKAEA) - I'd like to say a few words to clarify our position on the comparison of calculated and measured reactivities about which I reported earlier. While we do use the Goldstein-Cohen method for our design studies, all of our observations on the discrepancies between calculation and experiment have been based on what I would call exact methods. I feel that the discrepancies are real and not due to some inaccuracy or misapplication of the methods on our part.

Secondly, with respect to a well defined lower cutoff for resonance integrals, we are in agreement. But, I think an upper energy limit should also be considered since one is never quite sure where the $1/E$ spectrum runs out.