Variational Determination of the Neutron Integral Transport Equation Eigenvalues Using Space Asymptotic Trial Functions

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An approximate determination of the critical eigenvalue of the neutron transport equation in integral form, within both the one speed and energy multigroup models, for a homogeneous medium, is achieved by means of a variational technique. The space asymptotic solutions for both the direct and adjoint problems are used as trial functions. A variational procedure is also developed and numerically exploited within the Fourier transformed domain, where noticeable theoretical features can be demonstrated. It is evidenced that excellent results can be obtained with little computational effort, and a set of critical calculations in plane geometry is presented and discussed. © 1988 Academic Press, Inc.

1. INTRODUCTION AND SCOPE OF THE WORK

The determination of the eigenvalue of the stationary neutron transport equation is one of the main problems of nuclear reactor physics. Actually at least four different eigenvalue formulations have been devised in the past, each of them retaining some special physical characteristics and possibility of interpretation [1].

Although in practical applications it looks like the k_{eff} -eigenvalue has deserved a little more attention, we shall here always refer to the so called γ -eigenvalue [2], since, besides any physical considerations, often it can be handled in a more comprehensive way for both theoretical and numerical studies. The γ -eigenvalue is also easily introduced in the frame of transport multienergy-group isotropic scattering system of integral equations over the vacuum bounded volume V, which we shall consider here, as

$$\Phi_{g}(\mathbf{r}) = \frac{1}{\gamma} \int_{V} \left[\sum_{g'=1}^{G} \chi_{g} v \Sigma_{fg'} \phi_{g'}(\mathbf{r}') + \sum_{g'=1}^{G} \Sigma_{g' \to g} \Phi_{g'}(\mathbf{r}') \right] \frac{e^{-\Sigma_{g}|\mathbf{r}-\mathbf{r}'|}}{4\pi |\mathbf{r}-\mathbf{r}'|^{2}} d\mathbf{r}'$$
$$= \frac{1}{\gamma} \int_{V} \sum_{g'=1}^{G} \sigma_{g' \to g} \phi_{g'}(\mathbf{r}') \frac{e^{-\Sigma_{g}|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|^{2}} d\mathbf{r}', \qquad g = 1, ..., G$$
(1)

or, more concisely, in operator form:

$$\Phi_{g} = \frac{1}{\gamma} \sum_{g'=1}^{G} \hat{H}_{g'g} \Phi_{g'}.$$
 (2)

When $\gamma = 1$ the physical system is said to be "critical."

0021-9991/88 \$3.00 Copyright © 1988 by Academic Press, Inc. All rights of reproduction in any form reserved. The nomenclature is standard in reactor physics, as may be found in [3, 4], for instance. We shall propose the extension of the variational approach commonly employed for calculations of the one speed equation γ -eigenvalues [5] to multienergy-group cases, thus constituting the background for the extension of the related computational techniques.

As trial functions we propose the use of the direct and adjoint space asymptotic neutron distributions, which are easily computed and retain a large physical significance in the transport model. We shall thus present direct asymptotic theory [6] and work out explicitly the adjoint one.

Some calculations will then be presented and discussed. Finally a formal procedure to symmetrize the operator, hence giving a more definite and reliable basis to the whole variational frame, will be outlined and employed for a few calculations, trying to put into evidence its main implications.

Our interest is mainly restricted here to the physical comprehension of transport phenomena, rather than to pure mathematical considerations. We actually look forward to theoretical investigations oriented to get an insight to extend the methodology to future effective applications, such as finite differences and elements, boundary elements, and synthesis methods, which can overcome the shortcoming of asymptotic theory, that is, the possibility of describing only materially homogeneous systems.

2. VARIATIONAL METHODS APPLIED TO THE DETERMINATION OF NEUTRON TRANSPORT EIGENVALUES

Variational methods represent quite a versatile tool for the formulation and investigation of a great deal of physical problems [7]. Many approximate techniques may be derived in a very neat and elegant fashion.

The field of transport theory has stimulated the deduction of quite a few variational principles for the solution of typical problems [3, 4, 8, 9, 10], the reformulation of known approximations [11], or the formulation of new ones [12]. However, the application of variational techniques for the calculation of the eigenvalues of the linear integral transport equation in its most general energy dependent form presents a few theoretical problems, specially connected to the fact that the transport operator is not self-adjoint. That implies, in particular, among other difficulties, that functionals do not take on minimum or maximum values, but rather show stationary saddle points [11, 13]. That is, partially, one of the reasons why variational principles have been especially employed in one speed transport, where the integral operator is self-adjoint (symmetric) [5]. Some applications to multi-group energy dependent problems have been presented in [13], although with regards to diffusion theory.

We are here involved in the determination of the γ -eigenvalue of the transport equation in the multienergy-group physical model. We shall therefore make use of

the extension of a classical Galerkin principle for the variational estimate of eigenvalues [9], namely

$$\gamma = \frac{\int_{\mathcal{V}} d\mathbf{r} \left(\sum_{g=1}^{G} \Phi_{g}^{+} \sum_{g'=1}^{G} \hat{H}_{g'g} \Phi_{g'} \right)}{\int_{\mathcal{V}} d\mathbf{r} \sum_{g=1}^{G} \Phi_{g}^{+}(\mathbf{r}) \Phi_{g}(\mathbf{r})} = \frac{(\Phi^{+}, \hat{\mathscr{H}}\Phi)}{(\Phi^{+}, \Phi)},$$
(3)

where Φ_g^+ denotes the adjoint flux, and we have introduced the classical definition, at least for the transport field, for the bilinear form expressing the "scalar product" of direct and adjoint space functions.

Owing to the already recalled non-symmetricity of the operator, it is not possible to draw definite conclusions on the bounds and generally specify the sign [14] of the error of the operation. It is foreseen that the choice of quite accurate trial functions Φ_g and Φ_g^+ is mandatory in order to obtain satisfactorily good results, since no consideration tells us which is the "optimum" trial function.

Actually asymptotic theory yields by far the "best" space-energy trial functions (both in the direct and adjoint spaces) we can hope for. Such a theory preserves, but for the physical boundaries of the system, all the peculiar transport features and its calculation is simple and fast. Asymptotic space functions have already been suggested as excellent trial functions within variational principles, at least for optically large enough systems, but always for one speed calculations only [9, 15]. As a matter of fact, the theoretical foundation for the transport eigenvalue problem might be settled if the equation could be, somehow, changed into a self-adjoint one (Ritz method). That is not obviously an easy task; it could, however, be satisfactorily overcome following one of the procedures suggested by Tonti [16], either "transform(ing) the given problem into another one with same solutions," or "chang(ing) the bilinear form," or, finally, "chang(ing) the function."

We shall try here to follow the first suggestion, as previously done by Magri [17] for linear problems, as the one at hand. That involves the inversion of the transport operators, which, of course, is an unsolvable problem. A tremendous simplification may be formally achieved in the Fourier transformed space, where typically space asymptotic theory operates. This procedure can give us a further insight and evidence also some peculiar and interesting features of eigenvalue critical equations. They shall be presented and highlighted in the last section of the paper.

3. DIRECT AND ADJOINT SPACE ASYMPTOTIC THEORY

Space asymptotic theory applied to diffusion and transport problems dates back to the heroic and fertile old times of nuclear reactor theory [3] and derives its justification from the need of preserving a correct description of the neutron migration phenomena and somewhat simplifying the mathematical framework. From time to time, it has proved to be a quite efficient and powerful tool, when used to derive numerical solutions to the transport problem [18] and to be always physically well established [19] to allow a deep insight into the problem itself. Besides, one must not forget one of the most important theoretical consequences of the model, i.e., the "First Fundamental Theorem of Reactor Physics," stating the space-energy separability of the total neutron flux [3], which has also a great deal of practical applications in the neutronic calculations of multiplying systems.

The limitations of the theory rely on the assumed space form for the angularly integrated solution, which, with a diffusion-like feature, obeys the classical Helmholtz equation with zero boundary conditions. That restricts its validity to optically large homogeneous material systems [20], where boundary effects, which are poorly described by the above assumptions, are of relative little importance.

From this background, the idea of its application as a trial function within a suitable variational procedure stems naturally. Therefore it is now necessary to give at least the well-known fundamentals of direct asymptotic transport and to present, formally and substantially, its adjoint version.

We suppose to know, either from previous theoretical analyses or experiments, the space-energy transfer kernel $P(\mathbf{r}' \to \mathbf{r}, g' \to g, \Omega)$, that gives the probability density that a fission neutron isotropically emitted at \mathbf{r}' within group g' will be finally injected, as a result of a last scattering, about \mathbf{r} and Ω within group g. Setting the average of the transfer kernel on the fission spectrum as

$$\mathscr{P}_{g}(\mathbf{r}' \to \mathbf{r}, \mathbf{\Omega}) = \sum_{g'=1}^{G} \chi_{g'} P(\mathbf{r}' \to \mathbf{r}, g' \to g, \mathbf{\Omega})$$
(4)

we can write a stationary direct transport balance integro-differential equation in the following quite unconventional form:

$$\Omega \cdot \nabla \Phi_{g}(\mathbf{r}, \Omega) + \Sigma_{g} \Phi_{g}(\mathbf{r}, \Omega)$$

$$= \frac{1}{\gamma_{a}} \left\{ \int_{V} d\mathbf{r}' \sum_{g'=1}^{G} \mathscr{P}_{g}(\mathbf{r}' \to \mathbf{r}, \Omega) v \Sigma_{fg'} \int_{\Omega'} \Phi_{g'}(\mathbf{r}', \Omega') d\Omega' + \frac{\chi_{g}}{4\pi} \sum_{g'=1}^{G} v \Sigma_{fg'} \int_{\Omega'} \Phi_{g'}(\mathbf{r}, \Omega') d\Omega' \right\},$$
(5)

where with γ_a we denote the eigenvalue coherent with asymptotic theory. It is widely known that the adjoint function, at least for the classical integro-differential equation, may be interpreted as the "importance function" [21, 22]. Within the scheme that we have used to obtain (5) above, we can also write the balance for importance $\Phi_e^+(\mathbf{r}, \Omega)$:

$$-\mathbf{\Omega} \cdot \nabla \Phi_{g}^{+}(\mathbf{r}, \mathbf{\Omega}) + \Sigma_{g} \Phi_{g}^{+}(\mathbf{r}, \mathbf{\Omega})$$

$$= \frac{1}{\gamma_{a}} \left\{ \int_{V} d\mathbf{r}' \sum_{g'=1}^{G} v \Sigma_{fg} \int_{\mathbf{\Omega}'} d\mathbf{\Omega}' \phi_{g'}^{+}(\mathbf{r}', \mathbf{\Omega}') \mathcal{P}_{g'}(\mathbf{r}' \to \mathbf{r}, \mathbf{\Omega}') + \frac{v \Sigma_{fg}}{4\pi} \sum_{g'=1}^{G} \chi_{g'} \int_{\mathbf{\Omega}'} \phi_{g'}^{+}(\mathbf{r}, \mathbf{\Omega}') d\mathbf{\Omega}' \right\}.$$
(6)

It is worth recalling the fact that (6) can be deduced formally from (5) with a simple mathematical adjoining operation, with no physical consideration whatsoever.

Both Eqs. (5) and (6) can now be treated in the frame of asymptotic theory, which, in short, implies:

(a) The extension of the space domain into infinity, thus formally simplifying the space dependence of the kernel, on the distance $|\mathbf{r} - \mathbf{r}'|$ alone, explicitly $\mathscr{P}_{\infty g}(|\mathbf{r} - \mathbf{r}'|, \mathbf{\Omega} \cdot ((\mathbf{r} - \mathbf{r}')/|\mathbf{r} - \mathbf{r}'|))$, and letting V cover the whole three-dimensional space \mathbf{R}^3 .

(b) The application of the Fourier transform from \mathbf{r} into \mathbf{k} to take care of the space dependence (and especially of the convolution integrals).

(c) The derivation of a solvability (criticality for $\gamma_a = 1$) condition for the homogeneous equation, which is exactly the same (as obvious) for (5) and (6), namely

$$\gamma_{a} = \sum_{g=1}^{G} \nu \Sigma_{fg} \int_{\Omega} \frac{(2\pi)^{3/2} \mathscr{P}_{\infty \mathscr{F}g}(|\mathbf{k}|, -\Omega \cdot \mathbf{k}/k) + \chi_{g}/4\pi}{\Sigma_{g} + i\mathbf{\Omega} \cdot \mathbf{k}} d\Omega.$$
(7)

Such a condition may be derived, as usual, when a non-everywhere vanishing solution for either Φ or Φ^+ is looked for. Equation (7) verified at all points of the sphere identified by $|\mathbf{k}| = B_M$.

(d) The use of all above results to state the separability theorem for the total flux and importance as

$$\Phi_{g}(\mathbf{r}) = \psi_{g}(B_{M}) F(\mathbf{r}; B_{M})$$

$$\Phi_{g}^{+}(\mathbf{r}) = \psi_{g}^{+}(B_{M}) F(\mathbf{r}; B_{M}).$$
(8)

It is well worth noticing the complete independence of spectra ψ_g and ψ_g^+ on the value of asymptotic eigenvalue γ_a ; only the buckling B_M actually affects such spectra.

The theory sets the space form of the solution (identical for direct and adjoint problems) from its Fourier transform as

$$F(\mathbf{r}; B_M) = \int_{\omega} d\boldsymbol{\omega} \ e^{-iB_M\boldsymbol{\omega} \cdot \mathbf{r}} \ U(B_M\boldsymbol{\omega})$$
(9)

leaving the "geometry function" U undefined. Once a choice is made, any specific geometry may be described. In the present work we have restricted our attention to isotropic scattering only. In this case, each group component of the direct spectrum will turn out to be a solution of the coupled algebraic system

$$\psi_{g} = \left[\sum_{g'=1}^{G} \Sigma_{g' \to g} \psi_{g'} + \frac{\chi_{g}}{(2\pi)^{3/2}}\right] \Gamma_{g}, \qquad g = 1, ..., G,$$
(10)

where by definition Γ_g is the Fourier transform of the transport kernel

$$\Gamma_g \equiv \Gamma_g(B_M) = \frac{1}{B_M} \tan^{-1} \frac{B_M}{\Sigma_g}.$$
 (11)

On the other side, the adjoint spectrum can be worked out as

$$\psi_{g}^{+} = v \Sigma_{fg} \Gamma_{g} \frac{4\pi}{1 - \sum_{g'=1}^{G} \chi_{g'} v \Sigma_{fg'} \Gamma_{g'}}.$$
 (12)

It turns out, in a straightforward way, that both ψ_g and ψ_g^+ are only dependent on the value of the buckling and are totally independent on the eigenvalue γ_a . That might not be true for other formulations of the eigenvalue itself. B_M identifies also the volume within \mathbf{R}^3 where the space asymptotic solution is physically meaningful, i.e., where $F(\mathbf{r}; B_M)$, from (9), does not change its sign.

Formulae (8) are exactly the ones that we shall be using in the following within our variational principle to determine direct and adjoint trial functions. This choice is obviously physically founded, since it preserves much of the transport features of the problem, so a good performance of the principle may be foreseen already at the present stage, at least for optically large systems.

4. RESULTS USING SPACE ASYMPTOTIC TRIAL FUNCTIONS

Now trial fuctions (8) can be inserted into the Galerkin variational principle, as stated by (3), to obtain explicit values for γ .

We shall first present some results for plane geometry (Table I) for the one speed case (G = 1), for which "exact" reference values are currently available. The table reports also some results obtained when the variational principle is used not in connection with the exact transport Eq. (1), but rather with its various order discrete

| Slab | Exact Reference | | | Variational | | |
|----------|--------------------|-----------|----------|-------------|----------|---------------|
| m. f. p. | [4] | Transport | S-2 | <i>S</i> -4 | S-8 | <i>S</i> -512 |
| 11.3310 | 0.980392 | 0.978569 | 0.977507 | 0.978541 | 0.978569 | 0.978569 |
| 6.6004 | 0.952381 | 0.946381 | 0.941212 | 0.946181 | 0.946378 | 0.946382 |
| 4.2268 | 0.909091 | 0.896138 | 0.880398 | 0.895127 | 0.896097 | 0.896132 |
| 2.5786 | 0.833333 | 0.809631 | 0.769302 | 0.804589 | 0.809389 | 0.809695 |
| 2.0000 | 0.783024 | 0.753733 | 0.696151 | 0.743909 | 0.753097 | 0.753730 |
| 1.4732 | 0.714286 | 0.679297 | 0.599830 | 0.660589 | 0.677447 | 0.679296 |
| 1.0240 | 0.625000 | 0.585696 | 0.483442 | 0.552972 | 0.580481 | 0.58569 |

TABLE I

Eigenvalues for the Monokinetic Integral Transport Equation in Plane Geometry

ordinate approximations. As it is well known [23], such approximations may be cast into integral form by simply substituting the exact kernel—in plane geometry $\frac{1}{2}E_1(\Sigma_i|x-x'|)$ —with an approximate one, obtained by a suitable superposition of exponentials—in plane geometry $\frac{1}{2}\sum_{\beta=1}^{n} (w_{\beta}/\mu_{\beta}) e^{-\Sigma_i|x-x'|/\mu_{\beta}}$. Sets $\{w_{\beta}\}$ and $\{\mu_{\beta}\}$ are constituted by weights and abscissae, respectively, of a numerical integration formula. If chosen according to Gauss-Legendre rule, classical discrete ordinate S_N , P_{N-1} model is to be found. We recall the reader's attention upon the fact that S_2 coincides with diffusion theory. For the approximate kernel cases, all space integrals in (3) can be analytically computed, since $F(\mathbf{r}; B_M) \equiv \cos(B_M x)$. If, on the other side, the exact transport kernel is used, the integrals may be computed to any wanted degree of accuracy through conventional integration routines [24].

As it can be seen in Table I, the accuracy of the variational techniques gets poorer and poorer as geometrical dimensions decrease. That is of no surprise, as asymptotic trial functions approach exact eigenfunctions only for optically large systems. It turns out that for optically small systems better results may be achieved using different trial functions, such as low order polynomials, for instance, using classical procedures such as the ones proposed in [2-4].

Tables II and III are devoted to three energy group calculations. Table II, besides

| -> | 1 | 2 | 3 |
|-------------------|----------|-----------------|---------------|
| | • | Common data | |
| Σ_{ρ} – | 0.23987 | 0.63517 | 1.2382 |
| 1g | 0.20109 | 0.03519 | 0.0 |
| 20 | 0.0 | 0.55464 | 0.050833 |
| 30 | 0.0 | 0.0 | 1.1109 |
| χ _g | 1.0 | 0.0 | 0.0 |
| | Case (a) | (critical thick | (ness 150 cm) |
| Σ_{tr} | 3.7266-3 | 1.4924-2 | 0.16784 |
| ,, ,, | 0.62134 | 0.27073 | 0.10793 |
| r [†] g | 0.08878 | 0.13459 | 0.77661 |
| | Case (b) | (critical thicl | (ness 100 cm) |
| | 3.8137-3 | 1.5273-2 | 0.17177 |
| 1, | 0.62225 | 0.27017 | 0.10758 |
| ,† g | 0.08855 | 0.13458 | 0.77686 |
| | Case (c) | (critical thic | kness 50 cm) |
| Σ_{fg} | 4.2881-3 | 1.7173-3 | 0.19313 |
| , , | 0.62710 | 0.26717 | 0.10573 |
| U [†] | 0.08730 | 0.13456 | 0.77814 |

TABLE II

Material Data and Normalized Asymptotic Critical Spectra for Three Group Calculations

Note. All data in c.g.s. unit system.

TABLE III

| Slab | | D. (| | | Variational | | |
|------|------|----------|-----------|----------|-------------|-------------|----------|
| (cm) | Case | values | Transport | S-2 | S-4 | <i>S</i> -8 | S-512 |
| 150 | a | 0.999966 | 0.999965 | 0.999975 | 0.999966 | 0.999965 | 0.999965 |
| 175 | a | 0.999743 | 0.999723 | 0.999728 | 0.999723 | 0.999723 | 0.999723 |
| 125 | а | 1.000329 | 1.000363 | 1.000380 | 1.000364 | 1.000363 | 1.000363 |
| 100 | b | 0.999840 | 0.999884 | 0.999918 | 0.999885 | 0.999884 | 0.999884 |
| 125 | b | 0.997953 | 0.999162 | 0.999180 | 0.999164 | 0.999163 | 0.999163 |
| 75 | b | 1.008412 | 1.001398 | 1.001486 | 1.001404 | 1.001401 | 1.001401 |
| 50 | с | 0.998741 | 0.999112 | 0.999941 | 0.999121 | 0.999113 | 0.999112 |
| 60 | с | 0.996888 | 0.996869 | 0.997052 | 0.996887 | 0.996882 | 0.996882 |
| 40 | с | 1.001881 | 1.003023 | 1.003651 | 1.003066 | 1.003048 | 1.003047 |

Three Energy Group Eigenvalues

Note. Case (a) 150 cm, case (b) 100 cm, case (c) 50 cm are asymptotic critical structures.

material data, reports also the asymptotic direct and adjoint critical spectra as calculated by formulae (10) and (12). When calculations for non-asymptotically critical reactors are performed, the spectra obtained using bucklings corresponding to actual geometries are of course used. Reference values concerning multigroup calculations have been obtained through a numerical iterative procedure, relying on the integral transport equation, initialised by space asymptotic results. Such eigenvalues can be trusted up to six significant figures.

The tables put into clear evidence both the good performance of asymptotic theory and the convergence trend of S_N calculations.

Finally, Tables IV and V report some results derived within the two group scheme.

5. Symmetrization Procedures and Results

A general problem defined by non-symmetric invertible operator \hat{L} with eigenvalue λ

$$\hat{L}u = \lambda u \tag{13}$$

can be converted into a symmetric one, through the same definition of the bilinear functional "scalar product," by formal application of a suitable operator \hat{S} as [16]

$$\hat{S}\hat{L}u = \lambda\hat{S}u.\tag{14}$$

The determination of \hat{S} may become quite cumbersome for some problems—transport is one of them, and it is analytically impossible, at least if operating within the physical phase space. However, since we will apply all the

| TABLE | E IV |
|-------|------|

| | | • |
|----------------------|--------------------|-------------------|
| $g \rightarrow$ | 1 | 2 |
| | Common da | ata |
| Σ, | 0.27502 | 1.27329 |
| $\Sigma_{1\sigma}$ | 0.24799 | 0.014141 |
| Σ_{2g} | 0.0 | 1.11757 |
| χ _g | 1.0 | 0.0 |
| | Case (a) (critical | thickness 150 cm) |
| $v\Sigma_{f\sigma}$ | 7.6376–3 | 0.21949 |
| Ψ. | 0.91681 | 0.08319 |
| ψ_{g}^{\dagger} | 0.13853 | 0.86147 |
| | Case (b) (critical | thickness 100 cm) |
| $v\Sigma_{fg}$ | 7.8261-3 | 0.22491 |
| Ψ | 0.91688 | 0.08312 |
| Ψ_{R}^{\dagger} | 0.13826 | 0.86174 |
| | Case (c) (critical | thickness 50 cm) |
| $v\Sigma_{fg}$ | 8.8361-3 | 0.25394 |
| ψ, | 0.91725 | 0.08275 |
| ψ_{a}^{\dagger} | 0.13682 | 0.86318 |
| 1.6 | | |

| Material Data | and | Normalized | Asymptotic | Critical S | Spectra for | Two | Group | Calculations |
|---------------|-----|------------|------------|------------|-------------|------|-------|--------------|
| Material Data | anu | Normanzeu | Asymptotic | Cincipal o | spectra for | 1 40 | Oloup | Calculations |

Note. All data in c.g.s. unit system.

| TABLE | v |
|-------|---|
| | |

| I wo Energy Group Eigenvalues | Two | Energy | Group | Eigenvalues | |
|-------------------------------|-----|--------|-------|-------------|--|
|-------------------------------|-----|--------|-------|-------------|--|

| Slab | | D (| | | Variational | | |
|----------------|------|---------------------|------------|-------------|-------------|----------|---------------|
| thickness (cm) | Case | Reference values | Transport | <i>S</i> -2 | S-4 | S-8 | <i>S</i> -512 |
| 150 | a | 0.999947 | 0.999955 | 0.999967 | 0.999955 | 0.999955 | 0.999955 |
| 175 | а | 0.999645 | 0.999636 | 0.999644 | 0.999636 | 0.999636 | 0.999636 |
| 125 | a | 1.000439 | 1.000478 | 1.000499 | 1.000479 | 1.000478 | 1.000478 |
| 100 | b | 0.999773 | 0.999849 | 0.999893 | 0.999851 | 0.999849 | 0.999849 |
| 125 | b | 0.998896 | 0.998903 | 0.998925 | 0.998904 | 0.998904 | 0.998903 |
| 75 | b | 1.001579 | 1.001835 | 1.001945 | 1.001841 | 1.001838 | 1.001837 |
| 50 | с | 0.998262 | 0.998845 - | 0.999228 | 0.998857 | 0.998846 | 0.998845 |
| 60 | С | 0.995762 | 0.995952 | 0.996174 | 0.995959 | 0.995959 | 0.995959 |
| 40 | c | 1.002517 | 1.003891 | 1.004674 | 1.003928 | 1.003906 | 1.003904 |

Note. Case (a) 150 cm, case (b) 100 cm, case (c) 50 cm are asymptotic critical structures.

information obtainable from space asymptotic theory, it seems appropriate trying to operate in the three-dimensional Fourier transformed space. Therefore, after introducing as $\tilde{\Phi}_g(\mathbf{k})$ the *F*-transforms of $\Phi_g(\mathbf{r})$ into \mathbf{k} , and observing the convolution nature of the integral appearing in (1), we can write

$$\widetilde{\boldsymbol{\Phi}}_{g}(\mathbf{k}) = \frac{1}{\gamma} \left(\sum_{g'=1}^{g} \sigma_{g' \to g} \widetilde{\boldsymbol{\Phi}}_{g'}(\mathbf{k}) \right) \boldsymbol{\Gamma}_{g}(|\mathbf{k}|), \qquad g = 1, ..., G.$$
(15)

Problem (15) can be written in the self evident compact matrix form, with a structure at all similar to (13)

$$\tilde{\mathbf{\Phi}} = \frac{1}{\gamma} \, \tilde{\mathcal{H}} \, \tilde{\mathbf{\Phi}},\tag{16}$$

where it must be noted that $\tilde{\mathcal{H}}$ is an algebraic matrix operator, parametrically dependent on $|\mathbf{k}|$. Without going on into the symmetrization procedure, already at the present stage, we might derive a variationally founded explicit eigenvalue formula, as it follows. Equation (16) can be formally written in the antitransformed space

$$\mathbf{\Phi} = \frac{1}{\gamma} \mathscr{F}^{-1} \{ \widetilde{\mathscr{H}} \widetilde{\mathbf{\Phi}} \}$$
(17)

and principle (3) applied:

$$\gamma = \frac{(\mathbf{\Phi}^+, \mathscr{F}^{-1}\{\widetilde{\mathscr{H}}\widetilde{\mathbf{\Phi}}\})}{(\mathbf{\Phi}^+, \mathbf{\Phi})}.$$
 (18)

If an asymptotic direct trial function vector $\mathbf{\Phi}$ is employed, since each of its components obeys the Helmholtz equation and thus has a Dirac's delta function behaviour with singularity for $|\mathbf{k}| = B_M$ in the Fourier transformed space, we can write (18) as

$$\gamma = \frac{(\mathbf{\Phi}^+, \tilde{\mathscr{H}}(B_M) \,\mathscr{F}^{-1}\{\tilde{\mathbf{\Phi}}\})}{(\mathbf{\Phi}^+, \mathbf{\Phi})} = \frac{(\mathbf{\Phi}^+, \tilde{\mathscr{H}}(B_M) \,\mathbf{\Phi})}{(\mathbf{\Phi}^+, \mathbf{\Phi})} \tag{19}$$

which constitutes a formula suitable for the estimation of γ . Coherently with space asymptotic theory, all space integrals in (19) will be carried out over the whole geometry space \mathbb{R}^3 . The space part will, however, cancel off.

Now the symmetrization procedure can be worked out in all details, to obtain the algebraic symmetrization operator, which does not present any difficulties and, for consciseness' sake, shall here be omitted. It can be shown that such operator coincides simply with $\tilde{\mathcal{H}}^+$. Therefore

$$\widetilde{\mathscr{H}}^{+}\widetilde{\mathbf{\Phi}} = \frac{1}{\gamma} \widetilde{\mathscr{H}}^{+} \widetilde{\mathscr{H}} \widetilde{\mathbf{\Phi}}$$
(20)

has the same solution as (16) and $\tilde{\mathscr{H}}^+\tilde{\mathscr{H}}$ is symmetric.

TABLE VI

| thickness (cm) | Case | Reference values | Asymptotic values | Formula (19) | Formula (21) |
|-------------------|------|---------------------|----------------------|-----------------|-----------------|
| 150 | a | 0.999947 | 0.999999 | 0.999999 | 0.999999 |
| 175 | а | 0.999645 | 0.994754 | 0.999480 | 0.999664 |
| 125 | а | 1.000439 | 1.008694 | 1.000862 | 1.000555 |
| 100 | b | 0.999773 | 0.999999 | 0.999999 | 0.999999 |
| 125 | b | 0.998896 | 0.984400 | 0.998419 | 0.998980 |
| 75 | b | 1.001579 | 1.033620 | 1.003403 | 1.002188 |
| 50 | с | 0.998262 | 0.999999 | 0.999999 | 0.999999 |
| 60 | с | 0.995762 | 0.953605 | 0.994770 | 0.996630 |
| 40 | с | 1.002517 | 1.084802 | 1.009522 | 1.006086 |

Two Group Eigenvalues with Symmetrization Procedures

An extended Ritz variational principle may be written, using the same formal trick which led us to (19), based on the properties of the transform of asymptotic Φ , namely

$$\gamma = \frac{(\mathbf{\Phi}, \tilde{\mathscr{H}}^+(B_M) \tilde{\mathscr{H}}(B_M) \mathbf{\Phi})}{(\mathbf{\Phi}, \tilde{\mathscr{H}}^+(B_M) \mathbf{\Phi})}.$$
(21)

The same cancellation of space integrals will occur here as in (19). Formulae (19) and (21) are peculiar criticality relationships, whose performance is shown in Table VI. It must be noted that they give coincident results with asymptotic theory only when $\gamma_a = \gamma = 1$.

Theoretically, formula (21) constitutes a by far better achievement in multigroup theory than any other variational estimate presented in the paper, since it is founded on a self-adjoint symmetric problem and, thus, can effectively be associated to a minimization of the functional employed, with all the formal and practical consequences that such a matter implies.

6. CONCLUSIONS

Some formulae suitable for estimating the neutron transport eigenvalue have been deduced, their physical meaning and significance discussed, and some selected results presented. These formulae have been derived using classical variational formulations, currently employed in transport theory, extended to the multienergygroup model.

In order to give a sound theoretical foundation to the whole variational framework, a symmetrization technique has been exploited in the Fourier transfor-

med domain. As trial functions within the variational functional the results of standard space asymptotic energy dependent theory have been employed.

Numerical results are excellent. Therefore it seems promising to extend the study and investigate the possibility of utilizing similar variational procedures in the attempt of generating efficient numerical techniques in order to solve problems with a material and geometrical complexity larger than the one here considered, such as the ones effectively encountered in practical nuclear reactor applications.

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