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Thirty years of point group theory applied to reactor physics

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Summary. — A brief survey of applications of point groups to reactor physics is given. First, the general principles of applications of point groups are summarized, this is followed by a short historical review. Two instances of applications in reactor physics are mentioned: the analytical solution to the few group diffusion theory is given based on symmetry considerations. The analytical solution has made it possible to investigate Selengut's principle and conclude that in general, in the solution process in region \mathcal{D} it is not possible to replace a heterogeneous domain $\mathcal{D}_h \subset \mathcal{D}$ by a homogeneous material so that the solution to the few group diffusion equation outside the replaced part, *i.e.* in $\mathcal{D} - \mathcal{D}_h$ would remain unchanged.

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1. – Introduction

Symmetry considerations have been present in reactor theory since the beginning as one of the first pioneers of neutron physics was E. P. Wigner. In the theory of reactor lattices the concept of Wigner-Seitz cell was borrowed from solid state physics. As early as 1948, in the discussion of the boundary condition of reactors, Weinberg and Schweinler [1] made use of the image pile concept. Symmetry considerations were suggested by Mark Goldsmidth [2] as early as in 1963. Case and Zweifel [3] discussed the symmetry of the transport equation. Nieva and Christensen [4] used symmetries in the design of control rods. Binnebeck [5] urged symmetry considerations based on analogy with quantum mechanical calculations.

In the last years of 1970s, the application of symmetries to reactor physics has gained a new impetus. Finite elements: Albert Fässler of ETH (Zürich) worked out a finite element method in which the structure of the solution was simpler because of the careful selection of the basis functions. In 1979, the present author proposed [6] a more elaborate use of group theory tools in homogenization and in the nodal methods. The first nodal program using group theory was written in 1980 at Eidg. Institute für Reaktorforschung, Würenlingen [7]. That time the solution of the diffusion equation was attacked by two methods. Those believing in mathematical methods clung to variants of the finite difference method (FD) and hoped for finding an effective acceleration method. The other camp searched for new solution methods, differing from FD in using higher-order approximation thus allowing for a coarser discretization of the spatial domain. Two competitive methods have appeared: the finite element method [8] and the nodal method. The former has been used in engineering practice successfully, the latter was a novelty and rather promising tool. We mention here two groups, Allan Henry's group at MIT [9] and Wagner's at KWU [10]. The former used trial functions composed of an exponential plus a quadratic term but those were solutions of a one-dimensional equation hence an iteration is needed along the three spatial directions. An analytical solution was badly needed to work out an effective coarse mesh procedure. KWU worked with polynomials.

Roy Axford proposed an independent approach that used a discretization scheme conforming to the symmetry of the spatial region [11]. He used Lie groups in his works.

In sect. 2, we summarize the applied principles of group theoretical considerations. In sect. 3, we formulate the reactor physical problems to be investigated and use the principles of sect. 3 to derive an analytical solution to the few group diffusion equation. In sect. 4, the analytical solution is applied to the investigation of the Selengut principle [12]. Finally, concluding remarks are given.

2. – Main principles of applied group theory

In physical problems, we encounter known quantities (like spatial distribution of known materials, given sources or boundary conditions) and from them we determine other quantities (like the neutron flux in a region). The mathematical term map is used to describe the relationship between the known and unknown things. An area where those maps are typical is the iteration. When we seek an iterative solution to a problem, we map the old solution to a new one(¹). When we solve a source problem, an equation connects the known source to the unknown solution. Formally, the solution process has the following ingredients: given normed vector spaces \mathbb{E}, \mathbb{F} , a linear operator $\mathbf{A} : \mathbb{E} \to \mathbb{F}$. When we have a group G whose action is defined on \mathbb{E} and \mathbb{F} , the procedure can be refined. G not only generates a splitting \mathbb{E}_i of \mathbb{E} , and \mathbb{F}_i of \mathbb{F} such that \mathbb{E}_i and \mathbb{E}_j as well as \mathbb{F}_i and \mathbb{F}_j are orthogonal when $i \neq j$ but also $g \in G$ transforms elements in \mathbb{E}_i and \mathbb{F}_i in the same way. Furthermore, when the map $\mathbf{A} : \mathbb{E} \to \mathbb{F}$ commutes with elements of G, *i.e.* $\mathbf{A}g = g\mathbf{A}$ holds for any $g \in G$, $\mathbf{A}\mathbb{E}_i$ belongs to the subspace \mathbb{F}_i that transforms under $g \in G$ as \mathbb{E}_i does. In that sense map \mathbf{A} preserves the splitting of space \mathbb{E} .

In connection with the above expressed idea, one needs a recipe to find a group G, to determine the splitting of a given space. In reactor physics, the two most frequently encountered equations are the diffusion and the linear Boltzmann equation. Those equations are known [3] to be invariant with respect to rotations and reflections, the basic constituents of the geometric symmetries of a regular, homogeneous domain. Hence, G can be the symmetry group of the spatial region under consideration provided the material distribution in V is symmetric and the scattering cross-section depends solely on the angle between the entering and exiting directions. Discretization is an often used technique in numerical solutions, and there we encounter two kinds of volumes: the volume of the reactor V and the volume of a discretized part V_i (often called node) in-

 $^(^{1})$ And when the iteration is convergent the difference between "new" and "old" diminishes as the iteration proceeds.

terrelated as $V = \bigcup_i V_i$. It is clear that analyzing the iteration $\mathbf{A} : \Psi_k(r) \to \Psi_{k+1}(r)$, where k is the subscript of the iteration, we refer to a map $\mathbf{A} : \Psi(V) \to \Psi(V)$ bringing a function over the entire V into a new function over the entire V. When we regard the entering current-exiting current relation in a given map, we have to consider the $\Psi(V_i) \to \Psi(V_i)$ map.

The technique of splitting a set is available in textbooks [13,14], the main points are summarized below. If someone is more allured by the net, a consultation with the web site GAP [15] is recommended. There complete information is available.

Theorem 2.1 (Splitting [13], [14] of space \mathbb{E}). Let \mathbb{E} consist of the square integrable functions $\Psi(r), r \in V$. A splitting of $\Psi(r)$ is given by

(1)
$$\Psi_i(r) = \frac{\ell_i}{|G|} \sum_{g \in G} \chi_i(g)^* \Psi(\mathbf{R}_g^{-1}r), \Psi_i(r) \in \mathbb{E}_i.$$

Here ℓ_i is the dimension of subspace i, |G| is the number of elements in group G, and \mathbf{R}_g is the transformation (a matrix) of r under symmetry g. Matrices $\mathbf{R}_g, g \in G$ form a matrix representation of G. $\chi_i(g)^*$ is the transpose of the character table of G. $\Psi_i(r)$ and $\Psi_i(r)$ are orthogonal when $i \neq j$.

A character table is a concise description of a group. Group elements are ordered into equivalence classes, they form the columns of the character table. Each row is associated with an irreducible subspace (irrep). For details, see [13, 14]. The character tables also can be found in textbooks and at the GAP web site. The next theorem claims that an operator \mathbf{A} commuting with G is a multiple of the identity operator. The theorem is formulated for matrices [13].

Theorem 2.2 (Schur Lemma). Let matrices $\mathbf{D}_g, g \in G$ be an irreducible matrix representation of the group G. If there is a matrix \mathbf{C} commuting with every matrix of the representation, i.e. $\mathbf{CD}_g = \mathbf{D}_g \mathbf{C}$ for any $g \in G$, then \mathbf{C} is a constant times the identity matrix.

Example 2.3 (Irreps of flux on the boundary). Let V be a square, and along its four faces the entering current be $I_i^-(r, E)$, i = 1, 4; or writing the entering current along the boundary as a single vector \underline{I}^- . Using (1), we decompose the entering currents into irreps and obtain

(2)
$$\underline{I}^{-} = c_{A1}^{-}(r, E)(1, 1, 1, 1) + c_{B1}^{-}(r, E)(1, -1, 1, -1) + c_{E1}^{-}(r, E)(0, -1, 0, 1) + c_{E2}^{-}(r, E)(-1, 0, 1, 0),$$

where the subscripts refer to the given subspace. When the entering currents are face averaged, the entering currents are $\underline{I}^- = (I_1^-, I_2^-, I_3^-, I_4^-)$ and using (1), the decomposition is

(3)
$$\underline{I}^{-} = c_{A1}^{-}(1, 1, 1, 1) + c_{B1}^{-}(1, -1, 1, -1) + c_{E1}^{-}(0, -1, 0, 1) + c_{E2}^{-}(-1, 0, 1, 0).$$

Note that the difference between the two decompositions is only in the coefficients, the pattern is the same. Note that the entering currents are, in either case, in a four dimensional space and the number of linearly independent components is four. The structure



Fig. 1. – Irreducible components on the boundary of a square.

obtained by decomposition (1) is independent of the physical model and is also called irrep, shown in fig. 1, where inward arrows and outward arrows refer to positive and negative numbers, respectively.

3. – Selected reactor physics problems

Most applications in reactor physics include two problems. In an iteration we solve an eigenvalue problem but in each node, we face a source problem because the entering currents are the exiting currents of the neighboring nodes. Also, volumetric source from other groups may be known. We assume that in a node the homogeneous problem has only the trivial solution as a node must be subcritical.

3.1. Source problem. – Let us consider a given, homogeneous volume V, with a known source Q(r), which may be the contribution from other energy groups. We have to solve

(4)
$$\mathbf{A}\Psi(r) = Q(r); \quad r \in V,$$

for $\Psi(r)$. We decompose the source into irreps using (1):

(5)
$$Q(r) = \sum_{i} Q_i(r) \quad \Psi(r) = \sum_{i} \Psi_i(r),$$

and instead of solving one big problem, we solve a couple of smaller problems:

(6)
$$\mathbf{A}\Psi_i(r) = Q_i(r).$$

Here i is the subscript of the irreducible components.

When the boundary condition is non-homogeneous [16], and the homogeneous problem has only the identically zero function as solution, we seek the solution of

(7)
$$\mathbf{A}\Psi(r) = 0, r \in V, \quad \mathbf{B}\Psi(r) = q(r), r \in \partial V.$$

The procedure is similar, we decompose q(r) into irreps and because \mathbf{A}, \mathbf{B} are linear operators, we split the original problem into smaller ones:

(8)
$$\mathbf{A}\Psi_i(r) = 0, r \in V, \quad \mathbf{B}\Psi_i(r) = q_i(r), r \in \partial V.$$



Fig. 2. – Irreducible components on the boundary of a regular hexagon.

Here subscript *i* labels the irreps of *q*. In reactor physics, ∂V consists of faces and it suffices to approximate q(r) along a face by a low-order polynomial. Polynomial approximation corresponds to a polynomial approximation along each face [17, 18].

3.2. Eigenvalue problem. – Now we consider the following eigenvalue problem in V:

(9)
$$\mathbf{A}\Psi(r) = \lambda\Psi(r),$$

and use the decomposition (1) of Ψ . Because of the orthogonality of the components, we get for each component i

(10)
$$\mathbf{A}\Psi_i(r) = \lambda \Psi_i(r).$$

When the eigenspace associated with λ is one dimensional, only one irrep is present in Ψ .

3.3. Analytical solution to the diffusion equation. – In diffusion theory, the energydependent neutron flux is a vector $\underline{\Phi}(r)$, its components are the group fluxes $\Phi_k(r)$, $k = 1, \ldots, NG$, where NG is the number of energy groups. The operator

(11)
$$\mathbf{A} = \mathbf{D}\Delta + \boldsymbol{\Sigma}$$

is used to describe the neutron balance in the energy groups. Here **D** is a diagonal matrix, its entry is the diffusion coefficient in the given energy group. Σ includes all processes resulting in energy change. We assume V to be homogeneous thus neither **D** nor Σ depend on the position. The general problem may involve volume source Q and boundary source q:

(12)
$$\mathbf{A}\Psi(r) = Q(r), \ r \in V$$

(13)
$$\Psi(r) = q(r), \ r \in \partial V.$$

We decompose Q and q into irreps, and solve the diffusion equation for each irrep separately. The irreps bear physical meanings. Regard for example the irreps of q for a square, shown in fig. 1. The first component (A1) models a symmetric surrounding, the second (E1) and third (E2) model the x and y component of a gradient field, and the fourth component (B1) is a representation of a cross-flow (second gradient). In a regular hexagon node, the cross-flow is even more complicated, see fig. 2. For a given irrep, the analytical solution is expressed by the eigenfunctions of the Laplace operator

(14)
$$\Delta f_k(r) = -\lambda_k^2 f_k(r), k = 1, \dots, NG,$$

and the eigenvectors of the Σ matrix:

(15)
$$\Sigma \underline{t}_k = \lambda_k^2 \underline{t}_k, k = 1, \dots, NG.$$

The general solution is [19]

(16)
$$\underline{\Phi}(r) = \sum_{k=1}^{NG} \underline{t}_k f_k(r) c_k \equiv \mathbf{T} \langle f(r) \rangle \mathbf{c},$$

where $\langle \rangle$ is a diagonal matrix, columns of matrix **T** are the vectors \underline{t}_k . The general form of the scalar eigenfunction of the Laplacian is

(17)
$$f_k(r) = \int_{|e|=1} w(e) \exp\left[i\lambda_k er\right] \mathrm{d}e.$$

In order to create a function transforming as a given irrep, we choose the weight function w(e) appropriately. Let the parameter of unit vector e be its direction θ . In a regular n-gon, we form a step function $w_k = w(\theta), (k-1)\pi/n \leq \theta \leq k\pi/n, k = 1, \ldots, 2n$. This can be done because a transformation \mathbf{R}_g of r in (17) amounts to a transformation of \mathbf{R}_g^{-1} applied to vector e. It suffices to give the index of the interval and the constant value of the weight on the interval. The weights are given in table I. Remember, in the symmetry group of the square there are five irreducible subspaces, four of them, viz, A1, A2, B1, B2 are one dimensional. In a two-dimensional subspace there are two basis vector pairs E1, E2 and E3, E4 that are equivalent from the point of view of symmetries. Here we give, in one energy group, some operators often used in diffusion theory:

(18)
$$\overline{\Phi} = \int_{V} \Phi(r) \mathrm{d}r - \text{integrated flux},$$

(19)
$$I^{-}(r) = \frac{1}{4} \left(\Phi(r) + 2D\partial_{n}\Phi(r) \right) + \text{entering current},$$

(20)
$$I^{+}(r) = \frac{1}{4} \left(\Phi(r) - 2D\partial_{n}\Phi(r) \right) - \text{exiting current},$$

(21)
$$J_{\rm net}(r) = I^+(r) - I^-(r) - {\rm net \ current}.$$

From the above-defined quantities, response matrix ${f R}$ is formed, *e.g.*,

$$J(r) = \mathbf{R}I(r),$$

and analogous expressions hold for the above expression integrated along a face or the entire boundary of V. When J(r) and $I^{\pm}(r)$ transform according to a given irreducible component, the response matrix **R** connecting them is diagonal (*i.e.* a number), see Schur's lemma. It means that if the boundary condition transforms according to a given irrep, any response matrix mentioned above is diagonal. Simply, any physical

Irrep 1 2 3 4 5 6 7	8
	1
$\alpha = 1, A_1$ I I I I I I I I I	
$\alpha = 2, A_2$ 1 -1 1 -1 1 -1 1	-1
$\alpha = 3, B_1$ 1 1 -1 -1 1 1 -	1 -1
$\alpha = 4, B_2$ 1 -1 -1 1 1 -1 -	1 1
$\boxed{\alpha = 5, E_1} \qquad 0 \qquad 0 \qquad -1 \qquad -1 \qquad 0 \qquad 0 \qquad 1$	1
$\alpha = 5, E_2$ -1 1 0 0 1 -1 0	0
$\alpha = 5, E_3 \qquad 0 \qquad 0 \qquad -1 \qquad 1 \qquad 0 \qquad 0 \qquad 1$	-1
$\boxed{\alpha = 5, E_4} -1 -1 0 0 1 1 0$	0

TABLE I. – Weight functions in a square for the irreducible subspaces.

quantity represented by an operator that commutes with the symmetries of V inherits the symmetry of the boundary condition.

Example 3.1 (Eight boundary currents). It is possible to average the entering currents over a half faces of the square, thus we have eight entering currents given on the boundary of the square. Then,

(22)
$$\underline{I}^{-} = (I_{1}^{-}, \dots, I_{8}^{-}).$$

The irreps are obtained again from (1), and they turn out to be the eight-tuples in the rows of table I, that we write as \underline{w}_i , here i refers to the row i in table I. Thus the decomposition of the entering current is

(23)
$$\underline{I}^{-} = \sum_{i=1}^{8} c_i^{-} \underline{w}_i.$$

As to the exiting current, the analogous expression is

(24)
$$\underline{I}^+ = \sum_{i=1}^8 c_i^+ \underline{w}_i.$$

The definition of the \mathbf{R} response matrix is

(25)
$$\underline{I}^+ = \mathbf{R}\underline{I}^-.$$

We know from the Schur lemma that the response matrix is diagonal when we use irreps thus $\mathcal{L}_{\mathcal{L}}$

(26)
$$c_i^+ = R_i c_i^-, i = 1, \dots, 4;$$

and because lines 5 and 6, 7 and 8 of table I are components of two, equivalent, two-dimensional irreps, $% \left(\frac{1}{2} \right) = 0$

(27)
$$\begin{pmatrix} c_i^+ \\ c_{i+1}^+ \end{pmatrix} = \begin{pmatrix} R_5 & R_6 \\ R_7 & R_8 \end{pmatrix} \begin{pmatrix} c_i^- \\ c_{i+1}^- \end{pmatrix}$$

		Moments	
Representation	m = 0	m = 1	m = 2
A_1	$(I_1^0 + I_2^0 + I_3^0 + I_4^0)/4$	0	$(I_1^2 + I_2^2 + I_3^2 + I_4^2)/4$
A_2	0	$(I_1^1 + I_2^1 + I_3^1 + I_4^1)/4$	0
B_1	$(I_1^0 - I_2^0 + I_3^0 - I_4^0)/4$	0	$(I_1^2 - I_2^2 + I_3^2 - I_4^2)/4$
B_2	0	$(I_1^1 - I_2^1 + I_3^1 + I_4^1)/4$	0
E_1	$(I_1^0 - I_3^0)/2$	$(I_1^1 - I_3^1)/2$	$(I_1^2 - I_3^2)/2$
E_2	$(I_2^0 - I_4^0)/2$	$(I_2^1 - I_4^1)/2$	$(I_2^2 - I_4^2)/2$

TABLE II. – Irreps of moments of partial currents.

for i = 5, 7. We have less matrix elements to be parametrized in a production code and the calculation is faster when irreps are used.

Let the moments of the entering currents with respect to Legendre polynomial of degree m along face k of the square be $I_k^m, m = 0, 1, 2$. Then $I_k^m, m > 0$ are overtones [18], as their face averages give zero. The irreducible components of the entering currents are shown in table II. We have 12 entering currents per energy group (four faces and three moments of entering current per face) that allows for the following approximation in (17):

(28)
$$w(e) = \sum_{j=1}^{8} w_j \delta(e - e_j) + \sum_{j=9}^{12} w_j \delta(e - e_j),$$

where e_j vectors make an orbit⁽²⁾ of a general position e vector under the symmetries of the square, and $e_j, j > 8$ form an orbit of length four (this is the case when e is on a symmetry line). Then using table II one can determine the w_i weights solving four sets of equations for the 12 weights. To carry out the calculations, we need the relationship between moments of entering currents and weights. The former are calculated from $f_k(r)$, which is connected to the weights as

(29)
$$f_k(r) = \int_{|e|=1} w(e) \exp[i\lambda_k er] de = \sum_{j=1}^8 w_j \exp[i\lambda_k e_i r] + \sum_{j=9}^{12} w_j \exp[i\lambda_k e_j r].$$

Consequently, any spatial moment is a linear expression in the weights w_j and the 12 moments at the boundary can be satisfied with a suitable choice of weights, to this end a system of linear equations has to be solved.

We remark only here that it is possible to include higher moments, and work out an algorithm that uses a solution that satisfies the diffusion equation at each point and also the boundary condition to a prescribed accuracy.

(²) Images $g \cdot e, g \in G$ are called orbit.

4. – Selengut principle

Selengut [12] formulated the following principle: if the response matrix of a given V can be substituted by the response matrix of a homogeneous material in V, there exist an equivalent homogeneous material with which one may replace V. This principle simplifies the calculation considerably and therefore has been widely used in reactor physics. Below we investigate [20, 17] and the Selengut principle more closely.

The analysis is based on the analytical solution derived in the previous section. The problem is considered in the few group approach, the boundary flux \underline{F} is a vector, as well as the volume-averaged flux $\underline{\Phi}$. Using that solution, we are able to derive matrices mapping into each other the volume-integrated fluxes, the surface-integrated partial and net currents. First we present the corresponding matrices. Our basis is the boundary flux, that we derive for each irrep *i* from (16) as

(30)
$$\underline{F}_i = \mathbf{T} \langle f_i \rangle \underline{c}_i$$

The normal component of the net current \underline{J}_{net} is given in irrep i as

(31)
$$\underline{J}_{\text{net},i} = -\mathbf{DT}\langle g_i \rangle \underline{c}_i.$$

We eliminate \underline{c}_i to get

(32)
$$\underline{J}_{\text{net},i} = -\mathbf{D}\mathbf{T}\langle g_i/f_i\rangle\mathbf{T}^{-1}\underline{F}_i \equiv \mathbf{R}_i\underline{F}_i.$$

Here

(33)
$$g_i = -\nabla \mathbf{n} f_i(r).$$

The volume-integrated flux $\underline{\Phi}$ is obtained after integration from (16) as

(34)
$$\underline{\bar{\Phi}} = \mathbf{T} \langle \overline{F}_{A1} \rangle c_{A1}, \overline{\bar{F}}_{A1} = \int f(r) \mathrm{d}r,$$

and the integration runs over a face. Note that only irrep A1 contributes to the average flux. After eliminating c_{A1} from (30), we get a response matrix to determine volume-integrated flux $\overline{\Phi}$ from face-integrated flux F_{A1} :

(35)
$$\underline{\bar{\Phi}} = \mathbf{T} \langle \overline{F}_{A1} / f_{A1} \rangle \mathbf{T}^{-1} \langle \overline{F} \rangle \equiv \mathbf{W} \langle \overline{F} \rangle.$$

This assures that V is completely described by matrix **W** and diagonal matrices $\langle F(r) \rangle, \langle f(r) \rangle, \langle g(r) \rangle$ for each irrep. For example, we are able to reconstruct the crosssection matrix Σ from them. Note that $\mathbf{WT} = \mathbf{T} \langle F/f \rangle$, the eigenvectors of matrix **W** are the eigenvectors of Σ . Now we need solely a numerical procedure to find the eigenvalues λ_k from $\langle F/f \rangle$.

The question is, under what conditions the above-mentioned calculations are feasible. We count the number of response matrices in the general case: the matrix elements we need to characterize V may be all different and the number of matrices depends on the shape of V. The number of irreducible components of the involved matrices depends on the geometry. In a square-shaped homogeneous V, we have four \mathbf{R}_i matrices and

one **W**. Altogether we have to determine 5NG * NG elements. In an inhomogeneous hexagonal volume, there are 6 * NG * NG matrix elements, whereas the homogeneous material is described by NG * (NG + 1) parameters as in a homogeneous material there are altogether NG * NG cross-sections and NG diffusion constants. Therefore Selengut's principle is not exact it may only be a good approximation under specific circumstances. The homogenization recipes [21] preserve only specific reaction rates but they do not provide general equivalence.

5. – Concluding remarks

The present work is a summary of applications of group theory in reactor physics. Since then, point groups have been used in the following areas of physics:

- Field reconstruction (error estimation, pinpoint false measurement, etc.). The field to be reconstructed can be classified by the symmetries of the core and there is a class that can be reconstructed without loss of information [22].
- Investigation of iteration process. In the usual iteration we approximate the volume source by a polynomial, the partial current at the boundary by another polynomials and the two approximations may turn out to be inconsistent [16].
- Algebraic description of a composite volume [23]. If one assigns a graph to a large discretized volume, it is possible to decide if two discretizations are isomorphic and the solution can be transplanted from one to the other.
- Transfer of measurements to other simply connected volumes. If the measured value belongs to a one-dimensional eigenspace of a linear operator, it is possible to derive the results of measurement on another simply connected region [24].

Further applications of point group theory include:

- Determination of Green's function for some finite 2D regions using Sunada's theorem [25].
- Non-symmetric operators. When material properties are space dependent, the operator itself has to be decomposed into irreps. This results in a product representation [26].
- Non-symmetric regions (domain reduction). Faster algorithm is obtained when the solution domain is reduced. Reduction is achievable even in an apparently completely asymmetric domain [26].
- Find equispectral volumes [23]; stability investigation of nonlinear equations [27].

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