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# Symmetries and the Coarse-Mesh Method

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If one has taken leave of the innate circumstances, motherland, parents and relations and has gone to a foreign country (e.g., to study there at a university), to associate there only with irrational friends, thus waisting ones whole time, then this is nonsensical. Therefore, one must always adhere to one's own task and follow the aim for which one has come, i.e., to learn and study and to concentrate only on this!

*Wenn man einmal die durch das (angeborene) Schicksal gegebenen Umstände, Heimat, Eltern und Verwandte, verlassen hat und in ein fremdes Land gegangen ist (um dort zum Beispiel an einer Universität zu studieren), jedoch in diesem fremden Lande nur mit unvernünftigen Freunden (in schlechter Gesellschaft) verkehrt und dadurch die ganze Zeit verschwendet, so ist dies verrückt. Deswegen muß man immer an der eigenen Aufgabe und an dem Ziel, für das man gekommen ist, festhalten, das heißt lernen, studieren und sich nur darauf konzentrieren!*

Summary

This report approaches the basic problem of the coarse-mesh method from a new side. Group theory is used for the determination of the space dependency of the flux. The result is a method called ANANAS after the analytic-analytic solution. This method was tested on two benchmark problems: one given by Melice and the IAEA benchmark. The ANANAS program is an experimental one. The method was intended for use in hexagonal geometry.

## 1. Introduction

The Diffusion Equation has a key role in reactor physics. One effective solution is the so called coarse-mesh (CM) method [1]. The so called analytic methods [2-5] have proved to be very effective in this field. These analytic methods use either the analytic solution of a onedimensional diffusion equation or create some particular solution of the 2D problem in an ad-hoc way. These ad-hoc considerations are not immediately applicable in hexagonal geometry. Another shortcoming of the analytic methods is that usually cross leakages are determined from the neighbouring nodes using some "natural" approximation.

This work describes a procedure which is applicable in both 2D and 3D both in rectangular and in other geometries. The cross leakage is determined without using neighbouring meshes and the order of the cross leakage is analytic. The analysis is based on group theory [6-9]. The basic idea is presented here for a 1D, rather trivial, problem.

Find the solution of the one-group diffusion equation over the $V = [-a; +a]$ interval

$$\hat{D}\,\phi(x) \equiv \left[-\frac{d^2}{dx^2} + \alpha^2\right]\phi(x) = 0 \qquad (1)$$

if $x \in V$

with the boundary condition

$$\phi(+a) = f_\ell \text{ and } \phi(-a) = f_r \qquad (2)$$

It is easy to see that eq. (1) is invariant under the $\hat{\delta} \equiv \{x \to -x\}$ transformation. Therefore if we have one solution to eq. (1) $u_1(x)$ the $u_2(x) \equiv u_1(-x)$ is also a solution.

Furthermore the $\hat{\mathcal{J}}$ operation has the following properties

$$\begin{aligned} \hat{\mathcal{J}}\, u_1 &= u_2 \\ \hat{\mathcal{J}}\, u_2 &= u_1 \end{aligned} \tag{3}$$

which suggest to represent $\hat{\mathcal{J}}$ as a 2x2 matrix. Let us denote $\mathcal{J}$ the matrix of the $\hat{\mathcal{J}}$ transformation then

$$\mathcal{J} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and it acts on column vectors of type

$$\begin{bmatrix} u_1(x) \\ u_2(x) \end{bmatrix}$$

$\mathcal{J}$ is brought into a diagonal form by the following similarity transformation:

$$S^{-1}\,\mathcal{J}S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{ where } S = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

and S changes the basis vectors as

$$S \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} u_1 - u_2 \\ u_1 + u_2 \end{bmatrix}$$

The elements of this vector are eigenfunctions of $\mathcal{J}$. The boundary condition can alsc be put into symmetric form:

$$\Phi(+a) = \frac{f_\ell + f_r}{2} + \frac{f_\ell - f_r}{2}; \quad \Phi(-a) = \frac{f_\ell + f_r}{2} - \frac{f_\ell - f_r}{2}$$

where both terms are transformed into (±1) times itself by $\mathcal{J}$. Making use of the linearity of eq. (1) and remembering that $u_1(x) = c\cdot\exp(\alpha x)$ is a solution to eq. (1) the general solution is

$$[c_1,\ c_2] \begin{bmatrix} u_1 - u_2 \\ u_1 + u_2 \end{bmatrix} = \begin{bmatrix} c_o \operatorname{sh}\alpha x \\ c_e \operatorname{ch}\alpha x \end{bmatrix} \tag{4}$$

and $c_o$ and $c_e$ are determined from the symmetric and antisymmetric boundary condition respectively:

$$c_e = \frac{f_\ell + f_r}{2} \qquad c_o = \frac{f_\ell - f_r}{2}$$

The summary of this procedure follows. The diffusion equation (1) is invariant under some coordinate transformations*. We found such a transformation which brings into diagonal form this operation - the S matrix. The solution can be decomposed into functions which are eigenfunction of the symmetry operations i.e. shax and chax. The boundary condition is also decomposed this way. The even function must satisfy the "even" boundary condition and the odd function must satisfy the "odd" boundary condition, this fixes the constants. The generalization of this procedure for 2D and 3D requires group theoretical considerations.

The second part is devoted to the group theory background**. The theorems will not be proved here since they have been proved for the Schrödinger equation which, from the viewpoint of the group theory, is not essentially different from the diffusion equation. As example the symmetry of the DE over a hexagonal region is given in 2D.

In part 3 the results of the previous part are applied to the formal solution of the DE.

In part 4, the ANANAS algorithm is presented which is the application of the previous results in a 2D rectangular geometry program.

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* The x→x transformation always is such a transformation but it has not been mentioned before as this is trivial.

** See Ref. 15

## 2. The symmetries of the Diffusion Equation

The diffusion equation is

$$\hat{D}\phi \equiv -D_g \nabla^2 \phi_g + \Sigma_g \phi_g = \sum_{g'=1}^{N} \left[ \frac{\nu\Sigma_{fg'}\chi_g}{k_{eff}} + (1-\delta_{gg'})\Sigma_{g'\to g} \right] \phi_{g'} + Q_g \quad \text{(DE)}$$

written in the usual form where

- $D_g$ is the diffusion coefficient in group g
- $\Sigma_g$ is the removal cross-section in group g
- $\chi_g$ is the fission yield in group g
- $\nu\Sigma_{fg}$ is the number of secondary neutrons from fission
- $\Sigma_{g'\to g}$ is the scattering cross-section from group g' to group g
- $k_{eff}$ is the effective multiplication factor
- $Q_g$ is the outer source
- N the number of the groups.
- $\delta_{gg'}$ Kronecker delta

The region V over which the (DE) is to be solved is arbitrary. Along the border ∂V a boundary condition is given. This boundary condition is assumed to be a linear $\hat{T}$ operator acting on the flux:

$$\hat{T}_g(\underline{x}_b) = F(\underline{x}_b); \quad \underline{x}_b \in \partial V \tag{5}$$

and $F(\underline{x}_b)$ is a given function. The $\hat{T}$ operator for diffusion theory prescribes the incoming current on the boundary:

$$\hat{T}\phi_g(\underline{x}_b) = \frac{1}{4}\left[\phi_g(\underline{x}_b) + 2D_g \frac{\partial\phi_g}{\partial n}(\underline{x}_b)\right] \tag{6}$$

where $\partial/\partial n$ denotes the normal derivative. $F_i$ is the surface of the i-th face. The volume V is bordered by $n_F$ faces.

There are some coordinate systems in which the (DE) has the same form. Our objective is to make use of the relations of these coordinate systems.

1. Definition

A symmetry transformation with respect to the DE is a linear coordinate transformation such that the form of the DE is the same in the old and the new coordinate systems and the transformation leaves the region V unchanged.

Examples:

We recall that any orthogonal transformation leaves the Laplacian unchanged thus the V region determines the symmetries. The V region usually has a regular shape (sphere, cylinder, cube, hexagonal pile, circle, square, rectangle, hexagon or a symmetric interval) and the following transformations are often symmetries:

| | | |
|---|---|---|
| Rotation | $\underline{x}' = R\,\underline{x}$ | $\det R = 1$ |
| Inversion | $\underline{x}' = -\underline{x}$ | |
| Reflection | $\underline{x}' = R\,\underline{x}$ | $\det R = -1$. |

2. Definition

The transformation operator $\hat{P}_R$ associated with the symmetry transformation R is definied by the following operator equation which must be an identity in $\underline{x}$

$$\hat{P}_R\, f(\underline{x}) \equiv f(R^{-1}x) \tag{7}$$

The effect of the coordinate transformation has been fixed but we need the next two theorems for the application of the group theory. The theorems are not proved here because their proof is

just verbatim repetition of the proofs available in several textbooks.

1. Theorem

If the product of two transformations is definied to mean their consequtive application then the $\{\hat{P}_R\}$ set of transformation is isomorphic with the matrix set $\{R\}$ describing these transformations. (Proof omitted).

2. Theorem

If $\{R\}$ is the set of the symmetry transformations of the DE then $\hat{P}_R$ commutes with $\hat{D}$ for all R and the set $\{\hat{P}_R\}$ is a group G called the group of the DE. (Proof omitted).

According to theorem 1 the symmetry transformations are associated with matrices. Theorem 2 assures that these matrices commute with the DE. Symmetry operations are divided into classes. Generally a physically significant characteristic can be ascribed to each class. E.g. in the group of symmetry transformations of the hexagon the rotations and reflections belong to separate classes.

3. Definition

A T set of symmetry operations form a class if for every $x \in G$

$$xTx^{-1} = T.$$

1. Assumption

It is assumed that one particular solution of the DE is given. Denote this solution $e_1(\underline{x})$. Such a particular solution can be given if the eigenvalues of the cross-section matrix of the DE

are known. If $\lambda_j$ is one of the eigenvalues then

$$e_1^{(j)}(x) = e^{\underline{k}x\lambda j} \qquad |\underline{k}| = 1; \quad j = 1,\ldots,N$$

is an elementary solution

Appling the symmetry transformations on this elementary solution a function space is spanned. The symmetry transformations may have a new interpretation which is more convenient for analysing the symmetry property of a function. This new interpretation assignes a matrix to a fiven transformation. Hereafter we may look for eigenfunctions which are invariant under some symmetry transformation.

3. Theorem

If $e_1^{(j)}(x)$ is an arbitrary function in some space then the set of $\{\hat{P}e_1^{(j)}(x)\}$ formed from all $\hat{P}\in G$ defines a subspace S invariant under the G group of symmetry transformations. (Proof omitted).

By virtue of the linearity of the DE each vector of this invariant subspace is the solution of the DE. Let us choose the $\{\hat{P}e_1^{(j)}(x)\}$ functions as basis in this invariant subspace. For $\hat{P}$ doesn't change the scalar product it comes from (7) that this basis consists of

$$e_i^{(j)}(x) = e^{\underline{k}_i\underline{x}\ j\lambda} \tag{8}$$

functions where $\underline{k}_i = P_i\underline{k}$. (9)

The number of $e^{(j)}$ functions is equal to the number of elements (h) in the G group of the DE. They are, in general, not necessarily linearly independent. Once this subspace is invariant under the group G the transformed function can be expressed by the coordinates:

$$(\hat{P}\underline{f}) = P \cdot \underline{f} \qquad \underline{f} \in S \tag{10}$$

thus the matrix of $\hat{P}$, denoted by P, expresses the image function $(\hat{P}f)$ with the old coordinates $(\underline{f})$. As the basis consists of h-columned vectors, the P matrix has hxh elements.

It is easy to see that any $\hat{P} \in G$ operation changes only the order of the $(e_1^{(j)}(x),\ldots, e_h^{(j)}(\underline{x}))$ column vector so the P matrices are hxh permutation matrices. Such a representation is called regular representation.

Carring out a coordinate transformation on the basis spanned by the $e_i^{(j)}(\underline{x})$ functions new matrices are obtained. Therefore it is important to distinguish equivalent and inequivalent representations. Naturally the question arises: which representation is the simplest?

4. Definition

Two representations $\{P\}$ and $\{Q\}$ of the group G are equivalent representations if there exists some matrix M such that $P_i = M\, Q_i\, M^{-1}$ for all $P_i \in \{P\}$, $Q_i \in \{Q\}$.

5. Definition

The characters $\chi^{(i)}(P)$ of a representation i are the traces of the matrices of the representation:

$$\chi^{(i)}(p) = \sum_{\ell} P_{\ell\ell}^{(i)} \tag{11}$$

As the trace is invariant under similarity transformation (cf. definition 4) it offers a criterion for distinguishing equivalent and inequivalent representations.

6. Definition

A representation $\{P^{(i)}\}$ is said to be irreducible if each P∈G is represented by a block diagonal matrix:

$$P^{(i)} = \begin{pmatrix} A_i & C \\ 0 & B_i \end{pmatrix}$$

From the irreducible representation we can learn the eigenfunctions of the symmetry operations. Theire determination is a formidable problem. The main difficulties are that usually the matrices do not commute and we have to block diagonalize h matrices of hxh elements.

Fortunately this problem has been solved [8]. The results are summarized in the sc called character tables. In physical applications the knowledge of the character table is more than enough. The character table says that the irreducible representation are eigenfunction of each symmetry operation with a given eigenvalue. These eigenvalues are given in the table. The eigenvalues of operations belonging to the same class are equal. Thus in the table not single operators but classes are given. Below the most important properties of the character table are given.

4. Theorem

The character table has the following properties:

a, it is a square table, i.e. the number of irreducible representations is equal to the number of classes.

b, the first column contains the dimensions of the representations.

c, the sum of the squares of the terms in the first column equal to the number of elements of the group.

d, the first row contains only elements 1

e, the component of a function $\psi$ which transforms according to

the i-th irreducible representation of the group G is

$$\hat{R}^i \psi = \frac{\ell i}{h} \sum_{\hat{P} \in G} \psi^i(\hat{P})^* \hat{P}_{\hat{R}}(\psi) \qquad (12)$$

where $\ell i$-the dimension of the i-th irreducible representation.

This list is not complete. Those interested in the details should consult one of the standard textbooks. [7-10]

Finally the last important theorems stating that any function can be decomposed into irreducible representations follow.

5. Theorem

If $\Phi^{(i)}$ is the set of $\ell i$ orthogonal vectors spanning the subspace $V_{si}$ and transforming according to the irreducible representation i of a group G of unitary operations, and if $\Phi^{(j)}$ is definied similarly, then all vectors in $V_{si}$ are orthogonal to all those in $V_{sj}$ when $i \neq j$. (Proof omitted).

6. Theorem

Any solution to the DE can be decomposed into linear combinations of functions transforming according to the irreducible representations of G. (Proof omitted).

Example

The group of the DE with a hexagon region includes the following operations (see Figure 1a):

identity operation $\equiv E$

rotation by $\pi/3$ $\equiv C_1$

rotation by $2\pi/3$ $\equiv C_2$

rotation by $\pi$ $\equiv D$

rotation by $-2\pi/3$ $\equiv C_2^{-1}$

rotation by $-\pi/3$ $\equiv C_1^{-1}$

reflection through $m_1$ plane $\equiv m_1$

$m_2$ $\equiv m_2$

$m_3$ $\equiv m_3$

reflection through $m_1'$ plane $\equiv m_1'$

$m_2'$ $\equiv m_2'$

$m_3'$ $\equiv m_3'$

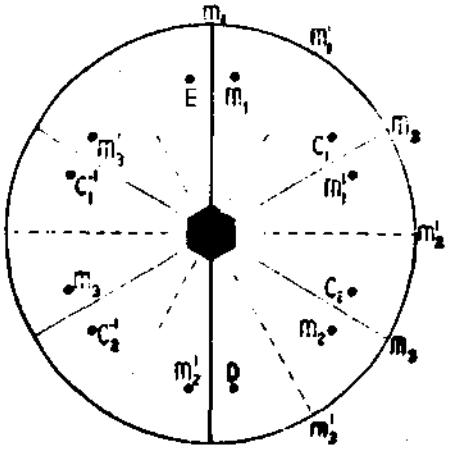


Figure 1a: The Symmetry operations of the DE over a hexagon.

This group called 6mm or $C_{6V}$ contains 12 elements. The operations belong to one of the 6 classes given in Table 1.

| Class symbol | Elements | $h_i$ |
|---|---|---|
| $\mathcal{C}_1$ | E | 1 |
| $\mathcal{C}_2$ | D | 1 |
| $\mathcal{C}_3$ | $C_2 + C_2^5$ | 2 |
| $\mathcal{C}_4$ | $C_1 + C_1^5$ | 2 |
| $\mathcal{C}_5$ | $m_1 + m_2 + m_3$ | 3 |
| $\mathcal{C}_6$ | $m_1' + m_2' + m_3'$ | 3 |

Table 1: Classes of the point group 6mm.

Let us assume that the $e_1(x)$ particular solution* is given so that the endpoint of the $\underline{k}$ vektor lies in E (see Figure 1a). Numbering the k vectors obtained by the symmetry operations applied on $\underline{k}$ according to the list of operations the basis of the invariant subspace is

$$\begin{bmatrix} e^{\underline{k}_1 \underline{x}\lambda} \\ e^{\underline{k}_2 \underline{x}\lambda} \\ \cdot \\ \cdot \\ \cdot \\ e^{\underline{k}_{12} \underline{x}\lambda} \end{bmatrix} \qquad (13)$$

and each symmetry operation is represented by a 12x12 matrix which permutes the basis vector (13). The unit matrix is the representation of E. For example $C_2$ is represented by the matrix

* This solution belongs to the eigenvalue $\lambda$.

$$
\begin{array}{cccccccccccc}
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0
\end{array}
\qquad (14)
$$

Let us turn now to the character table given in Table 2.

| Repr./Class | $C_1$ | $C_2$ | $2C_3$ | $2C_4$ | $3C_5$ | $C_6$ |
|---|---|---|---|---|---|---|
| $\Gamma_1$ | 1 | 1 | 1 | 1 | 1 | 1 |
| $\Gamma_2$ | 1 | 1 | 1 | 1 | -1 | -1 |
| $\Gamma_3$ | 1 | -1 | 1 | -1 | 1 | -1 |
| $\Gamma_4$ | 1 | -1 | 1 | -1 | -1 | 1 |
| $\Gamma_5$ | 2 | 2 | -1 | -1 | 0 | 0 |
| $\Gamma_6$ | 2 | -2 | -1 | 1 | 0 | 0 |

Table 2: The character table of the group 6mm.

This table shows that the group has four one-dimensional and two two-dimensional representations. The representation $\Gamma_1$ is eigenfunction of each operation with eigenvalue 1. Using (12) we can project out this representation; it is:

$$(1,1,\ldots 1)\begin{bmatrix} e^{\underline{k}_1\underline{x}^\lambda} \\ e^{\underline{k}_2\underline{x}^\lambda} \\ \cdot \\ \cdot \\ \cdot \\ e^{\underline{k}_{12}\underline{x}^\lambda} \end{bmatrix} \qquad (15)$$

The other representations can be projected out in a similar way. The symmetries are represented by 12x12 block diagonal matrices since the two-dimensional representation ($\Gamma_5$ and $\Gamma_6$) both appear twice when forming the irreducible representation. (Of course in the character table only the inequivalent representations are distinguished). The irreducible components have to be determined for each eigenvalue.

## 3. Solution to the DE

Using the above theorems we can construct a solution in the following way:

a, We take an arbitrary $\underline{k}$ vector
b, Form an invariant subspace according to theorem 3.
c, Using the character table we can project out the component of the solution which transforms according to the i-th irreducible representation (for every i).
d, According to theorem 6 the solution is a linear combination of the above determined irreducible representation.

The determination of the coefficients in the above mentioned linear combination can be given by considering the boundary conditions. Strictly speaking, the coarse-mesh methods using the general solution of the homogeneous equations should give a method for the determination of the constants in question and we have as many constants as the sum of the elements in the character table's first column. As this number is almost always greater than the number of the faces one boundary condition per face doesn't allow a full representation of the symmetry properties.

In part 2 several results were derived for the symmetry properties of the DE. We saw that the DE has the same form in some coordinate systems connected by a matrix transformation. We determined those functions which are eigenfunctions of these transformations the so called irreducible representations and showed how they can be determined.

In this part we apply the results to the diffusion equation as it is used in the coarse-mesh method. The problem is definied as follows:

Find such a solution of

$$\hat{D}\,\Phi(x,y) = 0 \tag{16}$$

over a region V, which satisfies the

$$\hat{T}\,\Phi(x_b,y_b) = F(x_b,y_b) \tag{17}$$

boundary condition at each $(x_b,y_b)$ point of the boundary of V.

2. Assumption

It is assumed that the boundary condition forming $\hat{T}$ operator is such that if $\hat{P}$ is a symmetry operation of $\hat{D}$ then $\hat{P}$ is a symmetry operation of $\hat{T}$, too.

This assumption assures that if $\hat{D}$ has the same form in coordinate systems transformed to each other by $\hat{P}$ then in these coordinate systems $\hat{T}$ also has the same form. Such a boundary condition is e.g. the given incoming partial current along the boundary.

Let us suppose that a $\underline{B}$ vector is given such that

$$\hat{D}\,e^{\underline{Bx}} = 0 \tag{18}$$

According to theorems 3,5,6 and 4 from $e^{\underline{Bx}}$ a set of functions $\Phi_i$ can be constructed transforming according to the i-th irreducible representation. What is more, the boundary condition $F(x_b,y_b)$ can also be decomposed into components transforming according to the irreducible representations. (The independent variables $x_B$ and $y_B$ are oppressed).

$$F = \sum_{i=1}^{n_c} c_i F_i \tag{19}$$

$n_c$ - number of classes

where $F_i$ transforms according to the i-th irreducible representation.

6. Definition

Applying the elements of the G group of the DE to $\underline{B}$ we obtain h (= the number of elements in G) different $B_i$ vectors. Each $\frac{2\pi}{h}$ sector contains one $\underline{B}_i$ vector. The sector $0 \leq \phi \leq \frac{2\pi}{h}$ is called the ground.

9. Theorem

The function

$$\psi_i(x) = \int_0^{2\pi/h} w(\phi) \cdot \Phi_i(\phi, \underline{x})\, d\phi \qquad (20)$$

satisfies the DE (16) and boundary condition (17) if $w(\Phi)$ is such that

$$F_i(x_b, y_b) = \int_0^{2\pi/h} w(\phi)\, \hat{T}\, \Phi_i(\phi, \underline{x}_b)\, d\phi \qquad (21)$$

$$\underline{x}_b \equiv (x_b, y_b) \in \partial V$$

Besides the $\psi_i$ solution transforms according to $\Phi_i$.

Proof:

Since $\psi_i$ is a linear combination of functions each transforming as $\Phi_i$ the last statement is true. As each $e^{\underline{Bx}}$ forming $\Phi_i(\phi, \underline{x})$ in eq. (21) satisfies the DE (16) and the DE is linear, any linear combinations of $\Phi_i(\phi, \underline{x})$ functions satisfies the DE. As to the boundary condition (17) first it will be shown that if (17) is fulfilled over the ground then it is fulfilled everywhere in $\partial V$.

Assume that

$$\hat{T}\,\psi_i = F_i$$

over the ground and apply P on (17):

$$\hat{P}\,\hat{T}\,\psi_i = \hat{P}\,F_i \tag{22}$$

but according to the Assumption 2.

$$\hat{T}\,\hat{P}\,\psi_i = \hat{P}\,\hat{T}\,\psi_i$$

thus

$$\hat{T}\,(\hat{P}\,\psi_i) = \hat{P}(F_i) \tag{23}$$

Here $\hat{P}$ is an operation which transforms any function form the ground to another sector. The fact that for every sector there exists at least one such a $\hat{P}$, follows from the definition of the symmetry operation. The application of the different $\hat{P}$ operations in (23) assures that (17) is fulfilled everywhere in $\partial V$. Therefore we have to prove that (17) is fulfilled over the ground. This condition gives an integral equation for $w(\phi)$. This is just equation (21).

Q.E.D.

Theorem 9 summarizes most of the benefits of the group theory. We are able to decompose the boundary condition into symmetry classes and to give the corresponding particular solution what is more we have a further result.

10. Theorem

The solution of the DE (16) with boundary condition (17) is

$$\phi(\underline{x}) = \sum_{i=1}^{n_c} c_i \psi_i(\underline{x}) \tag{24}$$

where $\psi_i(\underline{x})$ is given by (20) and $c_i$ by (19).

Proof:

Since $\psi_i(\underline{x})$ satisfies (16) so does $\Phi(\underline{x})$. On the boundary

$$\hat{T}\,\Phi(\underline{x}) = \sum_{i=1}^{n_c} c_i\,\hat{T}\,\psi_i(\underline{x}) = \sum_{i=1}^{n_c} c_i F_i(\underline{x}) = F(x)$$

so the boundary condition is fulfilled too.

Q.E.D.

All in all it was shown that using the symmetry properties of the considered node we can give the solution. To do so we must solve as many boundary condition problems as the number of classes ($n_c$). Most of the nodal methods use response matrices with $N \cdot n_f$ (N - number of the groups, $n_f$ - number of the faces). It is obvious that it is easier to solve $n_c$ times a set of equations with N unknowns than to solve one set of equations with $N \cdot n_f$ unknowns. In each problem we need the solution of (20) but as the ground is small (in case of a square h = 8, in case of a hexagon h = 12) we may hope that w can be well approximated over the ground by simple functions.

Face averaged incoming currents are the most frequently used boundary conditions in coarse-mesh methods. Although their efficiency has been proved several times let us emphasize again that their use doesn't allow a full representation of the symmetry. This means that the solution will not contain component(s) transforming according to some classe(s).

As to the application of the presented method, it can be applied in both 2D and 3D problems with an arbitrary number of groups. Though the geometry is indifferent, the reactor must contain only corresponding elements. In the next part a 2D algorithm is presented in rectangular geometry.

## 4. The ANANAS algorith

Let us consider the two-group diffusion equation over a two-dimensional rectangular node.

$$-D_g \nabla^2 \Phi_g + \Sigma_g \Phi_g = \chi_g \sum_{g'=1}^{2} \left[ \frac{\nu \Sigma_{fg'}}{k_{eff}} + (1-\delta_{gg'}) \Sigma_{g' \to g} \right] \Phi_{g'} + S_g, \quad g=1,2 \qquad (25)$$

The boundary condition fixes only the face averaged incoming currents:

$$I_{gus} = \frac{1}{\ell} \int_{-\frac{\ell}{2}}^{\ell/2} \frac{1}{4} \left[ \Phi_g(s \tfrac{\ell}{2}, v) + 2D_g \frac{\partial \Phi_g}{\partial n}(s \tfrac{\ell}{2}, v) \right] dv \qquad (26)$$

$u = x,y \qquad s = -1,+1 \qquad g = 1,2$

### a. The symmetry properties of the square

The symmetry properties are given in Ref. 8. The groups of the DE over a square form the group 4mm. This group contains 8 elements. (Figure 1 shows where a general vector with endpoint E is transformed to. The coordinate system is also given there, the z axis is oriented upward perpendicularly to the x,y, plane).

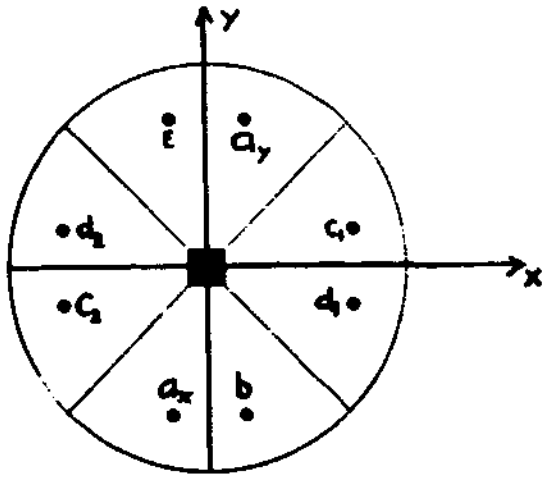


Figure 1: Stereogramm of the group 4mm.

E - identity

$a_x$ - rotation by $\pi$ about the x axis

$a_y$ - rotation by $\pi$ about the y axis

$d_1$ - rotation by $\pi$ about the x= y axis

$d_2$ - rotation by $\pi$ about the x=-y axis

b - rotation by $\pi$ about the z axis

$c_1$ - rotation by $3\pi/2$ about the z axis

$c_2$ - rotation by $\pi/2$ about the z axis

The group has 5 classes

$$C_e = E \quad C_b = b \quad C_c = c_1, c_2 \quad C_d = d_1, d_2$$

The character table is given in Table 3.

| Repr./Class | $C_e$ | $2C_a$ | $2C_d$ | $C_b$ | $2C_c$ |
|---|---|---|---|---|---|
| $\Gamma_1$ | 1 | 1 | 1 | 1 | 1 |
| $\Gamma_2$ | 1 | -1 | 1 | 1 | 1 |
| $\Gamma_3$ | 1 | 1 | -1 | 1 | -1 |
| $\Gamma_4$ | 1 | -1 | 1 | 1 | -1 |
| $\Gamma_5$ | 2 | 0 | 0 | -2 | 0 |

Table 3. The character table of the group 4mm.

The group 4 mm has four one dimensional and one two-dimensional irreducible representations. The full symmetry representation needs 6 constants but the use of the boundary condition (26) allows only 4 constants. It means that our solution will not contain some of the above representations. For finding the solution we follow the method given on page (18). The solution of (25) contains linear combinations of the elementary solutions which are eigenfunctions of the Laplacian with eigenvalue $\mu^2$ and $\nu^2$:

$$F_\mu(\underline{x}) = e^{\mu \underline{k} \underline{x}} \qquad (27)$$
$$F_\nu(\underline{x}) = e^{\nu \underline{k} \underline{x}}$$

$$\nu^2 = \frac{1}{2}\left[\beta_1^2 + \beta_2^2 + \sqrt{(\beta_1^2 - \beta_2^2)^2 + 4\delta_1\delta_2/D_1/D_2}\right] \qquad (28)$$

$$\mu^2 = \frac{1}{2}\left[-\beta_1^2 - \beta_2^2 + \sqrt{(\beta_1^2 - \beta_2^2)^2 + 4\delta_1\delta_2/D_1/D_2}\right] \qquad (29)$$

$$\beta_i = \Sigma_i/D_i \quad \delta_i = (\Sigma_i - \frac{\chi_i}{k_{eff}} \nu\Sigma_{fi})/D_i$$

We have to find the symmetry components of $F_\mu(\underline{x})$ and $F_\nu(\underline{x})$.

First we form an invariant subspace according to step b of page (13).

This space contains exponential functions with different $\underline{k}$-vectors. They are given in Figure 2. For projecting out the symmetry components we need their transformation (cf. (15)). This is given in Table 4.

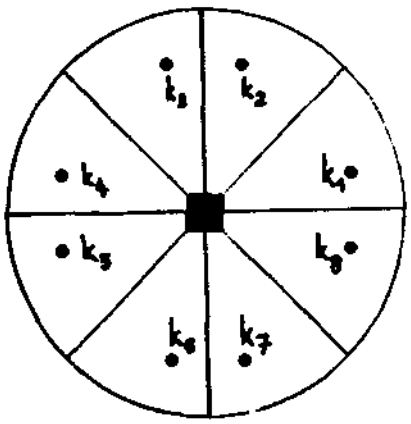


Figure 2: The end-points of the 8 $\underline{k}$ vectors.

| Starting-vector operation | $k_1$ | $k_2$ | $k_3$ | $k_4$ | $k_5$ | $k_6$ | $k_7$ | $k_8$ |
|---|---|---|---|---|---|---|---|---|
| E | $k_1$ | $k_2$ | $k_3$ | $k_4$ | $k_5$ | $k_6$ | $k_7$ | $k_8$ |
| $a_x$ | $k_8$ | $k_7$ | $k_6$ | $k_5$ | $k_4$ | $k_3$ | $k_2$ | $k_1$ |
| $a_y$ | $k_4$ | $k_3$ | $k_2$ | $k_1$ | $k_8$ | $k_7$ | $k_6$ | $k_5$ |
| $d_1$ | $k_2$ | $k_1$ | $k_8$ | $k_7$ | $k_6$ | $k_5$ | $k_4$ | $k_3$ |
| $d_2$ | $k_6$ | $k_5$ | $k_4$ | $k_3$ | $k_2$ | $k_1$ | $k_8$ | $k_7$ |
| b | $k_5$ | $k_6$ | $k_7$ | $k_8$ | $k_1$ | $k_2$ | $k_3$ | $k_4$ |
| $c_1$ | $k_3$ | $k_4$ | $k_5$ | $k_6$ | $k_7$ | $k_8$ | $k_1$ | $k_2$ |
| $c_2$ | $k_7$ | $k_8$ | $k_1$ | $1_2$ | $k_3$ | $k_4$ | $k_5$ | $k_6$ |

Table 4: The transformation rules for the k vectors.

Now we have to carry out the projection according to (15). The result is linear combination of exponentials irrespective of whether we use μ or ν. Let us introduce the notation

$$F_{is}(\underline{x}) = e^{s\underline{k}_i\underline{x}} \qquad s = \mu,\nu \qquad (30)$$

then the symmetrized function are

$$S_{is}(\underline{x}) = \sum_{i=1}^{8} \omega_{ij} F_{is}(\underline{x}) \qquad j = 1,\ldots 6 \qquad (31)$$

where the coefficients are given in Table 5. With this the symmetry components have been determined. We have to form the flux with them. The flux is a linear combination of the two $S_i(\underline{x})$ functions (one with $F_{i\mu}$ the other with $F_{i\nu}$).

$$\phi_{ig}(\underline{k}_1,\underline{x}) = c_{g\mu}^{(i)} S_{i\mu}(\underline{x}) + c_{g\nu}^{(i)} S_{i\nu}(\underline{x}) \quad g = 1,2 \qquad (32)$$

where $\phi_{ig}$ is the i-th symmetry component of the flux in group g, $c_{g\mu}^{(i)}$ and $c_{g\nu}^{(i)}$ are the so far unknown coefficients.

| g/i | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 2 | 1 | -1 | 1 | -1 | 1 | -1 | 1 | -1 |
| 3 | 1 | -1 | -1 | 1 | 1 | -1 | -1 | 1 |
| 4 | 1 | 1 | -1 | -1 | 1 | 1 | -1 | -1 |
| 5 | 1 | 1 | 1 | 1 | -1 | -1 | -1 | -1 |
| 6 | 1 | 1 | -1 | -1 | -1 | -1 | 1 | 1 |

Table 5: The $\omega_{ij}$ coefficients of the symmetrized $S_i$ functions.

For the determination of the coefficients the symmetry components of the boundary condition has to be determined. This goes according

to (15). In Table 4 $k_1 \equiv k_8$ $k_3 \equiv k_2$ $k_4 \equiv k_5$ $k_6 \equiv k_7$. The result is

$$\begin{bmatrix} I_{x\ell g} \\ I_{xrg} \\ I_{y\ell g} \\ I_{grg} \end{bmatrix} = m_{1g} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} + m_{3g} \begin{bmatrix} +1 \\ +1 \\ -1 \\ -1 \end{bmatrix} + m_{5a} \begin{bmatrix} 1 \\ -1 \\ 0 \\ 0 \end{bmatrix} + m_{5a} \begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix} \quad (33)$$

$$m_{1g} = (I_{x\ell g} + I_{xrg} + I_{y\ell g} + I_{yrg})/4 \quad (34a)$$

$$m_{3g} = (I_{x\ell g} + I_{xrg} - I_{y1g} - I_{yrg})/4 \quad (34b)$$

$$m_{5a} = (I_{x\ell g} - I_{xrg})/2 \quad (34c)$$

$$m_{5b} = (I_{y\ell g} - I_{yrg})/2 \quad (34d)$$

The column vectors transform according to $\Gamma_1$, $\Gamma_3$ and $\Gamma_5$ and since $\Gamma_5$ has two independent vectors it occurs twice. This decomposition clearly shows that the boundary condition doesn't contain components corresponding to $\Gamma_2$ and $\Gamma_4$.

Let us remember that (32) contains 2 unknown coefficients per group since we have the following relationship

$$c_{1\mu} = \frac{\delta_2}{D_1(\mu^2 + \beta_1^2)} \cdot c_{2\mu} \quad (35a)$$

$$c_{1\nu} = \frac{\delta_2}{D_1(\beta_1^2 - \nu^2)} \cdot c_{2\nu} \quad (35b)$$

The remaining two coefficients are determined from the boundary condition: each symmetry component of the flux must match the corresponding boundary condition-component. This condition will be met if

$$m_{ig} = c_{g\mu}^{(i)} \cdot H_{\mu g}^{(i)} + c_{g\nu}^{(i)} H_{g\nu}^{(i)} \quad g = 1,2 \quad i=1,3,5a,5b \tag{36}$$

where

$$H_{\mu g}^{(i)} = \frac{\sin \cdot k_{1x} \ell/2 \cdot \mu}{k_{1x} \ell/2 \cdot \mu} (\cos k_{1y} \ell/2 \mu - \mu D_g k_{1y} \sin k_{1y} \ell/2 \ \text{sign}(\mu^2)) +$$

$$+ \frac{\sin k_{1y} \ell/2 \mu}{k_{1x} \ell/2 \cdot \mu} (\cos k_{1x} \ell/2 \mu - 2\mu D_g k_{1x} \sin k_{1x} \ell/2 \cdot \mu \cdot \text{sign}(\mu^2)) \tag{37}$$

$$H_{\nu g}^{(i)} = \frac{\text{sh } k_{1x} \ell/2 \nu}{k_{1x} \ell/2 \nu} (\text{ch } k_{1y} \ell/2 \nu + 2D_g \nu k_{1y} \text{ sh} k_{1y} \ell/2 \mu) +$$

$$+ \frac{\text{sh } k_{1y} \ell/2 \nu}{k_{1y} \ell/2 \mu} (\text{ch } k_{1x} \ell/2 \nu + 2D_g \nu k_{1x} \text{ sh} k_{1x} \ell/2 \mu) \tag{38}$$

$$g = 1,2 \quad i = 1,3,5a, 5b.$$

and if $\mu^2 < 0$ the circular functions are replaced by hyperbolic ones in (37).

On solving (36) we obtained a particular solution which depends on $\underline{k}_1$. Let us denote it by $\phi_{ig}(\underline{k}_1, \underline{x})$. The general solution is a weighted integral for $\underline{k}_1$. But from Figure 2 it is clear that $\underline{k}_1$ is an arbitrary vector lying in the ground therefore the general solution is

$$\phi_{ig}(\underline{x}) = \int_{|\underline{k}_1|=1, \arg \underline{k}_1 \leq \pi/4} dk_1 \; \phi_{ig}(\underline{k}_1, \underline{x}) \cdot w(\underline{k}_1) \qquad (39)$$

The weight function is a solution to (23). At this point we have to compromize between a good approximation and efficiency. One can solve (23) using numerical techniques, the result is the w function at certain points. The more points we have the more accurate results we have but the more expressions like (37) and (38) have to be determined. In ANANAS we tried two possibilities:

a) Assuming $\underline{w}(k_1) \equiv 1$ we can carry out the integration indicated in (39). Using two-point Gaussian quadrature the results are surprisingly good. As an example the $k_{eff}$ dependence on the mesh size is given in Figure 3. The investigated benchmark was given by Melice [5].

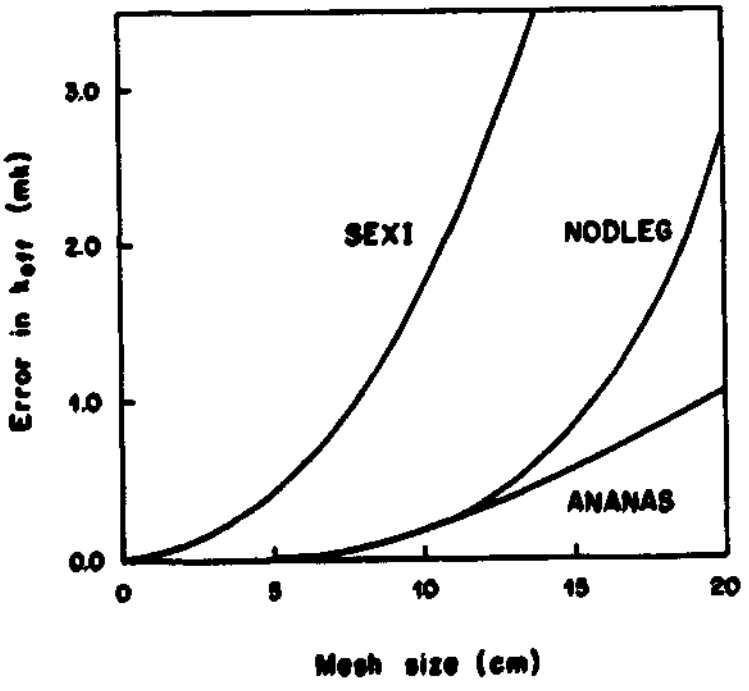


Figure 3: Mesh-size error in $k_{eff}$ for different approximations.

b) Since we have to use two numerical procedures: one for solving the integral equation (23) for w and another for the numerical integration in (39) we may hope that there exists one $\underline{k}_1$ vector which gives a good approximation. One guess is

$$\underline{k}_1 = (0.986258;\ 0.165213)$$

As illustration the 2D IAEA benchmark [11] results are given in Figure 4.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 0.7466 | 1.328 | 1.4705 | 1.225 | 0.6077 | 0.9388 | 0.9317 | 0.7487 |
| 0.7456 | 1.310 | 1.4537 | 1.211 | 0.6100 | 0.9351 | 0.9343 | 0.7549 |
| 0.13 | 1.40 | 1.16 | 1.18 | -0.39 | 0.40 | -0.28 | -0.82 |
| | 1.4465 | 1.491 | 1.323 | 1.078 | 1.035 | 0.9450 | 0.7283 |
| | 1.4351 | 1.480 | 1.315 | 1.070 | 1.036 | 0.9504 | 0.7358 |
| | 0.79 | 0.75 | 0.58 | 0.81 | -0.12 | -0.61 | -1.02 |
| | | 1.476 | 1.352 | 1.186 | 1.068 | 0.9710 | 0.6751 |
| | | 1.469 | 1.345 | 1.179 | 1.071 | 0.9752 | 0.6921 |
| | | 0.45 | 0.48 | 0.6 | -0.21 | -0.4 | -2.45 |
| | | | 1.197 | 0.9727 | 0.9024 | 0.8320 | |
| | | | 1.193 | 0.9670 | 0.9064 | 0.8461 | |
| | | | 0.36 | 0.59 | -0.44 | -1.67 | |
| | | | | 0.4660 | 0.6875 | 0.5838 | |
| | | | | 0.4706 | 0.6856 | 0.5972 | |
| | | | | -0.99 | 0.28 | -2.24 | |
| | | | | | 0.5655 | | |
| | | | | | 0.5849 | | |
| | | | | | -3.32 | | |

ANANAS
REF.
ERROR (%)

Figure 4: The 2D-IAEA Benchmark Power Distribution. (mesh size = 10cm).

According to our experiments the error only slightly depends on the $\underline{k}_1$ vector: it varies between 1% and 5%. This fact shows the power of the intuition of using only a second order cross-leakage. If someone is ready to devote computation time for accuracy, this method offers an "analytic" cross leakage approximation since in eq. (21) the left-hand side depends on the w function of the neighbouring node. This way an iterative method may serve for the determination of the weight functions in each node.

## 5. Comparison with other methods

Three methods are considered here. Melice [5] and Bonalumi [12] considered the transient and fundamental modes separately. For the transient modes the PWS (Plane Wave Superposition) approximation was used. The approximation corresponds to the choice of

$$w(\underline{k}_1) = \begin{cases} 1 & \text{if } \arg \underline{k}_1 = n\pi/2 \quad n = \text{integer} \\ 0 & \text{otherwise} \end{cases}$$

in (39). For the fundamental modes the NSB (Nodewise Seperable Buckling) approximation was used. In Melice's paper this means

$$w(\underline{k}_1) = \begin{cases} 1 & \text{if } \arg \underline{k}_1 = (2n+1)\pi/4 \quad n = \text{integer} \\ 0 & \text{otherwise} \end{cases}$$

while in Bonalumi's method three different directions were used. Both methods use leakages instead of partial currents which reduces the data transfer considerably. The third method [13] called SEXI used the PWS approximation for both nodes.

Finally we have to answer the question: is it possible to derive the above obtained flux form without group theory? The answer is yes, as it was shown by Maeder [14]. Using the Fourier-method one can derive the same relations with some differences. The integral equation for w (cf (20)) can be reduced only to the $|0, \pi/2|$ interval. In rectangular case this interval is two times larger than the ground. The second difference is that $N \cdot n_f$ coupled equations are obtained in contrast with the $n_f$ times N equations of ANANAS. We recall that face averaged boundary conditions are used in this part. In general the group-theory gives $N \cdot n_c$ equations. (Cf. Theorem 10 and the following remarks). Besides the Fourier method is confined to rectangular geometry.

## 6. Conclusions

By the investigation of the symmetry of the DE we could derive a set of particular solutions each transforming according to a given irreducible representation. These solutions involve a weight function which is the solution of an integral equation (cf. eq. (21)). This equation is to be solved over a relatively small interal, over the ground $|0, \pi/4|$. With a correct solution of this equation and the correct integration in the final flux (cf. (20) and (24)) an exact solution can be obtained.

A program was written using the symmetry considerations. This program (ANANAS) tried two approximations which represent a compromise between the accuracy and speed. The first one assumed equal weight in (20) and the integration in (24) was carried out using a two-point gaussian quadrature. The results are just at the acceptable level (5% power-error) in case of the 2D IAEA problem but the method shows one advantage: the order of the cross-leakage approximation doesn't depend on the neighbours. The second approximation determined numerically a favorable position of the initial $\underline{B}_1$ vector i.e. suitable $\Phi$ value in (20). In this case a two times faster algorithm can be obtained and as the 2D IAEA results witnessea it, the accuracy is better than in the first approximation.

Finally it should be emphasized that the possibilities of the method are far from being exhausted. Though weak points of the programmed algorithm offer an improvement its most prosperous application is in hexagonal geometry.

## Aknowledgement

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