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CALCULATION OF LARGE SYMMETRIC CORES

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## CALCULATION OF LARGE SYMMETRIC CORES

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## ABSTRACT

A rigorous mathematical extension of the buckling method is provided. The solution of the neutron transport equation is given as a power series of the buckling. The leading term of the solution has the well-known product form: it is the product of two functions, one determined by cell calculation /microflux/, the other by the solution of a diffusion equation /macroflux/. The microflux occurring in the second and third member is derived from a cell problem with heterogeneous boundary condition. The macroflux of the second and third member is the gradient and Laplacian of the macroflux occurring in the leading term. The coefficients of the diffusion equation for the macroflux are determined by the cross-sections of the transport equation averaged over the cell in the same manner as is given with asymptotic analysis.

## АННОТАЦИЯ

В работе описан метод обобщения лапласиана. Решение уравнения переноса дается лапласианом в виде степенного ряда. Первым членом этого ряда является часто встречающаяся при вычислении невозмущенных решеток формула Вигнера-Зейца. Микропотоки определяются из задачи собственного значения, относящегося к ячейке. Макропотоки определяются из единственного члена как решение диффузного уравнения с гомогенизированными членами. Способ гомогенизации соответствует методу асимптотического анализа.

## KIVONAT

A dolgozat a buckling módszer általánosítását adja. A transzport egyenlet megoldását a buckling hatványsoraként állítja elő. E sor első tagja a nem perturbált rácsok számításában gyakran felbukkanó Wigner-Seitz formula. A mikrofluxusok cellára vonatkozó sajátérték feladatból határozhatók meg. A makrofluxusok egyetlen tagból határozhatók meg egy homogenizált együtthatókkal felírt diffúziós egyenlet megoldásaként. A homogenizálás módja megegyezik az aszimptotikus analízis által megadott módszerrel.

And here, according to Trout, was the reason human beings could not reject ideas because they were bad; 'Ideas on Earth were badges of friendship or enmity. Their content did not matter. Friends agreed with friends, in order to express friendliness. Enemies disagreed with enemies, in order to express enmity.

K. VONNEGUT

## 1. INTRODUCTION

From the earliest days of reactor physics, difficulties in providing a neutron physical description for a complex power reactor were expected. What is really astonishing is that possible ways of overcoming these difficulties were also outlined<sup>1</sup>. It was proposed that the problem be separated into two and that the neutron flux be expressed as a product of two functions:

- the first giving a detailed picture of energy but a rough spatial description
- the second providing a fine description in space but a coarse picture of energy.

Today the best programs compete for the fourth and fifth digit in  $k_{\text{eff}}$  and a few tenths of a percent in power distribution<sup>2</sup>. For this reason there is abounding interest in knowing how well the great old recipe works. Its most common modern form is known as the buckling method<sup>3-10</sup>. The main point is the replacing of the transport equation by a diffusion equation that contains coefficients depending on the cross sections in the transport equation averaged over a cell. So far, no satisfactory

mathematical justification for this approximation has been published. Although the validity of the approximation is accepted, the nearly a dozen prescriptions for the coefficients in the diffusion equation have shown the lack of a firm theoretical foundation. The derivation of the diffusion coefficient involves hypothesized relationships between various quantities averaged over a cell. The obtained diffusion coefficients have sometimes been nonphysical in one sense or another.

In this paper the buckling method is derived in a mathematically rigorous way. The method is based strictly on the analysis of the neutron transport equation and on the symmetry properties of the core. The solution is given as a power series of the buckling. The first three members in the series are given explicitly. The first member is the product of two functions: the spatially periodic microflux is determined by a cell eigenproblem; the other term, the macroflux, by a diffusion equation whose coefficients depend on the result of cell calculations. The second member is the product of the macroflux gradient and a new microflux determined by a cell problem /not eigenproblem/ with inhomogeneous boundary conditions. The boundary condition is given by the cell eigenproblem's solution. The third member is the product of the Laplacian of the macroflux and a microflux that is determined by the solutions of the previous cell problems. The eigenvalue  $k_{eff}$  is expressed also as a power series of the buckling. It is shown that this power series may

not contain odd powers of the buckling components provided that the cell is symmetric. The zeroth and second order coefficient of this series can be expressed by the microfunctions and cross sections. Finally the coefficients of the diffusion equation are expressed by the microfunctions and by the coefficients in the transport equation.

Our method makes use of the trivial analogy between the structure of a reactor core and that of a solid material. In the case of the latter the Schrödinger equation is considered<sup>11</sup>. As both the neutron transport equation and the Schrödinger equation are eigenvalue problems they are closely related. TE is, however, a boundary value problem where boundary conditions have a vital role. In this paper only such boundary conditions are considered that can be fulfilled using "buckling constraint"<sup>12</sup>. The similarities of the two problems are summarized in Table 1. Making use of this remarkable similarity it will be shown in the following pages that several theorems /viz. Theorems 1,2,3,4/, valid for the Schrödinger equation<sup>11</sup> hold also for the TE notwithstanding that here only the TE is investigated. The theorems for the SE can be found in Ref.11.

## 2. THE PROBLEM TO BE SOLVED

The scope of our investigation is a core in which fuel pins and absorber rods are arranged in a regular way as for example in the simple core of Fig.1. We are looking for the neutron distribution in the core governed by the TE:

$$\underline{\Omega} \nabla \Psi(r, E, \underline{\Omega}) + \Sigma(r, E) \Psi(r, E, \underline{\Omega}) = S(r, E, \underline{\Omega}) \quad /1/$$

where the source is composed of downscatter and fission and is given by

$$S(r, E, \underline{\Omega}) = \int_0^{\infty} \int_{4\pi} \Sigma_s(r, E' \rightarrow E, \underline{\Omega} \cdot \underline{\Omega}') \Psi(r, E', \underline{\Omega}') d\underline{\Omega}' dE' \quad /2/$$

$$+ \frac{\kappa(r, E)}{4\pi} \int_0^{\infty} \int_{4\pi} \nu \Sigma_f(r, E') \Psi(r, E', \underline{\Omega}') d\underline{\Omega}' dE'$$

where the symbols need no explanation. Equation /1/ is often expressed as an eigenvalue problem. If the cross-sections-like operations are contracted into one  $\hat{\Sigma}$  operation as is customary<sup>12</sup>, we have

$$\left( \underline{\Omega} \nabla + \hat{\Sigma}(r, E, k_{eff}) \right) \Psi(r, E, \underline{\Omega}) = 0 \quad /3/$$

where

$$\hat{\Sigma}(r, E, k_{eff}) = \Sigma(r, E) + \int_0^{\infty} \int_{4\pi} \Sigma_s(r, E' \rightarrow E, \underline{\Omega} \cdot \underline{\Omega}') \cdot d\underline{\Omega}' dE'$$

$$+ \frac{\kappa(r, E)}{4\pi \cdot k_{eff}} \cdot \int_0^{\infty} \int_{4\pi} \nu \Sigma_f(r, E') \cdot d\underline{\Omega}' dE'$$



The boundary condition fixes the entering neutron density on the outer boundary of the core. Let  $\underline{R}$  denote a point on the boundary  $|\underline{R} \in \partial V|$ , then

$$\Psi(\underline{r}, E, \underline{\Omega}) = f(\underline{R}, E, \underline{\Omega}) \quad \text{if } \underline{\Omega} \cdot \underline{n} < 0 \quad |4|$$

where  $\underline{n}$  is the outward normal to the boundary of the core,  $f$  is some given function.

### 3. SYMMETRIES AND THEIR CONSEQUENCES

The fundamental problem in reactor physics is the following: given the TE of the core, find its highest eigenvalue and eigenfunction with given boundary conditions.

The neutron distribution in a finite core can be calculated by extending the core to infinity and finding the neutron distribution in this infinite system<sup>13</sup>. Most of the cores show noteworthy symmetry properties: they contain some symmetry planes or they have some rotational symmetry or both<sup>14</sup>. The core extended to infinity /in brief the infinite core/ possesses not only these kinds of symmetries but translational symmetry as well. Translational symmetry means that there are some vectors - the so called lattice vectors - shifting the infinite core into itself. The neutron density,  $\Psi$ , inherits these symmetry properties to some extent as will be shown below. The extension of the core to infinity is carried out by its periodic repetition thus the cross sections in the TE are extended in the following way:

$$\Sigma(\underline{r} + n_1 \underline{a}_1 + n_2 \underline{a}_2 + n_3 \underline{a}_3) = \Sigma(\underline{r}) \quad /5/$$

where  $\Sigma$  is any cross section in /1/ and  $\underline{a}_1$ ,  $\underline{a}_2$  and  $\underline{a}_3$  are the so called elementary translations joining the fuel rods in neighbouring cells;  $n_1$ ,  $n_2$  and  $n_3$  are integer. A common hexagonal cell is shown in Fig.2. A simple symmetric core made up from the cells of Fig.2. is shown in Fig.1.

1. Definition: A symmetry transformation with respect to the TE is a coordinate transformation such that the form of the TE is the same in the old and the new coordinate system.

Example: It is easy to see that  $\nabla^2$  is invariant with respect to rotations and reflections thus the symmetry operations are determined mostly by the space dependence of the cross sections in Eq./1/. The core of Fig.1. has the following symmetries: rotations by  $n \pi/3$ ,  $n=0,1,2,3,4,5$  about the z axis and reflections through 6 planes denoted by  $S_1, \dots, S_6$  in Fig.1. Although we do not intend to deal with cells or cores without symmetries the considerations presented here are valid for most of the PWR, BWR, LMFBR and HTR reactor types<sup>14</sup>.

Symmetry operations are denoted by  $\hat{P}$  and P stands for the matrix of this transformation, that is,

$$\underline{r}' = P\underline{r}$$

where  $\underline{r}$  is the coordinate in the old,  $\underline{r}'$  in the new coordinate system. A function is transformed according to the relation

$$Pf(\underline{r}) \equiv f(P^{-1}\underline{r})$$

First the infinite core solution is considered. Assume that a solution  $\Psi$  of the TE is given. This solution is not necessarily invariant with respect to the symmetries of the TE. If this is the case new solutions can be obtained from  $\Psi$  as is shown below.

Theorem 1. If  $\hat{P}$  is a symmetry of the TE and  $\Psi$  is a solution of the TE then  $\hat{P}\Psi$  is also a solution of the TE.

Proof: Apply  $\hat{P}$  to Eq./3/:  $\hat{P}[(\underline{\Omega}\nabla + \hat{\Sigma})\Psi] = \hat{P}(\underline{\Omega}\nabla + \hat{\Sigma}) \cdot \hat{P}\Psi$   
 and  $P$  is a symmetry thus  $\hat{P}(\underline{\Omega}\nabla + \hat{\Sigma}) = \underline{\Omega}\nabla + \hat{\Sigma}$  and we have  
 $(\underline{\Omega}\nabla + \hat{\Sigma}) \hat{P}\Psi = 0$  as was stated. Q.E.D.

It follows from Theorem 1. that the infinite core solution has translational invariance. Let  $\hat{P}_{\underline{l}}$  be a translation by a lattice vector  $\underline{l}$ . According to Theorem 1. the operation  $\underline{\Omega}\nabla + \hat{\Sigma}$  commutes with  $\hat{P}_{\underline{l}}$ . Thus the eigenfunctions of  $(\underline{\Omega}\nabla + \hat{\Sigma})$  are eigenfunctions of the translation operation too. The eigenproblem for  $\hat{P}_{\underline{l}}$  is expressed as

$$\Psi(\underline{r} + \underline{l}) = c_{\underline{l}} \cdot \Psi(\underline{r})$$

If  $\underline{l} = \underline{l}_1 + \underline{l}_2$  then

$$\Psi(\underline{r} + \underline{l}) = \Psi(\underline{r} + \underline{l}_1 + \underline{l}_2) = c_{\underline{l}_1} \cdot \Psi(\underline{r} + \underline{l}_2) = c_{\underline{l}_1} \cdot c_{\underline{l}_2} \cdot \Psi(\underline{r}).$$

Thus the eigenvalues of the translation are related as  $c_{\underline{l}} = c_{\underline{l}_1} \cdot c_{\underline{l}_2}$ .

The translation may be repeated any integer times and the solution remains finite only if  $|c_{\underline{l}}| = 1$ . Choosing

$$c_{\underline{l}} = e^{i \underline{B} \underline{l}}$$

where  $\underline{B}$  is a real, so far undefined, vector we have the following result:

Theorem 2. The operator of Eq./3/ commutes with the translation operation  $\hat{P}_{\underline{l}}$  so there exists a common eigenfunction system. This system consists of Bloch functions characterized by

$$f_{\underline{B}}(\underline{r} + \underline{l}) = e^{i \underline{B} \underline{l}} \cdot f_{\underline{B}}(\underline{r}) \quad /6/$$

For our purposes the following representation of the Bloch function is useful:

$$f_B(\underline{r}) = e^{i\underline{B}\underline{r}} \cdot u_B(\underline{r}) \quad /7/$$

where  $u_{\underline{B}}/\underline{r}/ = u_{\underline{B}}/\underline{r}+\underline{l}/$  if  $\underline{l}$  is a lattice vector.

Several authors <sup>4-10</sup> have assumed that the source in Eq./1/ has a Bloch form. It is an interesting fact that the solution of the SE has been sought in Bloch form since the 50'-s while the existence of such a solution was only assumed but not verified for the TE.

Before making the core finite let us consider the  $k_{\text{eff}}/B/$  and  $u_{\underline{B}}/\underline{r}/$  functions. Substituting Eq./7/ into Eq./3/ we have: Theorem 3. The  $u_{\underline{B}}/\underline{r}/$  function and the eigenvalue  $k_{\text{eff}}/B/$  are obtained from the following eigenproblem:

$$\left( \underline{\Omega} \nabla + \hat{\Sigma}(\underline{r}, E, k_{\text{eff}}) \right) u_{\underline{B}}(\underline{r}, E, \underline{\Omega}) = -i \underline{B} \underline{\Omega} u_{\underline{B}}(\underline{r}, E, \underline{\Omega}) \quad /8/$$

The boundary condition for this problem is that  $u_{\underline{B}}/\underline{r}/$  must be periodic in  $\underline{r}$ . There is an infinite number of  $k_{\text{eff}}$  values with which a nontrivial solution exists. For calculations the largest eigenvalue is of outstanding importance<sup>1</sup>: from now on only the largest eigenvalue is considered. The solution for the finite core is to be a combination of infinite core solutions<sup>13</sup>, i.e. of the Bloch functions. It is advantageous to select those infinite core solutions which belong to the same eigenvalue.

Theorem 4. The inverse function of the eigenvalue  $k_{\text{eff}}$  in the TE /3/ as a function of  $\underline{B}$  is not a single valued function. A given  $k_{\text{eff}}$  value belongs to those  $\underline{B}$  vectors which can be transformed into each other by one of the symmetries of the TE.

Proof: Apply a symmetry of the TE on both sides of Eq./8/. The operator on the LHS is invariant, the only change is that  $\underline{B} \rightarrow \underline{B}'$  and  $\underline{r} \rightarrow \underline{r}'$ . Thus Eq./8/ has the same form both in  $|\underline{B}'; \underline{r}'|$  and  $|\underline{B}; \underline{r}|$ . Remembering that  $k_{\text{eff}} = k_{\text{eff}}/|\underline{B}|$ , it is possible only if  $k_{\text{eff}}/|\underline{B}| = k_{\text{eff}}/|\underline{B}'|$ .

Q.E.D.

Thus the finite core solution is obtained as a linear combination of those Bloch functions which belong to the same vectors determined by a constant  $k_{\text{eff}}$  value. Let us denote the set of admissible  $\underline{B}$  vectors by  $\mathbb{R}$  then the solution is given by

$$\Psi(\underline{r}, E, \underline{\Omega}) = \int_{\mathbb{R}} W(\underline{B}) \cdot e^{i\underline{B}\underline{r}} u_{\underline{B}}(\underline{r}, E, \underline{\Omega}) d\underline{B} \quad /9/$$

The  $W/\underline{B}|$  function has to be chosen so that the boundary condition, Eq./4/, is met on the boundary of the finite core. To get rid of the transport boundary condition it is usual to assume that the neutron density can be taken<sup>15</sup> as the sum of a transient member decaying rapidly from the boundary of the core and an asymptotic member which is considerably greater than the transient almost everywhere:

$$\Psi(\underline{r}, E, \underline{\Omega}) = \Psi_a(\underline{r}, E, \underline{\Omega}) + \Psi_{tr}(\underline{r}, E, \underline{\Omega})$$

In this case the asymptotic member is a good approximation for most of the cells and it obeys some nicer boundary conditions, e.g. it vanishes on the boundary:

$$\Psi_a(\underline{B}, E, \underline{Q}) = 0 \quad \underline{R} \in \partial V$$

We shall return to the boundary condition in the next section. It is obvious that Eq./9/ gives a good approximation for the asymptotic member as it was built from infinite core solutions. Let us again emphasize that the set of admissible B vectors in Eq./9/ was determined by a cell eigenvalue problem, thus any B  $\in$   $\mathbb{R}$  is a possible material buckling.

#### 4. APPROXIMATION FOR LARGE CORES

The parameter  $\underline{B}$  in Eq./9/ has to be such that the boundary condition should be met, thus the admissible  $\underline{B}$  vectors are determined from geometrical considerations. Each  $\underline{B}$  is a possible geometrical buckling. A core is critical if the material bucklings and geometrical bucklings are the same. It can be seen that  $\underline{B}=0$  corresponds to an infinite core. Practice has proved that  $\underline{B} \ll 1$  is a good approximation for large reactors. This approximation means that a finite core can be considered as an infinite core and finiteness may be taken into consideration as a perturbation<sup>12,15</sup>. This approximation is formulated by taking into account the  $\underline{B}$  dependence as a power series. Let us begin with  $k_{\text{eff}}$ . According to Theorem 4. it may be written as

$$k_{\text{eff}}^{-1} = \lambda_0 + \sum_{i=1}^3 \lambda_{2i} \cdot B_i^2 + O(\underline{B}^4) \quad /10/$$

The expansion of the  $u_{\underline{B}}/\underline{r}$  function  $/\underline{r}=(x_1, x_2, x_3)/$  is

$$u_{\underline{B}}(\underline{r}) = u_0(\underline{r}) - i\underline{B} \cdot u_1(\underline{r}) + \sum_{i=1}^3 u_{2i}(\underline{r}) \cdot B_i^2 + O(\underline{B}^3) \quad /11/$$

where only the space variable is written explicitly. If we substitute Eq./10/ and Eq./11/ into Eq./8/ and compare the coefficients of  $\underline{B}$  powers, the following is obtained:

$$(\underline{\Omega} \nabla + \hat{\Sigma}_0(\lambda_0)) u_0(\underline{r}, E, \underline{\Omega}) = 0 \quad /12a/$$

$$(\underline{\Omega} \nabla + \hat{\Sigma}_0(\lambda_0)) u_1(\underline{r}, E, \underline{\Omega}) = \underline{\Omega} u_0(\underline{r}, E, \underline{\Omega}) \quad /12b/$$



$$(\underline{\Delta} + \hat{\Sigma}_0(\lambda_0)) u_{2i}(\underline{r}, E, \underline{\Omega}) = \Omega_i u_{1i}(\underline{r}, E, \underline{\Omega}) + \kappa_{2i} \cdot u_0(\underline{r}, E, \underline{\Omega}) \quad /12c/$$

where the  $\hat{\Sigma}(k_{\text{eff}})$  cross section are written as  $i = 1, 2, 3$

$$\hat{\Sigma}(\underline{r}, E, k_{\text{eff}}) = \hat{\Sigma}_0(\underline{r}, E, \lambda_0) + \hat{\Sigma}_2(\underline{r}, E) \cdot \sum_{i=1}^3 \kappa_{2i} B_i^2 + O(B^4) \quad /13/$$

and

$$\begin{aligned} \hat{\Sigma}_0(\underline{r}, E, k_{\text{eff}}) = \Sigma(\underline{r}, E) \cdot & \int_0^{\infty} \int_{4\pi} \Sigma_3(\underline{r}, E' \rightarrow E, \underline{\Omega}, \underline{\Omega}') \cdot d\underline{\Omega}' dE' \\ & + \kappa_0 \frac{\chi(\underline{r}, E)}{4\pi} \int_0^{\infty} \int_{4\pi} \nu \Sigma_f(\underline{r}, E') \cdot d\underline{\Omega}' dE' \quad /14a/ \end{aligned}$$

$$\hat{\Sigma}_2(\underline{r}, E) = \frac{\chi(\underline{r}, E)}{4\pi} \int_0^{\infty} \int_{4\pi} \nu \Sigma_f(\underline{r}, E') \cdot d\underline{\Omega}' dE' \quad /14b/$$

The boundary conditions belonging to Eq./12/ are determined from the symmetry properties of the functions  $u_i$ ,  $i=0,1,2$ , and from the fact that each  $u_i$  is periodic. Applying the symmetry operations of the TE to Eq./12/ we obtain the following for a cylindrical cell /vectors have only a radial component/:

$$u_0(\underline{r}_c, E, \mu) = u_0(\underline{r}_c, E, -\mu) \quad /15a/$$

$$u_1(\underline{r}_c, E, \mu) = -u_1(\underline{r}_c, E, -\mu) \quad /15b/$$

$$u_2(\underline{r}_c, E, \mu) = u_2(\underline{r}_c, E, \mu) \quad /15c/$$

where  $\underline{r}_c$  denotes the boundary of the cell and  $\mu$  is the angle variable in the cylindrical coordinate system. Equation /15a/ is the usually used white boundary condition, Eq./15b/ prescribes a cross-flow through the cell and Eq. /15c/ leads again to the white boundary condition<sup>10</sup>. From Eq./12a/ and Eq./15a/ the  $u_0$  function and the  $\lambda_0$  eigenvalue are to be determined. Equations /12b/ and /15b/ do not represent an eigenvalue problem. The source in Eq./12a/ is known so it can be solved for  $u_1(\underline{r}, E, \underline{\Omega})$  and the solution shows how a cell "responds" to a cross flow. Equations /12c/ and /15c/ again present an eigenvalue problem. The direction-dependent eigenvalues  $E_{2i}, i=1,2,3$  can be determined from the solvability condition<sup>16</sup>. Denote by  $u_0^+(\underline{r}, E, \underline{\Omega})$  the solution belonging to the adjoint of Eq./12a/. The Fredholm alternative states that Eq./12c/ has a unique solution only if the RHS of Eq./12c/ is orthogonal to  $u_0^+(\underline{r}, E, \underline{\Omega})$ :

$$\int_0^\infty \int_{4\pi} \int_{V_c} (\rho_i u_{1i}(\underline{r}, E, \underline{\Omega}) + \lambda_{2i} \hat{\Sigma}_2 u_0(\underline{r}, E, \underline{\Omega})) u_0^+(\underline{r}, E, \underline{\Omega}) d\underline{r} d\underline{\Omega} dE = 0 \quad /16/$$

Introducing the  $(f, g)$  notation for the integral\*

$$(f, g) = \int_0^\infty \int_{4\pi} \int_{V_c} f(\underline{r}, E, \underline{\Omega}) \cdot g(\underline{r}, E, \underline{\Omega}) d\underline{r} dE d\underline{\Omega}$$

we obtain for the  $\lambda_{2i}$  eigenvalues

$$\lambda_{2i} = \frac{(u_0^+ ; \rho_i u_{1i})}{(u_0 ; \hat{\Sigma}_2 u_0)} \quad i=1,2,3 \quad /17/$$

i.e. the second eigenvalue set  $\lambda_{2i}, i=1,2,3$  can be obtained from the averaged fission cross section and from the  $u_{1i}$  functions, characterizing the behaviour of the cell in a flux gra-

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\*Here  $V_c$  is the volume of a cell.

dient. As to the solution of the eigenproblem set Eqs./12/-/15/, it seems that three equations have to be solved. Below, it will be shown that this is not the case,  $u_1$  and  $u_{2i}$  can be obtained from two solutions of Eq./12a/.

Let us assume that  $u_0$  has been determined. A particular solution to Eq./12b/ is  $\underline{r} \cdot u_0 / \underline{r}, E, \underline{\Omega} /$  and let us denote  $p$  as a solution of the homogeneous part of Eq./12b/; or, what is the same, of Eq./12a/. Then

$$u_1(\underline{r}, E, \underline{\Omega}) = \underline{p}(\underline{r}, E, \underline{\Omega}) + \underline{r} \cdot u_0(\underline{r}, E, \underline{\Omega}) \quad /18/$$

A solution of Eq./12c/ is

$$u_{2i}(\underline{r}, E, \underline{\Omega}) = \underline{r}^2 \cdot \frac{1}{2} \cdot u_0(\underline{r}, E, \underline{\Omega}) + \chi_i u_{1i} + \lambda_{2i} q(\underline{r}, E, \underline{\Omega}) \quad /19/$$

as can be seen by substituting Eq./19/ into Eq./12c/. The function  $q / \underline{r}, E, \underline{\Omega} /$  satisfies the equation:

$$(\underline{\Omega} \nabla + \Sigma_0(\lambda_0)) q(\underline{r}, E, \underline{\Omega}) = \hat{\Sigma}_2 u_0(\underline{r}, E, \underline{\Omega}) \quad /20/$$

This equation can be obtained by differentiating Eq./12a/ with respect to  $\lambda_0$  /see Ref.17/, therefore

$$q(\underline{r}, E, \underline{\Omega}) = \frac{\partial u_0}{\partial \lambda_0}(\underline{r}, E, \underline{\Omega}) \quad /21/$$

thus the  $u_{2i}$  function can be expressed as

$$u_{2i}(\underline{r}, E, \underline{\Omega}) = 0.5 \cdot \underline{r}^2 \cdot u_0(\underline{r}, E, \underline{\Omega}) + \chi_i u_{1i}(\underline{r}, E, \underline{\Omega}) + \lambda_{2i} \frac{\partial u_0}{\partial \lambda_0}(\underline{r}, E, \underline{\Omega}) \quad /22/$$

According to Eqs./22/ and /18/ the solutions of the eigenproblem set (Eqs./12/-/15/) are built up from  $u_0 / \underline{r}, E, \underline{\Omega} /$  and  $p / \underline{r}, E, \underline{\Omega} /$ . The former is determined from the eigenproblem /12a/

/15a/, the latter is a solution of Eq./12a/ so that Eq./15b/ should be fulfilled for  $\underline{u}_1$  that fixes an inhomogeneous boundary condition for  $p$ . In cylindrical geometry

$$p(r_c, E, \mu) = -r_c \cdot u_0(r_c, E, \mu) \quad /23/$$

Now that we have determined the solutions of the cell problems we may turn back to the expression of the neutron density, Eq./9/. Substituting Eq./11/ into Eq./9/ we have the following expression for the solution of the TE over the whole core:

$$\begin{aligned} \Psi(r, E, \underline{\Omega}) = & \phi_M(r) \cdot u_0(r, E, \underline{\Omega}) + \nabla \phi_M(r) \cdot \underline{u}_1(r, E, \underline{\Omega}) + \\ & + \sum_{i=1}^3 \frac{\partial^2}{\partial x_i^2} \phi_M(r) \cdot u_{2i}(r, E, \underline{\Omega}) + O(B^3) \end{aligned} \quad /24/$$

where the macroflux  $\phi_M$  is given by

$$\phi_M(r) = \int_{\mathbb{R}} w(\underline{B}) e^{i \underline{B} \cdot r} d\underline{B} \quad /25/$$

According to Eq./24/ the flux can be given as a power series of  $\underline{B}$ . The first member in this series is the well known Wigner-Seitz formula. Since the macroflux has been determined from the translational symmetry of the core the macroflux has a diffusion character: it does not depend on  $\underline{\Omega}$ . Actually it can be seen that Theorem 5. The macroflux in the power series of the neutron density satisfies a one-group diffusion equation. This fact is independent from the energy dependence of the TE.

We have still to determine  $W/\underline{B}$  in Eq./25/. For a core that is invariant with respect to the symmetries of a cell,  $W/\underline{B}=1$ . For a more complicated core the determination of  $W/\underline{B}$  is a rather complicated problem. These difficulties are often overcome by the numerical solution of a diffusion equation the solution of which is the macroflux.

All in all the rigorous foundation of the buckling method has resulted in expressing the neutron density as a power series of  $\underline{B}$ . The derivation given here includes the former results<sup>8,10,12</sup>, obtained by assuming a Bloch type source in Eq./1/.\* So far, the only exact method, viz. asymptotic analysis<sup>15</sup>, has given only the first member in Eq./24/. Our analysis gives not only two further members in the power series of the neutron density but Eqs./22/ and /18/ give the solution of the first and second order cell problem by two solutions of the zeroth order cell problem:  $u_0/\underline{r}, E, \underline{\Omega}$  / is a solution of a cell eigenproblem,  $p/\underline{r}, E, \underline{\Omega}$  / is a solution of a cell problem with an inhomogeneous boundary conditions (see Eq./23/). The derivation presented here is applicable to 2D and 3D problems whereas most of the derivations<sup>8,10,12</sup> are confined to one-group slab problems. We have used only one assumption: the symmetry of the cell and the core. Most of the cores and cells applied in power plants fulfil this assumption.

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\*The authors of the cited papers gave only the first or the first and second members in /24/.

## 5. HOMOGENIZATION

In the previous section a formula was obtained for the neutron density in a symmetric core. The microfunctions occurring in Eq./24/ can be determined from cell calculations. The macroflux (cf.Eq./25/) is determined from the buckling constraint boundary condition. However simple the boundary condition may be, an analytic expression relating  $W(\underline{B})$  in Eq./25/ to the zig-zag like boundary of the core is out of the question even for a core of high symmetry. The so far only way is to find a diffusion equation with constant coefficients in a cell and to solve it with the help of some numerical techniques. Several authors have set out to create the homogenized coefficients with ad hoc assumptions<sup>3-10</sup>. Hypothesizing that some basic property is preserved in a heterogeneous medium is a common assumption<sup>3,8,9</sup>.

Because of the derivation which is based on the investigation of the TE only we arrived at an explicit form of the macroflux. According to Theorem 5. there is a diffusion equation the solution of which is just the macroflux. Let us write this diffusion equation as

$$\sum_{i=1}^3 \bar{D}_i \frac{\partial^2 \phi_M(\underline{r})}{\partial x_i^2} + \left( \frac{\bar{\nu} \bar{\Sigma}_f}{k_{eff}} - \bar{\Sigma}_a \right) \phi_M(\underline{r}) = 0 \quad /26/$$

where the coefficients are so far unknown, the corresponding boundary condition is the buckling constraint:

$$\Phi_M(\underline{R}) = 0 \quad R \in \partial V$$

/27/

The eigenvalue in Eq./26/ can be expressed by the cross sections as

$$k_{eff}^{-1} = \frac{\bar{\Sigma}_a}{\sqrt{\bar{\Sigma}_f}} \left[ 1 + \sum_{i=1}^3 \frac{\bar{D}_i}{\bar{\Sigma}_a} \cdot B_i^2 \right] + O(B^4) \quad /28/$$

When solving the cell problems /12/ we found that the eigenvalue is determined by cell properties as given by Eq./17/.  $\kappa_0$  is the multiplication factor in the infinite core and it can be obtained from the cell balance with white boundary condition:

$$\kappa_0 = \frac{(u_0^+; \Sigma_a u_0)}{(u_0^+; \sqrt{\Sigma_f} u_0)} \quad /29/$$

If we compare Eq./28/ with Eq./10/ a relationship is obtained between the sought homogenized coefficients of Eq./26/ and the averages in Eqs./29/ and /17/. The choice of

$$\bar{\Sigma}_a = (u_0^+; \Sigma_a u_0) / (u_0^+; u_0) \quad /30a/$$

$$\sqrt{\bar{\Sigma}_f} = (u_0^+; \sqrt{\Sigma_f} u_0) / (u_0^+; u_0) \quad /30b/$$

$$\bar{D}_i = (u_0^+; \Omega_i u_{ii}) / (u_0^+; u_0) \quad i = 1, 2, 3 \quad /30c/$$

is in agreement with Eqs./29/, /17/ and /28/. Equation /30/ shows that the cross-section-like quantities in the TE can be

averaged by the neutron density of the infinite core but the diffusion constant  $\bar{D}_1$ , as it has no counterpart in the TE, is determined through the  $u_1$  function. In other words the diffusion coefficient is determined from the response of the cell to a cross flow. The homogenization method /30/ is the same one as obtained with asymptotic analysis<sup>15</sup>. It is not our goal to compare the homogenization methods here.



## 6. CONCLUSIONS

We have shown that the buckling method leads to a solution of the energy dependent, multidimensional TE. The solution is given as a power series of the buckling, see Eq./24/. The first members in this series are formed from microfluxes and a macroflux. The microfluxes are: the solution of a cell eigenproblem  $u_0$  with white boundary condition, see Eqs./12a/ and /15a/, and the vector solution  $p$  of the same equation with known eigenvalue but inhomogeneous boundary condition /23/. The microfluxes of the second and third terms are available through Eqs./18/ and /22/.

The solution of the TE for a finite core is sought as a linear combination of the infinite core solution. It is shown that the infinite core solutions are Bloch functions. The macroflux is expressed by an integral, see Eq./24/. This macroflux always satisfies a one-group diffusion equation. The coefficients in this equation are given from the  $u_0$  and  $u_1$  microfunctions and the space dependent cross sections in the TE, see Eq./28/.

The result derived here partly confirm asymptotic analysis (the cell eigenvalue problems, the leading term in Eq./24/ are the same), partly generalize those results (the linear and quadratic terms are also given in /24/). It is reassuring that such different methods as asymptotic analysis and the buckling method lead to the same conclusions.

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	Schrödinger Equation	Transport Equation
Equation	$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V \right] \Psi = E \Psi$	$\left[ \underline{D} \nabla^2 + \hat{\Sigma}(k_{eff}) \right] \Psi = 0$
Properties of the medium	V-potential	$\hat{\Sigma}$ - cross section
Eigen-value	E - energy	$k_{eff}$
Eigen-function	$\Psi$ - wave function	$\Psi$ - neutron density
Auxiliary parameter	$\underline{k}$ - wave vector	$\underline{B}$ - buckling

Table 1. Corresponding quantities of the Schrödinger Equation /SE/ and the Transport Equation /TE/.

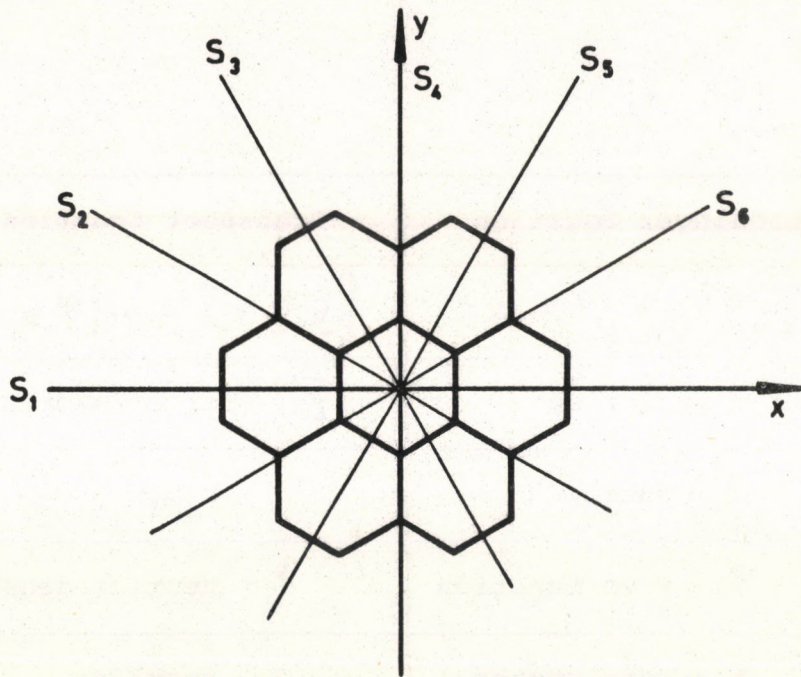


Fig. 1. A simple symmetric core with hexagonal cells .

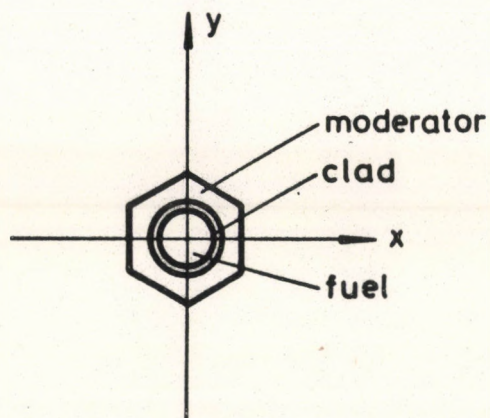
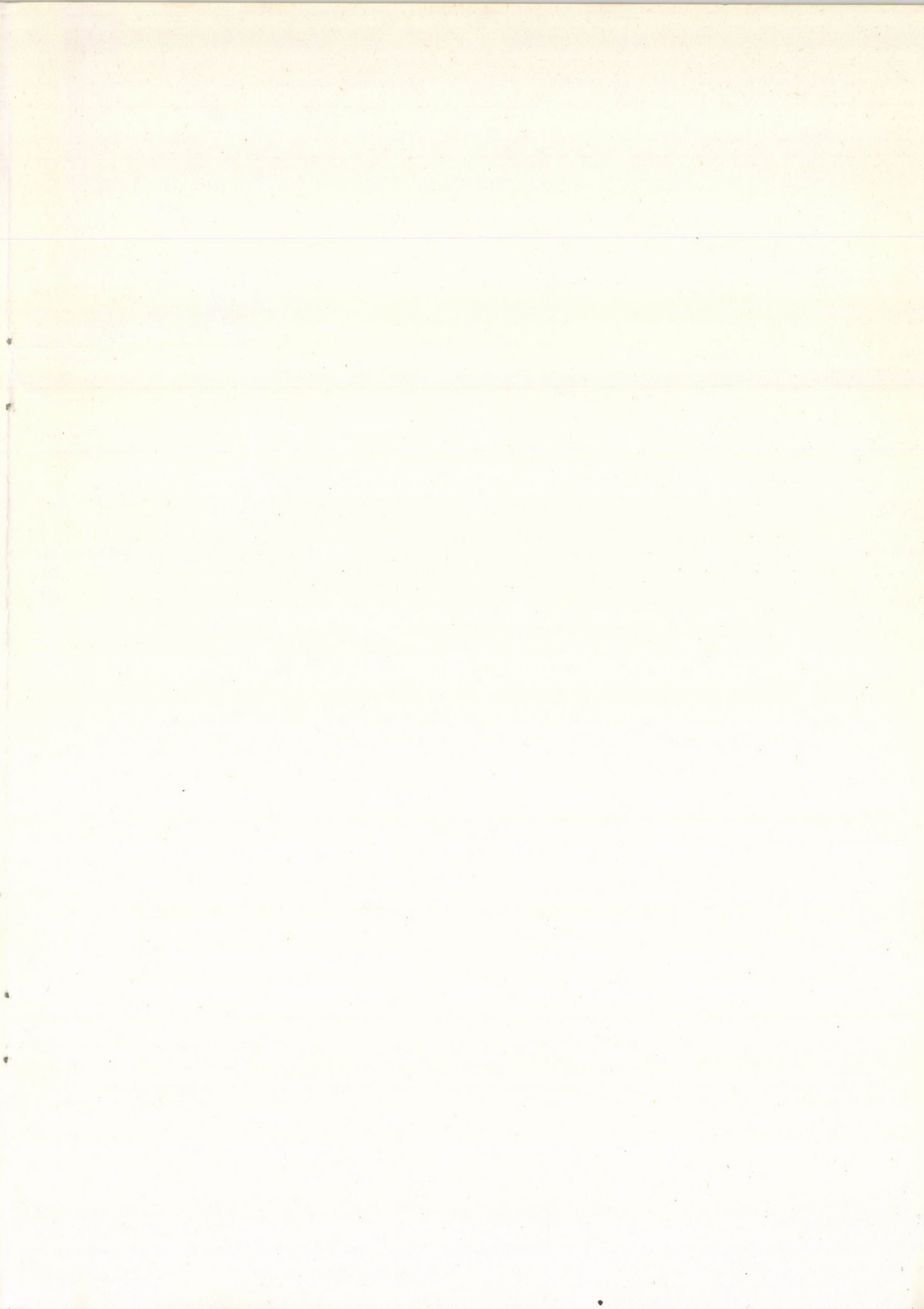
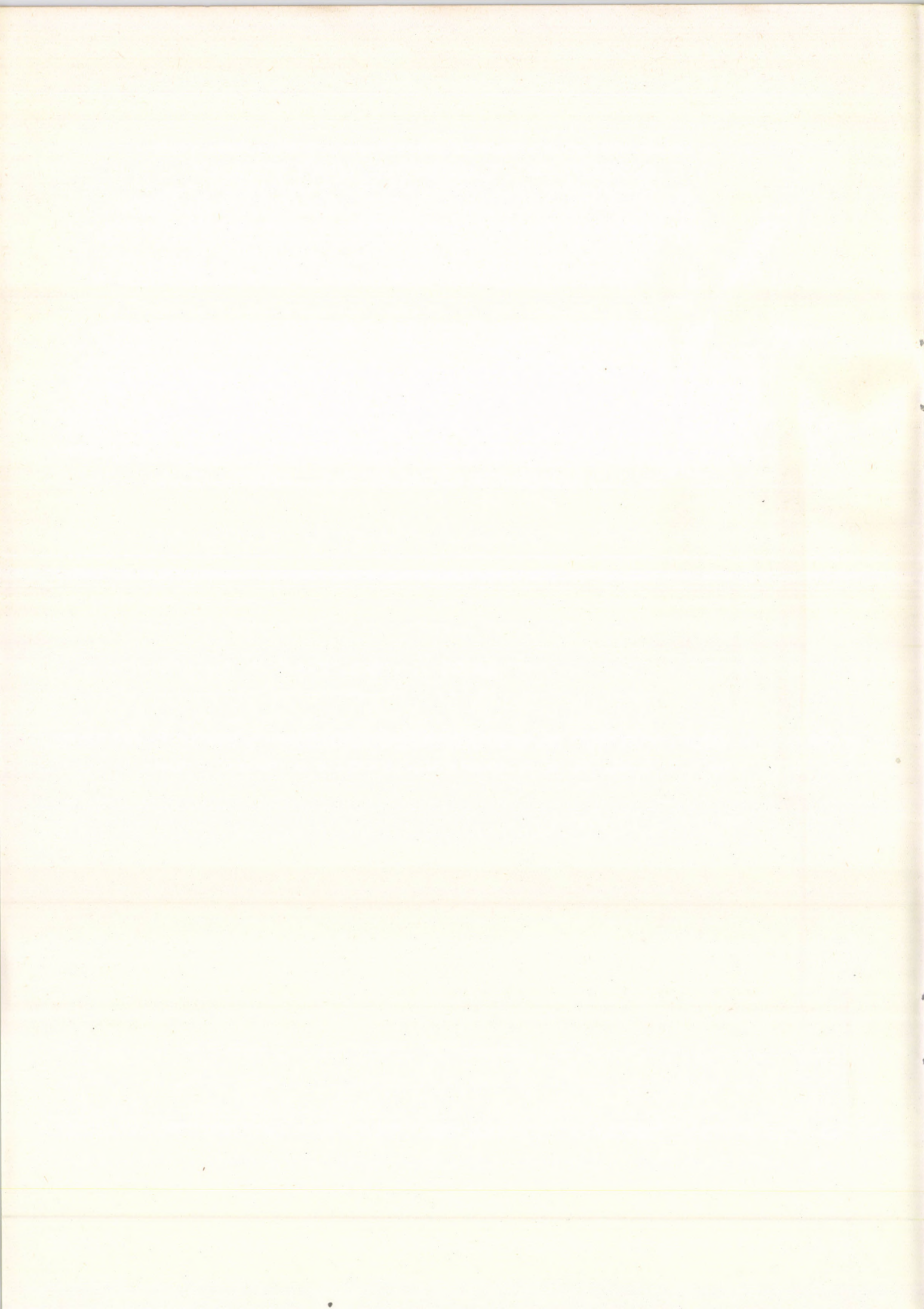


Fig. 2. A symmetric hexagonal cell.







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