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Abstract

The first flight collision probability for the square and hexagonal lattices is formulated as the extension of the probability in the cylindricalized cell, which was obtained previously by one of the authors. How the calculation time for the probability is made shorter is described, when the successive method is used for obtaining the length in the lattice system. The code for calculating the probability is also explained.

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Hiroshi Takahashi*

Takashi Nakayama**

* Division of Reactor Physics, Tokai Research Establishment

**Computing Center, Tokai Research Establishment

正方および六方格子系における衝突確率

要　　旨

著者の一人によって求められた円筒化近似系での衝突確率を計算する方法を拡張して，正方および六方格子においてこの確率を計算する方法を作った。格子系での各セル中を中性子が通る路の長さを逐次的に計算することによって，衝突確率をいかに短い時間で計算できるかが述べられており，さらにそれを計算するコードについて説明してある。

1964年7月

高　橋　　博*

中　山　　隆**

*　東海研究所原子炉物理部原子炉物理第1研究室

**　東海研究所計算センター室

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1. Introduction

In the applicability to complex systems, the method of the first flight collision probability (F. F. C. P.)[1], which is based on the integral neutron transport theory, has become more important than the differential theory. When the neutron transport equation is solved in the actual square and hexagonal lattices by the differential equation, the cylindrical cell approximation has often been used; one of the authors[1] formulated the integral transport equation for his cylindricalized cell. Chernick[2] showed, however, by the Pn method that the cylindricalized cell approximation is not accurate in the case of a closely packed lattice, and Newmarch[3] proved, by the integral formula mentioned above, that this inaccuracy is due to the perfectly reflected boundary condition for the neutrons on the circular cylindrical cell boundary. After these studies, many methods have been developed for this cylindricalized cell problem for the actual lattices.

As an exact method, Honeck[4] calculated the F. F. C. P. for the actual lattice system, by dividing the cell into many polygons, and Fukai[5] formulated the F. F. C. P. by extending the Ginsburg method for the Dancoff coefficient calculation. But these formulations require a long calculation time.

In the present paper, a simple exact formula for the F. F. C. P. in the actual square and hexagonal lattice is obtained as the extension of the cylindricalized-cell case. Although the length of neutron path in the actual lattice, from which the probability is calculated, is not the same, in all cells, as the cylindricalized cell, the length in a cell is easily obtained by the distance of neutron path from the center of cell before, because of the periodicity of the lattice. In the formula obtained, the property of the periodicity of the lattice system is used to reduce the calculation time. Also, the flat flux approximation in the subregions, which are divisions of many cylindrical rings and the outermost region, is used in

the same way as the usual F. F. C. P. . This approximation is exactly right in the case of Honeck's polygon method, if the cell is divided into a large number of subregions. But this method requires a long calculation time. This approximation holds accurately in the cylindrical cell in which the widths of subregion rings are narrow, because the flux in the system is cylindrically symmetry. But the flux in the actual lattice is not of a cylindrical symmetry. Consequently, even if the cell is divided into many subregions with narrow widths, the approximation is not exactly right. In spite of this, the approximation is used in the paper. In section 2, the general formula for the F. F. C. P. in the lattice system is derived. In section 3, it is explained how the length of the neutron path in each subregion is calculated in the F. F. C. P., using the perodic property of lattice system. In section 4, the code used in the calculation of the F. F. C. P. is described.

2. Formulation for the F. F. C. P. in a cylindrical rod lattice system

We consider a lattice system, consisting of infinitely long cylindrical rods and their cladding, as shown in Fig. 1. The first flight collision probability P_{ij} that the neutron born as a function $P_i(r, \alpha, \phi, \theta)$ in the i-th region with volume V_i will have its first collision in the j-th region, is expressed as follows;

$$P_{ij} = \frac{\int_{V_i} \int_{\Omega} P_i(r', \alpha, \phi, \theta)\, T_{ij}(r', \alpha, \phi, \theta) d\Omega dV}{\int_{V_i} \int_{\Omega} P_i(r', \alpha, \phi, \theta)\, d\Omega dV} \qquad (1)$$

where Ω is the solid angle, and the variables r', α, ϕ, θ, are illustrated in Fig. 1. In the case when the neutron path crosses the ith subregion twice, as shown in Fig. 1, the integration in terms of volume V is carried out over the both regions of $\overline{od_1}$ and of $\overline{d_2 d_3}$. These regions are suffixed by 1 and 2; the jth region also are suffixed as shown in Fig. 1. When the neutron path crosses the region once,

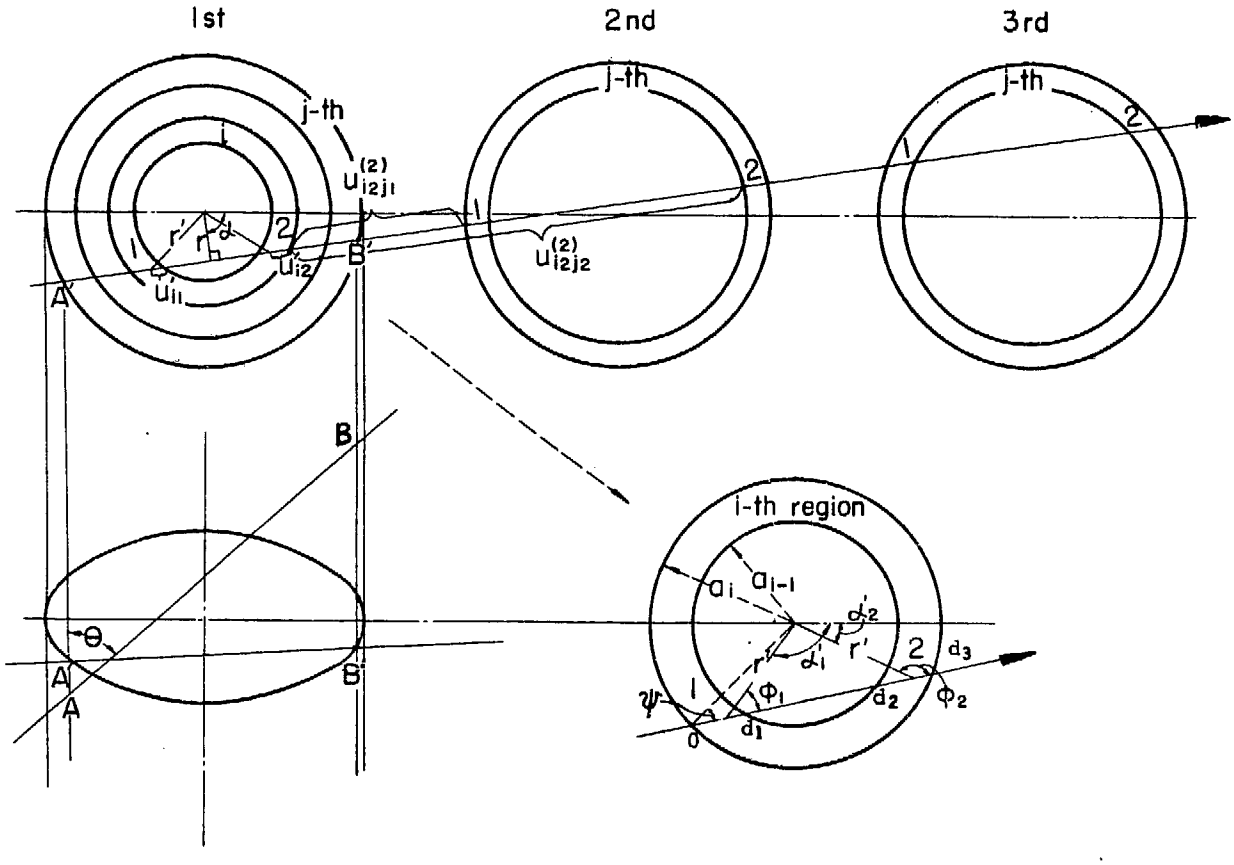


Fig. 1 The neutron path in the lattice system.

the neutron-path length is divided into two equal parts. The formula thus obtained is applicable in all cases including i = 1 and j = N+1.

The $T_{ij}(r', \alpha, \phi, \theta)$ in equation (1) is the collision probability for the neutron, which is born in the i-th region with function $P_i(r', \alpha, \phi, \theta)$. It is expressed as

$$T_{ikj}(r', \alpha, \phi, \theta) = \exp(-\frac{u'_{ik}}{\sin\theta}) \left\{ \exp(-\frac{u^{(1)}_{ikj1}}{\sin\theta}) \left[1 - \exp(-\frac{u^{(1)}_{j}}{\sin\theta}) \right] \right.$$

$$\left. + \sum_{q=2}^{\infty} \left[\exp(-\frac{u^{(q)}_{ikj1}}{\sin\theta}) + \exp(-\frac{u^{(q)}_{ikj2}}{\sin\theta}) \right] \left[1 - \exp(-\frac{u^{(q)}_{j}}{\sin\theta}) \right] \right\}$$

$$k = 1 \text{ and } 2 \qquad (2)$$

In the equation (2), are all the lengths of the neutron path projected into the plane perpendicular to the cylindrical axis, which were measured by the mean free path, the u'_{ik} is the length in the i_k-th region between the starting point (r', α'_k) and the point from which the path leaves the i_kth region. The $u^{(q)}_{ik, jk'}$ is the distance between the point where it leaves the i_kth region in the lst cell and the point where it enters the $j_{k'}$ in the qth cell, and the $u^{(q)}_{j}$ is the length of path in the j-th subregion in the q-th cell. These lengths are illustrated in Fig. 1.

The integration in terms of Ω and V in the equation is written as follows:

$$\widetilde{P}_{ij} = \frac{\int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} \cos\phi \, d\phi \int_0^{2\pi} d\alpha \int_0^{a_i} r' dr' \, P_i(r', \alpha, \phi, \theta) \, T_{ij}(r', \alpha, \phi, \theta)}{\int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} \cos\phi \, d\phi \int_0^{2\pi} d\alpha \int_0^{a_i} r' dr' \, P(r', \alpha, \phi, \theta)} \qquad (3)$$

The integration in terms of the variables (ϕ, r') is replaced by the integration in terms of the variable (ψ, x) shown in Fig. 1, by the following relations[4] between these variables.

$$\left. \begin{aligned} \frac{a_i}{\sin\phi} &= \frac{r'}{\sin\psi} \\ r'^2 &= a_i^2 + x^2 - 2 a_i x \cos\psi \end{aligned} \right\} \qquad (4)$$

The Jacobian of these variable is easily calculated

$$\left| \frac{\partial(\phi, r)}{\partial(\psi, x)} \right| = \frac{a_i \cos\psi}{r'} \tag{5}$$

and, we get

$$\tilde{P}_{ij} = \frac{a_i \int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\alpha \int_{-\pi/2}^{\pi/2} d\psi \cos\psi \left[\int_0^{d_1} dx + \int_{d_2}^{d_3} dx\right] P(x,\alpha,\psi,\theta) T_{ij}(x,\alpha,\psi,\theta)}{a_i \int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\alpha \int_{-\pi/2}^{\pi/2} d\psi \left[\int_0^{d_1} dx + \int_{d_2}^{d_3} dx\right] P(x,\alpha,\psi,\theta)} \tag{6}$$

It is difficult to get the closed form of the integration in terms of x, and so the flat flux approximation in the subregions has been often used. That is, the $P(x,\alpha,\psi,\theta)$ is replaced by a function, $P(\psi,\theta)$, independent of x and α. The subregions must be very small, so that the neutron flux in the regions may be approximated by the flat flux.

By integrating in terms of x, the equation (6) becomes

$$\begin{aligned}\tilde{P}_{ij} = a_i &\int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\alpha \int_{-\pi/2}^{\pi/2} d\psi \cos\psi\, P(\psi,\theta) \\ &\frac{\sin\theta}{\Sigma_i}\left[1 - \exp\left(-\frac{u_i^{(1)}}{\sin\theta}\right)\right]\left\{\left[\exp\left(-\frac{u_{i1j1}^{(1)}}{\sin\theta}\right) + \exp\left(-\frac{u_{i2j1}^{(1)}}{\sin\theta}\right)\right]\left[1 - \exp\left(-\frac{u_j^{(1)}}{\sin\theta}\right)\right]\right. \\ &+ \sum_{q=2}^{\infty}\left[\exp\left(-\frac{u_{i1j1}^{(q)}}{\sin\theta}\right) + \exp\left(-\frac{u_{i1j2}^{(q)}}{\sin\theta}\right) + \exp\left(-\frac{u_{i2j1}^{(q)}}{\sin\theta}\right) + \exp\left(-\frac{u_{i2j2}^{(q)}}{\sin\theta}\right)\right] \\ &\left.\times\left[1 - \exp\left(-\frac{u_j^{(q)}}{\sin\theta}\right)\right]\right\} \Big/ a_i \int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\alpha \int_{-\pi/2}^{\pi/2} d\psi \cos\psi\, P(\psi,\theta)\left[\overline{od_1} + \overline{d_2 d_3}\right]\end{aligned} \tag{7}$$

where $\overline{od_1}$ and $\overline{d_2 d_3}$ are the lengths of the od_1 are $d_2 d_3$. Although it is not difficult to calculate the equation (7) for the case of an anisotropic scattering medium[6], the isotropic scattering will be considered, because we deal with the simple F. F. C. P.. In this case, the integration in terms of θ is easily carried out and we get

$$P_{ij} = \frac{2a_i}{4\pi^2 \Sigma_i (a_i^2 - a_{i-1}^2)} \int_0^{2\pi} d\alpha \int_{-\pi/2}^{\pi/2} d\psi \cos\psi \left[F_0(\psi,\alpha) + F_1(\psi,\alpha)\right] \tag{8}$$

where

$$F_0(\psi,\alpha) = \sum_{\ell=1}^{2}\{K_{i3}(U_{ij}^1 + b_{\ell i}) - K_{i3}(U_{ij}^1 + b_{\ell i} + u_i^1) - K_{i3}(U_{ij}^1 + b_{\ell i} + u_j^1) + K_{i3}(U_{ij}^1 + b_{\ell i} + u_i^1) \quad (9)$$

$$F_1(\psi,\alpha) = \sum_{q=2}^{\infty}\sum_{\ell=1}^{2}\sum_{m=1}^{2} K_{i3}(U_{ij}^q + b_{\ell i} + c_{mi}^q) - K_{i3}(U_{ij}^q + b_{\ell i} + c_{mj}^q + u_i^1) - K_{i3}(U_{ij}^q + b_{\ell i} + c_{mi}^q + u_j^q) + K_{i3}(U_{ij}^q + b_{\ell i} + c_{mj}^q + u_i^1 + u_j^q) \quad (10)$$

and where, $K_{in}(x)$ is the Bickerley function defined by $K_{in}(x) = \int_0^{\frac{\pi}{2}} e^{-x/\sin\theta}(\sin\theta)^{n+1}d\theta$, and

$$\left.\begin{aligned} u_k^q &= \Sigma_k y_k^q a_0 \\ u_0^q &= \Sigma_0 y_0^q a_0 \\ b_{1i} &= 0\,, \qquad b_{2i} = 2\sum_{k=1}^{i-1} u_k^1 + u_i^1 \\ c_{1j}^q &= 0\,, \qquad c_{2j}^q = 2\sum_{k=1}^{j-1} u_k^q + u_j^q \\ U_{ij}^q &= U_{ij}^{(q-1)} + d_j^q \qquad q \geqslant 2 \\ U_{ij}^1 &= \sum_{k=i+1}^{j-1} u_k^1 \\ d_j^q &= \sum_{k=j}^{N} u_k^{(q-1)} + \sum_{k=j+1}^{N} u_k^q + u_\theta^{(q-1)} \end{aligned}\right\} \quad (11)$$

$a_0 y_k$ and $a_0 y_0/2$ are half the lengths of the neutron path in the kth and outermost regions, respectively; in the following section, how these lengths are calculated by the properties of the lattice are shown.

Since the lattice system is symmetric around the rod center, and the neutron path goes to the right in the study, the range of integration in terms of α over $0 \sim \pi/2$, is sufficient for the square lattice and over $0 \sim \pi/3$ for the hexagonal

lattice. At the same time, the range of integration in terms of ψ is limited to $0 \sim \pi/2$. For calculational convenience, the integration in terms of ψ is changed to the integration in terms of the distance from the neutron path to the rod center, by the following relation:

$$a_i \sin\psi = r \tag{12}$$

Finally, we get, for the square lattice,

$$P_{ij} = \frac{4}{\pi^2} \frac{1}{\sum (a_i^2 - a_{i-1}^2)} \int_0^{\pi/2} d\alpha \int_0^{a_i} dr \left[F_{0s}(r,\alpha) + F_{1s}(r,\alpha) \right] \tag{13}$$

and, for the hexagonal lattice,

$$P_{ij} = \frac{6}{\pi^2} \frac{1}{\sum_i (a_i^2 - a_{i-1}^2)} \int_0^{\pi/3} d\alpha \int_0^{a_i} dr_i \left[F_{0h}(r,\alpha) + F_{1h}(r,\alpha) \right] \tag{14}$$

where the suffices s and h are the values for the square and hexagonal lattices, respectively.

The F. F. C. P. P_{ij} for the case where the i or j is the inner or outermost region, is calculated by (13) and (14), because the length of the neutron path in these regions is divided into two equal lengths. The F. F. C. P. for this case is, however, simplified, in the square lattice.

$$\begin{aligned} P_{i\to 0} = \frac{4}{\pi^2} \frac{1}{(a_i^2 - a_{i-1}^2)} \int_0^{\pi/2} d\alpha \int_0^{a_i} dr \sum_{q=1}^{\infty} \sum_{\ell=1}^{2} \Big\{ & K_{i3}(U_{i0}^q + b_{\ell i}) \\ & - K_{i3}(U_{i0}^q + b_{\ell i} + u_i^1) - K_{i3}(U_{i0}^q + b_{\ell i} + u_0^1) \\ & + K_{i3}(U_{i0}^q + b_{\ell i} + u_i^1 + u_0^q) \Big\} \end{aligned} \tag{15}$$

$$\begin{aligned} P_{1\to j} = \frac{4}{\pi^2} \frac{1}{a_1^2} \int_0^{\pi/2} d\alpha \int_0^{a_i} dr \sum_{q=1}^{\infty} \sum_{m=1}^{2} \Big\{ & K_{i3}(U_{ij}^q + C_{mj}^q) \\ & - K_{i3}(U_{1j}^q + C_{rx,j}^q + u_j^1) - K_{i3}(U_{1j}^q + C_{mj}^q + 2u_1) \\ & + K_{i3}(U_{ij}^q + C_{mj}^q + u_j^1 + 2u_1) \Big\} \end{aligned} \tag{16}$$

$$P_{1\to 0} = \frac{4}{\pi^2}\frac{1}{a_1^2}\int_0^{\pi/2} d\alpha \int_0^{a_i} dr \sum_{q=1}^{\infty} \left\{ K_{i3}(U_{10}^q) - K_{i3}(U_{10}^q + u_0) - K_{i3}(U_{10}^q + 2u_1) + K_{i3}(U_{10}^q + u_0 + 2u_1) \right\} \quad (17)$$

where

$$\left.\begin{aligned} U_{i0}^1 &= \sum_{k=i+1}^{N} u_k^1 \\ U_{i0}^q &= U_{i0}^{(q-1)} + u_0^{(q-1)} + e_0^{(q-1)} \\ e_0^1 &= 0 \\ e_0^q &= 2\sum_{k=1}^{N} u_k^q \qquad \text{for } q \geqslant 2 \end{aligned}\right\} \quad (18)$$

The F. F. C. P. for the neutron from the jth region to the i-th region P_{ji} is calculated by the following reciprosity relation

$$P_{ij} V_i \Sigma_i = P_{ji} V_j \Sigma_j \quad (19)$$

and the F. F. C. P. for the neutron from the i-th region to the i-th reregion is calculated by the following relation

$$\sum_{j=1}^{N+1} P_{ij} = 1 \quad (20)$$

3. The Length of the neutron path in the square and hexagonal lattices

It has been shown in section 2 that the calculation of the F. F. C. P. for the lattice systems is easily carried out, if the lengths of the neutron path in the subregions are obtained for the system. In section 3, how the lengths in the subregions are calculated for the square and hexagonal lattices is shown. Since the lattice has a periodic property, if the relation between the distances for the adjoining two cells is obtained, the lengths in the cells following are successively calculated. This method is more simple than the method used in the Ginsburg's expression for the lattice system. First we consider the neutron path in the

square lattice as shown in Fig. 2. The cell is divided into N+1 subregions in such a way that the outer circle of the outermost Nth subregion touches that of the next cell (Fig. 2). The neutron path is determined uniquely by the distance from the center in the reference cell r^1 and by the angle α between $\overline{OA}$ and the reference direction. The length of the neutron path in the i-th subregion (whose number $i \leq N$) is a function only of the distance, r, of the neutron path from the cell center,

$$a_0 y_i^{(q)} = \sqrt{a_i^2 - r^{q2}} - \sqrt{a_{i-1}^2 - r^{q2}} \qquad i \leq N \tag{21}$$

The length of the neutron path in the (N+1)-th (0-th) outermost subregion is a function of r and α, and is calculated after obtaining the distance of the neutron path from the next-cell center. The distance in the next cell, r^{q+1}, is easily obtained as a simple function of the distance in the cell before, r^q, and the angle α; the lengths of the neutron path in the subregions are similarly determined successively.

For the square lattice, it is sufficient to consider the range of α, 0 to $\pi/2$, because of its symmetry. Then, a calculation of the distance of the neutron path in the next cell is made for the following three cases (Fig. 3). At a given value of θ, these cases depend on the distance, r^q, of the neutron path in the cell before.

For calculational simplicity, the distances of the cell centers are normalized to 2.

Thus,

1) $1 > r^q > 2 \sin\alpha - 1$

2) $0 \leq r^q < 1 - 2\cos\alpha$

3) $1 - 2\cos\alpha < r^q < 2\sin\alpha - 1$

And the distance of the neutron path in the next cell is determined as

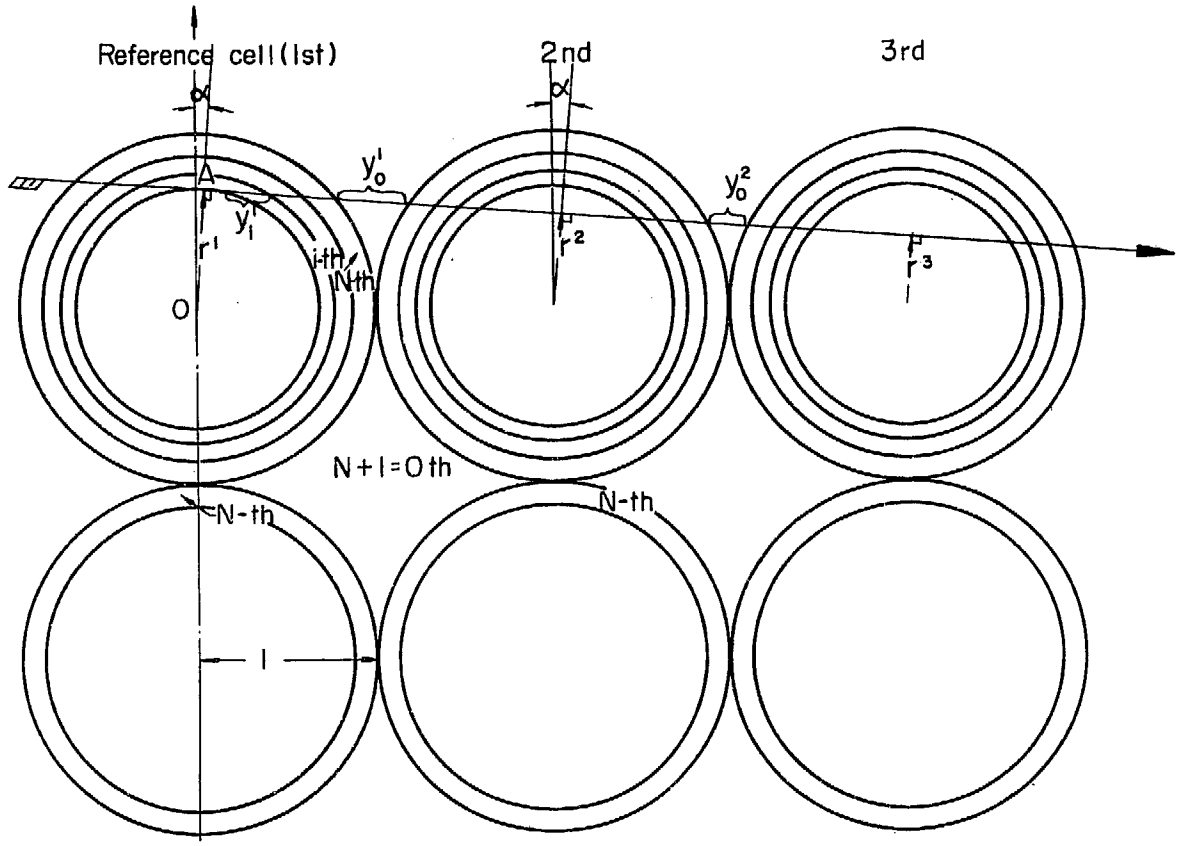
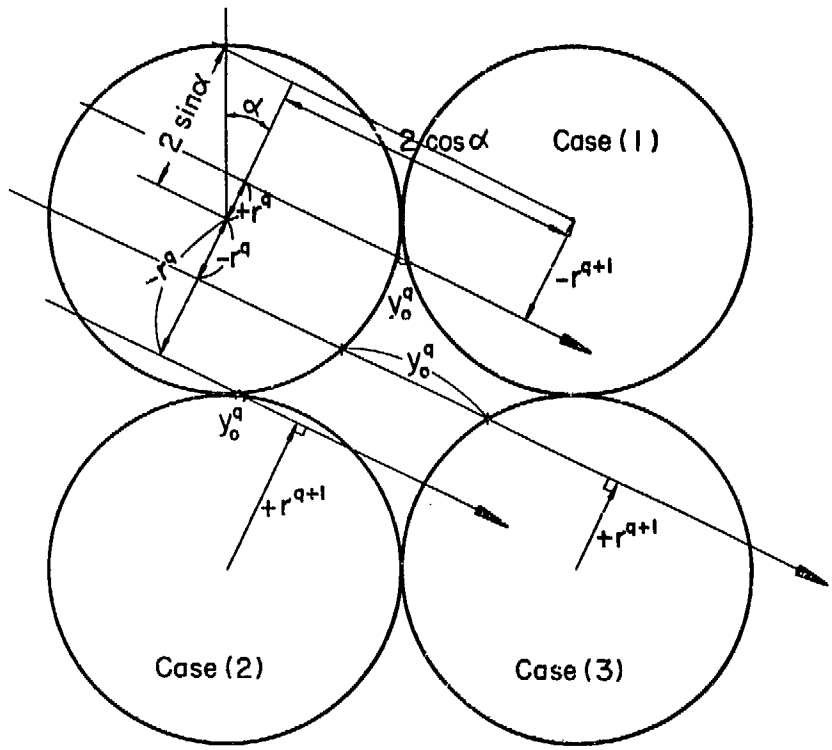
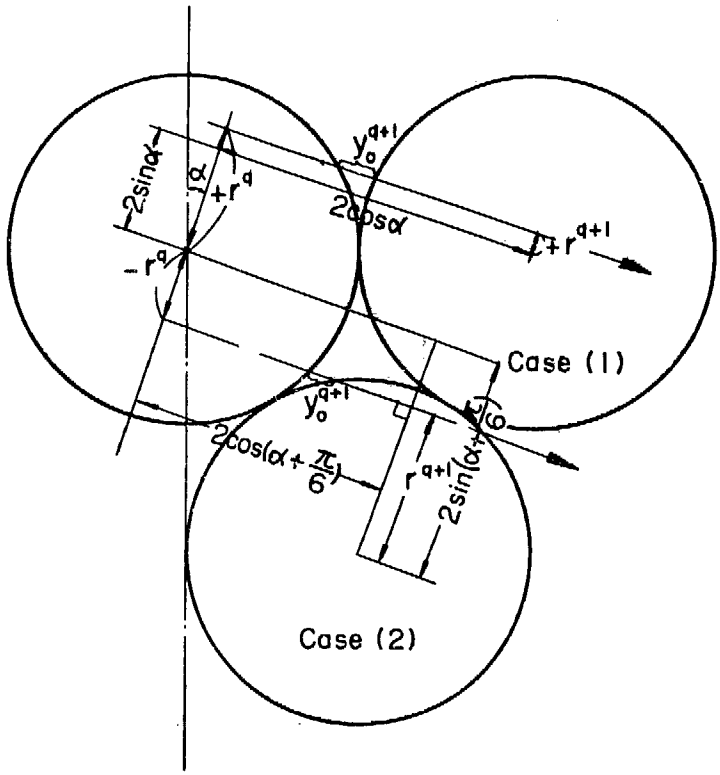


Fig. 2 The neutron path length in the normalized square lattice.



$$0 \leq \alpha \leq \frac{\pi}{2}$$

Fig. 3 Relation between the distances of the neutron paths from one and the next cells centers in square lattice.



$$0 \leq \alpha \leq \frac{\pi}{3}$$

Fig. 4 Relation between the distances of the neutron paths from one and the next cells centers in hexagonal lattice.

1) $r^{q+1} = r^q - 2\sin\alpha$

2) $r^{q+1} = r^q + 2\cos\alpha$

3) $r^{q+1} = r^q + 2(\cos\alpha - \sin\alpha)$

The length of the neutron path in the qth outermost region is

1) $y_0^q = 2\cos\alpha - \sqrt{1-r^{q2}} - \sqrt{1-r^{(q+1)2}}$

2) $y_0^q = 2\sin\alpha - \sqrt{1-r^{q2}} - \sqrt{1-r^{(q+1)2}}$

3) $y_0^q = 2(\cos\alpha + \sin\alpha) - \sqrt{1-r^{q2}} - \sqrt{1-r^{(q+1)2}}$

In the above expressions, the range of r^q is taken as $-1 < r^q < 1$. But if r^q is restricted to positive values, the expression for the case where r^q is negative must be used by changing the value α to $(\pi/2 - \alpha)$.

For the hexagonal lattice, two cases as shown in Fig. 4 should be considered. These cases depend on the distance, r^q, of the neutron path in cell before. Thus,

1) $1 \geq r^q > 2\sin\alpha - 1$

2) $r^q < 2\sin\alpha - 1$

The distance of the neutron path in the next cell is

1) $r^{q+1} = r^q - 2\sin\alpha$

2) $r^{q+1} = r^q - 2\sin(\alpha + \pi/6)$

The length of the neutron path in the outermost region is

1) $y_0^q = 2\cos\alpha - \sqrt{1-r^{q2}} - \sqrt{1-r^{(q+1)2}}$

2) $y_0^q = 2\cos(\alpha + \pi/6) - \sqrt{1-r^{q2}} - \sqrt{1-r^{(q+1)2}}$

If the r^q is restricted to positive values, the expressions for the case when r^q is negative, must be used by changing the value α to $(\pi/3 - \alpha)$.

When calculating on the computers, it is desirable to make tables for $r^{q+1}(r^q, \alpha)$ and $y^q(r^q, \alpha)$ and use the "look-up-the-table" method in order to reduce the calculation time.

In the cylindricalized cells in which the neutrons suffer perfect reflections at the cylindrical-cell boundary, the distances of the neutron path are the same in all the cells. The lengths of the neutron path are then periodic, and are independent of the angle α. Thus the expression very simple.

4. Calculation code GRAFA and concluding remark

The calculation code, GRAFA, for the first flight collision probability was written in the Fortran II of the IBM-7090 and the Fortran IV of the IBM-7044. This code can be used in the calculations for both the square and hexagonal lattice. The maximum number of subregions is 30. The tables for the length in the outermost region y^q and for the distance of the neutron path in the next cell r^{q+1} are made as a function of α and the distance in the cell before, r^q. The calculation of the F. F. C. P. is carried out by looking up these tables and a table for the lengths in the subregions, and so the accuracy depends on the finess of the tables. The maximum numbers of r_q and α are 30 and 10 respectively.

The code was used in the calculation of the thermal-neutron spectra for the square and hexagonal lattices, with the FIRST code, which was developed for the cylindrical cell system. The calculation time for the case where the numbers of the subregions and energy groups are 10 and 30, respectively, is less than 10 minutes.

In the paper, the method for the calculation of the F. F. C. P. for the square and hexagonal lattice systems has been described. As mentioned in section 2, the flat flux approximation, which is not exactly applicable in the actual lattices, is used. The use of the simple F. F. C. P. are limited to the isotropic-scattering medium, and so further study is desired on this problem.

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