lent to a linear integral equation with a symmetrical kernel, and the property of the system which is being evaluated is the average value of ϕ weighted by the inhomogeneous term $A_1(x)$ in the integral equation.

Imposing the two restrictions (a) and (b) has evidently limited us too greatly; while many physical systems admit of a description in terms of linear equations (which can always be written formally as an integral equation), they will generally involve unsymmetric kernels. Furthermore, while a weighted average of the state function is frequently of interest, one would like to be able to choose the weight function arbitrarily.

To overcome this difficulty, let us consider the possible descriptions, which admit the superposition principle and hence satisfy linear equations, of a scattering and absorbing medium in which neutrons are diffusing. (These considerations will also apply to more general physical systems.) One class of descriptions may be characterized as probability density distributions: the simplest example is the neutron density per unit phase space volume, but other possibilities are the flux, the absorption rate, and the collision rate. All of these descriptions are essentially equivalent since the calculation of any one from another is trivial. On the other hand, there is a second class of descriptions which may be characterized as probability distributions that a neutron at a given point in phase space will eventually undergo a particular process: for example, the probability of being absorbed, of escaping from the system, or of producing a second generation by causing a fission. While the members of this class are again essentially equivalent, it is usually not possible to obtain a description of one class from a description of the other class without solving again the equation defining the system.

We suppose, therefore, that for the case of a general linear system, the functional we are trying to evaluate will depend on a member of the second class of probability distributions, which we will denote by ϕ^+, as well as on a probability density distribution ϕ. As before, we can expand in a functional power series in both arguments and again terminate the series after the first term that leads to a nontrivial result:

$$F[\phi^+, \phi] = A_0 + \int dx A_1{}^+(x)\phi(x) + \int dx A_1(x)\phi^+(x) + \int dx \int dx' A_2(x, x')\phi^+(x)\phi(x') \tag{6}$$

Applying, now, requirement (b) leads to the following equations for the two arguments:

$$A_1(x) + \int dx' A_2(x, x')\phi(x') = 0 \tag{7}$$

$$A_1{}^+(x) + \int dx' A_2(x', x)\phi^+(x') = 0 \tag{8}$$

Using Eqs. (7) and (8) to simplify the expression for F results in

$$F[\phi^+, \phi] = A_0 + \int dx A_1{}^+(x)\phi(x) \tag{9}$$

when the arguments satisfy the two preceding equations.

In this case we have the following more general result: Imposing the requirements of simplicity and insensitivity on the calculation of a functional which depends on the two classes of state descriptions (probabilities and probability densities) implies that the theory describing the system must be in the form of a linear functional equation with no restrictions on the kernel, and that the class of functionals which can be computed in such theories consists of linear averages of the state description with an arbitrary weight function.

A restatement of this result is that the functional (6), regarded as dependent on two unknown functions ϕ and ϕ^+, is stationary in the neighborhood of the exact solutions and therefore constitutes a variational principle for Eqs. (7) and (8). It will provide an estimate of an arbitrary weighted average of the state function ϕ, provided that the weight function $A_1{}^+(x)$ is chosen as the inhomogeneous term of Eq. (8), which is recognized as the adjoint to Eq. (7). This is, in fact, just the functional proposed by Roussopoulos from formal considerations; the preceding discussion constitutes its derivation from the properties (a) and (b), which one can regard as plausible requirements to impose on a theory.

It is also clear from the preceding derivation that the functional F can be regarded as a Lagrangian for the theory, since the statement that F is stationary with respect to arbitrary small variations of its arguments permits us to deduce Eqs. (7) and (8) from the functional. Consequently, the procedure outlined here enables one to take a given linear theory and immediately write down a Lagrangian whose stationary property is equivalent to the equations of the theory, and which, at the same time, constitutes a variational principle for the estimation of an arbitrary linear functional of the state of the system.

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The Wigner-Seitz Cell; A Discussion and a Simple Calculational Method

A frequent problem in reactor design is the calculation of the thermal flux distribution in a fuel element and its associated moderator, i.e., the cell problem. For the sake of simplicity, a common design practice is to use a monoenergetic treatment, and the discussion in this letter is limited to this one-velocity approach. Because of the strong absorption in the fuel, P-1 (diffusion) theory is inadequate and a common practice is to employ a P-3 calculation. If the fuel element is cylindrical, the associated moderator (whose outside perimeter is frequently square or hexagonal) is often transformed, for the purposes of calculation, into an

"equivalent" annulus by demanding that the area of the mathematical annulus be equal to the actual cross-sectional area of the moderator. This procedure is referred to as the Wigner-Seitz approximation and results in a much simpler one-dimensional (in space) problem. In this letter we give a brief discussion of the existing calculational methods for the Wigner-Seitz cell and suggest a new and simple method which appears to be quite accurate.

Until recently the boundary conditions associated with the Wigner-Seitz cell were taken to be reflection of all neutrons at the cell boundary; i.e., every neutron incident on the cell boundary is reflected according to Snell's Law. This boundary condition is motivated by the fact that at the actual (square or hexagonal) cell boundary, symmetry considerations demand a reflection boundary condition. For the P-3 Wigner-Seitz approximation, the reflection boundary condition, in the notation of (*1*), implies

$$\psi_{11} = \psi_{31} = \psi_{33} = 0. \tag{1}$$

That is, three of the six moments are equated to zero at the cell boundary. Thie (*2*) has shown, however, that for tight lattices (thickness of the moderator annulus less than one mean free path) the P-3 Wigner-Seitz cell calculation, using Eq. (1) as the boundary conditions, leads to an inordinately large disadvantage factor (ratio of average flux in the moderator to average flux in the fuel). Since the same behavior was observed in high order S-N calculations (with reflecting boundary conditions), Thie concluded that the error stemmed from the physical model used, i.e., the Wigner-Seitz approximation with reflecting boundary conditions. That is, reflection from the curved Wigner-Seitz boundary is an artificiality which cannot be realized physically by the neutrons. Said another way, in order for symmetry considerations to imply reflection at a cell boundary, one must have an infinite symmetric array of cells filling all space. Obviously for cylindrical cells the geometry does not allow a completely filled space.

In order to improve the results of a cell calculation while still retaining the one-dimensional simplicity of theWigner-Seitz model, at least two sets of boundary conditions, different from Eq. (1), have been proposed. Honeck (*3*) has suggested (and used successfully) that the directional flux return from the cell boundary with a nearly isotropic distribution. This is accomplished by adding an optically thick outer region of pure scatterer (of infinite mass in the energy dependent problem) to the Wigner-Seitz cell. Secondly, Clendenin (*4*) has shown that the P-3 calculation can be improved by retaining the simple Wigner-Seitz cell (no extra region) but modifying the boundary conditions. Since ψ_{11} is the neutron current, he argues that all cell calculations must set ψ_{11} equal to zero at the cell boundary. As a second condition, the gradient of the scalar flux was set equal to zero at the cell boundary. As with the reflecting boundary conditions, the motivation for this lies in the fact that symmetry demands a zero gradient at the actual (square or hexagonal) cell boundary. As pointed out by Clendenin, reflecting boundary conditions on the cylindrical surface do not imply that the derivative of the scalar flux vanishes, except in the special case of the P-1 approximation. Several alternatives were tried for the third required boundary condition; the results were quite insensitive to this choice.

We now note that both of these suggestions, i.e., isotropic flux return and a zero spatial gradient are contained in a very simple theory, namely, P-1 (diffusion) theory. Thus one might expect diffusion theory to be quite adequate in the moderator. However, due to the strong absorption in the fuel, diffusion theory underestimates the flux dip in this region. Based on these arguments, one might expect that a theory employing diffusion theory in the moderator and a more accurate transport description in the fuel would yield quite good results. Such a theory is that of Amouyal *et al.* (*5*) and the results reported by Thie (*2*) indeed support the validity of this conclusion.

We now suggest another calculational method which has the two desired characteristics at the cell boundary, and has certain advantages over the method of Amouyal *et al.* and the P-3 method of Clendenin. This calculation employs a modified diffusion theory as recently described in ref. *6*. The main characteristics of this diffusion theory are:

1. The scalar flux in a homogeneous region has the asymptotic transport theory behavior.

2. The current at an interface between two media is continuous.

3. The scalar flux has a finite discontinuity at an interface between two media. This tends to compensate for the transient (rapidly varying) flux in the vicinity of an interface.

Although the formalism in (*6*) is constructed for slab geometry, we assume that the results are applicable to cylindrical geometry by merely writing the Laplacian in cylindrical coordinates. Assuming a spatially constant source in the moderator and no source in the fuel, the equations we must solve are

$$D_1\left[\frac{d^2\varphi_1(r)}{dr^2} + \frac{1}{r}\frac{d\varphi_1(r)}{dr}\right] - \Sigma_1(1 - c_1)\varphi_1(r) + S = 0, \tag{2}$$

$$D_0\left[\frac{d^2\varphi_0(r)}{dr^2} + \frac{1}{r}\frac{d\varphi_0(r)}{dr}\right] - \Sigma_0(1 - c_0)\varphi_0(r) = 0, \tag{3}$$

where subscripts 0 and 1 refer to the fuel and moderator respectively, D is the diffusion coefficient, $\varphi(r)$ is the scalar flux, Σ is the collision cross section, c is the mean number of secondaries per collision, and S is the magnitude of the source. The diffusion coefficient is taken to be the asymptotic transport diffusion coefficient,

$$D = (1 - c)/\nu^2\Sigma, \tag{4}$$

where

$$\frac{2\nu}{c} = \ln\left(\frac{1 + \nu}{1 - \nu}\right). \tag{5}$$

In Eq. (4) we have assumed isotropic scattering. To account for anisotropy in the scattering, one makes the transport correction, i.e., replaces the scattering cross section, Σ_s, by $\Sigma_s(1 - \bar{\mu})$, where $\bar{\mu}$ is the average cosine of the scattering angle. With the radius of the fuel rod as R_0 and the radius of the Wigner-Seitz cell as R_1, the appropriate boundary conditions are

$$\frac{d\varphi_0(0)}{dr} = \frac{d\varphi_1(R_1)}{dr} = 0, \tag{6}$$

$$J(R_0) = -D_1\frac{d\varphi_1(R_0)}{dr} = -D_0\frac{d\varphi_0(R_0)}{dr}, \tag{7}$$

$$\varphi_1(R_0) - \varphi_0(R_0) = |J(R_0)|(\Delta I), \tag{8}$$

TABLE I

DISADVANTAGE FACTORS BY VARIOUS METHODS

Lattice[a]	1	2	3	4
$\Sigma_{tr}^1(R_1 - R_0) =$	0.504	0.336	0.278	0.185
P-1	1.051	1.039	1.036	1.030
[b]P-3 (Clendenin)	1.099	1.077	1.075	1.059
This work (Eq. 9)	1.105	1.093	1.090	1.084
Monte-Carlo	1.135 ± 0.031	—	—	1.137 ± 0.012
Amouyal	1.170	1.169	1.155	1.159
P-3 (Reflecting)	1.165	1.188	1.207	1.265

[a] All lattices are 1.5% enriched uranium with a fuel rod radius of $R_0 = 0.15$ in. Thie (*2*) gives more detailed information on the lattice characteristics.

[b] These results take $\psi_{31} = 0$ as the third boundary condition. The results with other choices for this third condition are substantially the same (see ref. *4*).

where ΔI is an integral whose magnitude depends on the mismatch in cross sections between the fuel and the moderator. This integral has been computed numerically and is tabulated in (*6*). Our solution for the cell disadvantage factor, d, defined as the ratio of the average flux in the moderator to the average flux in the fuel, is

$$d = F + G + (E - 1)\left[\frac{\Sigma_0(1 - c_0)R_0^2}{\Sigma_1(1 - c_1)(R_1^2 - R_0^2)}\right], \quad (9)$$

where E, F, and G are given by

$$E = \frac{\nu_1\Sigma_1(R_1^2 - R_0^2)}{2R_0} \cdot \left[\frac{I_0(\nu_1\Sigma_1 R_0)K_1(\nu_1\Sigma_1 R_1) + K_0(\nu_1\Sigma_1 R_0)I_1(\nu_1\Sigma_1 R_1)}{I_1(\nu_1\Sigma_1 R_1)K_1(\nu_1\Sigma_1 R_0) - K_1(\nu_1\Sigma_1 R_1)I_1(\nu_1\Sigma_1 R_0)}\right], \quad (10)$$

$$F = \frac{\nu_0\Sigma_0 R_0}{2} \cdot \frac{I_0(\nu_0\Sigma_0 R_0)}{I_1(\nu_0\Sigma_0 R_0)}, \quad (11)$$

$$G = \frac{\Sigma_0(1 - c_0)(\Delta I)}{2}, \quad (12)$$

where I_i and K_i are the usual modified Bessel functions of the first and second kind. The functions E and F have the usual physical interpretations as noted by Glasstone and Edlund (*7*). The occurrence of the function G, which arises from the discontinuity of the scalar flux at $r = R_0$, is the major difference between this formulation and the P-1 result given by (*7*). A second, but less important, difference is that ν is defined in P-1 theory as $\nu = \sqrt{3(1 - c)}$ instead of by Eq. (5). However, in the limit as c approaches one, i.e., in the moderator, the P-1 definition and Eq. (5) agree. Thus only in the fuel is this second difference felt.

Equation (9) was used to compute the disadvantage factor for the first four lattices analyzed by Thie (*2*). Table I gives these results along with a summary of the results of Thie (*2*) and Clendenin (*4*). We see that the formulation suggested in this letter leads to a disadvantage factor significantly greater than the P-1 result. This is, of course, in the proper direction since P-1 theory underestimates the flux dip in the fuel. We also note that our results compare very favorably with the P-3 results of Clendenin (*4*). If one takes the 2-D Monte-Carlo results as a reference, our results are slightly better than Clendenin's P-3 results. It is also interesting to note that our results are an underestimate of the disadvantage factor, while the method of Amouyal *et al.* is an overestimate (again taking the Monte-Carlo results as a reference).

With regard to taking the Monte-Carlo results as a reference calculation several points should be made. For the purposes of these calculations, Thie (*2*) mentions that the fuel rod was approximated by a square with the corners removed. For tight lattices, this approximation could lead to significant errors. Further, the disadvantage factor should decrease as the water to fuel ratio decreases. The Monte-Carlo results do not show this trend. It is interesting to note that the method of Amouyal *et al.* as reported by Thie does not entirely show this trend either (see lattices 3 and 4 in Table I), whereas results using Amouyal's method reported by Honeck (*8*) do show the proper trend. Finally, the statistical errors in $(d - 1)$ associated with the Monte-Carlo results are quite large; i.e., 23% for lattice 1 and 9% for lattice 4. All of these points make the validity of the Monte-Carlo results for reference purposes open to suspect. Perhaps a better reference would be the P-3 results of Clendenin (*4*) with which our proposed method gives quite good agreement.

The advantage of the calculation proposed here over Clendenin's P-3 calculation is simplicity if one is doing a hand calculation and a savings in machine time if a computer is involved. The advantages of our method over that of Amouyal *et al.* (*5*) are several:

1. While the treatment of the moderator by the two methods is essentially the same, our method treats the fuel in a slightly simpler fashion.
2. Our method gives a flux distribution in the fuel.
3. Our method is applicable to an arbitrary number of regions.
4. Our method is capable of treating multidimensional problems.

This last point should be emphasized. One of the incentives for using diffusion theory for multidimensional problems is the relatively small amount of computer time involved. The modified diffusion theory suggested in this letter is no more complex than the usual (P-1) diffusion theory, but appears to give P-3 accuracy. This conclusion is supported by other calculations not reported here. Thus it may be feasible to do two-dimensional cell problems in routine design work.

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