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ISOPERIMETRIC AND OTHER INEQUALITIES IN THE THEORY OF NEUTRON TRANSPORT, II

Lawrence Dresner

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Abstract

In a previous paper[1] some inequalities occurring in the one-velocity theory of neutron transport with isotropic scattering were derived. In the present paper some of the previous results are generalized to the case of linearly anisotropic scattering.

1. Introduction

1.1. In a previous paper[1] the author stated and proved fourteen theorems concerning five quantities of interest that arise in the one-velocity theory of neutron transport. These quantities are all set-functions referring to bare, homogeneous, convex solids with isotropic scattering. The purpose of the present paper is to lift the restriction of isotropic scattering; accordingly the case of linear anisotropy is considered here.

1.2. Of the five quantities considered in I, only two need be considered here: the first-collision probability P of neutrons from the persisting distribution and the nonescape (absorption) probability P_a of neutrons from a uniform, isotropic source in the solid. The other three, the first-collision probability P_c from a uniform, isotropic source, the buckling B^2, and P_{ad}, the diffusion-theoretic value of P_a, need not be considered here at all. This is true for the diffusion-theoretic quantities B^2 and P_{ad} because the form of diffusion theory does not change with a changing angular distribution of scattering although the constants involved in the theory do. Thus, the theorems regarding B^2 and P_{ad} hold with at most some alterations in the constants. That P_c is entirely independent of any anisotropy follows from the fact that the angular distribution of scattering cannot make itself felt until after the first scattering has occurred; the theorems of I regarding it hold without any changes at all.

1.3. The theorems proved in I about P and P_a are of five distinct types. The first type is the inclusion theorem; it compares values of P and P_a in two solids one of which can be entirely inscribed in the other. The second type is the symmetrization theorem; it compares values of P and P_a in two

solids related by some process of symmetrization.[2] From the symmetrization theorem isoperimetric theorems can easily be derived.[3] The third type of theorem is that related to the so-called second fundamental theorem of reactor physics[4] and arises from the convexity[5] of the Fourier transform of the infinite-medium transport kernel. The fourth type is the factorization theorem; it compares, for example, the values of P for a considered solid with the product of the respective values for certain other solids whose orthogonal intersection is the considered solid. The fifth and last type of theorem relates the values of P, P_a, and P_c for a given solid.

1.4. All of these theorems are proved in I using variational representations for P and P_a. These representations are of the maximum type, that is, the functional whose stationary value is P or P_a is always $\leq$ P or P_a respectively. This latter property is ultimately a consequence of the isotropy of scattering assumed in I; the most important direct effect of this assumption is to allow the ordinarily non-self-adjoint transport equation to be reduced to a self-adjoint form. This self-adjointness combined with some other properties is enough to prove the maximum property of the variational principles used in I. The maximum property fails when the restriction of isotropy is lifted, and since it is a central feature in all the proofs in I, its failure prevents the direct transcription of the proofs in I <u>mutatis mutandis</u>.

In the present paper two devices are used to circumvent the loss of the maximum property. The first of these depends on the extremum property of the variational principle against small variations in the trial functions and is essentially a form of perturbation theory. It runs as follows:

When a physical property of the solid (e.g., volume, shape, degree of anisotropy of the scattering) changes by a small amount, the change induced in either P or P_a is independent to first order of the induced changes in the flux. This fact allows the derivation of formulae for the derivatives of P and P_a with respect to the physical parameters of the solid that do not involve the variation of the flux although they involve the flux itself. Frequently, it can be shown from these formulae that the derivatives of P and P_a with respect to certain properties of the solid have only one sign; from this fact an inequality can be immediately constructed. The second device involves the construction of an auxiliary problem that is self-adjoint and in which a quantity P' exists that is always $<$ P and that can be represented by a variational principle of the maximum type.

1.5. Using these two devices, it has been possible to prove some but not all of the types of theorems proved in I. An inclusion theorem has been proven for P and P_a identical with that of I. No symmetrization theorems have been proven nor has it been possible to prove an isoperimetric theorem; in fact, all that has been shown is that P and P_a are stationary against small, volume-preserving deformations of a sphere. A theorem of the third type mentioned above (that related to the second fundamental theorem) which is analogous to that of I has been proved. No factorization theorem has been proved. None of the three relations given in I between P, P_a, and P_c has been proved, but one new type of theorem has been proved, viz., one comparing the values of P (or P_a) corresponding to different degrees of anisotropy.

2. The Integral Transport Equation

2.1. Neutron transport in an infinite homogeneous medium is governed by the integro-differential Boltzmann equation[6]

$$\text{div}\,[\vec{\Omega}\psi(\vec{r},\vec{\Omega})] + \psi(\vec{r},\vec{\Omega}) = c\int f(\vec{\Omega}\cdot\vec{\Omega}')\,\psi(\vec{r},\vec{\Omega}')\,d\Omega' + Q/4\pi \qquad (1)$$

where $\psi(\vec{r},\vec{\Omega})$ is the collision density at $\vec{r}$ of neutrons traveling in a direction specified by the unit vector $\vec{\Omega}$, $f(\vec{\Omega}\cdot\vec{\Omega}')$ is the normalized angular distribution of secondary neutrons resulting from collision of primaries of direction $\vec{\Omega}'$, c is the number of secondary neutrons produced per collision, and $Q/4\pi$ is a uniform, isotropic, external source. Here, as in the rest of the paper, the unit of length has been chosen equal to the mean free path in the medium. When (1) is applied to a finite, homogeneous solid V the following boundary condition must be added to it:

$$\psi(\vec{r}_s,\vec{\Omega}) = 0 \qquad \text{if } \vec{n}\cdot\vec{\Omega} < 0, \qquad (2)$$

where $\vec{r}_s$ is any point on the surface S of V, and $\vec{n}$ is the outward normal at $\vec{r}_s$.

If Q = 0, Eqs. 1 and 2 describe the criticality of the solid V. Among the solutions of Eqs. 1 and 2 there will be a persisting distribution $\psi(\vec{r},\vec{\Omega})$, which is positive everywhere in V.[7] The value of c corresponding to it is the critical multiplication; its reciprocal c^{-1} is equal to P, the first-collision probability of neutrons from this persisting distribution.

2.2. When $f(\vec{\Omega}\cdot\vec{\Omega}') = (4\pi)^{-1}$, i.e., when the scattering is isotropic as considered in I, Eqs. 1 and 2 can be transformed into the following integral equation:

$$\phi(\vec{r}) = c\int_V \frac{\exp(-|\vec{r}-\vec{r}'|)}{4\pi\,|\vec{r}-\vec{r}'|^2}\,\phi(\vec{r}')\,d^3r' \qquad (3)$$

where $\phi(\vec{r}) = \int \psi(\vec{r},\vec{\Omega})d\Omega$. A similar transformation is possible when $f(\vec{\Omega}\cdot\vec{\Omega}')$

is a polynomial in $\vec{\Omega}\cdot\vec{\Omega}'$; the manner of making this transformation is fully explained by Davison,[8] but for the sake of completeness it will be sketched briefly here.

If $\vec{\Omega}$ is imagined to be held fixed, then

$$\text{div}\,[\vec{\Omega}\psi(\vec{r},\vec{\Omega})] = \vec{\Omega}\cdot\nabla\psi(\vec{r},\vec{\Omega}) = \frac{\partial\psi(\vec{r},\vec{\Omega})}{\partial s} \tag{4}$$

where s is the path length along any chord C of the solid V that points in the direction $\vec{\Omega}$. Substituting Eq. 4 into Eq. 1 converts the LHS of the latter into a first-order linear differential operator that can be inverted to give

$$\psi(\vec{r},\vec{\Omega}) = \int_0^s e^{-(s-s')}\, R(\vec{r}',\vec{\Omega})\, ds' \tag{5}$$

where $R(\vec{r},\vec{\Omega})$ represents the entire RHS of Eq. 1. In Eq. 5 the positive direction along C has been chosen in the direction of $\vec{\Omega}$, and the point s = 0 has been chosen as that intersection of C with S at which $\vec{\Omega}$ points into V. The point $\vec{r}'$ is given by

$$\vec{r}' = \vec{r} - (s - s')\,\vec{\Omega} \tag{6}$$

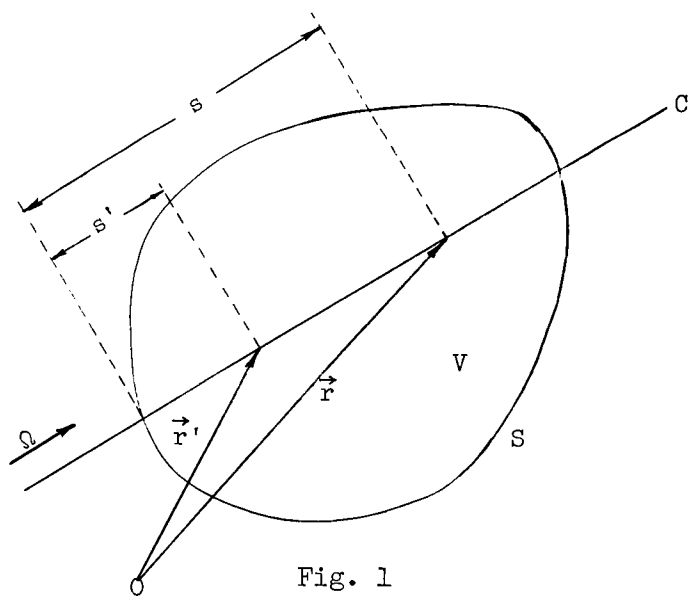

Fig. 1

In accordance with these definitions, it follows from Eq. 5 that $\psi(\vec{r},\vec{\Omega}) = 0$ when $s = 0$, as it should, since when $s = 0$ $\vec{r}$ is on S and $\vec{\Omega}$ points into V. If we now introduce the variable $\rho = s - s'$ we can rewrite Eq. 5 as

$$\psi(\vec{r},\vec{\Omega}) = \int_0^{s(\vec{r},\vec{\Omega})} e^{-\rho} \; R(\vec{r},\vec{\Omega}) \, d\rho \tag{7}$$

where $s(\vec{r},\vec{\Omega})$ is the distance from the point $\vec{r}$ to S in direction $-\vec{\Omega}$. Eq. 7 may be written out more fully by replacing R by its value from Eq. 1. It then becomes

$$\psi(\vec{r},\vec{\Omega}) = \int_0^{s(\vec{r},\vec{\Omega})} e^{-\rho} \; d\rho \left[c \int f(\vec{\Omega}\cdot\vec{\Omega}') \;\; \psi(\vec{r}',\vec{\Omega}') \, d\Omega' + Q/4\pi \right] \tag{8}$$

2.3. The case of linear anisotropy, which is dealt with in this paper, corresponds to a linear form for the function f, i.e.,

$$f(\vec{\Omega}\cdot\vec{\Omega}') = (4\pi)^{-1} \, (1 + 3\bar{\mu}\vec{\Omega}\cdot\vec{\Omega}') \quad , \tag{9}$$

where $\bar{\mu}$ is the average cosine of the scattering angle, that is, the angle between $\vec{\Omega}'$ and $\vec{\Omega}$. If Eq. 9 is introduced into Eq. 8 the latter becomes

$$\psi(\vec{r},\vec{\Omega}) = \int_0^{s(\vec{r},\vec{\Omega})} e^{-\rho} \, d\rho \left[\frac{c}{4\pi} \;\; \phi(\vec{r}') + \frac{c}{4\pi} \, 3\bar{\mu} \; \vec{\Omega}\cdot\vec{j}(\vec{r}') + Q/4\pi \right] \tag{10}$$

where the flux $\phi(\vec{r})$ is defined by

$$\phi(\vec{r}) = \int \psi(\vec{r},\vec{\Omega})\, d\Omega \tag{11}$$

and the current vector $\vec{j}(\vec{r})$ is defined by

$$\vec{j}(\vec{r}) = \int \vec{\Omega}\psi(\vec{r},\vec{\Omega})\, d\Omega \tag{12}$$

2.4. A pair of coupled integral equations for ϕ and $\vec{j}$ can now be derived from Eq. 10 by multiplication by 1 and $\vec{\Omega}$, respectively, and integration over $\vec{\Omega}$. To carry these steps out it is first necessary to note that

$$\vec{\Omega} = (\vec{r} - \vec{r}\,')/\rho \tag{13a}$$

$$\rho = |\vec{r} - \vec{r}\,'| \tag{13b}$$

and

$$\int d\Omega \int_0^{s(\vec{r},\vec{\Omega})} \ldots \rho^2 d\rho = \int_V \ldots d^3r' \tag{13c}$$

Then we can easily obtain from Eq. 10 the coupled pair:

$$\phi(\vec{r}) = c \int_V \frac{e^{-|\vec{r} - \vec{r}\,'|}}{4\pi|\vec{r} - \vec{r}\,'|^2} \left\{ \phi(\vec{r}\,') + 3\bar{\mu}\, \frac{(\vec{r} - \vec{r}\,')}{|\vec{r} - \vec{r}\,'|} \cdot \vec{j}(\vec{r}\,') \right\} d^3r' \tag{14a}$$

$$+ Q \int_V \frac{e^{-|\vec{r} - \vec{r}\,'|}}{4\pi|\vec{r} - \vec{r}\,'|^2}\, d^3r'$$

$$\vec{j}(\vec{r}) = c\int_V \frac{e^{-|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|^2}\left\{\frac{(\vec{r}-\vec{r}')}{|\vec{r}-\vec{r}'|}\,\phi(\vec{r}') + 3\bar{\mu}\,\frac{(\vec{r}-\vec{r}')}{|\vec{r}-\vec{r}'|}\,\frac{(\vec{r}-\vec{r}')}{|\vec{r}-\vec{r}'|}\cdot\vec{j}(\vec{r}')\right\} d^3r'$$

$$+ Q\int_V \frac{e^{-|\vec{r}-\vec{r}'|}}{4\pi\,|\vec{r}-\vec{r}'|^2}\,\frac{(\vec{r}-\vec{r}')}{|\vec{r}-\vec{r}'|}\,d^3r' \qquad (14b)$$

3. <u>The Variational Principle for P</u>

When $Q = 0$, Eqs. 14a and 14b define an eigenvalue problem for $c = P^{-1}$. By making use of the notation

$$K = \int_V \frac{e^{-|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|^2}\;\ldots\;d^3r' \;, \qquad (15a)$$

$$K\vec{\omega} = \int_V \frac{e^{-|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|^2}\,\frac{(\vec{r}-\vec{r}')}{|\vec{r}-\vec{r}'|}\;\ldots\;d^3r' \;, \qquad (15b)$$

etc., this eigenvalue problem can be written in the form

$$M\Phi = P\Phi \qquad (16a)$$

where Φ is the column vector

$$\begin{pmatrix} \phi(\vec{r}) \\ \vec{j}(\vec{r}) \end{pmatrix}$$

and the operator-matrix M is given by

$$M = \begin{pmatrix} K & 3\bar{\mu}\,K\vec{\omega} \\ K\vec{\omega} & 3\bar{\mu}\,K\vec{\omega}\vec{\omega} \end{pmatrix} \qquad (16b)$$

The adjoint of M is the operator-matrix.

$$M^{+} = \begin{pmatrix} K & -K\vec{\omega} \\ -3\bar{\mu}\ K\vec{\omega} & 3\bar{\mu}\ K\vec{\omega}\vec{\omega} \end{pmatrix} \tag{17a}$$

The minus signs occur here because in forming the adjoint of an integral operator the two arguments $\vec{r}$ and $\vec{r}'$ must be exchanged. The adjoint flux, $\phi^{+}(\vec{r})$, and current, $\vec{j}^{+}(\vec{r})$, are defined by Eq. 16a with M replaced by M^{+}. It is easily seen that

$$\phi^{+}(\vec{r}) = \phi(\vec{r}) \tag{17b}$$

$$\vec{j}^{+}(\vec{r}) = -3\bar{\mu}\vec{j}(\vec{r}) \tag{17c}$$

As is well known, a stationary expression for the eigenvalue P is

$$P = \frac{(\Phi^{+}, M\Phi)}{(\Phi^{+}, \Phi)} \tag{18}$$

When rewritten using 15a, b, 16b, and 17b, c, this equation becomes

$$P = \frac{\displaystyle\int_V d^3r \int_V d^3r' \left\{ \phi(\vec{r}) + 3\bar{\mu}\,\frac{(\vec{r}' - \vec{r})}{|\vec{r}' - \vec{r}|} \cdot \vec{j}(\vec{r}) \right\} \frac{e^{-|\vec{r} - \vec{r}'|}}{4\pi\,|\vec{r} - \vec{r}'|^2} \left\{ \phi(\vec{r}') + 3\bar{\mu}\,\frac{(\vec{r} - \vec{r}')}{|\vec{r} - \vec{r}'|} \cdot \vec{j}(\vec{r}') \right\}}{\displaystyle\int_V \left\{ \phi^2(\vec{r}) - 3\bar{\mu}\ j^2(\vec{r}) \right\} d^3r} \tag{19}$$

That this expression for P is stationary can now also be demonstrated directly by the usual methods of variational calculus; the work is straightforward.

4. Dependence of P on $\bar{\mu}$

4.1. Let ϕ^* and $\vec{j}^*$ satisfy (14a,b) with $Q = 0$ for a certain value of $\bar{\mu} = \bar{\mu}^*$ corresponding to a value of $P = P^*$. If $\bar{\mu}$ is given an increment $\delta\bar{\mu}$, i.e., if $\bar{\mu} = \bar{\mu}^* + \delta\bar{\mu}$, ϕ will equal $\phi^* + \delta\phi$ and $\vec{j}$ will equal $\vec{j}^* + \delta\vec{j}$. However, because Eq. 19 is a stationary expression for P, the first-order terms in $\delta\phi$ and $\delta\vec{j}$ in the expression for δP vanish identically. The first derivative of P with respect to $\bar{\mu}$ may therefore be calculated exactly by ordinary differentiation of Eq. 19 treating ϕ and $\vec{j}$ as constants that are equal respectively to ϕ^* and $\vec{j}^*$. The result of this differentiation is

$$\frac{1}{P^*}\frac{dP^*}{d\bar{\mu}} = -\frac{3\int_V j^{*2}(\vec{r})\, d^3r}{\int_V \left\{ \phi^{*2}(\vec{r}) - 3\bar{\mu} j^{*2}(\vec{r}) \right\} d^3r} , \qquad (20)$$

where use has been made of the fact that ϕ^* and $\vec{j}^*$ satisfy (14a,b) with $Q = 0$.

The numerator in the fraction in Eq. 20 is clearly positive, being the square of a real quantity. The denominator is also positive; this we show by noting that

$$\phi^2(\vec{r}) - 3\bar{\mu}\, j^2(\vec{r}) = 4\pi \int \psi(\vec{r},-\vec{\Omega})\, f(\vec{\Omega}\cdot\vec{\Omega}')\, \psi(\vec{r},\vec{\Omega}')\, d\Omega\, d\Omega' . \qquad (21)$$

Thus

$$\frac{dP^*}{d\bar{\mu}} < 0 \tag{22}$$

<u>and P is a monotone decreasing function of $\bar{\mu}$.</u>

4.2. It has been mentioned in the introduction that the variational principle for P is neither of the maximum nor of the minimum type. That this is so can be proven directly from Eq. 22 as follows. Let us assume that Eq. 19 is a variational principle of the maximum type. Then when $\bar{\mu} = \bar{\mu}^*$,

$$P^* \geqq J[\phi, \vec{j}] \tag{23}$$

where J is the functional appearing on the RHS of Eq. 19. Choosing $\phi = \phi_{iso}$ and $\vec{j} = 0$ where ϕ_{iso} is the solution of Eq. 14a when $\bar{\mu} = Q = 0$, we get from Eq. 23

$$P^* \geqq P_{iso} \tag{24}$$

where P_{iso} is the value of P corresponding to $\bar{\mu} = 0$. If we choose $\bar{\mu}^* > 0$, however, it follows from Eq. 22 that

$$P^* \leqq P_{iso}; \tag{25}$$

thus P* cannot be of the maximum type. A similar proof holds when the

variational principle is assumed to be of the minimum type, except that $\bar{\mu}$* must be chosen negative.*

5. Dependence of P on the Size and Shape of V

5.1. The dependence of P on the size and shape of V can be obtained by a procedure similar to that of Section 4. Let us begin by introducing the characteristic function $f(\vec{r})$ of the solid V, defined by

$$f(\vec{r}) = 1 \qquad \vec{r} \in V \tag{26a}$$

$$f(\vec{r}) = 0 \qquad \vec{r} \notin V \tag{26b}$$

Let us now consider a one-parameter family of convex solids $V(\epsilon)$ with characteristic functions $f(\vec{r},\epsilon)$ whose boundary surfaces vary continuously with ϵ. Let us denote the solutions of Eqs. 14a, b for these solids by $\phi(\vec{r},\epsilon)$ and $\vec{j}(\vec{r},\epsilon)$. With this notation Eq. 19 can be rewritten

$$P(\epsilon) = \int d^3r \int d^3r' \, f(\vec{r},\epsilon)\, f(\vec{r}',\epsilon) \left\{ \phi(\vec{r},\epsilon) + 3\bar{\mu} \frac{(\vec{r}' - \vec{r})}{|\vec{r}' - \vec{r}|} \cdot \vec{j}(\vec{r},\epsilon) \right\}$$

$$\times \quad \frac{e^{-|\vec{r} - \vec{r}'|}}{4\pi\, |\vec{r} - \vec{r}'|^2} \left\{ \phi(\vec{r}',\epsilon) + 3\bar{\mu} \frac{(\vec{r} - \vec{r}')}{|\vec{r} - \vec{r}'|} \cdot \vec{j}(\vec{r}',\epsilon) \right\} \Big/ \int f(\vec{r},\epsilon) \tag{27}$$

$$\times \quad \left\{ \phi^2(\vec{r},\epsilon) - 3\bar{\mu}\, j^2(\vec{r},\epsilon) \right\} d^3r$$

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*It may be argued that this proof does not preclude the possibility that Eq. 19 is a maximum principle for $\bar{\mu} < 0$ and a minimum principle when $\bar{\mu} > 0$. We can eliminate this possibility, however, as follows: Choose functions ϕ and $\vec{j}$ which are not solutions of Eq. 14a, b for any $\bar{\mu}$. Then P would be $> J(\bar{\mu})$ when $\bar{\mu} < 0$ and $< J(\bar{\mu})$ when $\bar{\mu} > 0$. Since J and P are both continuous functions of $\bar{\mu}$, P(0) would then equal J(0). But since ϕ and $\vec{j}$ are not solutions of Eq. 14 for any $\bar{\mu}$, $P(0) > J(0)$, for the variational principle is in fact of the maximum type when $\bar{\mu} = 0$ (see I).

Again because Eq. 27 is stationary with respect to first order variations in Φ and $\vec{j}$, the derivative of P with respect to ϵ may be calculated only by differentiating f:

$$\frac{1}{P}\left(\frac{dP}{d\epsilon}\right) = \frac{\int \frac{\partial f(\vec{r},\epsilon)}{\partial \epsilon}\left\{\Phi^2(\vec{r},\epsilon) - 3\bar{\mu}\, j^2(\vec{r},\epsilon)\right\} d^3r}{\int f(\vec{r},\epsilon)\left\{\Phi^2(\vec{r},\epsilon) - 3\bar{\mu}\, j^2(\vec{r},\epsilon)\right\} d^3r} \tag{28}$$

Use has again been made of the fact that Φ and $\vec{j}$ satisfy Eq. 14a, b.

5.2. If the family of solids $V(\epsilon)$ is such that $V(\epsilon_2)$ can be inscribed in $V(\epsilon_1)$ if $\epsilon_1 > \epsilon_2$, then $\frac{\partial f(\vec{r},\epsilon)}{\partial \epsilon} > 0$. Thus $dP/d\epsilon > 0$, from which it follows that <u>if a solid V_2 can be inscribed in another solid V_1, $P(V_1) \geq P(V_2)$.</u>

5.3. If the family of solids $V(\epsilon)$ is such that all members of it have the same volume V, then

$$0 = \frac{\partial V}{\partial \epsilon} = \frac{\partial}{\partial \epsilon}\int f(\vec{r},\epsilon)\, d^3r = \int \frac{\partial f(\vec{r},\epsilon)}{\partial \epsilon}\, d^3r \tag{29}$$

Now $\partial f(\vec{r},\epsilon)/\partial\epsilon$ is different from zero only on the surface of $V(\epsilon)$ (where it behaves like a delta function); thus if $\Phi^2(\vec{r},\epsilon) - 3\bar{\mu}j^2(\vec{r},\epsilon)$ were the same at every point of the surface of V, $dP/d\epsilon$ would be zero. This condition is certainly fulfilled if $V(\epsilon)$ is a sphere. Hence, <u>P is stationary against any infinitesimal, volume - preserving deformation of a sphere</u>.

Furthermore, it follows from Eqs. 28 and 29 that $\Phi^2 - 3\bar{\mu}j^2$ must be the same at every point on the surface of any solid for which P is stationary against any infinitesimal, volume-preserving deformation. The author

believes but has not proven that the only solid for which $\phi^2 - 3\bar{\mu}j^2$ is the same at every point on the surface is a sphere. If this were so, then among all solids of a given volume, P would be an extremum only for the sphere. It is physically obvious that this extremum would have to be a maximum, and the isoperimetric theorem would be proved: Of all solids of a given volume, P is greatest for the sphere.

Analogous remarks apply to the infinite right circular cylinder.

6. The Connection with the Second Fundamental Theorem

6.1. If Q = 0 in Eq. 14 and V is all space, one may introduce the Fourier transforms

$$\phi(\vec{k}) = \int \phi(\vec{r})\, e^{i\vec{k}\cdot\vec{r}}\, d^3r \tag{30a}$$

$$\vec{j}(\vec{k}) = \int \vec{j}(\vec{r})\, e^{i\vec{k}\cdot\vec{r}}\, d^3r \tag{30b}$$

and manipulate* Eq. 14 into the form

$$P_\infty\, \phi(\vec{k}) = \kappa(k)\, \phi(\vec{k}) + 3\bar{\mu}i\, \frac{1 - \kappa(k)}{k}\, \frac{\vec{k}}{k} \cdot \vec{j}(\vec{k}) \tag{31a}$$

$$P_\infty\, \frac{\vec{k}}{k} \cdot \vec{j}(\vec{k}) = i\, \frac{1 - \kappa(k)}{k}\, \phi(\vec{k}) + 3\bar{\mu}\, \frac{1 - \kappa(k)}{k^2}\, \frac{\vec{k}}{k} \cdot \vec{j}(\vec{k}) \tag{31b}$$

where $\kappa(k) = (\arctan k)/k$ and P_∞ denotes the infinite-medium eigenvalue. From Eq. 31 it follows that P_∞ is then the root of the secular equation

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*See Appendix 1.

$$0 = \begin{vmatrix} \kappa(k) - P_\infty & i3\bar{\mu}\,\dfrac{1-\kappa(k)}{k} \\ i\,\dfrac{1-\kappa(k)}{k} & 3\bar{\mu}\,\dfrac{1-\kappa(k)}{k^2} - P_\infty \end{vmatrix} \tag{32}$$

To each infinite medium solution there corresponds but one value of $k = |\vec{k}|$. Thus the infinite medium flux $\phi(\vec{r})$ satisfies the wave equation

$$\nabla^2 \phi(\vec{r}) + k^2\phi(\vec{r}) = 0 \tag{33}$$

6.2. The so-called second fundamental theorem of reactor physics is a method of estimation of P for finite solids based on the infinite medium equation 32. It consists of setting $k = B$ where B^2 is the lowest eigenvalue of Eq. 33 and some arbitrary boundary condition. This boundary condition generally has the form of a requirement that $\phi(\vec{r})$ vanish on some surface, usually chosen to be just outside the physical surface of the solid being considered. With a proper choice of boundary condition, the numerical accuracy of this method is quite high, but the method involves an unavoidable element of arbitrariness.

This latter feature is removed in the following theorem, which we shall prove in the following sections: <u>Let a solid V with surface S be given. Let B^2 be the lowest eigenvalue of Eq. 33 with the boundary condition $\phi(\vec{r}) = 0$ if $\vec{r} \epsilon S$. Then if $P(V)/[1-P(V)] \geqq 3\bar{\mu} \geqq 0$, $P(V) \geqq P_\infty(B)$.</u>

6.3. We begin by rewriting Eq. 14a. We make use of the identity

$$\frac{e^{-r}}{4\pi r^2}\left(\frac{\vec{r}}{r}\right) = -\nabla \int_r^\infty \frac{e^{-r'}}{4\pi r'^2}\,dr' = -\nabla \frac{E_2(r)}{4\pi r} \tag{34a}$$

where

$$E_2(u) = \int_1^\infty e^{-uv} \frac{dv}{v^2} \tag{34b}$$

Then

$$\int_V \frac{e^{-|\vec{r} - \vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|^2} \frac{(\vec{r} - \vec{r}')}{|\vec{r} - \vec{r}'|} \cdot \vec{j}(\vec{r}')\, d^3r' = \int_V \vec{j}(\vec{r}') \cdot \nabla_{r'} \frac{E_2(|\vec{r} - \vec{r}'|)}{4\pi\, |\vec{r} - \vec{r}'|}\, d^3r'$$

$$= -\int_V \frac{E_2(|\vec{r} - \vec{r}'|)}{4\pi\, |\vec{r} - \vec{r}'|} \nabla_{r'} \cdot \vec{j}(\vec{r}')\, d^3r' + \int_S \frac{E_2(|\vec{r} - \vec{r}'|)}{4\pi\, |\vec{r} - \vec{r}'|} \vec{j}(\vec{r}') \cdot d\vec{S}' \tag{35}$$

where the last integral is a surface integral over the surface S of V. $\nabla \cdot \vec{j}$ may be expressed in terms of ϕ through the equation of continuity which follows from Eq. 1 by integration over Ω:

$$\nabla \cdot \vec{j}(\vec{r}) = (c - 1)\, \phi(\vec{r}) + Q \tag{36}$$

Substituting Eqs. 36 and 35 in 14a ($Q = 0$), we get:

$$P\phi(\vec{r}) = \int_V \left\{ \frac{e^{-|\vec{r} - \vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|^2} - 3\bar{\mu}(c-1) \frac{E_2(|\vec{r} - \vec{r}'|)}{4\pi\, |\vec{r} - \vec{r}'|} \right\} \phi(\vec{r}')\, d^3r' \tag{37}$$

$$+ 3\bar{\mu} \int \frac{E_2(|\vec{r} - \vec{r}'|)}{4\pi\, |\vec{r} - \vec{r}'|} \vec{j}(\vec{r}') \cdot d\vec{S}'$$

6.4. Let us now consider an auxiliary problem defined by the self-adjoint integral equation

$$P'\chi(\vec{r}) = \int_V \left\{ \frac{e^{-|\vec{r} - \vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|^2} - 3\bar{\mu}(c - 1) \frac{E_2(|\vec{r} - \vec{r}'|)}{4\pi|\vec{r} - \vec{r}'|} \right\} \chi(\vec{r}')\, d^3r' \qquad (38)$$

In Eqs. 37 and 38 c has exactly the same value; in 37 $c = P^{-1}$, but in Eq. 38, of course, no such simple relation holds between P' and c. Let us for the moment consider only those cases in which $(c - 1)^{-1} \geq 3\bar{\mu} \geq 0$. In this case the eigenvalues $c'_n = (P'_n)^{-1}$ are all real and positive and form a discrete set; furthermore, to the lowest of these eigenvalues c'_o there corresponds an eigenfunction $\chi_o(\vec{r})$ which is everywhere positive in V (see Appendix 2). Thus a variational principle of the maximum type holds for P'_o (henceforth we will drop the subscript zero and only be concerned with the lowest mode):

$$P' \geqq \frac{\int_V d^3r \int_V d^3r'\, \chi(\vec{r}) \left\{ \frac{e^{-|\vec{r} - \vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|^2} - 3\bar{\mu}(c - 1) \frac{E_2(|\vec{r} - \vec{r}'|)}{4\pi|\vec{r} - \vec{r}'|} \right\} \chi(\vec{r}')}{\int_V \chi^2(\vec{r})\, d^3r} \qquad (39)$$

where $\chi(\vec{r})$ is now arbitrary.

6.5. If we multiply Eq. 37 by $\chi(\vec{r})$, Eq. 38 by $\phi(\vec{r})$, integrate over $\vec{r}$ and subtract, we obtain

$$(P-P')\int_V \phi(\vec{r})\ \chi(\vec{r})\ d^3r = 3\bar{\mu}\int_V\int_S \chi(\vec{r})\ \frac{E_2(|\vec{r}-\vec{r}'|)}{4\pi|\vec{r}-\vec{r}'|}\ \vec{j}(\vec{r}')\cdot d\vec{S}'\ d^3r \qquad (40)$$

now since $\vec{j}(\vec{r})\cdot\vec{n} = \int \psi(\vec{r},\vec{\Omega})\vec{\Omega}\cdot\vec{n}\ d\Omega$ and since for a point on the surface S only values of $\vec{\Omega}$ for which $\vec{\Omega}\cdot\vec{n} > 0$ contribute to the integral, the integrand on the RHS of Eq. 40 is positive. Thus if $\bar{\mu} \geq 0$,

$$P \geq P' \qquad (41)$$

6.6. Let us now introduce the Fourier transform

$$\chi(\vec{k}) = \int_V \chi(\vec{r})\ e^{i\vec{k}\cdot\vec{r}}\ d^3r \qquad (42)$$

into Eq. 39. Then it becomes*

$$P' = \frac{\int |\chi(\vec{k})|^2 \left\{ \kappa(k) - 3\bar{\mu}(c-1)\frac{1-\kappa(k)}{k^2} \right\} d^3k}{\int |\chi(\vec{k})|^2\ d^3k}$$

If $3\bar{\mu}(c-1) \leq 7/5$ the quantity in braces in Eq. 43 is a positive, convex-downwards, decreasing function of k^2.** Therefore, by theorem 204 of Hardy <u>et al</u>.

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*See Appendix 2.
**See Appendix 3.

$$P' \geqq \kappa(k_o) - 3\bar{\mu}\,(c - 1)\,\frac{1 - \kappa(k_o)}{k_o^2} \tag{44a}$$

where

$$k_o^2 = \frac{\int |\chi(\vec{k})|^2\, k^2\, d^3k}{\int |\chi(\vec{k})|^2\, d^3k} \tag{44b}$$

If we invert the transforms in Eq. 44b, noting that

$$i\nabla\chi(\vec{r}) = (2\pi)^{-3} \int \vec{k}\, \chi(\vec{k})\, e^{-i\vec{k}\cdot\vec{r}}\, d^3k \tag{45}$$

we find

$$k_o^2 = \frac{\int_V |\nabla\chi(\vec{r})|^2\, d^3r}{\int_V \chi^2(\vec{r})\, d^3r} \tag{46}$$

The RHS of Eq. 45 can only converge if $\chi(\vec{r}) = 0$ on S, the surface of V, for otherwise since $\chi(\vec{r}) = 0$ outside of V (see Eq. 42), $\nabla\chi(\vec{r})$ will have an infinite singularity on S. Since the trial function $\chi(\vec{r})$ is arbitrary we now choose it to vanish on S. Now because the RHS of Eq. 44 is a monotone decreasing function, the best value of k_o will be the smallest possible. Under the boundary condition $\chi(\vec{r}) = 0$ on S, the minimum of Eq. 46 is achieved for that trial function $\chi(\vec{r})$ which satisfies the wave equation

$$\nabla^2\, \chi(\vec{r}) + B^2\chi(\vec{r}) = 0, \tag{47}$$

and the minimum value of k_o is just B. Combining this fact with Eq. 44 and Eq. 41, we obtain

$$P \geqq \kappa(B) - 3\bar{\mu}\left(\frac{1}{P} - 1\right)\frac{1 - \kappa(B)}{B^2} \tag{48a}$$

or

$$P^2 - P\left(\kappa + 3\bar{\mu}\,\frac{1 - \kappa}{B^2}\right) + 3\bar{\mu}\left(\frac{1 - \kappa}{B^2}\right) \geqq 0 \ . \tag{48b}$$

With an equality sign Eq. 48b is just the equation determining P_∞; this follows from Eq. 32. If we call the larger and smaller roots of Eq. 48b P_∞ and P'_∞, respectively, then either $P \geqq P_\infty$ or $P \leqq P'_\infty$. When $\bar{\mu} = 0$ we know that $P \geqq P_\infty$;[1] hence by the continuity of these functions, this conclusion must be true for finite $\bar{\mu}$.

6.7. The proof given above depends upon the two conditions $P/(1-P) \geqq 3\bar{\mu} \geqq 0$. The condition $3\bar{\mu} \geqq 0$, although sufficient, is not necessary. For since P exceeds P_∞ in a finite solid by a finite amount when $\bar{\mu} = 0$, it must also do so for sufficiently small negative values of $\bar{\mu}$. This raises the question of whether the theorem is true for all negative values of $\bar{\mu}$. A comparison shown in Table 1 of P values previously calculated by the author for slabs with the corresponding values of P_∞ supports the validity the theorem for all negative $\bar{\mu}$. No proof of this validity, however, has yet been found.

The other condition, which may be rewritten $P \geqq 3\bar{\mu}/(1 + 3\bar{\mu})$, limits the applicability of the theorem to solids larger than a certain size.

Table 1. Comparison of P(V) and $P_\infty(B)$ for Slabs

Thickness	$\bar{\mu}$	P_∞	P
0.2	-0.3333	0.1222	0.2685
0.2	-0.2500	0.1167	0.2667
0.2	-0.1666	0.1106	0.2648
0.2	-0.0833	0.1038	0.2630
0.2	0.	0.0959	0.2611
0.2	0.0833	0.0862	0.2592
0.2	0.1666	0.0725	0.2574
0.2	0.2500		0.2555
0.2	0.3333		0.2537
0.4	-0.3333	0.2285	0.4097
0.4	-0.2500	0.2192	0.4063
0.4	-0.1666	0.2089	0.4030
0.4	-0.0833	0.1973	0.3997
0.4	0.	0.1838	0.3964
0.4	0.0833	0.1674	0.3931
0.4	0.1666	0.1448	0.3898
0.4	0.2500		0.3865
0.4	0.3333		0.3831
1.0	-0.3333	0.4701	0.6407
1.0	-0.2500	0.4561	0.6353
1.0	-0.1666	0.4404	0.6299
1.0	-0.0833	0.4226	0.6244
1.0	0.	0.4019	0.6190
1.0	0.0833	0.3768	0.6136
1.0	0.1666	0.3441	0.6081
1.0	0.2500	0.2913	0.6027
1.0	0.3333		0.5973
2.0	-0.3333	0.7013	0.8059
2.0	-0.2500	0.6886	0.8002
2.0	-0.1666	0.6744	0.7945
2.0	-0.0833	0.6580	0.7887
2.0	0.	0.6390	0.7830
2.0	0.0833	0.6163	0.7773
2.0	0.1666	0.5878	0.7715
2.0	0.2500	0.5489	0.7658
2.0	0.3333	0.4817	0.7601

Table 1 (Continued)

Thickness	$\bar{\mu}$	P_∞	P
4.0	-0.3333	0.8810	0.9185
4.0	-0.2500	0.8743	0.9144
4.0	-0.1666	0.8666	0.9103
4.0	-0.0833	0.8579	0.9062
4.0	0.	0.8476	0.9021
4.0	0.0833	0.8355	0.8980
4.0	0.1666	0.8207	0.8939
4.0	0.2500	0.8019	0.8898
4.0	0.3333	0.7767	0.8857
8.0	-0.3333	0.9642	0.9730
8.0	-0.2500	0.9619	0.9709
8.0	-0.1666	0.9593	0.9689
8.0	-0.0833	0.9563	0.9668
8.0	0.	0.9528	0.9648
8.0	0.0833	0.9487	0.9628
8.0	0.1666	0.9437	0.9607
8.0	0.2500	0.9376	0.9587
8.0	0.3333	0.9298	0.9566
20.0	-0.3333	0.9939	0.9949
20.0	-0.2500	0.9935	0.9944
20.0	-0.1666	0.9930	0.9939
20.0	-0.0833	0.9925	0.9934
20.0	0.	0.9918	0.9929
20.0	0.0833	0.9911	0.9924
20.0	0.1666	0.9902	0.9919
20.0	0.2500	0.9892	0.9914
20.0	0.3333	0.9878	0.9909

The numerical results given in Table 1 indicate that for positive $\bar{\mu}$ P_∞ decreases relatively more rapidly than P with decreasing size. Hence, it is likely that even when the condition $P \geqq 3\bar{\mu}/(1 + 3\bar{\mu})$ is violated, $P \geqq P_\infty$.

6.8. The result proved above is the most important application of Eq. 37. Another result of less practical utility that can be obtained from Eq. 37 is the following: <u>If P_o is the value of $P = c - 1$ for a solid V when $\bar{\mu} = 0$, then</u>

$$P > P_o[1 - 3\bar{\mu}(c - 1)] \qquad \bar{\mu} > 0$$

$$P < P_o[1 - 3\bar{\mu}(c - 1)] \qquad \bar{\mu} < 0$$

To prove this, we begin by noting that $E_2(r) \leqq e^{-r}/r$. Then, if $\bar{\mu} > 0$,

$$P\phi(\vec{r}) \geq [1 - 3\bar{\mu}(c - 1)] \int_V \frac{e^{-|\vec{r} - \vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|^2} \phi(\vec{r}')\, d^3r' \tag{49}$$

Now

$$P_o\chi(\vec{r}) = \int_V \frac{e^{-|\vec{r} - \vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|^2} \chi(\vec{r}')\, d^3r' \tag{50}$$

where $\chi(\vec{r})$ is now the value of $\phi(\vec{r})$ corresponding to $\bar{\mu} = 0$. Multiplying Eq. 49 by $\chi(\vec{r})$, Eq. 50 by $\phi(\vec{r})$, integrating over $\vec{r}$, and dividing gives the desired result. When $\bar{\mu} < 0$ an analogous proof holds except the sense of the inequality in Eq. 49 is reversed.

7. The Variational Principle for P_a

7.1. In I it was shown that if H was a positive, Hermitian operator and ϕ^* was the solution of the equation $H\phi^* = S$, where S is some source, that

$$\frac{|(S,\phi)|^2}{(\phi,H\phi)}$$

is a variational expression of the maximum type for the inner product (S,ϕ^*). From this functional a variational expression of the maximum type can be constructed for P_a, the average absorption (nonescape) probability.

When the scattering is anisotropic the relevant operator, M, is no longer Hermitian. The procedure of I can still be followed, however, and will yield a stationary principle for P_a but not one of the maximum type. We begin by noting that if

$$\Phi^* - cM\Phi^* = S \tag{51a}$$

the functional

$$J = \frac{(\Phi^+,S)(S^+,\Phi)}{(\Phi^+,\Phi)-(\Phi^+,cM\Phi)} \tag{51b}$$

is stationary around $\Phi = \Phi^*$, $\Phi^+ = \Phi^{*+}$, and is equal to (S^+,Φ^*). Here the

meaning of the adjoint of a column vector is given by Eq. 17b, c. To prove the stationary character of (Eq. 51b) the result $M^+\Phi^+ = (M\Phi)^+$, verifiable by direct computation, must be used to show that $\Phi^{*+} - cM^+\Phi^{*+} = S^+$.

7.2. Let us now apply Eq. 51b to Eq. 14a, b in the case that $Q = 1/V$. This choice corresponds to a uniform, isotropic source of unit total strength in V. c is now to be interpreted as the scattering fraction and is therefore ≤ 1. In this case the source vector has the form

$$S = \frac{1}{V}\begin{pmatrix} K \\ K\vec{\omega} \end{pmatrix}$$

where the operand of the operators K and $K\vec{\omega}$ is understood to be 1. Substitution of Eq. 52 into Eq. 51b and use of the definitions 15, 16, and 17, yields for the functional J the result:

$$J = \left(\frac{1}{V} \int_V d^3r \int_V d^3r' \; \frac{e^{-|\vec{r} - \vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|^2} \left\{ \phi(\vec{r}') + 3\bar{\mu} \; \frac{(\vec{r} - \vec{r}')}{|\vec{r} - \vec{r}'|} \cdot \vec{j}(\vec{r}') \right\} \right)^2 \Bigg/$$

$$\left[\int_V \left\{ \phi^2(\vec{r}) - 3\bar{\mu} \; j^2(\vec{r}) \right\} d^3r - c \int_V d^3r \int_V d^3r' \left\{ \phi(\vec{r}) + 3\bar{\mu} \; \frac{(\vec{r}' - \vec{r})}{|\vec{r}' - \vec{r}|} \cdot \vec{j}(\vec{r}) \right\} \right.$$

$$\left. \frac{e^{-|\vec{r} - \vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|^2} \left\{ \phi(\vec{r}') + 3\bar{\mu} \; \frac{(\vec{r} - \vec{r}')}{|\vec{r} - \vec{r}'|} \cdot \vec{j}(\vec{r}') \right\} \right] \tag{53}$$

The value of J when $\Phi = \Phi^*$ can be obtained from Eq. 53 by use of Eq. 14a, b and is

$$J[\Phi^*] = \frac{1}{Vc}\left[\int_V \phi^*(\vec{r})\, d^3r - \frac{1}{V}\int_V d^3r \int_V d^3r' \frac{e^{-|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|^2}\right] \tag{54a}$$

Now with the source normalization chosen as it has been, the nonescape probability P_a is just equal to $(1 - c)\int_V \phi^*(r)d^3r$. Using this fact as well as the fact that the double integral in Eq. 54 is just P_c, the first-collision probability from a uniform, isotropic source in V, Eq. 54 can be written as

$$P_a = (1 - c)\,(VcJ[\Phi^*] + P_c) \tag{54b}$$

Replacing $J[\Phi^*]$ by $J[\Phi]$ in Eq. 54b then gives a stationary expression for P_a, as may now be verified by the usual methods of variational calculus.

8. Dependence of P_a on $\bar{\mu}$

Proceeding as we did in Section 4.1 we show that

$$\frac{dP_a}{d\bar{\mu}} = -\,3(1 - c)cV\int_V j^2(\vec{r})\, d^3r \quad , \tag{55}$$

a quantity which is clearly negative. Thus P_a is a monotone decreasing function of $\bar{\mu}$. The variational principle for P_a can now be shown to be neither of the maximum or of the minimum type by using the argument of Section 4.2.

9. Dependence of P_a on the Size and Shape of V

By introducing the characteristic function $f(\vec{r})$ of V as in Section 5, one can derive the result

$$\frac{dP_a}{d\epsilon} = (1 - c) \int_V \frac{\partial f(\vec{r},\epsilon)}{\partial \epsilon} \left\{ 2\phi(\vec{r}) + Vc\,[\phi^2(\vec{r}) - 3\bar{\mu}\;\; j^2(\vec{r})] \right\} d^3r \qquad (56)$$

From Eq. 56 it follows that (1) <u>if a solid V_1 can be inscribed in another solid V_2, $P_a(V_1) \overset{<}{=} P_a(V_2)$ and (2) P_a is stationary against any infinitesimal, volume-preserving deformation of a sphere.</u>

10. Concluding Remarks

The theorems just proven represent on the whole a less satisfying body of knowledge than their analogues in I. For example, in the present paper it has not been possible to prove either the symmetrization theorem or the isoperimetric theorem for P and P_a although it seems certain that both are true. Furthermore, the proof of the inequality between $P_\infty(B)$ and P(V), which is related to the second fundamental theorem of reactor physics, is at present marred by two restrictive but apparently superfluous conditions. The author feels that these particular difficulties can be remedied, however, and looks forward to the time when some interested reader effects a cure.

Other instances in which the present paper is less satisfactory than I concern the questions of whether a factorization theorem holds for P or whether any general inequality relates the values of P, P_a, and P_c. Here the author makes no conjecture but hopes as before some interested reader will find an answer.

Appendix 1

Since the integral kernels in Eq. 14 are difference kernels, the form Eq. 31 results from Fourier transformation of Eq. 14 by a straightforward application of the convolution theorem. The main work of this appendix will then be the evaluation of the Fourier transforms of the various kernels appearing in Eq. 14. One other kernel appearing in Eq. 38 will also be transformed. The first of these is $e^{-r}/4\pi r^2$ and is relatively easy to transform. Introducing spherical coordinates,

$$\kappa(k) = \int e^{i\vec{k}\cdot\vec{r}}\left(\frac{e^{-r}}{4\pi r^2}\right) d^3r = 1/2\int_0^{\pi} \sin\phi d\phi \int_0^{\infty} e^{ikr\cos\phi - r}\, dr \qquad (1.1)$$

The r-integration is easily done and after the change of variables $\nu = \cos\phi$ yields

$$\kappa(k) = 1/2 \int_{-1}^{+1} \frac{d\mu}{1 - ik\mu} \qquad (1.2)$$

$$= \int_0^1 \frac{d\mu}{1 + k^2\mu^2} = \frac{\arctan k}{k}$$

The second kernel to be transformed $(e^{-r}/4\pi r^2)(\vec{r}/r)$. Owing to the symmetry of this kernel, its Fourier transform must be parallel to the vector $\vec{k}$. Thus

$$\vec{\kappa}_1(\vec{k}) = \int e^{i\vec{k}\cdot\vec{r}}\left(\frac{e^{-r}}{4\pi r^2}\right)\frac{\vec{r}}{r}\, d^3r = \frac{\vec{k}}{k}\int e^{i\vec{k}\cdot\vec{r}}\left(\frac{e^{-r}}{4\pi r^2}\right)\frac{\vec{k}\cdot\vec{r}}{kr}\, d^3r \qquad (1.3)$$

Proceeding exactly as before, we reduce $\vec{\kappa}_1(\vec{k})$ to

$$\vec{\kappa}_1(\vec{k}) = \frac{\vec{k}}{k} \int_{-1}^{+1} \frac{\mu d\mu}{2(1-ik\mu)} = i\,\frac{\vec{k}}{k^2}\left(1 - \frac{1}{2}\int_{-1}^{+1} \frac{d\mu}{1 - ik\mu}\right) = i\,\frac{\vec{k}}{k}\left(\frac{1 - \kappa(k)}{k}\right) \tag{1.4}$$

The next kernel to be transformed is the dyadic $(e^{-r}/4\pi r^2)(\vec{r}\vec{r}/rr)$. Again by considering the symmetry of the kernel it can be seen that the transform must be a linear combination of the unit dyadic $\vec{\vec{I}}$ and the dyadic $\vec{k}\,\vec{k}$. Thus we can write

$$\kappa_2(\vec{k})\,\vec{\vec{I}} + \kappa_3(\vec{k})\,\vec{k}\,\vec{k} = \int e^{i\vec{k}\cdot\vec{r}} \left(\frac{e^{-r}}{4\pi r^2}\right)\frac{\vec{r}\,\vec{r}}{r\,r}\,d^3r \tag{1.5}$$

This operator actually appears in Eq. 31 in the form

$$\frac{\vec{k}}{k}\cdot\left\{\kappa_2(\vec{k})\;\vec{\vec{I}} + \kappa_3(k)\,\vec{k}\,\vec{k}\right\}\cdot\vec{j}(\vec{k}), \tag{1.6}$$

which can be rewritten as

$$\frac{\vec{k}\cdot\vec{j}(\vec{k})}{k}\left\{\kappa_2(\vec{k}) + \kappa_3(\vec{k})\right\} \tag{1.7}$$

It follows from Eq. 5.1 by pre- and postmultiplication by $\frac{\vec{k}}{k}$ that

$$\kappa_2(\vec{k}) + \kappa_3(\vec{k}) = \int e^{i\vec{k}\cdot\vec{r}}\left(\frac{e^{-r}}{4\pi r^2}\right)\left(\frac{\vec{k}\cdot\vec{r}}{kr}\right)^2 d^3r \tag{1.8}$$

This reduces to

$$\kappa_2(\vec{k}) + \kappa_3(\vec{k}) = \int_{-1}^{+1} \frac{\mu^2 d\mu}{2(1-ik\mu)} = \frac{1}{2ik} \int_{-1}^{+1} \left(\frac{1}{1 - ik\mu} - 1 \right) \mu d\mu \tag{1.9}$$

$$= \frac{1 - \kappa(k)}{k^2}$$

The last kernel to be transformed is one appearing in Eq. 38, viz., $E_2(r)/4\pi r$. Now using Eq. 34b, it can be shown that

$$\int e^{i\vec{k}\cdot\vec{r}} \frac{E_2(r)}{4\pi r} d^3r = \int_1^{\infty} \frac{dv}{v^2} \int_{-1}^{+1} \frac{d\mu}{2(v-ik\mu)^2}$$

$$= \int_1^{\infty} \frac{dv}{v^2(v^2 + k^2)} = \frac{1 - \kappa(k)}{k^2} \tag{1.10}$$

Appendix 2

In this appendix we shall consider some of the spectral properties of the Fredholm equation

$$\chi(\vec{r}) = c' \int_V \left\{ \frac{e^{-|\vec{r} - \vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|^2} - a \frac{E_2(|\vec{r} - \vec{r}'|)}{4\pi|\vec{r} - \vec{r}'|} \right\} \chi(\vec{r}') \, d^3r' , \quad 1 \geq a \geq 0 \quad (2.1)$$

The discussion here is patterned after that of Davison[9] in the case $a = 0$.

The statements we are trying to prove about this equation are that its eigenvalue spectrum in a finite solid V is composed of discrete, real, positive eigenvalues c'_n, that the eigenfunction corresponding to the lowest of these is everywhere positive in V, and that a variational principle of the maximum type holds for $c_0'^{-1}$ (see Eq. 39). Now the fact that the eigenvalues are real follows from the symmetry of the kernel. To prove they are discrete, Davison reasons as follows: If the bracketed kernel were nonsingular, then by a well-known theorem its eigenvalue spectrum in a finite solid would be discrete. Since the kernel is singular at $\vec{r} = \vec{r}'$, this theorem cannot be directly applied. However, if any iterate of the kernel is nonsingular, then this iterated kernel will have a discrete eigenvalue spectrum in V. Since the eigenvalues of the iterated kernel are just a fixed power of the eigenvalues of the original kernel, these latter are also discrete. Now the kernel (1.2) is $\leq \frac{1}{4\pi} |\vec{r} - \vec{r}'|^{-2}$; a discussion given by Morse and Feshbach[10] shows that the third iterates of such kernels are nonsingular.

That the eigenvalues are all positive can be shown by Fourier transforming Eq. 1.2. If $\chi_n(\vec{r})$ is the (real) eigenfunction corresponding to the eigenvalue c_n', then

$$c_n'^{-1} = \frac{\int |\chi_n(\vec{k})|^2 \left\{\kappa(k) - a\,\frac{1 - \kappa(k)}{k^2}\right\} d^3k}{\int |\chi_n(k)|^2\, d^3k} \tag{2.2}$$

In obtaining Eq. 2.2, we have used the result

$$\int e^{i\vec{k}\cdot\vec{r}} \left(\frac{E_2(r)}{4\pi r}\right) d^3r = \frac{1 - \kappa(k)}{k^2} \tag{2.3}$$

which has been derived in detail in Appendix 1. In Appendix 3 it will be shown that $\kappa(k) \geq (1 - \kappa(k)/k^2$; thus $c_n'^{-1} \geq 0$ as long as $a \leq 1$. Since the c_n' are a real, positive, discrete set, they can be ordered starting with a lowest, viz., $c_o' \leq c_1' \leq c_2' - \ldots$.

Davison next notes that under the circumstances already known to prevail, the kernel in Eq. 2.1 can be written in a bilinear Hilbert-Schmidt series, $\sum_{n=o}^{\infty} \chi_n(\vec{r})\, \chi_n(\vec{r})/c_n'$, irrespective of whether χ_n form a complete set. Furthermore, any function $\chi(\vec{r})$ may be expanded as $\chi(\vec{r}) = \sum_{n=o}^{\infty} a_n \chi_n(\vec{r}) + p(\vec{r})$, where $p(\vec{r})$ is orthogonal to every χ_n and vanishes if they form a complete

set. Substituting these two series in the Rayleigh quotient on the RHS of Eq. 39 shows that this quotient is always less than $c_o'^{-1} = P_o'$.

The last link in the chain, namely, showing the lowest eigenfunction $\chi_o(\vec{r})$ is positive everywhere in V, is fashioned as follows by Davison: Suppose that $\chi_o(\vec{r})$ is the exact eigenfunction corresponding to $c_o' = P_o'^{-1}$ and suppose that it is not everywhere positive. Then use of the trial function $|\chi_o(\vec{r})|$ on the RHS of Eq. 39 will make the Rayleigh quotient even larger than $P_o' = c_o'^{-1}$, which is not allowed. Hence $\chi_o(\vec{r})$ is in fact positive everywhere in V. It is worth noting that this conclusion depends on the condition $a \leq 1$, since for the argument to be valid, the kernel can never be negative. The condition $a \leq 1$ suffices for this since $e^{-r} \geq E_2(r)/r$.

Appendix 3

In this Appendix, we prove that if $a \leq 7/5$, then the function $F(k) = \kappa(k) - a[1 - \kappa(k)]/k^2$ is a positive, convex-downwards, decreasing function of k^2. We perform the proof in three parts.

<u>Part 1.</u> If $a \leq 3$, $F(k) \geq 0$. Proof: By cross multiplication and expansion it is possible to prove that

$$\frac{1}{1 + k^2} \geq \frac{1 - \frac{1}{3} k^2}{(1 + \frac{1}{3} k^2)^2} \tag{3.1}$$

Integration of Eq. 3.1 between the limits 0 and k gives the result

$$\arctan k \geq \frac{k}{1 + \frac{1}{3}k^2} , \tag{3.2}$$

from which it follows by a simple rearrangement that

$$\kappa(k) \geq 3 \frac{1 - \kappa(k)}{k^2} \tag{3.3}$$

Equality is achieved when $k = 0$. Thus since κ and $(1 - \kappa)/k^2$ are always positive, $a = 3$ is the largest value for which $F(k)$ is also always positive.

<u>Part 2.</u> If $a \leq \frac{5}{3}$, $\frac{dF}{d(k^2)} \leq 0$. Proof: It will be enough to show that $dF/dk \leq 0$. First we consider $d\kappa/dk$.

$$\frac{d\kappa}{dk} = \frac{1}{k(1 + k^2)} - \frac{\arctan k}{k^2} = \frac{1}{k^2} \left(\frac{k}{1 + k^2} - \arctan k \right) \leq 0 \tag{3.4}$$

The last inequality is a trivial consequence of Eq. 2.3. Next we consider $[1-\kappa(k)]/k^2$.

$$\frac{d}{dk}\left(\frac{1-\kappa(k)}{k^2}\right) = \frac{3}{k^4}\left(\arctan k - k\,\frac{1+\frac{2}{3}k^2}{1+k^2}\right) \tag{3.5}$$

To show this is less than zero, we start from the identity

$$\frac{1}{1+k^2} \leq \frac{1+k^2+\frac{2}{3}k^4}{(1+k^2)^2} \tag{3.6}$$

which yields on integration the result

$$\arctan k \leq k\,\frac{1+\frac{2}{3}k^2}{1+k^2} \tag{3.7}$$

Finally, we consider $F(k) = \kappa(k) - \frac{5}{3}\left(\frac{1-\kappa(k)}{k^2}\right)$. From Eqs. 3.4 and 3.5 it follows that

$$\frac{dF}{dk} = \frac{k^2+5}{k^4}\left(\frac{k}{1+k^2} + \frac{\frac{2}{3}k^2}{(1+k^2)(1+k^2/5)} - \arctan k\right) \tag{3.8}$$

Now by partial integration we can easily show that

$$\arctan k = \int_0^k \frac{dx}{1+x^2} = \frac{k}{1+k^2} + \int_0^k \frac{2x^2dx}{(1+x^2)^2} \tag{3.9}$$

Thus dF/dk will be negative if

$$\int_0^k \frac{2x^2dx}{(1+x^2)^2} \geq \frac{\frac{2}{3}k^2}{(1+k^2)(1+k^2/5)} \tag{3.10}$$

(10.3) can be verified by noting that

$$\frac{\frac{2}{3}k^2}{(1+k^2)(1+k^2/5)} = \int_0^k \frac{2x^2}{(1+x^2)^2} \cdot \frac{1+\frac{2}{5}x^2 - \frac{x^4}{15}}{1+\frac{2}{5}x^2+\frac{x^4}{25}}\, dx \qquad (3.11)$$

Since $dF/dk = 0$ when $k = 0$ and $a = 5/3$, and since $\frac{d\kappa}{dk}$ and $\frac{d}{dk}\left(\frac{1-\kappa}{k^2}\right)$ are ≤ 0, $5/3$ is the largest value of a for which $dF/dk \leq 0$ for all k.

<u>Part 3.</u> If $a \leq 7/5$, $d^2F/d(k^2)^2 \geq 0$. Proof: Let us first consider κ. Now

$$\frac{d^2\kappa}{d(k^2)} = \frac{3}{4k^5}\left(\arctan k - \frac{1+\frac{5}{3}k^2}{(1+k^2)^2}\right) \qquad (3.12)$$

From Eq. 9.3 it follows that

$$\arctan k \geq \frac{k}{1+k^2} + \frac{1}{(1+k^2)^2}\int_0^k 2x^2dx = k\,\frac{1+5k^2/3}{(1+k^2)^2}\,; \qquad (3.13)$$

thus $d^2\kappa/d(k^2)^2$ is ≥ 0.

Next we consider $[1-\kappa(k)]/k^2$.

$$\frac{d^2}{d(k^2)^2}\left(\frac{1-\kappa(k)}{k^2}\right) = \frac{15}{4k^7}\left(k\,\frac{1+\frac{5}{3}k^2+\frac{8}{15}k^4}{(1+k^2)^2} - \arctan k\right) \qquad (3.14)$$

A second partial integration of Eq. 9.3 gives

$$\arctan k = k \frac{1 + \frac{5}{3} k^2}{(1 + k^2)^2} + \frac{8}{3} \int_0^k \frac{x^4 dx}{(1 + x^2)^3} \tag{3.15}$$

The derivative under consideration will be positive if

$$\frac{k^5/5}{(1 + k^2)^2} \geqq \int_0^k \frac{x^4 dx}{(1 + x^2)^3} \tag{3.16}$$

This last inequality can be proven by noting that

$$\frac{k^5/5}{(1 + k^2)^2} = \int_0^k \frac{x^4 + \frac{1}{5} x^6}{(1 + x^2)^3} dx \tag{3.17}$$

Finally we consider $F(k) = \kappa(k) - \frac{7}{5}\left(\frac{1 - \kappa(k)}{k^2}\right)$. Now

$$\frac{d^2F}{d(k^2)^2} = \frac{3(k^2 + 7)}{4k^7} \left(\arctan k - k \frac{1 + \frac{5}{3} k^2}{(1 + k^2)^2} - \frac{\frac{8}{15} k^5}{(1 + k^2)^2(1 + k^2/7)} \right) \tag{3.18}$$

The positivity of the parenthesis is equivalent to the inequality

$$\int_0^k \frac{x^4 dx}{(1 + x^2)^3} \geqq \frac{k^5/5}{(1 + k^2)^2(1 + k^2/7)} \tag{3.19}$$

Eq. 19.3 can be proven by noting that

$$\frac{k^5/5}{(1 + k^2)^2 (1 + k^2/7)} = \int_0^k \frac{x^4}{(1 + x^2)^3} \cdot \frac{1 + \frac{2}{7} x^2 - \frac{x^4}{35}}{1 + \frac{2}{7} x^2 + \frac{x^4}{49}} \, dx \qquad (3.20)$$

Since $d^2F/d(k^2)^2 = 0$ when $k = 0$ and $a = 7/5$, and since $d^2\kappa/d(k^2)^2$ and $\frac{d^2}{d(k^2)^2}\left(\frac{1 - \kappa}{k^2}\right)$ are both positive, $7/5$ is the largest value of a for which $d^2F/d(k^2)^2$ is ≥ 0 for all k.

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