October 15, 1971 FRA-TM-21

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Weston M. Stacey, Jr.

Argonne National Laboratory
Applied Physics Division
9700 South Cass Avenue
Argonne, Illinois 60439

FRA TECHNICAL MEMORANDUM NO. 21

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Work performed under the auspices of the U. S. Atomic Energy Commission.

Variational Estimates and Generalized Perturbation Theory for the Ratios of Linear and Bilinear Functionals

WESTON M. STACEY, JR.
Applied Physics Division, Argonne National Laboratory
Argonne, Illinois 60439

ABSTRACT

Variational functionals are presented which provide an estimate of ratios of linear and bilinear functionals of the solutions of the direct and adjoint equations (inhomogeneous and homogeneous) governing linear systems. These variational functionals are used as the basis for a generalized perturbation theory for estimating the effects of changes in system parameters upon these ratios of linear and bilinear functionals. The relation of the present theory to the variational theory of Pomraning and to the generalized perturbation theory of Usachev and Gandini is discussed. Potential applications of the theory to nuclear reactor physics are outlined.

I. INTRODUCTION

If a variational functional can be written for a given property of a linear system, then that property can be computed to second-order accuracy (with respect to errors in the solution function) by evaluating the variational functional. For example, a variational functional for the eigenvalue of the linear system described by the equation[1]

$$(A - \lambda B)\phi_\lambda = 0 \tag{1}$$

is[2]

$$\lambda\left[\phi_\lambda^*,\phi_\lambda\right] = \frac{\left\langle \phi_\lambda^*, A\phi_\lambda \right\rangle}{\left\langle \phi_\lambda^*, B\phi_\lambda \right\rangle}, \tag{2}$$

where ϕ_λ^* must satisfy the adjoint equation

$$\left(A^* - \lambda B^*\right)\phi_\lambda^* = 0 . \tag{3}$$

A, B, A^*, and B^* are linear operators satisfying $\langle u,Av\rangle = \langle A^*u,v\rangle$, $\langle u,Bv\rangle = \langle B^*u,v\rangle$. If functions $\tilde{\phi}$ and $\tilde{\phi}^*$ which differ from the solutions to Eqs. (1) and (3) by $\delta\phi$ and $\delta\phi^*$, respectively, are used to evaluate Eq. (2), it may be shown that

$$\delta\lambda \equiv \lambda\left[\tilde{\phi}_\lambda^*,\tilde{\phi}_\lambda\right] - \lambda\left[\phi_\lambda^*,\phi_\lambda\right] = 0 + \text{order}\left\langle \delta\phi^*,\delta\phi \right\rangle.$$

Similarly, a variational estimate of the linear functional $\langle S^*,\phi\rangle$ of the solution to the inhomogeneous equation

$$(A - B)\phi = S \tag{4}$$

is given by the Roussopolos functional[3]

$$R\left[\phi^*,\phi\right] = \left\langle S^*,\phi\right\rangle + \left\langle \phi^*,[S - (A - B)\phi]\right\rangle \tag{5}$$

or the Schwinger functional[4]

$$J[\phi^*,\phi] = \frac{\left\langle S^*,\phi\right\rangle \left\langle \phi^*,S\right\rangle}{\left\langle \phi^*,(A - B)\phi\right\rangle}, \tag{6}$$

where ϕ^* satisfies

$$\left(A^* - B^*\right)\phi^* = S^* . \tag{7}$$

Selengut[5] demonstrated that these latter two functionals are equivalent.

Pomraning[6] suggested the variational functional

$$P_1[\psi^*,\phi] = G[\phi] + \left\langle \psi^*,[S - (A - B)\phi]\right\rangle \tag{8}$$

for estimating the arbitrary linear functional $G[\phi]$ of the solution of Eq. (4). He demonstrated that ψ^* must satisfy

$$\left(A^* - B^*\right)\psi^* = G'[\phi] , \tag{9}$$

where the prime indicates the functional derivative.

Pomraning[7] also suggested the variational functional

$$P_2\left[\theta^*,\phi_\lambda\right] = G\left[\phi_\lambda\right] + \left\langle \theta^*,(A - \lambda B)\phi_\lambda\right\rangle \tag{10}$$

for estimating an arbitrary linear functional $G\left[\phi_\lambda\right]$ of the eigensolution of Eq. (1). He showed that θ^* must satisfy

$$\left(A^{*} - \lambda B^{*}\right)\theta^{*} = -G'\left[\phi_\lambda\right] . \tag{11}$$

A necessary condition for Eq. (11) to have a solution is that the RHS is orthogonal to the eigensolutions of Eq. (1) or

$$\left\langle \phi_\lambda , G'\left[\phi_\lambda\right] \right\rangle = 0 ,$$

which is just the basic property of homogeneous functionals.

In many practical situations, the property of interest is the ratio of two linear or bilinear functionals of the solution to the direct [Eqs. (1) or (4)] and/or adjoint [Eqs. (3) or (7)] equations describing the system. While Pomraning's functionals may be specialized to accommodate the case of ratios of linear functionals of the solution to the direct equations, no variational functionals have been presented which are suitable for estimating ratios of linear functionals of the solution to the adjoint equation or ratios of bilinear functionals of the solutions of the direct and adjoint equations.

The primary purpose of this paper is to present variational functionals which may be used to estimate ratios of linear and bilinear functionals of the direct and adjoint solutions of the equations which govern linear systems. A secondary purpose is to develop a perturbation theory from the variational functionals, which, for eigenvalue problems, is identical to the generalized perturbation theory developed from physical arguments for reactor physics problems by Usachev[8] and extended by Gandini.[9] Thus, an ancilliary result is the provision of a firmer theoretical basis for the generalized perturbation theory, in addition to extending that theory to systems governed by inhomogeneous equations.

II. LINEAR FLUX RATIOS — INHOMOGENEOUS SYSTEMS

Consider the problem of estimating the ratio of linear functionals of the solution ϕ of Eq. (4)

$$R_{ij} \equiv \frac{\left\langle \Sigma_i \phi \right\rangle}{\left\langle \Sigma_j \phi \right\rangle}, \tag{12}$$

where Σ_i and Σ_j are scalar operators. A direct estimate of R_{ij} from Eq. (12) with a function $\tilde{\phi}$ which differed from the solution of Eq. (4) by a function $\delta\phi$ would introduce an error $\delta R_{ij} \propto \left\langle \delta\phi \right\rangle$; i.e. a first-order error.

However, the variational functional

$$F_1[\psi^*,\phi] = \frac{\left\langle \Sigma_i \phi \right\rangle}{\left\langle \Sigma_j \phi \right\rangle} \left\{ 1 - \left\langle \psi^*, [(A - B)\phi - S] \right\rangle \right\} \tag{13}$$

provides an estimate of R_{ij} with error $\delta R_{ij} \propto \left\langle \delta\psi^*, \delta\phi \right\rangle$; i.e. of second order. Here $\delta\phi$ is the difference between the trial function $\tilde{\phi}$ used to evaluate Eq. (13) and the solution of Eq. (4), and $\delta\psi^*$ is the difference between the trial function $\tilde{\psi}^*$ used to evaluate Eq. (13) and the solution of

$$\left(A^* - B^*\right)\psi^* = \frac{\Sigma_i}{\left\langle \Sigma_i \phi \right\rangle} - \frac{\Sigma_j}{\left\langle \Sigma_j \phi \right\rangle}. \tag{14}$$

The proof of this follows from the easily verifiable fact that F_1 is stationary (i.e. $\delta F_1 = 0$ to first order) about functions ψ^* and ϕ which satisfy Eqs. (14) and (4), respectively, and the stationary value is R_{ij}. Pomraning's results[6] reduce to this form when $G[\phi] = R_{ij}$.

II. LINEAR FLUX RATIOS -- INHOMOGENEOUS SYSTEMS

Consider the problem of estimating the ratio of linear functionals of the solution ϕ of Eq. (4)

$$R_{12} = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle} , \tag{12}$$

where Σ_1 and Σ_2 are scalar operators. A linear estimate of R_{12} from Eq. (12) with a function ϕ which differed from the solution of Eq. (4) by a function $\delta\phi$ would introduce an error $\delta R_{12} \sim (\delta\phi)$; i.e. a first-order error.

However, the variational functional

$$F_1[\phi^*,\phi] = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle}\left\{1 + \left\langle \phi^*, [(A - B)\phi - S]\right\rangle\right\} \tag{13}$$

produces an estimate of R_{12} with error $\delta R_{12} \sim (\delta\phi^*, \delta\phi)$; i.e., of second order. Here $\delta\phi$ is the difference between the trial function ϕ used to evaluate Eq. (13) and the solution of Eq. (4), and $\delta\phi^*$ is the difference between the trial function ϕ^* used to evaluate Eq. (13) and the solution of

$$\left(A^* - B^*\right)\phi^* = \frac{\Sigma_1}{\langle \Sigma_1 \phi \rangle} - \frac{\Sigma_2}{\langle \Sigma_2 \phi \rangle} . \tag{14}$$

The proof of this follows from the easily verifiable fact that F_1 is stationary (i.e., $\delta F_1 = 0$ to first order) about functions ϕ^* and ϕ which satisfy Eqs. (14) and (4), respectively, and the stationary value is R_{12}. Pomraning's results[8] reduce to this form when $S(x) = \Sigma_2$.

A perturbation theory for changes in R_{ij} corresponding to changes in the system parameters can be derived from the difference

$$\delta R_{ij} = F_1'[\psi^*,\phi] - F_1[\psi^*,\phi] . \tag{15}$$

The prime indicates that the perturbed values Σ_i', Σ_j', A', B', S' are used in Eq. (13) to evaluate F', while the unperturbed values are used to evaluate F. Trial functions which approximate (or are equal to) the unperturbed solutions to Eqs. (4) and (14) are used to evaluate both F' and F. The result, accurate to second order, is

$$\frac{\delta R_{ij}}{R_{ij}} = \frac{\left\langle \delta\Sigma_i\phi \right\rangle}{\left\langle \Sigma_i\phi \right\rangle} - \frac{\left\langle \delta\Sigma_j\phi \right\rangle}{\left\langle \Sigma_j\phi \right\rangle} - \left\langle \psi^*,[(\delta A - \delta B)\phi - \delta S] \right\rangle , \tag{16}$$

where $\delta A \equiv A' - A$, etc. If the solution ϕ did not change with the introduction of the perturbation, the first two terms in Eq. (16) would rigorously describe the change $\delta R_{ij}/R_{ij}$. A conventional estimate (one in which the unperturbed flux is used) based on Eq. (12) yields just the first two terms. Thus, the final term in Eq. (16) accounts for the effect of the perturbation upon the solution ϕ, and represents a refinement upon conventional methods.

III. LINEAR FLUX RATIOS — HOMOGENEOUS SYSTEMS

Consider again the problem of estimating R_{ij}, this time with ϕ_λ, the fundamental eigensolution of Eq. (1). Again, a direct estimate from Eq. (12) would yield a first-order error δR_{ij}. The variational functional

$$F_2\left[\psi^*,\phi_\lambda\right] = \frac{\left\langle \Sigma_i\phi_\lambda \right\rangle}{\left\langle \Sigma_j\phi_\lambda \right\rangle}\left[1 - \left\langle \psi^*,(A - \lambda B)\phi_\lambda \right\rangle\right] \tag{17}$$

provides an estimate of R_{ij} accurate to second order with respect to the differences $\delta\phi$ and $\delta\psi^*$ between the trial functions used in evaluating Eq. (17) and the solutions of Eq. (1) and

$$\left(A^* - \lambda B^*\right)\psi^* = \frac{\Sigma_i}{\left\langle \Sigma_i \phi_\lambda \right\rangle} - \frac{\Sigma_j}{\left\langle \Sigma_j \phi_\lambda \right\rangle}, \tag{18}$$

respectively. Proof follows from consideration of the stationarity conditions for F_2. Pomraning's results[7] reduce to this form when $G[\phi] = R_{ij}$.

Equation (18) has a solution because the RHS is orthogonal to ϕ_λ, the fundamental eigensolution of Eq. (1). The method of successive approximations yields a solution to Eq. (18) of the form (see Appendix for proof of convergence)

$$\psi^* = \sum_{n=0}^{\infty} \psi_n^*, \tag{19}$$

where

$$A^* \psi_0^* = \frac{\Sigma_i}{\left\langle \Sigma_i \phi_\lambda \right\rangle} - \frac{\Sigma_j}{\left\langle \Sigma_j \phi_\lambda \right\rangle}, \tag{20a}$$

$$A^* \psi_n^* = \lambda B^* \psi_{n-1}^*, \qquad n > 0. \tag{20b}$$

A mutual orthogonality relation can be constructed from Eqs. (20) and Eq. (1)

$$0 = \frac{\langle \Sigma_i \phi_\lambda \rangle}{\langle \Sigma_i \phi_\lambda \rangle} - \frac{\langle \Sigma_j \phi_\lambda \rangle}{\langle \Sigma_j \phi_\lambda \rangle} = \langle A^* \psi_0^*, \phi_\lambda \rangle = \langle \psi_0^*, A\phi_\lambda \rangle$$

$$= \langle \psi_0^*, \lambda B\phi_\lambda \rangle = \langle \lambda B^* \psi_0^*, \phi_\lambda \rangle = \langle A^* \psi_1^*, \phi_\lambda \rangle$$

$$= \langle \psi_1^*, A\phi_\lambda \rangle = \langle \psi_1, \lambda B\phi_\lambda \rangle = \ldots = \langle \psi_n^*, \lambda B\phi_\lambda \rangle = \ldots .$$

Thus, the ψ_n^*, and hence ψ^*, are biorthogonal to ϕ_λ with respect to the operator B. This suggests that Eqs. (20) be replaced by

$$A^* \xi_0^* = \frac{\Sigma_i}{\langle \Sigma_i \phi_\lambda \rangle} - \frac{\Sigma_j}{\langle \Sigma_j \phi_\lambda \rangle}, \tag{21a}$$

$$A^* \xi_n^* = \lambda B^* \psi_{n-1}^*, \qquad n > 0, \tag{21b}$$

$$\psi_n^* = \xi_n^* - \frac{\langle \xi_n^*, B\phi_\lambda \rangle}{\langle \phi_\lambda^*, B\phi_\lambda \rangle} \phi_\lambda^*, \tag{21c}$$

where the second term in Eq. (21c) was added to remove any fundamental mode contamination which may arise from numerical roundoff.

A perturbation theory for changes in R_{ij} corresponding to changes in the system parameters can be derived from the difference

$$\delta R_{ij} = F_2' \left[\psi^*, \phi_\lambda \right] - F_2 \left[\psi^*, \phi_\lambda \right], \tag{22}$$

where both F_2' and F_2 are evaluated with approximations to the solutions of Eqs. (1) and (18) for the unperturbed system parameters, while perturbed and unperturbed system parameters are used in Eq. (17) to evaluate F_2' and F_2, respectively. The result, accurate to second order, is

$$\frac{\delta R_{ij}}{R_{ij}} = \frac{\left\langle \delta\Sigma_i \phi_\lambda \right\rangle}{\left\langle \Sigma_i \phi_\lambda \right\rangle} - \frac{\left\langle \delta\Sigma_j \phi_\lambda \right\rangle}{\left\langle \Sigma_j \phi_\lambda \right\rangle} - \left\langle \psi^*, [\delta A - \delta(\lambda B)]\phi_\lambda \right\rangle \quad , \tag{23}$$

where, again, $\delta A \equiv A' - A$, etc. As before, the third term in Eq. (23) accounts for the effect of the perturbation upon the eigensolution, ϕ_λ, and represents a refinement upon conventional theory, which would approximate $\delta R_{ij}/R_{ij}$ with the first two terms of Eq. (23).

Usachev[8] obtained a perturbation expression equivalent to Eq. (23), and prescriptions equivalent to Eqs. (19) and (21), from physical arguments for the case of neutron transport within a critical nuclear reactor. It is indicative of the power of variational principles that the straightforward derivation given above led to the same results as the convoluted physical arguments of Usachev.

IV. LINEAR ADJOINT RATIOS — INHOMOGENEOUS SYSTEMS

Now consider the problem of estimating the ratio of linear functionals of the solution of Eq. (7)

$$R^*_{ij} \equiv \frac{\left\langle \phi^* s_i \right\rangle}{\left\langle \phi^* s_j \right\rangle} , \tag{24}$$

where s_i and s_j are scalar operators. A direct estimate from Eq. (24) results in errors δR^*_{ij} which are first order in the difference $\delta\phi^*$ between the trial function used to evaluate Eq. (24), $\tilde{\phi}^*$, and the solution of Eq. (7), ϕ^*.

The variational functional

$$F_3\left[\phi^*,\psi\right] = \frac{\left\langle \phi^* s_i \right\rangle}{\left\langle \phi^* s_j \right\rangle}\left\{1 - \left\langle \left[\left(A^* - B^*\right)\phi^* - S^*\right], \psi \right\rangle\right\} \tag{25}$$

provides a second-order estimate of R^*_{ij} relative to the functions $\delta\phi^*$ mentioned above and $\delta\psi$, which is the difference between a trial function $\tilde{\psi}$ used to evaluate Eq. (25) and the solution to

$$(A - B)\psi = \frac{s_i}{\left\langle \phi^* s_i \right\rangle} - \frac{s_j}{\left\langle \phi^* s_j \right\rangle} . \tag{26}$$

Proof of this follows from consideration of the stationarity properties of F_3.

A perturbation theory for changes in R_{ij} corresponding to changes in the system parameters can be derived from the difference

$$\delta R^*_{ij} = F_3'\left[\phi^*,\psi\right] - F_3\left[\phi^*,\psi\right] , \tag{27}$$

where both F_3' and F_3 are evaluated with approximations to the solutions of the unperturbed Eqs. (7) and (26), F_3' is evaluated with the perturbed system parameters, and F_3 is evaluated with the unperturbed system parameters. The result, accurate to second order, is

$$\frac{\delta R^*_{ij}}{R^*_{ij}} = \frac{\left\langle \phi^* \delta s_i \right\rangle}{\left\langle \phi^* s_i \right\rangle} - \frac{\left\langle \phi^* \delta s_j \right\rangle}{\left\langle \phi^* s_j \right\rangle} - \left\langle \left[\left(\delta A^* - \delta B^*\right)\phi^* - \delta S^*\right], \psi \right\rangle . \tag{28}$$

Because the first two terms in Eq. (28), which correspond to the conventional method of estimation, are exact in the case where the perturbation does not change the adjoint, the third term in Eq. (28) represents a refinement to account for the effect of the perturbation on the adjoint.

$$F_3\left[\phi^*,\psi\right] = \frac{\left\langle \phi^* S_1 \right\rangle}{\left\langle \phi^* S_j \right\rangle}\left\{1 - \left\langle \left[\left(A^* - B^*\right)\phi^* - S^*\right], \psi \right\rangle \right\} \tag{25}$$

provides a second-order estimate of R^*_{1j} relative to the functions $\delta\phi^*$ mentioned above and $\delta\psi$, which is the difference between a trial function ψ used to evaluate Eq. (25) and the solution to

$$(A - B)\psi = \frac{S_1}{\left\langle \phi^* S_1 \right\rangle} - \frac{S_j}{\left\langle \phi^* S_j \right\rangle} . \tag{26}$$

Proof of this follows from consideration of the stationarity properties of F_3.

A perturbation theory for changes in R^*_{1j} corresponding to changes in the system parameters can be derived from the difference

$$\delta R^*_{1j} = F_3'\left[\phi^*,\psi\right] - F_3\left[\phi^*,\psi\right] , \tag{27}$$

where both F_3' and F_3 are evaluated with approximations to the solutions of the unperturbed Eqs. (7) and (26), F_3' is evaluated with the perturbed system parameters, and F_3 is evaluated with the unperturbed system parameters. The result, accurate to second order, is

$$\frac{\delta R^*_{1j}}{R^*_{1j}} = \frac{\left\langle \phi^* \delta S_1 \right\rangle}{\left\langle \phi^* S_1 \right\rangle} - \frac{\left\langle \phi^* \delta S_j \right\rangle}{\left\langle \phi^* S_j \right\rangle} - \left\langle \left[\left(\delta A^* - \delta B^*\right)\phi^* - \delta S^*\right], \psi \right\rangle . \tag{28}$$

Because the first two terms in Eq. (28), which correspond to the conventional method of estimation, are exact in the case where the perturbation does not change the adjoint, the third term in Eq. (28) represents a refinement to account for the effect of the perturbation on the adjoint.

V. LINEAR ADJOINT RATIOS — HOMOGENEOUS SYSTEMS

In this case, a variational estimate of R^*_{ij} is sought for the case in which the ratio involves linear functionals of the fundamental eigensolution, ϕ^*_λ, of Eq. (3). The variational functional

$$F_4\left[\phi^*_\lambda,\psi\right] = \frac{\left\langle \phi^*_\lambda s_i \right\rangle}{\left\langle \phi^*_\lambda s_j \right\rangle}\left[1 - \left\langle \phi^*_\lambda,(A - \lambda B)\psi \right\rangle\right] \tag{29}$$

provides a second-order estimate of R^*_{ij} relative to the difference $\delta\phi^*_\lambda$ between the trial function used to evaluate Eq. (29) and the solution to Eq. (3), and the difference $\delta\psi$ between the trial function used to evaluate Eq. (29) and the solution to

$$(A - \lambda B)\psi = \frac{s_i}{\left\langle \phi^*_\lambda s_i \right\rangle} - \frac{s_j}{\left\langle \phi^*_\lambda s_j \right\rangle} . \tag{30}$$

Proof follows from the stationarity properties of F_4.

Equation (30) has a solution because the RHS is orthogonal to ϕ^*_λ, the fundamental eigensolution of Eq. (3). The method of successive approximation applied to Eq. (30) yields a solution of the form (see Appendix for proof of convergence)

$$\psi = \sum_{n=0}^{\infty} \psi_n , \tag{31}$$

where

$$\psi_n = \xi_n - \frac{\left\langle \phi^*_\lambda, B\xi_n \right\rangle}{\left\langle \phi^*_\lambda, B\phi_\lambda \right\rangle}\phi_\lambda \tag{32}$$

and the ξ_n are generated recursively

$$A\xi_0 = \frac{s_i}{\left\langle \phi_\lambda^* s_i \right\rangle} - \frac{s_j}{\left\langle \phi_\lambda^* s_j \right\rangle} , \tag{33a}$$

$$A\xi_n = \lambda B\psi_{n-1} , \qquad n > 0 . \tag{33b}$$

The second term in Eq. (32) is included to remove fundamental mode contamination which may arise from numerical roundoff. (A mutual biorthogonality relation exists which requires that $\left\langle \phi_\lambda^*, B\psi_n \right\rangle = 0$, $n \geq 0$.)

A perturbation theory may be derived, similar to the previous section, from the difference

$$\delta R_{ij}^* = F_4' \left[\phi_\lambda^*, \psi \right] - F_4 \left[\phi_\lambda^*, \psi \right] , \tag{34}$$

where the unperturbed trial solutions are used to evaluate F_4' and F_4. Perturbed system parameters are used to evaluate F_4', while F_4 is evaluated with the unperturbed parameters. The result, accurate to second order, is

$$\frac{\delta R_{ij}^*}{R_{ij}^*} = \frac{\left\langle \phi_\lambda^* \delta s_i \right\rangle}{\left\langle \phi_\lambda^* s_i \right\rangle} - \frac{\left\langle \phi_\lambda^* \delta s_j \right\rangle}{\left\langle \phi_\lambda^* s_j \right\rangle} - \left\langle \phi_\lambda^*, \left[\delta A - \delta(\lambda B) \right] \psi \right\rangle \tag{35}$$

The reasoning of the previous section indicates that the third term in Eq. (35) is a refinement upon conventional theory which accounts for the effect of the perturbation on the adjoint. Gandini[9] obtained an expression equivalent to Eq. (35), and algorithms equivalent to Eqs. (31) through (33), in his extension of Usachev's generalized perturbation theory.

VI. BILINEAR RATIOS — INHOMOGENEOUS SYSTEMS

In many practical situations an estimate of the ratio of bilinear functionals of the solutions ϕ of Eq. (4) and ϕ^* of Eq. (7)

$$\rho_{ij} \equiv \frac{\left\langle \phi^*, H_i \phi \right\rangle}{\left\langle \phi^*, H_j \phi \right\rangle} . \tag{36}$$

is required. Here H_i and H_j are arbitrary linear operators. A direct estimate from Eq. (36) leads to errors which are of first order in $\delta\phi^*$ and $\delta\phi$, the differences between the trial functions $\tilde{\phi}^*$ and $\tilde{\phi}$ used to evaluate Eq. (36) and the solutions to Eqs. (7) and (4), respectively.

The variational functional

$$F_5\left[\phi^*, \Gamma^*, \phi, \Gamma\right] = \frac{\left\langle \phi^*, H_i \phi \right\rangle}{\left\langle \phi^*, H_j \phi \right\rangle} \left\{ 1 - \left\langle \Gamma^*, \left[(A - B)\phi - S\right] \right\rangle - \left\langle \left[\left(A^* - B^*\right)\phi^* - S^*\right], \Gamma \right\rangle \right\} \tag{37}$$

provides an estimate of ρ_{ij} which is accurate to second order in $\delta\phi^*$, $\delta\phi$ and the functions $\delta\Gamma^*$ and $\delta\Gamma$, which are the differences between the trial functions $\tilde{\Gamma}^*$ and $\tilde{\Gamma}$ used to evaluate Eq. (37) and the solutions of

$$\left(A^* - B^*\right)\Gamma^* = \frac{H_i^* \phi^*}{\left\langle \phi^*, H_i \phi \right\rangle} - \frac{H_j^* \phi^*}{\left\langle \phi^*, H_j \phi \right\rangle} \tag{38}$$

and

$$(A - B)\Gamma = \frac{H_i \phi}{\left\langle \phi^*, H_i \phi \right\rangle} - \frac{H_j \phi}{\left\langle \phi^*, H_j \phi \right\rangle} , \tag{39}$$

respectively. Proof follows from the stationarity properties of F_5.

A perturbation theory for changes in ρ_{ij} corresponding to perturbation in the system parameters can be derived from the difference

$$\delta\rho_{ij} = F_5'\left[\phi^*, \Gamma^*, \phi, \Gamma\right] - F_5\left[\phi^*, \Gamma^*, \phi, \Gamma\right] , \tag{40}$$

where both F_5' and F_5 are evaluated with approximations to Eqs. (4), (7), (38), and (39) for the unperturbed system, and F_5' is evaluated with the perturbed parameters while F_5 is evaluated with the unperturbed parameters. The result, accurate to second order, is

$$\frac{\delta\rho_{ij}}{\rho_{ij}} = \frac{\left\langle \phi^*, \delta H_i \phi \right\rangle}{\left\langle \phi^*, H_i \phi \right\rangle} - \frac{\left\langle \phi^*, \delta H_j \phi \right\rangle}{\left\langle \phi^*, H_j \phi \right\rangle} - \left\langle \Gamma^*, [(\delta A - \delta B)\phi - \delta S] \right\rangle$$

$$- \left\langle \left[\left(\delta A^* - \delta B^*\right)\phi^* - \delta S^*\right], \Gamma \right\rangle . \tag{41}$$

The first two terms in Eq. (41) correspond to the conventional theory, and would be exact if the perturbation did not alter ϕ^* or ϕ. The third and fourth terms are refinements which account for the effect of the perturbation upon ϕ and ϕ^*, respectively.

VII. BILINEAR RATIOS — HOMOGENEOUS SYSTEMS

Consider again the problem of estimating ρ_{ij} of Eq. (36), this time with ϕ_λ^* and ϕ_λ, the fundamental eigensolutions of Eqs. (3) and (1), respectively. As before, a direct estimate from Eq. (36) would have an error which was first order in $\delta\phi_\lambda^*$ and $\delta\phi_\lambda$, the differences between the

trial functions $\tilde{\phi}_\lambda^*$ and $\tilde{\phi}_\lambda$ used to evaluate Eq. (36) and the solutions of Eqs. (3) and (1), respectively.

The variational functional

$$F_6\left[\phi_\lambda^*,\Gamma^*,\phi_\lambda,\Gamma\right] = \frac{\left\langle \phi_\lambda^*,H_i\phi_\lambda\right\rangle}{\left\langle \phi_\lambda^*,H_j\phi_\lambda\right\rangle}\left[1 - \left\langle \phi_\lambda^*,(A-\lambda B)\Gamma\right\rangle - \left\langle \Gamma^*,(A-\lambda B)\phi_\lambda\right\rangle\right] \quad (42)$$

provides an estimate of ρ_{ij} which is accurate to second order in $\delta\phi_\lambda^*$, $\delta\phi_\lambda$, and the differences $\delta\Gamma^*$ and $\delta\Gamma$ between the trial functions used to evaluate Eq. (42) and the solutions of

$$\left(A^* - \lambda B^*\right)\Gamma^* = \frac{H_i^*\phi_\lambda^*}{\left\langle \phi_\lambda^*,H_i\phi_\lambda\right\rangle} - \frac{H_j^*\phi_\lambda^*}{\left\langle \phi_\lambda^*,H_j\phi_\lambda\right\rangle} \quad (43)$$

and

$$(A - \lambda B)\Gamma = \frac{H_i\phi_\lambda}{\left\langle \phi_\lambda^*,H_i\phi_\lambda\right\rangle} - \frac{H_j\phi_\lambda}{\left\langle \phi_\lambda^*,H_j\phi_\lambda\right\rangle}, \quad (44)$$

respectively. Proof follows from the stationarity properties of F_6.

Equation (43) has a solution because the RHS is orthogonal to ϕ_λ, the fundamental eigensolution of Eq. (1). Application of successive approximations to Eq. (43) yields (see Appendix for proof of convergence)

$$\Gamma^* = \sum_{n=0}^{\infty} \Gamma_n^*, \quad (45)$$

where

$$\Gamma_n^* = \xi_n^* - \frac{\left\langle \xi_n^*,B\phi_\lambda\right\rangle}{\left\langle \phi_\lambda^*,B\phi_\lambda\right\rangle}\phi_\lambda^*, \quad (46)$$

and the ξ_n^* are generated recursively

$$A^*\xi_0^* = \frac{H_i^*\phi_\lambda^*}{\left\langle \phi_\lambda^*, H_i\phi_\lambda \right\rangle} - \frac{H_j^*\phi_\lambda^*}{\left\langle \phi_\lambda^*, H_j\phi_\lambda \right\rangle}, \tag{47a}$$

$$A^*\xi_n^* = \lambda B^*\Gamma_{n-k}^*, \quad n > 0. \tag{47b}$$

Similarly, a solution to Eq. (44) may be constructed from

$$\Gamma = \sum_{n=0}^{\infty} \Gamma_n, \tag{48}$$

where

$$\Gamma_n = \xi_n - \frac{\left\langle \phi_\lambda^*, B\xi_n \right\rangle}{\left\langle \phi_\lambda^*, B\phi_\lambda \right\rangle}\phi_\lambda \tag{49}$$

and the ξ_n are generated recursively

$$A\xi_0 = \frac{H_i\phi_\lambda}{\left\langle \phi_\lambda^*, H_i\phi_\lambda \right\rangle} - \frac{H_j\phi_\lambda}{\left\langle \phi_\lambda^*, H_j\phi_\lambda \right\rangle}, \tag{50a}$$

$$A\xi_n = \lambda B\Gamma_{n-1}, \quad n > 0. \tag{50b}$$

The second terms in Eqs. (46) and (49) are included to remove any fundamental mode contamination which may arise from numerical roundoff. (Mutual biorthogonality relations exist which require that $\left\langle \Gamma_n^*, B\phi_\lambda \right\rangle = 0$, $\left\langle \phi_\lambda^*, B\Gamma_n \right\rangle = 0$, $n \geq 0$.)

A perturbation theory for changes in ρ_{ij} corresponding to perturbations in the system parameters can be derived from the difference

$$\delta\rho_{ij} = F_6'\left[\phi_\lambda^*, \Gamma^*, \phi_\lambda, \Gamma\right] - F_6\left[\phi_\lambda^*, \Gamma^*, \phi_\lambda, \Gamma\right] . \tag{51}$$

As before, F_6' and F_6 are both evaluated with trial functions which approximate the solution of the unperturbed Eqs. (1), (3), (43), and (44). Perturbed parameters are used to evaluate F_6', while unperturbed parameters are used to evaluate F_6. The result, accurate to second order, is

$$\frac{\delta\rho_{ij}}{\rho_{ij}} = \frac{\left\langle \phi_\lambda^*, \delta H_i \phi_\lambda \right\rangle}{\left\langle \phi_\lambda^*, H_i \phi_\lambda \right\rangle} - \frac{\left\langle \phi_\lambda^*, \delta H_j \phi_\lambda \right\rangle}{\left\langle \phi_\lambda^*, H_j \phi_\lambda \right\rangle} - \left\langle \phi_\lambda^*, [\delta A - \delta(\lambda B)]\, \Gamma \right\rangle$$

$$- \left\langle \Gamma^*, [\delta A - \delta(\lambda B)]\, \phi_\lambda \right\rangle . \tag{52}$$

Again, the first two terms in Eq. (52) correspond to the conventional result. The third and fourth terms are refinements which account for the effect of the perturbation upon ϕ_λ^* and ϕ_λ, respectively.

Gandini[9] obtained a perturbation expression equivalent to Eq. (52) and algorithms equivalent to Eqs. (45) through (50) in his extension of Usachev's generalized perturbation theory.

VIII. POSSIBLE APPLICATIONS TO NUCLEAR REACTOR PHYSICS

Potential applications to problems in reactor physics are considered to illustrate the use of the theory presented in the previous sections. Hopefully, these examples will suggest applications in other fields by analogy.

Frequently the solution to a problem slightly different from the problem of interest is either available or readily obtainable and one would like to use this solution to compute a ratio of functionals for the problem of interest, or one would like to assess the change in the ratio of functionals corresponding to the changes leading from the problem for which a solution is available to the problem of interest. In the former case, the variational functionals F_1 through F_6 provide a more accurate estimate of the ratio of functionals than would be obtained by a direct evaluation of the ratio using the available solution. In the latter case, the perturbation expressions provide a means, accurate to second order, of assessing the change in the ratio of functionals without the necessity of calculating the solution for the problem of interest. Changes in material composition, material arrangement, mathematical model, nuclear data, source, and fuel temperature arise in reactor analysis.

Material composition changes occur when one material is substituted for another (e.g. insertion of a control rod, experimental device, detector, etc.) and when changes in isotopic composition due to fission, activation, and radioactive decay take place. Changes in material arrangement may arise from thermal expansion or changes in the loading pattern. In a somewhat different vein, the material in a reactor may be homogenized in the calculational model to facilitate obtaining a solution. This homo-

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Material composition changes occur when one material is substituted for another (e.g. insertion of a control rod, experimental device, detector, etc.) and when changes in isotopic composition due to fission, activation, and radioactive decay take place. Changes in material arrangement may arise from thermal expansion or changes in the loading pattern. In a somewhat different vein, the material in a reactor may be homogenized in the calculational model to facilitate obtaining a solution. This homogenized solution could be used, together with the actual heterogeneous material configuration, in a variational functional to obtain an estimate of a ratio in the actual system, or in a perturbation expression to assess the difference between the ratio in the fictictious homogenized model and in the actual heterogeneous model. (Variational and perturbation expressions for the eigenvalue have been applied to this end.[11,12])

In the same vein, a simplified mathematical model may be used to obtain an approximate solution. This solution may be used in a variational functional constructed for a more rigorous mathematical model to obtain an estimate of a ratio. Alternately, the perturbation expression, with δA and δB corresponding to the differences between the more rigorous and approximate operators, could be used with the approximate solution to assess the effect of the difference between the more rigorous and approximate models on the ratio. Replacing high-order neutron transport approximations with low-order approximations, such as diffusion theory, and neglecting anisotropy in the neutron angular scattering distributions, are typical simplifications.

Perturbation expressions of the form presented in this paper have been used to assess the effect of nuclear data uncertainties upon ratios of functionals, both for the purpose of assessing the implied uncertainty in the performance of nuclear reactors[13,14] and for adjusting averaged cross sections to obtain agreement with integral experiments.[14,15] Use of the variational functionals would allow an estimate of the corresponding ratios when new data became available without the necessity of obtaining a solution corresponding to the new data.

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reactors. In this case Σ_i and Σ_j are the cross sections appropriate to the reactions, distributed or localized in space and energy according to the dictates of the problem. The functionals can also provide an estimate of relative local flux or power peaking if $\Sigma_i = \delta\left(r - r_i\right)$ or $\Sigma_f\delta\left(r - r_i\right)$ and $\Sigma_j = 1$ or Σ_f, respectively. $\delta\left(r - r_i\right)$ is the Dirac delta, r is the spatial variable, and Σ_f is the macroscopic fission cross section distributed in space and energy. Another use of these functionals is to estimate the relative neutron flux above some energy E_{min}. In this case, $\Sigma_i = U\left(E - E_{min}\right)$ and $\Sigma_j = 1$, where U is the step function.

An estimate of the relative importance of neutron sources s_i and s_j to the reaction rate $\left\langle S^*,\phi\right\rangle$ in a subcritical reactor is provided by the variational functional F_3. Both F_3 (subcritical) and F_4 (critical) provide an estimate of the relative local adjoint when $s_i = \delta\left(r - r_i\right)$ and $s_j = 1$.

The variational functionals F_5 (subcritical) and F_6 (critical) provide an estimate of reactivity worths, effective delayed neutron fraction, and effective prompt-neutron lifetime, depending upon the choice of H_i and H_j. When H_i is the change in the neutron balance operator $-\Delta(A - \lambda B)$ (critical) or $-\Delta(A - B)$ (subcritical) due to a sample inserted into a reactor, and H_j is the integral operator

$$\chi(E) \int_0^\infty dE' \; \nu\Sigma_f(E',r) \; ,$$

then the variational functionals provide an estimate of the reactivity worth of the sample. Here E is the neutron energy, ν is the number of neutrons per fission, and χ is the energy distribution of fission neutrons.

When H_i is the integral operator

$$\chi_d(E) \int_0^\infty dE' \; \nu\beta\Sigma_f(E',r),$$

and H_j remains the same, an estimate of the effective delayed neutron fraction is provided by the variational functionals. Here, β is the fraction of delayed fission neutrons and χ_d is the distribution in energy of these delayed neutrons. If H_i is the inverse neutron speed, and H_j remains the same, F_5 and F_6 provide an estimate of the prompt-neutron lifetime. A ratio of reactivity worths results when both H_i and H_j are changes in the neutron balance operator.

Thus, there are many potential applications of the theory to nuclear reactor physics, only a few of which have been examined to date. Certainly, fruitful applications must exist in other fields as well.

APPENDIX

The method of successive approximations was used to construct a solution to the flux importance equation

$$(A - \lambda B)\chi = S \qquad (A.1)$$

of the form

$$\chi = \sum_{n=0}^{\infty} \chi_n , \qquad (A.2)$$

where

$$A\chi_0 = S , \qquad (A.3)$$

$$A\chi_n = \lambda B\chi_{n-1} , \quad n > 0 . \qquad (A.4)$$

Solving Eqs. (A.3) and (A.4)

$$\chi_n = A^{-1}\lambda B\chi_{n-1} = \left(A^{-1}\lambda B\right)^n A^{-1}S , \quad n \geq 0 , \qquad (A.5)$$

and substituting in Eq. (A.2) yields

$$\chi = \sum_{n=0}^{\infty} (A^{-1}\lambda B)^n A^{-1}S . \qquad (A.6)$$

It was shown previously that

$$\left\langle \phi_\lambda^*, S \right\rangle = 0 ,$$

where ϕ_λ^* is the fundamental (i = 0) eigenfunction of

$$\left(A^* - \lambda_i B^*\right)\phi_i^* = 0 . \qquad (A.7)$$

Thus, S can be represented by an expansion in the higher harmonic ($i > 0$) eigenfunctions ϕ_i of

$$\left(A - \lambda_i B\right)\phi_i = 0 \; . \tag{A.8}$$

Writing

$$S = \sum_{i=1}^{\infty} a_i \lambda_i B \phi_i \; ,$$

it follows that

$$\left(A^{-1}\lambda B\right)^n A^{-1} S = \sum_{i=1}^{\infty} a_i \left(\frac{\lambda_0}{\lambda_i}\right)^n \phi_i \; .$$

For the multigroup diffusion equations there are positivity proofs[17] which assure that $\lambda_0 < \lambda_i$, $i \geq 1$. Thus, the sum in Eq. (A.6) converges, and may be written

$$\chi = \sum_{n=0}^{\infty} \left(A^{-1}\lambda B\right)^n A^{-1} S = \left(I - A^{-1}\lambda B\right)^{-1} A^{-1} S = \left(A - \lambda B\right)^{-1} S \; , \tag{A.9}$$

which is the solution of Eq. (A.1).

A similar proof obtains for the adjoint importance solution.

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