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On the Derivation of a Variational Principle for Linear Systems

A variational principle due to Roussopoulos (*1*) makes it possible to estimate the weighted average of an arbitrary linear functional of the solution to a given linear operator equation. It can be shown (*2*) that most of the familiar variational principles for linear equations (for example, those used by Marshak, Schwinger, Kourganoff, and Rayleigh) can be derived from Roussopoulos' principle as special cases. However, since it is still necessary to postulate arbitrarily the form of this functional, it is desirable to derive it from simpler or more intuitive considerations. The following is an attempt to do this.

We consider a specified physical system (such as a reactor) whose state is described by a function $\phi(x)$, where x denotes the relevant phase space coordinates of the system (that is, the independent variables such as position, energy, angle, and time). In general, there will be many ways of describing the given system, each with its corresponding state function and associated linear or nonlinear equation which the state function satisfies. While the conventional equations describing neutron diffusion are linear, it is possible to choose a nonlinear description, as in the invariant embedding method of Bellman. On the other hand, a problem such as the propagation of a one-dimensional shock wave in compressible gas dynamics, which seems inherently nonlinear, can be linearized by interchanging the independent and dependent variables as first shown by Riemann. In both cases, the alternative descriptions involve no approximations and are completely equivalent to the original ones; they are, however, more convenient for some purposes.

We shall take the standpoint that our objective in choosing an appropriate description of the system is not primarily to calculate the particular state function ϕ in all its detail; we are interested, instead, in determining a single numerical quantity depending on the state (for example, the absorption rate in a particular region of a reactor, or the multiplication constant). We shall denote this quantity by $F[\phi]$ to indicate that it is a functional of the state description; that is, it depends on the state throughout the system phase space. As yet we have specified neither the state description nor the dependence on the state of the quantity we want to calculate. Regardless of the form of this dependence, however, the quantity can be expanded in a functional power series (*3*)

$$F[\phi] = \sum_{n=0}^{\infty} \frac{1}{n!} \cdot \int dx_1 \cdots \int dx_n \, A_n(x_1 \cdots x_n)\phi(x_1) \cdots \phi(x_n) \tag{1}$$

where the integrations extend over the region in phase space defining the system. The kernels are given by

$$A_n(x_1 \cdots x_n) = \left. \frac{\delta^n F[\phi]}{\delta\phi(x_1) \cdots \delta\phi(x_n)} \right|_{\phi=0} \tag{2}$$

and are the nth functional derivatives of F evaluated for $\phi = 0$. (This expansion can be obtained by considering that ϕ is specified at a finite number of points, regarding F as an ordinary function of these variables, expanding it in a Taylor series, and letting the number of points at which ϕ is evaluated become infinite.)

At this point, we shall impose two requirements on this formalism and determine what specializations in the theory they will lead to.

(a) The first requirement is simplicity. We would like to choose a description of the system in such a way that the dependence on the state function, of the number we are primarily interested in, is as simple as possible. To this end, we shall assume that the higher terms in the functional power series are rapidly decreasing and that we can truncate the series after the quadratic term.

(b) The second requirement is insensitivity. That is, we would like the value of F to depend only weakly on its argument so that it will be insensitive to errors made in an approximate calculation of the state function. More formally, we shall require that if a small error $\delta\phi$ is made in the state, the corresponding error δF will vanish to first order.

To determine the consequences of these two requirements, we have to calculate the variation in F from Eq. (1) and set it equal to zero. The result is

$$\delta F = \int dx \, \delta\phi(x) \left[A_1(x) + \int dx' A_2(x, x')\phi(x') \right] = 0. \tag{3}$$

Now since this holds for arbitrary variations of ϕ (provided they are sufficiently small), it follows that ϕ must satisfy the following equation:

$$A_1(x) + \int dx' A_2(x, x')\phi(x') = 0 \tag{4}$$

which is of the form of a general linear inhomogeneous integral equation, with a kernel which is symmetric (since the functional derivatives are symmetric in their arguments) but which is otherwise arbitrary. Suppose now that we use Eq. (4) to simplify the calculation of the functional F by substituting it into the right side of Eq. (1) (the sum now goes only from zero to two). The result is

$$F[\phi] = A_0 + \frac{1}{2} \int dx A_1(x)\phi(x), \tag{5}$$

where ϕ is now the particular function which satisfies Eq. (4).

We thus have the following result: Imposing the requirements of simplicity and insensitivity implies that the theory which has been used to describe the system is equiva-

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