

An Analogy Between the Variational Principles of Reactor Theory and those of Classical Mechanics*

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A formal parallelism is shown to exist between two classical variational principles governing the time behavior of mechanical systems and two principles relating to the λ -mode eigenvalue problem of neutron group diffusion theory. By identifying the space variable with the time variable and space derivatives (gradients and divergences) with time derivatives, the 'usual' variational principle of diffusion theory is shown to be analogous to Hamilton's principle and the diffusion equations are analogous to the Lagrange equations. Hamilton's canonical equations are then analogous to the diffusion equations in first-order form, and the analog of the principle involving the canonical integral is a principle closely related to one proposed recently by Selengut and Wachspress.

A well-known variational principle in reactor theory^{1,2} is

$$\delta \int_R \left[\nabla u^{*T} \cdot D \nabla u + u^{*T} \left(A - \frac{1}{\lambda} M \right) u \right] d\tau = 0, \quad (1)$$

in which the matrix notation of group diffusion theory is used; R is the volume of the reactor, D is a diagonal matrix of group diffusion coefficients, A is the matrix of absorption and group transfer cross sections, M is the fission matrix, $1/\lambda$ is a Lagrange multiplier, superscript T denotes a transpose and u and u^* are column matrices

$$u(\mathbf{r}) = \begin{bmatrix} u_1 \\ \vdots \\ u_G \end{bmatrix}, \quad u^*(\mathbf{r}) = \begin{bmatrix} u_1^* \\ \vdots \\ u_G^* \end{bmatrix}, \quad (2)$$

whose elements are continuous real valued functions on R . If the admissible functions are further required to satisfy a homogeneous boundary condition (for example $u = u^* = 0$) on the surface of R then Eq. (1) holds if and only if

$$-\nabla \cdot D \nabla u + \left(A - \frac{1}{\lambda} M \right) u = 0 \quad (3a)$$

$$-\nabla \cdot D \nabla u^* + \left(A - \frac{1}{\lambda} M^T \right) u^* = 0. \quad (3b)$$

Equation (3a) is the usual group diffusion-theory eigenvalue problem, and Eq. (3b) is the adjoint eigenvalue problem. Thus Eq. (1) is satisfied if and only if u is the flux, u^* is the adjoint flux and λ is the effective multiplication constant.

Selengut and Wachspress³ have recently proposed another variational principle, which we write in the following slightly modified form:

$$\delta \int_R \left\{ [u^{*T} v^{*T}] \begin{bmatrix} \left(A - \frac{1}{\lambda} M \right) & \\ & 0 \quad -D^{-1} \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} + [v^T v^{*T}] \begin{bmatrix} \cdot \nabla u^* \\ \cdot \nabla u \end{bmatrix} \right\} d\tau = 0 \quad (4)$$

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¹D. S. SELENGUT, "Variational Analysis of Multi-dimensional Systems," HW59126 Quarterly Physics Report, (1958).

²S. KAPLAN, *Nucl. Sci. Eng.*, 13, 22-31 (1962).

³E. L. WACHSPRESS, "Variational Synthesis with Discontinuous Trial Functions," Int'l. Conf. on the Appl. of Computing Methods to Reactor Problems, Argonne National Laboratory, Paper #6, (May 1965).

in which v and v^* are columns

$$v = \begin{bmatrix} v_1 \\ \vdots \\ v_G \end{bmatrix}, \quad v^* = \begin{bmatrix} v_1^* \\ \vdots \\ v_G^* \end{bmatrix}$$

of vector-valued (in the usual three-dimensional vector sense) functions on R . This principle has for its stationary conditions

$$\left(A - \frac{1}{\lambda} M\right)u - \nabla \cdot v = 0 \tag{5a}$$

$$\nabla u - D^{-1}v = 0 \tag{5b}$$

$$\left(A^T - \frac{1}{\lambda} M^T\right)u^* - \nabla \cdot v^* = 0 \tag{6a}$$

$$\nabla u^* - D^{-1}v^* = 0 \tag{6b}$$

These equations are again the group diffusion and adjoint equations, but now written in first-order form (through the substitutions $v = D\nabla u$, $v^* = D\nabla u^*$). Thus it may appear that nothing has been gained. However, Selengut and Wachspress have argued³ that if it is suitably interpreted the principle (4) may be regarded as operating on an admissible domain, which includes discontinuous functions, u , u^* , v , v^* . To accomplish this they assign to the functional with discontinuous arguments a value equal to the limit of the values it takes on for a series of arguments that are continuous but approach the discontinuous ones. The continuity requirements of diffusion theory then appear as part of the stationary conditions of Eq. (4). This raises the intriguing possibility that the principle (4) can be used to develop a 'cell theory' or a general method of representing a reactor as a small number of large interacting pieces. We shall not pursue these possibilities here, although they may be very important to reactor analysis. In the present paper we limit ourselves to displaying a simple formal analogy which is interesting in itself and may possibly have some conceptual or pedagogical value.

For this purpose let us next consider a finite dimensional mechanical system having generalized coordinates $q_1(t), \dots, q_N(t)$, which are functions of time. Using the notation

$$q = \begin{bmatrix} q_1 \\ \vdots \\ q_N \end{bmatrix}$$

we write the Lagrangian of the system as $L(q, \dot{q}, t)$. The Lagrangian is a scalar valued function of the coordinates, q , the velocities, \dot{q} , and the time. As the basic law governing the behavior of the system we take Hamilton's principle

$$\delta \left\{ \int_{t_0}^{t_1} L(q, \dot{q}, t) dt \right\} = 0 \tag{7}$$

from which it follows that the true motion of the system satisfies Lagrange's equations

$$-\frac{d}{dt} \frac{\partial L}{\partial \dot{q}} + \frac{\partial L}{\partial q} = 0 \tag{8}$$

In Eq. (8) we have written the derivative of a scalar, L , with respect to a column q . By this we mean

$$\frac{\partial L}{\partial q} = \begin{bmatrix} \frac{\partial L}{\partial q_1} \\ \vdots \\ \frac{\partial L}{\partial q_N} \end{bmatrix}$$

and similarly for $\frac{\partial L}{\partial \dot{q}}$. We shall use this notation extensively in what follows.

We now desire to place Eq. (1) into correspondence with Eq. (7). To do this we think of u and u^* as the generalized coordinates, and we let the space variable, r , in Eq. (1) play the role of the time variable, t , in Eq. (7). The space derivatives ∇u , ∇u^* must then be analogous to the time derivatives \dot{q} . Thus we regard the integrand in Eq. (1) as a Lagrangian

$$L[u, u^*, \nabla u, \nabla u^*, r] = \left[\nabla u^{*T} \cdot D\nabla u + u^{*T} \left(A - \frac{1}{\lambda} M \right) u \right], \tag{9}$$

and therefore rewrite Eq. (1) as

$$\delta \left\{ \int_R L[u, u^*, \nabla u, \nabla u^*, r] dr \right\} = 0. \tag{1a}$$

Taking the variation, we obtain the corresponding Lagrange equations

$$-\nabla \cdot \frac{\partial L}{\partial \nabla u^*} + \frac{\partial L}{\partial u^*} = 0 \tag{10a}$$

$$-\nabla \cdot \frac{\partial L}{\partial \nabla u} + \frac{\partial L}{\partial u} = 0. \tag{10b}$$

These equations must of course be exactly the diffusion equations (3). This can be verified by inserting the explicit form, Eq. (9) of L into Eqs. (10) and noting that

$$\frac{\partial L}{\partial u^*} = \left(A - \frac{1}{\lambda} M \right) u \tag{11a}$$

$$\frac{\partial L}{\partial u} = \left(A^T - \frac{1}{\lambda} M^T \right) u^* \tag{11b}$$

and

$$\frac{\partial L}{\partial \nabla u^*} = D\nabla u \tag{12a}$$

$$\frac{\partial L}{\partial \nabla u} = D\nabla u^*. \tag{12b}$$

Next let us review the derivation of the Hamilton canonical formulation of the mechanics problem⁴. The first step is to define the conjugate momenta

$$p = \frac{\partial L}{\partial \dot{q}}(q, \dot{q}, t) \quad (13)$$

and the Hamiltonian function

$$H(q, p, t) = p^T \dot{q} - L(q, \dot{q}, t), \quad (14)$$

where on the right-hand side of Eq. (14) it is understood that \dot{q} is eliminated in terms of q, p and t by means of Eq. (13). Differentiation of H and use of Eqs. (8) and (13) yields Hamilton's canonical equations

$$\frac{\partial H}{\partial q} = \frac{\partial \dot{q}^T}{\partial q} p - \frac{\partial \dot{q}^T}{\partial q} \frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = -\dot{p} \quad (15a)$$

$$\frac{\partial H}{\partial p} = \dot{q} + \frac{\partial \dot{q}^T}{\partial p} p - \frac{\partial \dot{q}^T}{\partial p} \frac{\partial L}{\partial \dot{q}} = \dot{q}, \quad (15b)$$

which may be thought of as the equations of motion in first-order form. We have arrived at these from the variational principle (7) via the transformations (13) and (14). They may also be arrived at directly as the stationary condition of the variational principle

$$\delta \left\{ \int_{t_0}^{t_1} [p^T \dot{q} - H(q, p, t)] dt \right\} = 0, \quad (16)$$

in which p and q are varied independently. The integral in Eq. (16) is called the canonical integral⁴.

We now imitate the steps (13 to 15) using the Lagrangian (9). Thus we define.

$$p = \frac{\partial L}{\partial \nabla u} = D \nabla u^* \quad (17a)$$

$$p^* = \frac{\partial L}{\partial \nabla u^*} = D \nabla u \quad (17b)$$

$$H(u, u^*, p, p^*, r) = p^T \cdot \nabla u + p^{*T} \cdot \nabla u^* - L(u, u^*, \nabla u, \nabla u^*, r), \quad (18)$$

and, in analogy to Eq. (15), we find that

$$\frac{\partial H}{\partial u} = - \frac{\partial L}{\partial u} = - \nabla \cdot p \quad (19a)$$

$$\frac{\partial H}{\partial u^*} = - \frac{\partial L}{\partial u^*} = - \nabla \cdot p^* \quad (19b)$$

$$\frac{\partial H}{\partial p} = \nabla u \quad (19c)$$

$$\frac{\partial H}{\partial p^*} = \nabla u^*. \quad (19d)$$

Just as we showed that the Lagrange equations (10) were the same as the diffusion equations (3), we now show that the canonical equations (19) are the diffusion equations (5) and (6) in first-order form. To do this we use Eq. (9) in Eq. (18) and eliminate $\nabla u, \nabla u^*$ by means of Eq. (17). This yields the Hamiltonian in explicit form

$$H(u, u^*, p, p^*, r) = p^{*T} \cdot D^{-1} p - u^{*T} \left(A - \frac{1}{\lambda} M \right) u. \quad (20)$$

Putting this into Eq. (19) yields

$$- \nabla \cdot p = - \left(A^T - \frac{1}{\lambda} M^T \right) u^*$$

$$D^{-1} p = \nabla u^*$$

$$- \nabla \cdot p^* = - \left(A - \frac{1}{\lambda} M \right) u$$

$$D^{-1} p^* = \nabla u,$$

which are exactly Eqs. (5) and (6) with the identifications $p^* = v, p = v^*$.

Finally let us write down the analog of Eq. (16),

$$\delta \int_R \left\{ [p^T p^{*T}] \begin{bmatrix} \cdot \nabla u \\ \cdot \nabla u^* \end{bmatrix} - H(u, u^*, p, p^*, r) \right\} d\tau = 0, \quad (21)$$

and note that the stationary conditions for this principle are exactly Eqs. (19). If we insert the form (20) of the Hamiltonian into Eq. (21), we obtain Eq. (4).

Thus we arrive at our major point, that if the reactor theory variational principle (1) be placed into analogy with Hamilton's principle in mechanics then the Selengut-Wachspress principle (4) plays the role of the principle (16) involving the canonical integral. We summarize this and our various other analogies in Table I.

⁴C. LANCZOS, *The Variational Principles of Mechanics*, University of Toronto Press (1949).

TABLE I
Summary of Analogies

Name	Classical Mechanics	Reactor Theory	
		In terms of L, H	Explicit
Hamilton's Principle	$\delta \int_{t_0}^{t_1} L(q, \dot{q}, t) dt = 0$	$\delta \int_R L(u, u^*, \nabla u, \nabla u^*, \tau) d\tau = 0$	$\delta \int_R [\nabla u^{*T} D \nabla u + u^{*T} (A - \frac{1}{\lambda} M) u] d\tau = 0$
Lagrange's Equations	$-\frac{d}{dt} \frac{\partial L}{\partial \dot{q}} + \frac{\partial L}{\partial q} = 0$	$-\nabla \cdot \frac{\partial L}{\partial \nabla u} + \frac{\partial L}{\partial u} = 0$ $-\nabla \cdot \frac{\partial L}{\partial \nabla u^*} + \frac{\partial L}{\partial u^*} = 0$	$-\nabla \cdot D \nabla u^* + (A^T - \frac{1}{\lambda} M^T) u^* = 0$ $-\nabla \cdot D \nabla u + (A - \frac{1}{\lambda} M) u = 0$
Legendre Transformation	$p = \frac{\partial L}{\partial \dot{q}}$ $H(q, p, t) = p^T \dot{q} - L(q, \dot{q}, t)$	$p = \frac{\partial L}{\partial \nabla u}, p^* = \frac{\partial L}{\partial \nabla u^*}$ $H(u, u^*, p, p^*, \tau)$ $= p^T \cdot \nabla u + p^{*T} \cdot \nabla u^* - L(u, u^*, \nabla u, \nabla u^*, \tau)$	$p = D \nabla u^*, p^* = D \nabla u$ $H = p^{*T} \cdot D^{-1} p - u^{*T} (A - \frac{1}{\lambda} M) u$
Canonical Equations	$\dot{q} = \frac{\partial H}{\partial p}$ $-\dot{p} = \frac{\partial H}{\partial q}$	$\nabla u = \frac{\partial H}{\partial p}, \nabla u^* = \frac{\partial H}{\partial p^*}$ $-\nabla p = \frac{\partial H}{\partial u}, -\nabla p^* = \frac{\partial H}{\partial u^*}$	$\nabla u = D^{-1} p^*, \nabla u^* = D^{-1} p$ $-\nabla p = - (A^T - \frac{1}{\lambda} M^T) u^*,$ $-\nabla p^* = - (A - \frac{1}{\lambda} M) u$
Canonical Integral	$\delta \int_{t_0}^{t_1} [p^T \dot{q} - H] dt = 0$	$\delta \int_R [p^T \cdot \nabla u + p^{*T} \cdot \nabla u^* - H] d\tau = 0$	$\delta \int_R [p^T \cdot \nabla u + p^{*T} \cdot \nabla u^* - p^{*T} \cdot D^{-1} p + u^{*T} (A - \frac{1}{\lambda} M) u] d\tau = 0$