69-4260

MADSEN, Larry Charles, 1942-

HAMILTONIAN FORMALISM APPLIED TO MULTIDIMENSIONAL REACTOR SYSTEMS AND RELATED CONCEPTS.

Iowa State University, Ph.D., 1968
Engineering, nuclear

University Microfilms, Inc., Ann Arbor, Michigan

HAMILTONIAN FORMALISM APPLIED TO MULTIDIMENSIONAL REACTOR SYSTEMS AND RELATED CONCEPTS

by

Larry Charles Madsen

A Dissertation Submitted to the
Graduate Faculty in Partial Fulfillment of
The Requirements for the Degree of
DOCTOR OF PHILOSOPHY

Major Subject: Nuclear Engineering

Approved:

Signature was redacted for privacy.
In Charge of Major Work

Signature was redacted for privacy.
In Charge of Major Work

Signature was redacted for privacy.
Head of Major Department

Signature was redacted for privacy.
Dean of Graduate College

Iowa State University
Ames, Iowa

1968

TABLE OF CONTENTS

INTRODUCTION

The Hamiltonian and Lagrangian formulation of a dynamic system is an elegant approach which facilitates the solution of certain problems and provides a framework for considering certain abstract philosophical implications. The basic importance of the Hamiltonian system and the canonical transformations lies in the invariances of the Hamiltonian system base. That is, if the motion of a system is governed by a set of partial differential equations, the motions can be represented by a collection of canonical mappings of the conjugate variables. These mappings preserve the form of the canonical equations and effectively change the basis of the system through the mapping of the conjugate variables.

Scientific inquiry into these subtleties began in the late eighteenth century and continued through the nineteenth century, when a dramatic change in intellectual climate stimulated such thinkers as Euler, Gauss, Lagrange, Hamilton and others to visualize a closer relationship between mathematics and philosophy. In contrast to their eighteenth century predecessers, these men found it impossible to regard the physical sciences as purely empirical disciplines. Basic new ideas were beginning to emerge from physics and mathematics which required fundamental re-evaluation of the relationship between experience and "reality". The results of their speculations have left the scientific community a

legacy of unverified theoretical conclusions.

For problems in describing reactor systems, the flux shape can be visualized as a three-dimensional surface undergoing change as time progresses. At any point of the reactor, the flux trajectory can be followed in time. The totality of these trajectories form a hypersurface in space-time which is effectively the solution of the equations of motion for the system. The trajectories can be characterized by a first order equation, commonly called the Hamilton-Jacobi equation. The canonical equations are the characteristic equations of this first order equation, which allows it to be derived from a canonical transformation approach. The solution of the Hamilton-Jacobi equation then defines a generating function that generates the solution surface from the initial values of the conjugate variables.

The problems in considering a realistic description of a large reactor, together with its accompanying operating system are indeed formidable. The objective of this study is to formulate these problems with a Hamiltonian approach and to develop some of the relationships that exist because of this formulation.

The generalized form of the Hamilton-Jacobi equation is developed and the mathematical and geometrical implications of the equation are discussed. Related concepts from classical mechanics such as Poisson brackets and the conservation laws generated by Noether's theorem are developed for contin-

uous systems. The canonical transformation is shown to be a fundamental concept in the description of the evolution of a dynamical system. The relationships generated by the canonical transformation are the heart of the Hamiltonian formulism, and gives rise to the Hamilton-Jacobi equation. This central theme has been absent in the recent articles promoting the analogy between classical mechanics and reactor theory.

After the general mathematical presentation of the Hamiltonian formulism and the related Hamilton-Jacobi theory, the results are applied to reactor systems. This is generally restricted to the derivation of the forms of the equations and the illustration of the relationship to certain other techniques and methods. This limitation is due to the difficulty in actually solving the Hamilton-Jacobi equation except for certain special cases. Hence, the practical aspects of the theory is restricted to separable solutions and to perturbation type solutions.

The theory presented in this work provides a method for extending Turley's (1) work to time-dependent problems. It also provides a basis for developing connections with the solution to the Hamilton-Jacobi equation and other techniques such as Lie series and Laplace transformations. The solution of two examples from reactor theory will be obtained by solving the corresponding Hamilton-Jacobi equation.

LITERATURE REVIEW

The first use of variational principles as a basic tool for the formulation of reactor physics problems can be attributed to Selengut (2). He illustrated that a Lagrangian functional could be defined so that invoking Hamilton's principle yielded the original equations under consideration. Also the variational principle could be used to develop an approximation theory for the calculation of various terms of interest in reactor physics. Selengut's work was based on time-independent equations and Lewins (3) extended the variational representation to time-dependent problems through his concept of the adjoint function. The addition of an independent field, i.e., the adjoint flux, was shown to be necessary to formulate Hamilton's principle for time-dependent systems described by the diffusion equation.

Following these two papers, a number of articles appeared pretaining to the inclusion of boundary conditions and the possiblity of different forms of the Lagrangian (4-10). Dickson's (11) thesis is the first to consider the Hamiltonian and the possibility of the constants of motion associated with it. The next discussion of the basic formulism appears in an article by Kaplan (12) where he constructs the analogy between the equations of reactor theory and those of classical mechanics. This work was based on time-dependent considerations. Clancy and Tavel (13) extended the analogy to time-

dependent diffusion theory and observed that in one form of the Lagrangian the momenta were redundant variables. However, they did not pursue this observation for any implication this might have relating to the physical process under investigation. Kaplan and Davis (14) have discussed the notion of canonical and involutory transformations for the transport equation. They show by the canonical transformation the equivalence of various variational formulations that have been previously used in the literature. The involutory transformation is used to relate a minimum problem to an equivalent maximum problem. Tavel, Clancy, and Pomraning (15) have utilized Noether's theorem from classical and quantum mechanics to construct analogies and generate some conservation laws for reactor problems. They suggest that more complex transformations could lead to more significant results.

The literature illustrates that the full exploitation of the variational principle as extended to reactor theory has not been realized. This thesis is an attempt to emphasis the fundamental aspects of the Hamiltonian formulation in dynamical systems and to consider the application to reactor theory.

LAGRANGIAN AND HAMILTONIAN FORMULISM

In the introduction, the utilization of concepts from classical mechanics was discussed. In this section, the Lagrangian and Hamiltonian formulation of a general dynamic system will be derived from a general form of Hamilton's principle.

Lagrangian Formulation

Hamilton's principle is a realization first discovered in the study of classical systems, and its development appears in many works (16-23). Here it will be postulated that the reactor systems obey a general form of Hamilton's principle and that the corresponding equations can be derived from it. The most commonly used equation to describe the space-time behavior of a reactor has been the time-dependent diffusion equation.

$$\nabla \cdot D \nabla \phi + \nu \Sigma_f \phi - \Sigma_a \phi + S = \frac{1}{v} \frac{\partial \phi}{\partial t} \qquad (1.1)$$

The notation is standard and is listed in Appendix A. There are more general equations that can be used, but this one will be the subject of investigation in the sequel. However, it does serve to remind one to review the limitations of the use of diffusion theory. The conclusions one makes when considering a phenomenon must be tempered by a consideration of the model used and the equations used to describe the model.

A general reactor system can be described by considering a dynamical field with components $\phi(x_\omega)$ which are real-valued functions, where the x_ω are coordinates specifying location in space and time, i.e., the quadtuple (x_1, x_2, x_3, x_4) corresponds to (x,y,z,t). The integral I is defined by

$$I = \int_T \mathcal{L}\left(x_\omega, \phi_\mu(x_\omega), \frac{\partial \phi_\mu(x_\omega)}{\partial x_\omega}\right) d\gamma \qquad (1.2)$$

where $\mathcal{L}$ is a Lagrangian density function and T is the hypervolume determined by the coordinates $\{x_\omega\}$. A general form of Hamilton's principle can be written as

$$\delta I = \delta \int_T \mathcal{L}\, d\gamma = 0 \qquad (1.3)$$

where δI denotes the first variation of the functional integral I. The stationarity of this integral gives rise to the Euler-Lagrange equations associated with the Lagrangian density $\mathcal{L}$. This variational principle serves to distinguish the field among all possible fields by leading to the correct Euler-Lagrange equations.

To derive the Euler-Lagrange equations, consider the field components undergoing small changes of the form

$$\phi_\mu(x_\omega) \Longrightarrow \phi_\mu(x_\omega) + \delta\phi_\mu \qquad (1.4)$$

The variation of the integral I can be written as

$$\delta I = \int_T \mathcal{L}\left(x_\omega, \phi_\mu + \delta\phi_\mu, \frac{\partial}{\partial x_\omega}(\phi_\mu + \delta\phi_\mu)\right) d\gamma - \int_T \mathcal{L}\left(x_\omega, \phi_\mu, \frac{\partial \phi_\mu}{\partial x_\omega}\right) \qquad (1.5)$$

If the Lagrangian density of the first term is expanded in a Taylor's series about the Lagrangian of the unvaried variables, δI can be written to the first order in the small variations $\delta\phi_\mu$ as

$$\delta I = \int_{\tau} \sum_{\mu=1}^{n} \left\{ \frac{\partial \mathcal{L}}{\partial \phi_\mu} \delta \phi_\mu + \sum_{\omega=1}^{4} \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \phi_\mu}{\partial x_\omega} \right)} \delta \left(\frac{\partial \phi_\mu}{\partial x_\omega} \right) \right\} d\tau \qquad (1.6)$$

The second term of the integrand is integrated by parts and the generalized form of Green's theorem is used to convert Eq. 1.6 into the form

$$\delta I = \int_{\tau} \sum_{\mu=1}^{n} \left\{ \frac{\partial \mathcal{L}}{\partial \phi_\mu} - \sum_{\omega=1}^{4} \frac{\partial}{\partial x_\omega} \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \phi_\mu}{\partial x_\omega} \right)} \right\} \delta \phi_\mu \, d\tau + \int_{\Sigma} \sum_{n=1}^{n} \left(\sum_{\omega=1}^{4} \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \phi_\mu}{\partial x_\omega} \right)} \ell_\omega \right) \delta \phi_\mu \, d\sigma \qquad (1.7)$$

where the ℓ_ω are the direction cosines of the outward directed normal to the hypersurface Σ at any point. If the variation of the field components is zero on the hypersurface, then the expression of δI yields the Euler-Lagrange equations.

$$\frac{\partial \mathcal{L}}{\partial \phi_\mu} - \sum_{\omega=1}^{4} \frac{\partial}{\partial x_\omega} \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \phi_\mu}{\partial x_\omega} \right)} = 0 \qquad (\mu = 1, 2, \cdots n) \qquad (1.8)$$

This set of equations can be written in a more compact form by defining the functional derivative of $\mathcal{L}$ by

$$\frac{\delta \mathcal{L}}{\delta \phi_\mu} \triangleq \frac{\partial \mathcal{L}}{\partial \phi_\mu} - \sum_{\omega=1}^{4} \frac{\partial}{\partial x_\omega} \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \phi_\mu}{\partial x_\omega} \right)} \qquad (1.9)$$

Equation 1.8 then can be written as

$$\frac{\delta \mathcal{L}}{\delta \phi_\mu} = 0 \qquad (\mu = 1, 2 \cdots n) \qquad (1.10)$$

The Euler-Lagrange equations have been written in a general form. Later in this study, the time coordinate will be singled out as a special coordinate and the Euler-Lagrange equations will take a more familiar form. The Hamiltonian formulation of the field equations will now be derived from an equivalent form of Hamilton's integral.

Hamiltonian Formulation

The fundamental significance of the Hamiltonian formulation lies in the concept of "momenta" as additional independent field variables. This gives rise to a more symmetric form of the field equations commonly called the canonical equations. The momentum density components corresponding to field component ϕ_μ is given by

$$\pi_\mu^{\ \omega} = \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \phi_\mu}{\partial x_\omega}\right)} \tag{1.11}$$

Then the Hamiltonian density is defined as

$$\mathcal{H} = \sum_{\mu=1}^{n} \sum_{\omega=1}^{4} \pi_\mu^{\ \omega} \frac{\partial \phi_\mu}{\partial x_\omega} - \mathcal{L} \tag{1.12}$$

and the integral I can be expressed in terms of $\mathcal{H}$ as

$$I = \int_T \left\{ \sum_{\mu=1}^{n} \sum_{\omega=1}^{4} \pi_\mu^{\ \omega} \frac{\partial \phi_\mu}{\partial x_\omega} - \mathcal{H} \right\} d\tau \tag{1.13}$$

The canonical equations are derived in a manner similiar to the derivation of the Euler-Lagrange equations by considering small independent variations in the field and momentum components. The variation of I becomes

$$\delta I = \int_T \left[\sum_{\mu=1}^{n} \sum_{\omega=1}^{4} \left\{ \pi_\mu^{\ \omega} \delta\left(\frac{\partial \phi_\mu}{\partial x_\omega}\right) + \delta \pi_\mu^{\ \omega} \frac{\partial \phi_\mu}{\partial x_\omega} \right\} - \delta \mathcal{H} \right] d\tau \tag{1.14}$$

If the terms involving variation of derivatives of the variables are integrated by parts and Green's theorem utilized, δI becomes

$$\delta I = \int_T \sum_{\mu=1}^{n} \left[\sum_{\omega=1}^{4} \frac{\partial \pi_\mu^{\ \omega}}{\partial x_\omega} \delta \phi_\mu + \sum_{\omega=1}^{4} \frac{\partial \phi_\mu}{\partial x_\omega} \delta \pi_\mu^{\ \omega} - \frac{\partial \mathcal{H}}{\partial \phi_\mu} \delta \phi_\mu - \right.$$
$$\left. - \sum_{\omega=1}^{4} \frac{\partial \mathcal{H}}{\partial \pi_\mu^{\ \omega}} \delta \pi_\mu^{\ \omega} \right] d\tau = 0 \tag{1.15}$$

if the surface integral vanishes. For independent variations of ϕ_μ and π_μ^ω Eq. 1.15 can only be zero if the coefficients of $\delta\phi_\mu$ and $\delta\pi_\mu^\omega$ vanish. This gives the canonical equations

$$\frac{\partial \phi_\mu}{\partial x_\omega} = \frac{\partial \mathcal{H}'}{\partial \pi_\mu^\omega} \qquad (\omega = 1,2\cdots 4\,;\ \mu = 1,2\cdots n) \tag{1.16}$$

$$\sum_{\omega=1}^{4} \frac{\partial}{\partial x_\omega} \pi_\mu^\omega = -\frac{\partial \mathcal{H}'}{\partial \phi_\mu} \qquad (\mu = 1,2,\cdots n) \tag{1.17}$$

which are analogous to Hamilton's equations in classical mechanics (16, 17, 21). It should be noted that the development just given has abstracted the concept of momentum to include all the derivatives of the field components. It is the usual practice to write the momenta only as the time derivatives. If the integral I is written as

$$I = \int_{t_1}^{t_2} dt \iiint_V \left[\sum_{\mu=1}^{n} \pi_\mu \dot{\phi}_\mu - \mathcal{H}(x_\omega, \phi_\mu, \nabla\phi_\mu, \pi_\mu, \nabla\pi_\mu)\right] d\vec{\tau} \tag{1.18}$$

with the momenta defined now as

$$\pi_\mu = \frac{\partial \mathcal{L}}{\partial \dot{\phi}_\mu} \tag{1.19}$$

then the canonical equations become

$$\dot{\phi}_\mu = \frac{\partial \mathcal{H}}{\partial \pi_\mu} - \sum_{\alpha=1}^{3} \frac{\partial}{\partial x_\alpha} \frac{\partial \mathcal{H}}{\partial\left(\frac{\partial \pi_\mu}{\partial x_\alpha}\right)} \qquad (\mu = 1,2\cdots n) \tag{1.20}$$

$$\dot{\pi}_\mu = -\frac{\partial \mathcal{H}}{\partial \phi_\mu} + \sum_{\alpha=1}^{3} \frac{\partial}{\partial x_\alpha} \frac{\partial \mathcal{H}}{\partial\left(\frac{\partial \phi_\mu}{\partial x_\alpha}\right)} \qquad (\mu = 1,2,\cdots n) \tag{1.21}$$

where the coordinate x_4 has been equated with the time t. Also, terms involving the spatial derivatives of π_μ have been added to Eq. 1.21 to achieve a symmetrical form. The Hamiltonian density derived from the the Lagrangian density that depends only on the field components and their first deriv-

atives does not contain terms of this type and so Eq. 1.21 reduces to the proper form. However, the Hamiltonian density need not be considered to be derived in this manner. In general, the form of the Hamiltonian density could have been assumed and the Lagrangian density derived from it. Mercier (21) considers this case in more detail.

The canonical field equations represent the motion of a dynamical system as does the previously derived Euler-Lagrange equations, but the defining function space manifolds are different in concept. In the canonical case, the field components and momenta represent a kind of a duality between their corresponding function spaces. This is due to the independent status given to the momenta in the Hamiltonian formulation.

CANONICAL TRANSFORMATIONS

Canonical transformation is the name given to a class of transformations that preserve the form of the canonical equations. It is through transformations of this type that the true significance of the Hamiltonian formulation is revealed

The problem to be solved is the transformation that connects the following sets of canonical equations.

$$\left.\begin{aligned} \frac{\partial \phi_\mu}{\partial \chi_\omega} &= \frac{\partial \mathcal{H}}{\partial \pi_\mu{}^\omega} \\ \sum_{\omega=1}^{4} \frac{\partial \pi_\mu{}^\omega}{\partial \chi_\omega} &= -\frac{\partial \mathcal{H}}{\partial \phi_\mu} \end{aligned}\right\} \Leftrightarrow \left\{\begin{aligned} \frac{\partial \bar{\Phi}_\mu}{\partial \chi_\omega} &= \frac{\partial \mathcal{K}}{\partial \Pi_\mu{}^\omega} \\ \sum_{\omega=1}^{4} \frac{\partial \Pi_\mu{}^\omega}{\partial \chi_\omega} &= -\frac{\partial \mathcal{K}}{\partial \bar{\Phi}_\mu} \end{aligned}\right. \tag{2.1}$$

Hamilton's principle is required to hold in both systems and the form of the canonical equations is to remain unchanged. If the mapping between old and new variables is

$$\left.\begin{aligned} \bar{\Phi}_\mu &= \bar{\Phi}_\mu(\chi_\beta, \phi_\eta, \pi_\eta{}^\beta) \\ \Pi_\mu{}^\omega &= \Pi_\mu{}^\omega(\chi_\beta, \phi_\mu, \pi_\eta{}^\beta) \end{aligned}\right\} \begin{matrix} (\mu, \eta = 1,2,\cdots n) \\ (\omega, \beta = 1,2,3,4) \end{matrix} \tag{2.2}$$

then the requirement on Hamilton's principle yields the relationship

$$\delta \int_\tau \left\{ \left[\sum_{\mu=1}^{n} \sum_{\omega=1}^{4} \pi_\mu{}^\omega \frac{\partial \phi_\mu}{\partial \chi_\omega} - \mathcal{H} \right] - \left[\sum_{\mu=1}^{n} \sum_{\omega=1}^{4} \Pi_\mu{}^\omega \frac{\partial \bar{\Phi}_\mu}{\partial \chi_\omega} - \mathcal{K} \right] \right\} d\gamma - \delta \int_\tau \circledcirc\!\!\ominus \, d\gamma = 0 \tag{2.3}$$

where the last integral is an "independent integral". An independent integral is one in which the variation vanishes identically along the path of the motion. It can be considered analogous to a total differential in a one dimensional

case. One form that may be written for Θ is the four- divergence of a function $\mathcal{F}$ that in general depends on both the old and new variables. Because of the relationship between the field components and the momenta in each system, the function $\mathcal{F}$ need only be a function of one set of the new variables and one set of the old variables. This gives rise to four different forms of $\mathcal{F}$ to be considered. These are

$$\left.\begin{aligned} \mathcal{F}^{(1)} &= \mathcal{F}^{(1)}[\chi_\omega, \phi_\mu, \Phi_\mu] \\ \mathcal{F}^{(2)} &= \mathcal{F}^{(2)}[\chi_\omega, \phi_\mu, \Pi_\mu{}^\omega] \\ \mathcal{F}^{(3)} &= \mathcal{F}^{(3)}[\chi_\omega, \pi_\mu{}^\omega, \Phi_\mu] \\ \mathcal{F}^{(4)} &= \mathcal{F}^{(4)}[\chi_\omega, \pi_\mu{}^\omega, \Pi_\mu{}^\omega] \end{aligned}\right\} \quad \begin{matrix}(\mu = 1,2\cdots n)\\ (\omega = 1,2,3,4)\end{matrix} \qquad (2.4)$$

As an example of the derivation of the transformation equations, consider $\mathcal{F}^{(2)}$. The independent integral can be written for this case as

$$\int_T \sum_{\omega=1}^{4} \frac{d}{d\chi_\omega} \mathcal{F}_\omega^{(2)}\, d\tau = \int_T \sum_{\omega=1}^{4} \left\{ \frac{\partial \mathcal{F}_\omega^{(2)}}{\partial \chi_\omega} + \sum_{\mu=1}^{n} \frac{\partial \mathcal{F}_\omega^{(2)}}{\partial \phi_\mu} \frac{\partial \phi_\mu}{\partial \chi_\omega} + \sum_{\mu=1}^{n} \sum_{\alpha=1}^{4} \frac{\partial \mathcal{F}_\omega^{(2)}}{\partial \Pi_\mu^\alpha} \frac{\partial \Pi_\mu^\alpha}{\partial \chi_\omega} \right\} d\tau \qquad (2.5)$$

When Eq. 2.5 is substituted into Eq. 2.3, and the terms collected, the result is the following expression.

$$\delta \int_T \Big[\sum_{\mu=1}^{n} \sum_{\omega=1}^{4} \Big\{ \Big[\pi_\mu{}^\omega - \frac{\partial \mathcal{F}_\omega^{(2)}}{\partial \phi_\mu} \Big] \frac{\partial \phi_\mu}{\partial \chi_\omega} - \Big[\Phi_\mu - \sum_{\alpha=1}^{4} \frac{\partial \mathcal{F}_\omega^{(2)}}{\partial \Pi_\mu^\alpha} \Big] \frac{\partial \Pi}{\partial \chi_\omega} \Big\} - \mathcal{H} + \mathcal{K} - \sum_{\omega=1}^{4} \frac{\partial \mathcal{F}_\omega^{(2)}}{\partial \chi_\omega} \Big] d\tau = 0 \qquad (2.6)$$

If the variation of these integrals is to be zero for both sets of variables, the the integrands must satisfy the expression

$$\Big[\Big\{ \pi_\mu{}^\omega - \frac{\partial \mathcal{F}_\omega^{(2)}}{\partial \phi_\mu} \Big\} \frac{\partial \phi_\mu}{\partial \chi_\omega} - \Big\{ \Phi_\mu - \sum_{\alpha=1}^{4} \frac{\partial \mathcal{F}_\omega^{(2)}}{\partial \Pi_\mu^\alpha} \Big\} \frac{\partial \Pi_\mu{}^\omega}{\partial \chi_\omega} - \mathcal{H} + \mathcal{K} - \sum_{\omega=1}^{4} \frac{\partial \mathcal{F}_\omega^{(2)}}{\partial \chi_\omega} \Big] = 0 \qquad (2.7)$$

from which the transformation relations follow, i.e.,

$$\pi_\mu^{\ \omega} = \frac{\partial \mathcal{F}_\omega^{(2)}}{\partial \phi_\mu} \tag{2.8}$$

$$\Phi_\mu = \sum_{\alpha=1}^{4} \frac{\partial \mathcal{F}_\omega^{(2)}}{\partial \Pi_\mu^{\ \alpha}} \tag{2.9}$$

$$\mathcal{K} = \mathcal{H} + \sum_{\omega=1}^{4} \frac{\partial \mathcal{F}_\omega^{(2)}}{\partial x_\omega} \tag{2.10}$$

This set indicates that $\mathcal{F}^{(2)}$ is a generating function of the transformation. This means that if $\mathcal{F}$ is given, then the transformation is completely specified.

The transformation relationship for the other three forms that the generating function can take are as follows.

Form $\mathcal{F}^{(1)}$:

$$\left.\begin{aligned} \pi_\mu^{\ \omega} &= \frac{\partial \mathcal{F}_\omega^{(1)}}{\partial \phi_\mu} \\ \Pi_\mu^{\ \omega} &= -\frac{\partial \mathcal{F}_\omega^{(1)}}{\partial \Phi_\mu} \\ \mathcal{K} &= \mathcal{H} + \sum_{\omega=1}^{4} \frac{\partial \mathcal{F}_\omega^{(1)}}{\partial x_\omega} \end{aligned}\right\} \quad \begin{matrix}(\mu = 1,2,\cdots n)\\ (\omega = 1,2,3,4)\end{matrix} \tag{2.11}$$

Form $\mathcal{F}^{(3)}$:

$$\left.\begin{aligned} \phi_\mu &= -\sum_{\omega=1}^{4} \frac{\partial \mathcal{F}_\omega^{(3)}}{\partial \pi_\mu^{\ \omega}} \\ \Pi_\mu^{\ \omega} &= -\frac{\partial \mathcal{F}_\omega^{(3)}}{\partial \Phi_\mu} \\ \mathcal{K} &= \mathcal{H} + \sum_{\omega=1}^{4} \frac{\partial \mathcal{F}_\omega^{(3)}}{\partial x_\omega} \end{aligned}\right\} \quad \begin{matrix}(\mu = 1,2,\cdots n)\\ (\omega = 1,2,3,4)\end{matrix} \tag{2.12}$$

Form $\mathcal{F}^{(4)}$:

$$\left.\begin{aligned} \phi_\mu &= -\sum_{\omega=1}^{4} \frac{\partial \mathcal{F}^{(4)}}{\partial \pi_\mu^{\ \omega}} \\ \Phi_\mu &= \sum_{\omega=1}^{4} \frac{\partial \mathcal{F}_\omega^{(4)}}{\partial \Pi_\mu^{\ \omega}} \\ \mathcal{K} &= \mathcal{H} + \sum_{\omega=1}^{4} \frac{\partial \mathcal{F}_\omega^{(4)}}{\partial x_\omega} \end{aligned}\right\} \quad \begin{matrix}(\mu = 1,2,\cdots n)\\ (\omega = 1,2,3,4)\end{matrix} \tag{2.13}$$

It is noted that in every case, the new Hamiltonian density differs from the old one by the explicit dependence of the coordinates.

HAMILTON-JACOBI THEORY

In this section, the Hamilton-Jacobi equation will be derived from a special consideration of a canonical transformation. A generalization of Hamilton's principle function will be shown to lead to the Hamilton-Jacobi equation. A brief discussion will follow on the general solution of the Hamilton-Jacobi equation and the central position that the Hamilton-Jacobi equation plays in the theory of dynamical systems.

Derivation by Canonical Transformation

In classical mechanics, the Hamilton-Jacobi equation is derived by considering a special canonical transformation where the new coordinates and the new momenta are constants. The solution of the Hamilton-Jacobi equation then can be interpreted as the generating function of the motion from the known initial conditions.

In extending the Hamilton-Jacobi theory to continuous fields, the requirement is that the new conjugate variables be known functions. That is, the new variables reduce to

$$\overline{\Phi}_\mu = \alpha_\mu(\chi_\alpha) \qquad (\alpha = 1,2,3,4) \tag{3.1}$$

$$\overline{\Pi}_\mu^{\ \omega} = \beta_\mu^{\ \omega}(\chi_\alpha) \qquad (\alpha, \omega = 1,2,3,4) \tag{3.2}$$

where the reference has been made for time t=0. If this is the case, the determination of the proper generating function will be equivalent to solving the equations of the field.

From the results of the previous section, the generating function of the form

$$S_\omega = S_\omega(\chi_\sigma, \phi_\mu, \alpha_\mu) \qquad (\sigma, \omega = 1,2,3,4) \tag{3.3}$$

yields the following transformation equations.

$$\pi_\mu^{\ \omega} = \frac{\partial S_\omega}{\partial \phi_\mu} \tag{3.4}$$

$$\Pi_\mu^{\ \omega} = -\frac{\partial S_\omega}{\partial \alpha_\mu} = -\beta_\mu^{\ \omega} \tag{3.5}$$

$$\sum_{\omega=1}^{4} \frac{\partial S_\omega}{\partial \chi_\omega} + \mathcal{H}' = \mathcal{K} \tag{3.6}$$

If the new Hamiltonian density is zero for the new variables, the generalized form of the Hamilton-Jacobi equation is obtained.

$$\sum_{\omega=1}^{4} \frac{\partial S_\omega}{\partial \chi_\omega} + \mathcal{H}\left(\chi_\sigma, \phi_\mu, \frac{\partial S_\sigma}{\partial \phi_\mu}\right) = 0 \tag{3.7}$$

Thus the transformation that transforms the Hamiltonian to zero yields canonical equations which can be immediately integrated. Equation 3.7 is a first order partial differential equation involving functionals and is in general very difficult to solve. However, the form of a complete integral can be obtained from an extension of the theory of first order partial differential equations. Because of the use that will be made in the sequel of the Hamilton-Jacobi equation, it is useful to derive a time-preferred formulation of the equation. The momenta are now considered as only the time derivatives of the field components, i.e.,

$$\pi_\mu = \frac{\partial}{\partial \dot{\phi}_\mu} \mathcal{L}(\chi_\omega, \phi_\mu, \nabla\phi_\mu, \dot{\phi}_\mu) \tag{3.8}$$

The spatial derivatives are carried along without any special notation. The integral I can be separated into two domains of integration if the hyperspace is representable as a hyper-

cylinder or its topological equivalent. This gives rise to the form of Hamilton's integral written in Eq.1.18. The corresponding canonical equations were given in Eqs. 1.20 and 1.21. The derivation of the Hamilton-Jacobi equation for this case proceeds in the same manner as the general case. The assumption is made that the independent integral is now only a function of a total time derivative, the spatial portion vanishing identically on the spatial boundary. This gives

$$\frac{\partial S}{\partial t} + \mathcal{H}\left(t, x, y, z, \phi_\mu, \nabla\phi_\mu, \frac{\partial S}{\partial \phi_\mu}\right) = 0 \qquad (3.9)$$

as the corresponding Hamilton-Jacobi equation. An alternate derivation of this equation based on physical considerations will be made in the next section when the analog of Hamilton's principle function is considered.

Hamilton's Principle Function

Another way of deriving the Hamilton-Jacobi equation is via the concept of Hamilton's principle function (24, 25). This is more geometrical in nature than the derivation by canonical transformation and as a result has a more direct physical interpretation. Hamilton's principle function is defined as the action integral over the hyperspace T expressed as a function of the value of the coordinates and field components at the boundary, i.e.,

$$S(\mathcal{P}', \mathcal{P}^*) = \int_{\mathcal{P}'}^{\mathcal{P}^*} \mathcal{L}\left(x_\omega, \phi_\mu, \frac{\partial \phi_\mu}{\partial x_\omega}\right) d\tau \qquad (3.10)$$

where P' and P* denote two locations in the hyperspace. Figure 3.1 illustrates the basic concept by representing the hypersurfaces defined by the parameters Σ' and Σ^* by two curves with the points P' and P* lying on these surfaces. The curve connecting the points P' and P*, denoted by Γ, is a natural trajectory or solution curve of the field equations. The action integral is taken along this curve and may be equivalently represented in the Hamiltonian notation as

$$S = \int_{P'}^{P^*} \left[\sum_{\mu=1}^{n} \sum_{\omega=1}^{4} \pi_\mu{}^\omega \frac{\partial \phi_\mu}{\partial x_\omega} - \mathcal{H} \right] d\tau \qquad (3.11)$$

The variation in S can be written as the difference of the integrals

$$\delta S = \int_{\Sigma^*} \mathcal{L}^*(x_\omega^*, \phi_\mu^*, \frac{\partial \phi_\mu^*}{\partial x_\omega^*}) d\tau - \int_{\Sigma'} \mathcal{L}'(x_\omega', \phi_\mu', \frac{\partial \phi_\mu}{\partial x_\omega}) d\tau \qquad (3.12)$$

where the coordinates as well as the field components are allowed to vary. Equation 3.12 can be written in terms of an integral with fixed limits and a term due to variation at the boundary.

$$\delta S = \int_{P'}^{P^*} \delta \mathcal{L} \, d\tau + \mathcal{L} \, \delta\tau \Big|_{x_\omega'}^{x_\omega^*} \qquad (3.13)$$

The first term in this expression vanishes except for a boundary term because of the path of integration. At this point, it is useful to introduce two types of variations. The total variation consists of the intrinsic variation due to the variation in the field components plus the variation in the field components due to variation in the coordinates, i.e.,

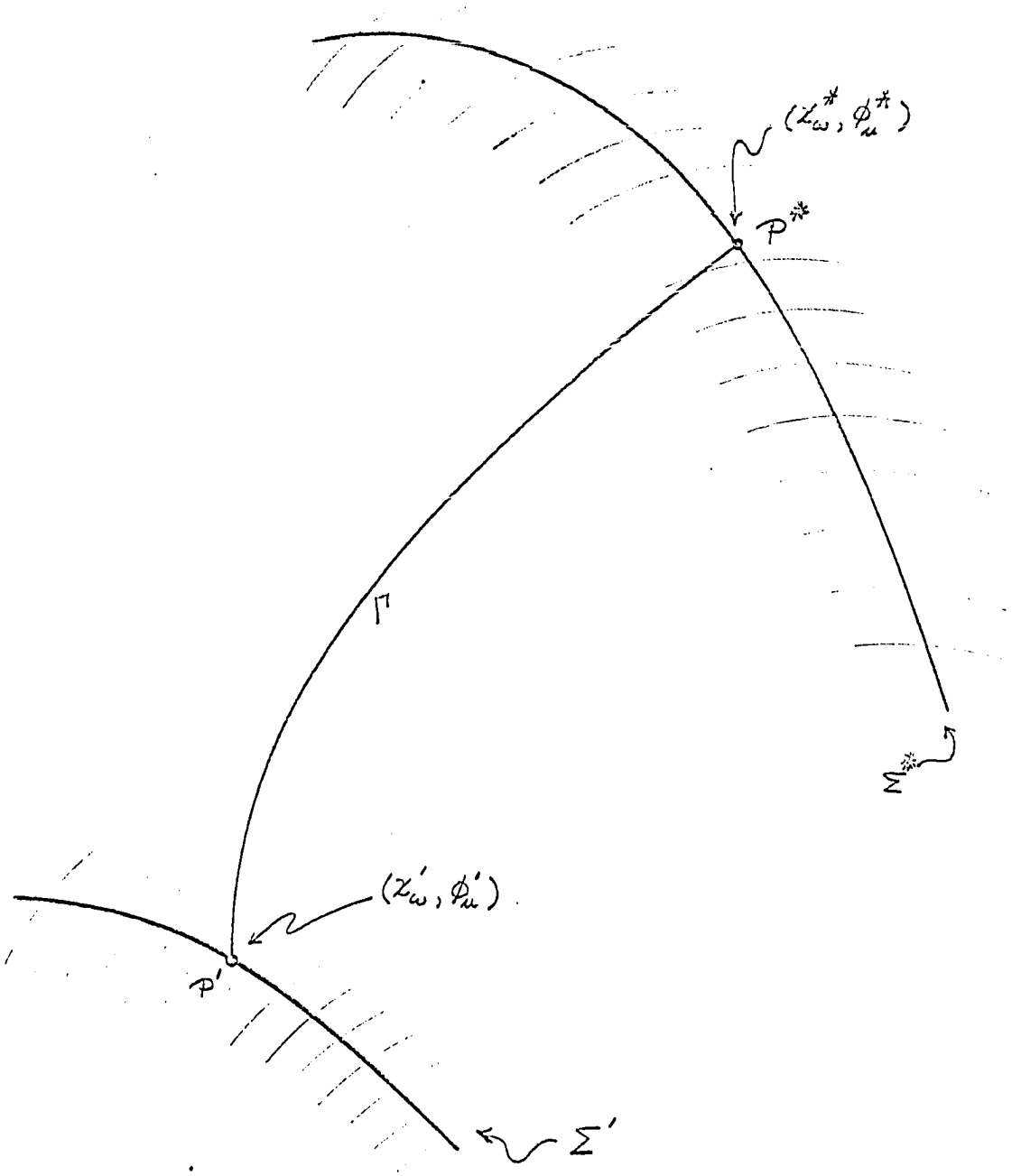

Fig. 3.1. Geometry of Hamilton's principle function in the space of $\{z_\omega, \phi_\mu\}$.

$$\delta\phi_\mu = \Delta\phi_\mu + \sum_{\omega=1}^{4'} \frac{\partial\phi_\mu}{\partial\chi_\omega}\,\delta\chi_\omega \tag{3.14}$$

Equation 3.13 can then be written as

$$\delta S = \int_{P'}^{P^*} \Delta\left[\sum_{\mu=1}^{n}\sum_{\omega=1}^{4'} \pi_\mu{}^\omega \frac{\partial\phi_\mu}{\partial\chi_\omega} - \mathcal{H}\right] d\tau + \left[\sum_{\mu=1}^{n}\sum_{\omega=1}^{4'} \pi_\mu{}^\omega \delta\phi_\mu - \mathcal{H}\,\delta\tau\right]_{\chi_\omega'}^{\chi_\omega^*} \tag{3.15}$$

If the variation in S is computed based on the functional dependence of S, another expression for δS becomes

$$\delta S = \sum_{\mu=1}^{4'} \frac{\partial S}{\partial \chi_\omega'}\,\delta\chi_\omega' + \sum_{\mu=1}^{n} \frac{\partial S}{\partial \phi_\mu'}\,\delta\phi_\mu' + \sum_{\omega=1}^{4'} \frac{\partial S}{\partial \chi_\omega^*}\,\delta\chi_\omega^* + \sum_{\mu=1}^{n} \frac{\partial S}{\partial \phi_\mu^*}\,\delta\phi_\mu^* \tag{3.16}$$

and comparing with Eq. 3.15 yields the set of equations

$$\sum_{\omega=1}^{4'} \frac{\partial S}{\partial \chi_\omega^*} = -\mathcal{H}^* \quad ; \quad \frac{\partial S}{\partial \phi_\mu^*} = \sum_{\omega=1}^{4'} \pi_\mu^{*\omega}(\chi_\alpha^*) \tag{3.17}$$

$$\sum_{\omega=1}^{4'} \frac{\partial S}{\partial \chi_\omega'} = \mathcal{H}' \quad ; \quad \frac{\partial S}{\partial \phi_\mu'} = -\sum_{\omega=1}^{4'} \pi_\mu'^{\omega}(\chi_\alpha') \tag{3.18}$$

These equations are the generalized equivalent to the equations that Hamilton (24) obtained in his original work. If the time coordinate is singled out from the other coordinates and this is the only coordinate allowed to vary, the time-preferred equivalents to Eqs. 3.17 and 3.18 are

$$\frac{\partial S}{\partial t^*} = -\mathcal{H}^* \quad ; \quad \frac{\partial S}{\partial \phi_\mu^*} = \pi_\mu^* \tag{3.19}$$

$$\frac{\partial S}{\partial t'} = \mathcal{H}' \quad ; \quad \frac{\partial S}{\partial \phi_\mu'} = -\pi_\mu' \tag{3.20}$$

The results just obtained are similiar to those obtained in deriving the Hamilton-Jacobi equation by canonical transformation. However, there are now two sets of equations to be satisfied by S. If the principle function had been taken

from an integral with fixed lower boundary, the results of a similiar development as above would have given the expressions in Eqs. 3.4, 3.5, and 3.6. The second equation of the Hamilton-Jacobi type becomes redundant in the sense that S need now only satisfy one equation.

The two viewpoints that have been used to derive the Hamilton-Jacobi equation have different physical interpretations. The principle function serves to relate two arbitrary points in the hyperspace, and thus in effect is a transformation between two states of the system. This gives rise to the two sets of equations that the principle function must satisfy. On the other hand, the canonical transformation was choosen to reduce the problem to some known state, i.e., the initial state. This last viewpoint is the one taken for computational purposes since one is generally interested in solving for the state of a dynamical system in terms of its initial configuration.

There are other techniques for obtaining the Hamilton-Jacobi equation. One method is based on the Pffafian form of the equations of motion. This is based on a theory of differential forms and is similiar in approach to that of the canonical transformations. Flanders (26) and Pars (27) discuss this in their works. Caratheodory (28) and Rund (29) derive the Hamilton-Jacobi equation from considerations of imbedding theorems for geodesic fields and the concept of equivalent integrals.

Solution of Hamilton-Jacobi Equation

There is not a set method of solving the Hamilton-Jacobi equation explicitly for a given field equation. A general form of the solution can be written as a complete integral as based on the theory of first order equations.

A complete integral of the Hamilton-Jacobi equation consists of a functional plus an additive constant, i.e.,

$$S = \Lambda(x_\omega, \phi_\mu, \beta_\mu^\omega) + C \qquad (3.21)$$

where the β_μ^ω are a set of constants. From Courant and Hilbert (30), the complete solution depends on as many arbitrary constants as independent variables. A knowledge of the complete integral yields the solution to the canonical equations by differentiation and elimination. The additive constant in Eq. 3.21 appears because S occurs in the Hamilton-Jacobi equation only as a differentiated quantity and may be arbitrary to this extent without violating the conditions for a solution. Thus it is seen that the generating function that satisfies the Hamilton-Jacobi equation which is expressed in terms of the initial arbitrary constants is a complete integral. This complete integral effectively defines the solution of the equations once the initial conditions are given. The solution of the Hamilton-Jacobi equation then is of primary importance in determining the solution of a dynamical system. The problem is to find solutions of the Hamilton-Jacobi equation without first solving the original equations of motion.

The discussion of the principle function indicated that the solution of the Hamilton-Jacobi equation was the integral

$$S = \int \mathcal{L}\left(x_\omega, \phi_\mu, \frac{\partial \phi_\mu}{\partial x_\omega}\right) d\tau \qquad (3.22)$$

But this integral cannot be evaluated without first knowing the solution to the equations of motion. This form will be used to develop a perturbation approximation when the theory is applied to reactor systems.

The solution of the Hamilton-Jacobi equation can be made easier if a separation of variables can be preformed. In practice, only when such a separation can be made is the Hamilton-Jacobi technique a useful computational tool. This is generally the case for any method of solving multivariate problems. The existence and uniqueness of general solutions to partial differential equations is usually not of any help in the computation of an explicit solution. One is generally forced to simplify the problem by assuming solutions that can be represented by some combination of solutions of ordinary differential equations

If the Hamiltonian is not an explicit function of the coordinates $\{x_\omega\}$, the solution of the Hamilton-Jacobi equation may be written as

$$S = \sum_{\omega=1}^{q} \alpha_\omega x_\omega + W(\phi_\mu, \pi_\mu{}^\omega) \qquad (3.23)$$

This gives rise to the conditions for conservation of the Hamiltonian when Eq. 3.23 is substituted into the Hamilton-Jacobi equation.

There are other special cases when the Hamilton-Jacobi equation may be separated. If the principle function can be written as a sum of terms each involving only one of the field components

$$W = \sum_{\mu=1}^{n} W_\mu (\phi_\mu, \alpha_1, \cdots \alpha_n) \tag{3.24}$$

then the Hamilton-Jacobi equation is split into a set of equations of the form

$$\mathcal{H}_\mu \left(\phi_\mu, \frac{\partial W_\mu}{\partial \phi_\mu}, \alpha_1 \cdots \alpha_n\right) = \alpha_\mu \tag{3.25}$$

Also if some of the variables are cyclic, i.e., they do not appear in the Lagrangian density, then W is simplified since the canonical transformation to cyclic coordinates is then an identity transformation (16). Whittaker (31) discusses this point further. Basically the conditions for separability are those occuring for separability in other techniques of solution. The form of the Lagrangian and the system of coordinates are the joint properties that determine separability.

INFINITESIMAL TRANSFORMATIONS, POISSON BRACKETS, AND CONSERVATION LAWS

In this section, the infinitesimal canonical transformation will be used to illustrate that the Hamiltonian is the generator of the actual motion. Poisson brackets are introduced to allow notational convenience and are shown to be a means for testing conserved quantities. The derivation of a density conservation law leeds to consideration of the components of the stress-energy-momentum tensor. Lastly, a continuous transformation of the coordinates and field components is shown to lead to results predicted by Noether's theorem.

Infinitesimal Transformations

From the results obtained in the discussion of canonical transformations, the following generating function is easily shown to be an identity transformation.

$$\mathcal{F} = \sum_{\mu=1}^{n} \sum_{\omega=1}^{4} \phi_\mu \Pi_\mu^{\ \omega} \tag{4.1}$$

If an infinitesimal quantity is added to Eq. 4.1 in the form of an arbitrary functional and infinitesimal parameter, the result is

$$\mathcal{F}' = \sum_{\mu=1}^{n} \sum_{\omega=1}^{4} \phi_\mu \Pi_\mu^{\ \omega} + \epsilon \mathcal{G}(x_\omega, \phi_\mu, \Pi_\mu^{\ \omega}) \tag{4.2}$$

The transformation equations yield the following relations.

$$\pi_\mu^{\ \omega} = \Pi_\mu^{\ \omega} + \epsilon \frac{\partial \mathcal{G}}{\partial \phi_\mu} \tag{4.3}$$

$$\Phi_\mu = \phi_\mu + \epsilon \sum_{\omega=1}^{4} \frac{\partial \mathcal{G}}{\partial \Pi_\mu^{\ \omega}} \tag{4.4}$$

If $\mathcal{G}$ is replaced by $\mathcal{H}$ and ϵ by dx_ω, and the canonical equations utilized, Eqs. 4.3 and 4.4 become

$$\pi_\mu{}^\omega = \Pi_\mu{}^\omega - \sum_{\omega=1}^{4} \frac{\partial \pi_\mu{}^\omega}{\partial x_\omega} dx_\omega \tag{4.5}$$

$$\Phi_\mu = \phi_\mu + \sum_{\omega=1}^{4} \frac{\partial \phi_\mu}{\partial x_\omega} dx_\omega \tag{4.6}$$

This result is the infinitesimal motion as generated by the actual motion. Thus the Hamiltonian is the generator of the motion. For the time-preferred case, similiar results are obtained, i.e.,

$$\mathcal{I}' = \sum_{\mu=1}^{n} \phi_\mu \Pi_\mu + \epsilon \mathcal{H}(t, x_i, \phi_\mu, \nabla\phi_\mu, \pi_\mu) \tag{4.7}$$

$$\pi_\mu = \Pi_\mu + \frac{\delta \mathcal{H}}{\delta \phi_\mu} dt = \Pi_\mu - \dot{\pi}_\mu dt \tag{4.8}$$

$$\Phi_\mu = \phi_\mu + \frac{\delta \mathcal{H}}{\delta \Pi_\mu} dt = \phi_\mu + \dot{\phi}_\mu dt \tag{4.9}$$

where ϵ has been replaced by dt and functional derivatives employed. The motion of a dynamical system can be thought of as a succession of infinitesimal canonical transformations generated by the Hamiltonian. This indicates that the canonical transformations may possess the properties of a group. For certain types of fields this is indeed the case, and in quantum mechanics it is used (32).

Now consider the generating function of the form,

$$\mathcal{I} = \sum_{\mu=1}^{n} \sum_{\omega=1}^{4} \phi_\mu \beta_\mu{}^\omega + \delta S(x_\omega, \phi_\mu, \beta_\mu{}^\omega) \tag{4.10}$$

where the infinitesimal portion is represented by the variation of the functional S. The transformation equations give

$$\pi_\mu{}^\omega = \beta_\mu{}^\omega + \frac{\partial \delta S}{\partial \phi_\mu} \tag{4.11}$$

and

$$\alpha_\mu = \phi_\mu + \sum_{\omega=1}^{4} \frac{\partial \delta S}{\partial \beta_\mu{}^\omega} \tag{4.12}$$

This form of the transformation will be used in considering the relationship of the Hamilton-Jacobi theory to the evolution operator technique in the next section. For the time-preferred case, the equations equivalent to Eqs. 4.3 and 4.4 are

$$\pi_\mu = \beta_\mu + \frac{\delta(\delta S)}{\delta \phi_\mu} = \beta_\mu + \delta t \frac{\delta \mathcal{H}}{\delta \beta_\mu} \tag{4.13}$$

$$\phi_\mu = \alpha_\mu + \frac{\delta(\delta S)}{\delta \beta_\mu} = \alpha_\mu + \delta t \frac{\delta \mathcal{H}}{\delta \beta_\mu} \tag{4.14}$$

which follow from the expression obtained previously, i.e.,

$$\delta S = \mathcal{H}\, \delta t \tag{4.15}$$

Poisson Brackets

Following Goldstein (16), the Poisson brackets for a continuous field can be written as

$$[F, J] \triangleq \sum_{\mu=1}^{n} \left(\frac{\delta F}{\delta \phi_\mu} \frac{\delta J}{\delta \pi_\mu} - \frac{\delta F}{\delta \pi_\mu} \frac{\delta J}{\delta \phi_\mu} \right) \tag{4.16}$$

where F and J are two functionals defined as the spatial integrals of their corresponding density functions. This is generally the desirable notation when working with the time-preferred formulation. For example, the total time derivative of the functional G

$$G = \iiint \mathcal{G}(t, x_i, \phi_\mu, \nabla \phi_\mu, \pi_\mu, \nabla \pi_\mu)\, d\vec{x} \tag{4.17}$$

can be written as

$$\frac{dG}{dt} = \frac{\partial G}{\partial t} + [G, H] \tag{4.18}$$

using the canonical equations and the Poisson brackets. A Poisson bracket may be defined for density functions also, but the use of functional derivatives of the density functions must be qualified due to the fact that they appeared previously because of the variation of an integral quantity. The special form of the functional derivative is essentially due to the integration by parts of the derivative terms. Thus one must be careful in applying functional derivatives to density type quantities. In light of this, the Poisson bracket for density functions is defined as

$$\{\mathcal{F}, \mathcal{G}\} \triangleq \sum_{\mu=1}^{n} \left[\frac{\partial \mathcal{F}}{\partial \phi_\mu} \frac{\partial \mathcal{G}}{\partial \pi_\mu} - \frac{\partial \mathcal{F}}{\partial \pi_\mu} \frac{\partial \mathcal{G}}{\partial \phi_\mu} \right] \tag{4.19}$$

If the canonical equations were to be expressed in terms of density brackets, a corresponding definition would be required for the derivatives of the density functions, i.e.,

$$\{\mathcal{F}, \mathcal{G}\}_{,i} \triangleq \sum_{\mu=1}^{n} \left[\frac{\partial \mathcal{F}}{\partial\left(\frac{\partial \phi_\mu}{\partial x_i}\right)} \frac{\partial \mathcal{G}}{\partial\left(\frac{\partial \pi_\mu}{\partial x_i}\right)} - \frac{\partial \mathcal{F}}{\partial\left(\frac{\partial \pi_\mu}{\partial x_i}\right)} \frac{\partial \mathcal{G}}{\partial\left(\frac{\partial \phi_\mu}{\partial x_i}\right)} \right] \tag{4.20}$$

Then the canonical equations can be written as

$$\dot{\phi}_\mu = \{\phi_\mu, \mathcal{H}\} - \sum_{i=1}^{3} \frac{\partial}{\partial x_i} \left\{ \frac{\partial \phi_\mu}{\partial x_i}, \mathcal{H} \right\}_{,i} \tag{4.21}$$

$$\dot{\pi}_\mu = \{\pi_\mu, \mathcal{H}\} - \sum_{i=1}^{3} \frac{\partial}{\partial x_i} \left\{ \frac{\partial \pi_\mu}{\partial x_i}, \mathcal{H} \right\}_{,i} \tag{4.22}$$

These equations can also be written in terms of the Poisson bracket of Eq. 4.16 as

$$\dot{\phi}_\mu = [\phi_\mu, H] \tag{4.23}$$

$$\dot{\pi}_\mu = [\pi_\mu, H] \tag{4.24}$$

The two sets of equations are equivalent because H is defined as the spatial integral of $\mathcal{H}$, and the derivation of the equations were originally from Hamilton's integral.

The notational convenience of the Poisson bracket is obvious, but it is the special properties of this bracket which make it important in dynamics. From Eq. 4.17 the condition for a functional to be constant in time is that its Poisson bracket with H is zero when the functional does not depend explicitly on time. This gives rise to the expression

$$[G, H] = 0 \tag{4.25}$$

for dynamical quantities that are conserved. The question of conservation laws for fields and density functions will be considered next.

Conservation Laws

Derivation of a density conservation law

From the functional form of the time-preferred Hamiltonian density,

$$\mathcal{H} = \mathcal{H}(t, x_i, \phi_\mu, \nabla\phi_\mu, \pi_\mu, \nabla\pi_\mu) \tag{4.26}$$

the total time derivative is computed.

$$\frac{d\mathcal{H}}{dt} = \frac{\partial\mathcal{H}}{\partial t} + \sum_{\mu=1}^{n} \frac{\partial\mathcal{H}}{\partial\phi_\mu}\dot{\phi}_\mu + \sum_{\mu=1}^{n} \frac{\partial\mathcal{H}}{\partial(\nabla\phi_\mu)} \frac{\partial\nabla\phi_\mu}{\partial t} + \sum_{\mu=1}^{n} \frac{\partial\mathcal{H}}{\partial\pi_\mu}\dot{\pi}_\mu + \sum_{\mu=1}^{n} \frac{\partial\mathcal{H}}{\partial(\nabla\pi_\mu)} \frac{\partial\nabla\pi_\mu}{\partial t} \tag{4.27}$$

From the definition of $\mathcal{H}$ in terms of the Lagrangian density $\mathcal{L}$ and the use of the Euler-Lagrange equations, the intermediate result is obtained,

$$\frac{d\mathcal{H}}{dt} = \sum_{\mu=1}^{n} \left\{ \left(\dot{\pi}_\mu - \frac{\partial \mathcal{L}}{\partial \phi_\mu} \right) \dot{\phi}_\mu - \sum_{\omega=1}^{n} \frac{\partial \mathcal{L}}{\partial (\nabla \phi_\mu)} \frac{\partial \dot{\phi}_\mu}{\partial x_\omega} \right\} + \frac{\partial \mathcal{H}}{\partial t} \qquad (4.28)$$

from which the following form of Eq. 4.27 is easily derived.

$$\frac{d\mathcal{H}}{dt} = -\sum_{\mu=1}^{n} \sum_{i=1}^{3} \left[\left(\frac{\partial}{\partial x_i} \frac{\partial \mathcal{L}}{\partial (\nabla \phi_\mu)} \right) \dot{\phi}_\mu + \frac{\partial \mathcal{L}}{\partial (\nabla \phi_\mu)} \frac{\partial \dot{\phi}_\mu}{\partial x_i} \right] + \frac{\partial \mathcal{H}}{\partial t} \qquad (4.29)$$

The quantity Q_i is defined by

$$Q_i = \sum_{\mu=1}^{n} \frac{\partial \mathcal{L}}{\partial (\nabla \phi_\mu)} \dot{\phi}_\mu \qquad (i = 1,2,3) \qquad (4.30)$$

The expression for $\frac{d\mathcal{H}}{dt}$ can be written as

$$\frac{d\mathcal{H}}{dt} = -\nabla \cdot \vec{Q} + \frac{\partial \mathcal{H}}{\partial t} \qquad (4.31)$$

where $\vec{Q}$ is the vector with components Q_i. If $\mathcal{H}$ is a conserved quantity, i.e., the total time derivative is zero, then Eq. 4.31 becomes

$$\nabla \cdot \vec{Q} - \frac{\partial \mathcal{H}}{\partial t} = 0 \qquad (4.32)$$

which has the form of a continuity equation. Another density functional analogous to Q_i can be defined as

$$V_i = -\sum_{\mu=1}^{n} \frac{\partial \mathcal{L}}{\partial \dot{\phi}_\mu} \frac{\partial \phi_\mu}{\partial x_i} \qquad (i = 1,2,3) \qquad (4.33)$$

which is seen to be the opposite combination of derivatives from $\vec{Q}$. If the time derivative of V_i is computed and the terms manipulated algebraically, the intermediate result is

$$\frac{dV_i}{dt} = -\sum_{\mu=1}^{n}\left\{\frac{\partial \mathcal{L}}{\partial \phi_\mu}\frac{\partial \phi_\mu}{\partial x_i} - \sum_{j=1}^{3}\frac{d}{dx_j}\left(\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \phi_\mu}{\partial x_j}\right)}\right)\frac{\partial \phi_\mu}{\partial x_i} + \frac{\partial \mathcal{L}}{\partial \dot{\phi}_\mu}\frac{\partial \dot{\phi}_\mu}{\partial x_i}\right\} \quad (4.34)$$

by using the Euler-Lagrange equations. Further reduction results in the expression

$$\frac{dV_i}{dt} = \frac{\partial \mathcal{L}}{\partial x_i} + \sum_{j=1}^{3}\frac{d}{dx_j}\sum_{\mu=1}^{n}\left\{\frac{\partial \mathcal{L}}{\partial(\nabla_j \phi_\mu)}\frac{\partial \phi_\mu}{\partial x_i} - \delta_{ij}\mathcal{L}\right\} \quad (4.35)$$

where δ_{ij} is the Kronecker delta.

Morse and Feshbach (33) give the expression

$$\mathcal{W}_{rs} = \sum_{\mu=1}^{n}\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \phi_\mu}{\partial x_s}\right)}\frac{\partial \phi_\mu}{\partial x_r} - \delta_{rs}\mathcal{L} \qquad (r,s=1,2\cdots 4) \quad (4.36)$$

from which the components of the stress-energy-momentum tensor can be computed. Comparison with the expressions for $\vec{Q}$ and $\vec{V}$ reveal that these are the same type of terms. Writing out the tensor in tabular form following Morse and Feshbach gives

$$\mathfrak{M} = \begin{pmatrix} \mathcal{W}_{11} & \mathcal{W}_{12} & \mathcal{W}_{13} & V_1 \\ \mathcal{W}_{21} & \mathcal{W}_{22} & \mathcal{W}_{23} & V_2 \\ \mathcal{W}_{31} & \mathcal{W}_{32} & \mathcal{W}_{33} & V_3 \\ Q_1 & Q_2 & Q_3 & \mathcal{H} \end{pmatrix} \quad (4.37)$$

Hence $\mathcal{H}$ is the (4,4) component of $\mathfrak{M}$, and the vector $\vec{Q}$ corresponds to components (4,1), (4,2), and (4,3) of $\mathfrak{M}$. Likewise, the components of $\vec{V}$ are the (1,4), (2,4), and (3,4) components of the stress-energy-momentum tensor. These components have special significance in connection with mechanical and elastic systems. For instance the $\vec{Q}$ is usually

called the field intensity or energy flow vector, and V is generally known as the field momentum vector. The significance of these terms in connection with reactor theory will be discussed in the next section.

A continuous transformation

The transformation depending on the continuous parameter α is expressed by the mapping

$$\begin{aligned} x_\omega^* &= \Psi(x_\omega, \phi_\mu, \nabla\phi_\mu, \dot{\phi}_\mu; \alpha) \\ \phi_\mu^* &= \Xi(x_\omega, \phi_\mu, \nabla\phi_\mu, \dot{\phi}_\mu; \alpha) \end{aligned} \tag{4.38}$$

where for $\alpha=0$ the transformation reduces to the identity transformation. If the notation for variations introduced in Eq. 3.14 is used and if a Taylor's series expansion to first order terms is made of Eq. 4.38 about $\alpha=0$, the variations to be used are

$$\delta x_\omega = x_\omega^* - x_\omega \tag{4.39}$$

$$\delta\phi_\mu^* = \phi_\mu^*(x_\omega) - \phi_\mu(x_\omega) + \sum_{\omega=1}^{4} \frac{\partial\phi_\mu}{\partial x_\omega}\,\delta x_\omega \tag{4.40}$$

The variation in the functional integral I can be written as

$$\delta I = \int_{T^*} \mathcal{L}\left(x_\omega^*, \phi_\mu^*, \frac{\partial\phi_\mu^*}{\partial x_\omega^*}\right) dx_\omega^* - \int_T \mathcal{L}\left(x_\omega, \phi_\mu, \frac{\partial\phi_\mu}{\partial x_\omega}\right) dx_\omega \tag{4.41}$$

where T* is the transformed region of integration, i.e., the transformation carries the hypersurface $\Sigma: \{x_\omega, \phi_\mu \in T\}$ into the hypersurface $\Sigma^*: \{x_\omega^*, \phi_\mu^* \in T^*\}$. Equation 4.41 can be written in terms of the Jacobian of the transformation as

$$\delta I = \int_T dx_\omega \left[\mathcal{L}(x_\omega^*, \phi_\mu^*, \nabla\phi_\mu^*, \dot{\phi}_\mu^*)\, J(x_\omega^*, x_\omega) - \mathcal{L}(x_\omega, \phi_\mu, \nabla\phi_\mu, \dot{\phi})\right] \tag{4.42}$$

where to first order in α , the Jacobian $J(x^*_\omega, x_\omega)$ can be written as

$$J(x^*_\omega, x_\omega) \approx 1 + \alpha \sum_{\beta=1}^{4} \frac{\partial}{\partial x_\beta} \left(\frac{\partial \Psi_\beta}{\partial \alpha} \Big|_{\alpha=0} \right) + O(\alpha^2) \quad (4.43)$$

A Taylor's series expansion of the resulting first term in Eq. 4.42 gives the following expression for δI

$$\delta I = \int_T \Big[\sum_{\omega=1}^{4} \frac{\partial \mathcal{L}}{\partial x_\omega} \delta x_\omega + \sum_{\mu=1}^{n} \frac{\partial \mathcal{L}}{\partial \phi_\mu} \delta \phi_\mu^* + \sum_{\mu=1}^{n} \sum_{\omega=1}^{4} \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \phi_\mu}{\partial x_\omega} \right)} \delta^* \left(\frac{\partial \phi_\mu}{\partial x_\omega} \right) + \alpha \mathcal{L}(x^*_\omega, \phi^*_\mu, \nabla \phi^*_\mu, \dot{\phi}^*_\mu) \sum_{\beta=1}^{4} \frac{\partial}{\partial x_\beta} \left(\frac{\partial \Psi_\beta}{\partial \alpha} \right) \Big] d x_\omega \quad (4.44)$$

where only terms of first order in α are retained. Terms of the form

$$\delta^* \left(\frac{\partial \phi_\mu}{\partial x_\omega} \right) = \frac{\partial \left(\phi_\mu^*(x_\omega^*) - \phi_\mu(x_\omega^*) \right)}{\partial x_\omega^*} + \frac{\partial \left(\phi_\mu(x_\omega^*) - \phi_\mu(x_\omega) \right)}{\partial x_\omega} \quad (4.45)$$

and to first order in α

$$\delta^* \left(\frac{\partial \phi_\mu}{\partial x_\omega} \right) \approx \alpha \left[\frac{\partial}{\partial x_\omega} \left(\frac{\partial \approx (x_\omega)}{\partial \alpha} \right)_{\alpha=0} + \sum_{\beta=1}^{4} \frac{\partial^2 \phi_\mu(x_\omega)}{\partial x_\beta \partial x_\omega} \left(\frac{\partial \Psi}{\partial \alpha} \right)_{\alpha=0} \right] \quad (4.46)$$

are substituted into Eq. 4.44 and algebraic reduction gives the result

$$\delta I = \int_T \sum_{\mu=1}^{n} \Big[\frac{\partial \mathcal{L}}{\partial \phi_\mu} - \sum_{\omega=1}^{4} \frac{\partial}{\partial x_\omega} \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \phi_\mu}{\partial x_\omega} \right)} \Big] \delta \phi_\mu \, d x_\omega + \int_T \sum_{\mu=1}^{n} \sum_{\omega=1}^{4} \frac{\partial}{\partial x_\omega} \left(\frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \phi_\mu}{\partial x_\omega} \right)} \delta \phi_\mu + \mathcal{L} \delta x_\omega \right) d x_\omega \quad (4.47)$$

The first integral is the same as obtained in deriving the Euler-Lagrange equations. The second integral is a divergence term similiar to that encountered in the derivation of the Hamilton-Jacobi equation. If δI is required to vanish along the path of the motion, Eq. 4.47 becomes

$$\int_T \sum_{\mu=1}^{n} \sum_{\omega=1}^{4} \frac{\partial}{\partial x_\omega} \left(\frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \phi_\mu}{\partial x_\omega} \right)} \delta \phi_\mu + \mathcal{L} \delta x_\omega \right) d x_\omega = 0 \quad (4.48)$$

If the domain T is considered arbitrary, then Eq. 4.48 implies that the integrand vanishes, i.e.,

$$\frac{\partial}{\partial x_\omega}\left(\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \phi_\mu}{\partial x_\omega}\right)}\delta\phi_\mu + \mathcal{L}\,\delta x_\omega\right) = 0 \qquad (4.49)$$

which is the form usually taken as representing Noether's theorem. Gel'fand and Fomin (34) and Rund (29) consider Noether's theorem in more detail.

APPLICATION TO REACTOR SYSTEMS

In this section the previous theory will be discussed with respect to its application to nuclear reactor systems. The Hamiltonian for some of the field equations used to describe a reactor will be derived. The discussion of a continuity equation leads to a consideration of reactor invariants and the calculation of the components of the stress-energy-momentum tensor. The action integral is discussed with respect to reactor theory and the relationship between the Hamilton-Jacobi approach and the evolution operator, Lie series, and Laplace transform methods is investigated. Lastly the solution of sample problems from reactor theory are obtained by solving their corresponding Hamilton-Jacobi equation.

Reactor Hamiltonians

Time-dependent diffusion equation

The time-dependent diffusion equation and its corresponding adjoint are

$$\nabla \cdot D \nabla \phi - \Sigma_a \phi + \nu \Sigma_f \phi = \frac{1}{v} \frac{\partial \phi}{\partial t} + S_{ext} \qquad (5.1)$$

$$\nabla \cdot D \nabla \phi^* - \Sigma_a \phi^* + \nu \Sigma_f \phi^* = -\frac{1}{v} \frac{\partial \phi^*}{\partial t} + S^*_{ext} \qquad (5.2)$$

where the notation is standard and listed in Appendix A. There are several Lagrangians that can be used which yield Eqs. 5.1 and 5.2 upon invoking Hamilton's principle. These can all be obtained from a general form of the Lagrangian

density written as

$$\mathcal{L} = \left[\nabla\phi^* \cdot D\nabla\phi - \phi^* A\phi - \left\{\nu^{-1}\lambda\phi^*\dot{\phi} + (1-\lambda)\nu^{-1}\phi\dot{\phi}^*\right\} + S_{ext}\phi^* - S^*_{ext}\phi\right] \tag{5.3}$$

by setting λ equal to 0, $\frac{1}{2}$, or 1. The variational principle has been used primarily for the calculation of coefficients in assumed solutions to Eqs. 5.1 and 5.2. For example, if the flux is assumed to be of the form

$$\phi(\vec{r},t) = \sum_{n=0}^{\infty} a_n(t)\,\psi_n(\vec{r}) \tag{5.4}$$

where the $\psi(\vec{r})$ are known functions, the equations for determining the unknown coefficients a_n are obtained by using the stationarity of the Hamilton integral (4, 5, 8, 9, 10).

The momenta for the diffusion equation can be defined for the time-preferred formulation as

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = \nu^{-1}\lambda\,\phi^* \tag{5.5}$$

$$\pi^* = \frac{\partial \mathcal{L}}{\partial \dot{\phi}^*} = -\nu^{-1}(1-\lambda)\phi \tag{5.6}$$

where λ again takes on the corresponding values used in defining the Lagrangian. The Hamiltonian is derived from its definition in Eq. 1.12 which gives the symmetric result

$$\mathcal{H} = \nu\left\{-\left[\nabla\pi \cdot D\nabla\phi - D\nabla\pi^* \cdot \nabla\phi\right] + A(\pi\phi - \pi^*\phi^*)\right\} - S_{ext}\phi^* + S^*_{ext}\phi \tag{5.7}$$

This expression for $\mathcal{H}$ reduces to a simplier form on substitution of the expression for the momenta.

$$\mathcal{H} = \left[-\nabla\phi^* \cdot D\nabla\phi + \phi^* A\phi - S_{ext}\phi^* + S^*_{ext}\phi\right] \tag{5.8}$$

This expression for $\mathcal{H}$ can be used to compute the canonical equations. This calculation gives back the original equa-

tions, i.e.,

$$\dot{\phi} = \frac{\delta \mathcal{H}}{\delta \pi} = v\nabla\cdot D\nabla\phi + vA\phi - v S_{ext} \tag{5.9}$$

$$\dot{\pi} = -\frac{\delta \mathcal{H}}{\delta \phi} = -v\nabla\cdot D\nabla\phi^* - vA\phi^* + v S^*_{ext} \tag{5.10}$$

The momenta and flux variables are seen not to be independent of each other. This is characteristic of the variational formulation of the equations of a "dissipative" system. That is, the linearity in the first time derivative in the Lagrangian density causes the transformation to canonical variables to be somewhat obscured. This can be seen from the Hamiltonian of Eq. 5.8 where the momenta terms have been eliminated and $\mathcal{H}$ appears as a function of the flux and the adjoint flux. This is an artifical elimination due to the relationship of the variables. If the canonical equations are rederived from Hamilton's principle using the relationship between the variations of the momenta and the fluxes,

$$\delta\pi = \frac{\partial \pi}{\partial \phi^*}\,\delta\phi^* \tag{5.11}$$

$$\delta\pi^* = \frac{\partial \pi^*}{\partial \phi}\,\delta\phi \tag{5.12}$$

together with the usual argument for the independent variations of ϕ and ϕ^*, then the canonical equations can be written as

$$\dot{\phi}\left[\frac{\partial \pi}{\partial \phi^*} - \frac{\partial \pi^*}{\partial \phi}\right] = \frac{\delta \mathcal{H}}{\delta \phi^*} \tag{5.13}$$

$$\dot{\phi}^*\left[\frac{\partial \pi^*}{\partial \phi} - \frac{\partial \pi}{\partial \phi^*}\right] = \frac{\delta \mathcal{H}}{\delta \phi} \tag{5.14}$$

These equations reduce to the original equations when the expressions for $\frac{\partial \pi}{\partial \phi^*}$ and $\frac{\partial \pi^*}{\partial \rho}$ are calculated from Eqs. 5.5 and 5.6.

The Hamilton-Jacobi equation calculated from Eq. 3.9, using the Hamiltonian of Eq. 5.8, is

$$\frac{\partial S}{\partial t} + \left[-\nabla \left(v \frac{\partial S}{\partial \phi} \right) \cdot D \nabla \phi + v \frac{\partial S}{\partial \phi} A\phi + v \bar{\Sigma}_{sxt} \frac{\partial S}{\partial \phi} \right] - \bar{\Sigma}^*_{sxt} \phi = 0 \tag{5.15}$$

where the source terms in the original equations have been written with an overbar to further distinguish then from S. For the source free equations and when A and D are constants, Eq. 5.15 reduces to

$$\frac{\partial S}{\partial t} + v \left[-\nabla \frac{\partial S}{\partial \phi} \cdot D \nabla \phi \right] + \frac{\partial S}{\partial \phi} A\phi = 0 \tag{5.16}$$

This form of the equation will be used later in solving the diffusion equation.

Time-dependent group equations

The Hamiltonian for the time-dependent group diffusion equations is similiar to that just obtained for the one-group case. The group equations written in matrix form are

$$[v]^{-1} \frac{\partial}{\partial t} \vec{\psi} = \nabla \cdot [D] \nabla \vec{\psi} + [A] \vec{\psi} \tag{5.17}$$

$$-[v]^{-1} \frac{\partial}{\partial t} \vec{\psi}^* = \nabla \cdot [D]^T \nabla \vec{\psi}^* + [A]^T \vec{\psi}^* \tag{5.18}$$

where $\vec{\psi}$ and $\vec{\psi}^*$ denote the column vectors made up to the group fluxes and the group adjoint fluxes. The elements of the matrices [A], [v] and [D] are assumed constant or at least

piece-wise constant. A Lagrangian corresponding to Eqs. 5.17 and 5.18 is

$$\mathcal{L} = \nabla\vec{\psi}^{*T}\cdot[D]\nabla\vec{\psi} - \vec{\psi}^{*T}[A]\vec{\psi} + [v]^{-1}\dot{\vec{\psi}}^{*T}\vec{\psi} \qquad (5.19)$$

The momenta derived from Eq. 5.19 and denoted by P and P* are

$$\vec{p} = \frac{\partial\mathcal{L}}{\partial\dot{\vec{\psi}}} = 0 \qquad (5.20)$$

$$\vec{p}^{*} = \frac{\partial\mathcal{L}}{\partial\dot{\vec{\psi}}^{*}} = [v]^{-1}\vec{\psi} \qquad (5.21)$$

and the corresponding Hamiltonian becomes

$$\mathcal{H} = -[v]\left\{\nabla\vec{\psi}^{*T}\cdot[D]\nabla\vec{\psi} + \vec{\psi}^{*T}[A]\vec{\psi}\right\} \qquad (5.22)$$

The canonical equations can be written down directly as

$$\dot{\vec{\psi}} = \frac{\delta\mathcal{H}}{\delta\vec{p}^{*}} = [v]\nabla\cdot[D]\nabla\vec{\psi} + [A]\vec{\psi} \qquad (5.23)$$

$$\dot{\vec{p}}^{*} = -\frac{\delta\mathcal{H}}{\delta\vec{\psi}} = -\nabla\cdot[D]\nabla\vec{\psi}^{*} - [A]^{T}\vec{\psi}^{*} \qquad (5.24)$$

which checks the Hamiltonian by yielding the original equations. The generator of the Hamilton-Jacobi equation is now a function of the vector flux and vector momenta so that the Hamilton-Jacobi equation for the multi-group equations is

$$\frac{\partial S}{\partial t} - \nabla\vec{\psi}^{*T}\cdot[D]\nabla\frac{\partial S}{\partial\vec{\psi}^{*}} + \vec{\psi}^{*T}[A]\frac{\partial S}{\partial\vec{\psi}^{*}} = 0 \qquad (5.25)$$

Diffusion equation with delayed neutrons

The one-group diffusion equation with delayed neutrons

and its associated precusor equation are (35)

$$\nabla \cdot D \nabla \phi + [(1-\beta)\nu\Sigma_f - \Sigma_a]\phi + \sum_{i=1}^{6} \lambda_i C_i = \frac{1}{v}\frac{\partial \phi}{\partial t} \qquad (5.26)$$

$$\frac{\nu\Sigma_f \beta_i \phi}{\ell} - \lambda_i C_i = \frac{\partial C_i}{\partial t} \qquad (i=1,2\cdots 6) \qquad (5.27)$$

To define the appropiate Lagrangian and Hamiltonian, the equations adjoint to these are needed. These are

$$\nabla \cdot D \nabla \phi^* + [(1-\beta)\nu\Sigma_f - \Sigma_a]\phi^* + \frac{\nu\Sigma_f \beta_i}{\ell} C_i^* = -\frac{1}{v}\frac{\partial \phi}{\partial t} \qquad (5.28)$$

$$\lambda_i \phi^* - \lambda_i C_i^* = -\frac{\partial C_i^*}{\partial t} \qquad (i=1,2,\cdots 6) \qquad (5.29)$$

The momenta can be defined in the usual manner, using appropiate subscripts for the neutron and precusor terms.

$$\pi_n = \frac{1}{2}\phi^* \quad ; \quad \pi_n^* = -\tfrac{1}{2}\phi \qquad (5.30)$$

$$\pi_i = \frac{v}{2} C_i^* \quad ; \quad \pi_i^* = -\frac{v}{2} C_i \qquad (5.31)$$

The Hamiltonian becomes

$$\mathcal{H} = -vD\nabla\phi \cdot \nabla\pi_n + R\pi_n\phi - v\sum_{i=1}^{6}\lambda_i \pi_i C_i + v\sum_{i=1}^{6}\lambda_i C_i \pi_n + \sum_{i=1}^{6}\frac{\nu\Sigma_f\beta_i}{\ell}\pi_i\phi \qquad (5.32)$$

where the symbol R denotes the combination of coefficients

$$R = v[(1-\beta)\nu\Sigma_f - \Sigma_a] \qquad (5.33)$$

A check of the Hamiltonian in Eq. 5.32 by computing the canonical equations yields the original equations. The symmetric form of $\mathcal{H}$ has been used here because it makes the derivation easier to follow. The Hamilton-Jacobi equation can be written directly as

$$\frac{\partial S}{\partial t} - v D \nabla\phi \cdot \nabla \frac{\partial S}{\partial \phi} + \Sigma \frac{\partial S}{\partial \phi}\phi - v\sum_{i=1}^{6} \lambda_i \frac{\partial S}{\partial C_i} C_i + v\sum_{i=1}^{6} \lambda_i C_i \frac{\partial S}{\partial \phi} + \sum_{i=1}^{6} \frac{k_{eff}\beta_i}{\ell} \frac{\partial S}{\partial C_i}\phi = 0 \quad (5.34)$$

Point reactor kinetics equations

The point reactor kinetics equations are derived from the general space-time equations, Eqs. 5.26 and 5.27 by defining appropriately averaged quantities (36). These equations are generally written as follows

$$\frac{dn}{dt} = \left[\frac{k_{eff}(1-\beta)-1}{\ell}\right] n + \bar{\lambda} C \quad (5.35)$$

$$\frac{dC}{dt} = k_{eff}\frac{\beta}{\ell} n - \bar{\lambda} C \quad (5.36)$$

The corresponding adjoint equations are

$$-\frac{dn^*}{dt} = \left[\frac{k_{eff}(1-\beta)-1}{\ell}\right] n^* + k_{eff}\frac{\beta}{\ell} C^* \quad (5.37)$$

$$-\frac{dC^*}{dt} = \bar{\lambda} n^* - \bar{\lambda} C^* \quad (5.38)$$

A Hamiltonian can be written directly from the relationship to Eq. 5.32

$$\mathcal{H} = \left[\frac{k_{eff}(1-\beta)-1}{\ell}\right] n \pi_n + \bar{\lambda}\pi_n C + \frac{k_{eff}\beta}{\ell} n\pi_c - \bar{\lambda}\pi_c C \quad (5.39)$$

with the definition for the momenta

$$\pi_n = n^* \quad ; \quad \pi_n^* = 0 \quad (5.40)$$

$$\pi_c = C^* \quad ; \quad \pi_c^* = 0 \quad (5.41)$$

Here the unsymmetrical form for $\mathcal{H}$ has been used, as it is more compact for notational purposes. A check on $\mathcal{H}$ by computing the canonical equations is easily seen to give the

original set. The Hamilton-Jacobi equation becomes

$$\frac{\partial S}{\partial t} + \left[\frac{k_{eff}(1-\beta)-1}{\ell}\right] n \frac{\partial S}{\partial n} + \bar{\lambda} \frac{\partial S}{\partial n} C + \frac{k_{eff}\beta}{\ell} n \frac{\partial S}{\partial C} - \bar{\lambda} \frac{\partial S}{\partial C} C = 0 \tag{5.42}$$

Reactor with xenon feedback

Consider the two group diffusion equation without delayed neutrons, but with xenon and iodine feedback as given in many of the standard references (37, 38). These equations are in general nonlinear, involving products of the field components. If these equations are linearized by considering a perturbation approximation about the steady state flux and the equilibrium xenon and iodine concentrations, the result can be written in matrix form as

$$\frac{\partial}{\partial t}\begin{pmatrix} I \\ X \\ \phi_f \\ \phi_s \end{pmatrix} = \begin{pmatrix} -\lambda_I & 0 & \gamma_I \Sigma_{ff} & \gamma_I \Sigma_{fs} \\ \lambda_I & -\mathcal{P}_1 & \mathcal{P}_2 & \mathcal{P}_3 \\ 0 & -\nu_f \sigma_{xf} \phi_{of} & \nu_f \mathcal{L}_f & \nu_f \nu \Sigma_{fs} \\ 0 & -\nu_s \sigma_{xs} \phi_{os} & \nu_s \Sigma_\ell & \nu_s \mathcal{L}_s \end{pmatrix} \begin{pmatrix} I \\ X \\ \phi_f \\ \phi_s \end{pmatrix} + [\mathcal{R}_o] \tag{5.43}$$

or more compactly as

$$\frac{\partial}{\partial t}\vec{\psi} = \dot{M}\vec{\psi} + \mathcal{R}_o \tag{5.44}$$

with the terms making up the matrix M being given in Appendix A. The Lagrangian can be written in an unsymmetrical form by analogy with the Lagrangian of the multi-group equations.

$$\mathcal{L} = \vec{\psi}^{*T}\dot{\vec{\psi}} - \vec{\psi}^{*T} M \vec{\psi} + \vec{\psi}^{*T}\mathcal{R}_0 + \vec{\psi}^{T}\mathcal{R}_0^{*} \tag{5.45}$$

The corresponding momenta are

$$\vec{\pi}^{*} = \frac{\partial \mathcal{L}}{\partial \dot{\vec{\psi}}^{*}} = 0 \tag{5.46}$$

$$\vec{\pi} = \frac{\partial \mathcal{L}}{\partial \dot{\vec{\psi}}} = \vec{\psi}^{*} \tag{5.47}$$

Then the Hamiltonian becomes simply

$$\mathcal{H} = \vec{\psi}^{*T} M \vec{\psi} + \vec{\psi}^{*T}\mathcal{R}_0 - \vec{\psi}^{T}\mathcal{R}_0^{*} \tag{5.48}$$

where the matrix notation has disguised its complexity. The Hamilton-Jacobi equation can be written in an equally simple form as

$$\frac{\partial S}{\partial t} + \left(\frac{\partial S}{\partial \pi}\right)^{T} M \vec{\psi} + \left(\frac{\partial S}{\partial \pi}\right)^{T} \mathcal{R}_0 - \vec{\psi}^{T}\mathcal{R}_0^{*} = 0 \tag{5.49}$$

Telegrapher's equation

The telegrapher's equation has been used in reactor theory to describe wave phenomena and as a better approximation to the transport equation than diffusion theory. The form of the equation normally used in reactor theory is as follows (39, 40)

$$\frac{3D}{v^2}\frac{\partial^2}{\partial t^2}\phi + \frac{1}{v}(1 + 3D\Sigma_a)\frac{\partial \phi}{\partial t} = D\nabla^2\phi + A\phi \tag{5.50}$$

where the definition of the terms is the same as in the dif-

fusion equation. The equation adjoint to Eq. 5.50 is

$$\frac{3D}{v^2}\frac{\partial^2\phi^*}{\partial t^2} - \frac{1}{v}(1+3D\Sigma_a)\frac{\partial\phi^*}{\partial t} = D\nabla^2\phi^* + A\phi^* \qquad (5.51)$$

A Lagrangian constructed by analogy from the Lagrangian for the diffusion equation is proposed as

$$\mathcal{L} = D\nabla\phi^*\cdot\nabla\phi - \phi^* A\phi + \phi^* v^{-1}(1+3D\Sigma_a)\dot{\phi} - \frac{3D}{v^2}\dot{\phi}^*\dot{\phi} \qquad (5.52)$$

As a check, the Euler-Lagrange equations are computed from Eq. 1.8 and are found to yield the oringinal equations, i.e.,

$$\sum_{\omega=1}^{4}\frac{d}{dx_\omega}\frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\phi_u}{\partial x_\omega}\right)} - \frac{\partial\mathcal{L}}{\partial\phi} = 0 \qquad (5.53)$$

becomes

$$\nabla\cdot D\nabla\phi - \frac{d}{dt}\left(\frac{3D}{v^2}\dot{\phi}\right) + A\phi - v^{-1}(1+3D\Sigma_a)\dot{\phi} = 0 \qquad (5.54)$$

which is the same as Eq. 5.50. The momenta defined in the usual manner become

$$\pi = \frac{\partial\mathcal{L}}{\partial\dot{\phi}} = \frac{3D}{v^2}\dot{\phi}^* + \phi^* v^{-1}(1+3D\Sigma_a) \qquad (5.55)$$

$$\pi^* = \frac{\partial\mathcal{L}}{\partial\dot{\phi}^*} = \frac{3D}{v^2}\dot{\phi} \qquad (5.56)$$

from which the Hamiltonian can be derived as

$$\mathcal{H} = \pi^*\dot{\phi}^* - D\nabla\phi^*\cdot\nabla\phi + \phi^* A\phi \qquad (5.57)$$

and the Hamilton-Jacobi equation can be written as

$$\frac{\partial S}{\partial t} + \frac{\partial S}{\partial\phi^*}\dot{\phi}^* - D\nabla\phi^*\cdot\nabla\phi + \phi^* A\phi = 0 \qquad (5.58)$$

Reactor Invariants and Conservation Laws

A continuity equation

A continuity equation can be easily derived from the diffusion equation and its adjoint as written in Eqs. 5.1 and 5.2 by multiplying by ϕ^* and ϕ respectively and subtracting the resulting expressions. This gives the result

$$\frac{1}{v}\frac{\partial}{\partial t}(\phi\phi^*) = \phi^*\nabla\cdot D\nabla\phi - \phi\nabla\cdot D\nabla\phi^* \qquad (5.59)$$

By standard vector identities, Eq. 5.59 can be rewritten in the form of a continuity equation as

$$\frac{\partial}{\partial t}(\phi\phi^*) = v\nabla\cdot D[\phi^*\nabla\phi - \phi\nabla\phi^*] \qquad (5.60)$$

If the combination $\phi\phi^*$ is denoted by ρ , and the vector $\vec{J}$ is set equal to $[\phi^*\nabla\phi - \phi\nabla\phi^*]$, then Eq. 5.60 takes on the more traditional form of a continuity equation

$$\frac{\partial}{\partial t}\rho - v\nabla\cdot D\vec{J} = 0 \qquad (5.61)$$

This is another way of expressing the balance equation for a reactor. The time rate of change of the density-like quantity ρ is equal to the spatial divergence of the current-type vector $\vec{J}$. In fluid flow, a similiar type of equation relates the time rate of change of mass to the divergence of the mass velocity vector (33). If ρ is interpreted as a probability density analogous to the combination of wave functions in quantum mechanics, the continuity equation relates the divergence of the probable current density to the time rate of change of the probability density. That this is a

a valid interpretation for the diffusion equation can be argued from the inherent statistical nature of the neutron multiplication processes. Also the physical concept of the adjoint function as an importance function may lend some weight to this viewpoint. Ussachof (41) defined the importance function as the change in the power level of a just critical reactor when one neutron is introduced. Thus the point of introduction becomes important in determining the resulting change in the power. From another point of view, the adjoint variables can be interpreted as mirror or dual variables much like the method of treating dissipative systems in elementary classical mechanics. In this sense, the overall system is treated as two subsystems where losses in one appear as gains in the other.

The Poisson brackets allows a way of testing for a conserved quantity. From its definition, the Poisson bracket of $\phi\phi^*$ with $\mathcal{H}$ is

$$[\phi\phi^*, \mathcal{H}] = \left[\frac{\partial(\phi\phi^*)}{\partial\phi} \frac{\delta\mathcal{H}}{\delta\phi^*} - \frac{\partial(\phi\phi^*)}{\partial\phi^*} \frac{\delta\mathcal{H}}{\delta\phi} \right] \qquad (5.62)$$

which becomes

$$[\phi\phi^*, \mathcal{H}] = v^{-1} \frac{d}{dt} (\phi\phi^*) = \nabla \cdot D\vec{J} \qquad (5.63)$$

which is the same as Eq. 5.61. If the continuity equation is integrated over the spatial volume of the reactor and Gauss's theorem invoked on the divergence term, the result is

$$\frac{\partial}{\partial t}\iiint_V \rho\, dV = v \oint_S D\vec{J}\cdot d\vec{S} \qquad (5.64)$$

The usual boundary conditions on the diffusion equation are that the flux and the adjoint flux go to zero on the extrapolated boundary. If this is invoked, the total time derivative of the integral of ρ is zero. From experience in the solution of the diffusion equation for constant coefficients, the time derivative of the quantity ρ itself is zero because of the nature of the separable solutions. That is, separable type solutions yield equal and opposite signed eigenvalues for the flux and the adjoint flux and the time coefficients in the product $\phi\phi^*$ cancel each other. This could have also been inferred from Eq. 5.62 since the Poisson bracket

$$[(\phi^* \nabla\phi - \phi\nabla\phi^*), \mathcal{H}] \qquad (5.65)$$

reduces to zero under constant coefficient conditions. During material changes in the reactor, the product $\phi\phi^*$ will in general not be conserved. Equation 5.64 would imply in this situation that the boundary condition of zero flux on the extrapolated boundary is violated. This may well be the case since during material changes, the assumption of constant coefficients is not valid and the solution will be in general nonseparable. Thus it appears that the boundary conditions for a nonseparable solution are not compatible with the vanishing of the flux on the extrapolated surface.

Stess-energy-momentum tensor components

From the previous discussion of the components of the stress-energy-momentum tensor, certain density relations were developed. It is useful to examine the corresponding components for the time-dependent diffusion equation. From the Lagrangian of Eq. 5.3 in the symmetric form, the components of $\vec{Q}$ are

$$\sum_{i=1}^{3} Q_i = \sum_{i=1}^{3} \sum_{\mu=1}^{n} \frac{\partial \mathcal{L}}{\partial(\nabla \phi_\mu)} \dot{\phi}_\mu = D[\nabla \phi^* \dot{\phi} + \nabla \phi \dot{\phi}^*] \tag{5.66}$$

If $\mathcal{L}$ does not depend explicitly on the coordinates, i.e., for constant coefficients in the diffusion equation, the relation analogous to Eq. 4.31 is

$$-\nabla \cdot [D \dot{\phi} \nabla \phi^* + D \dot{\phi}^* \nabla \phi] + \frac{d\mathcal{H}}{dt} = 0 \tag{5.67}$$

This is the same result as Tavel, Clancy and Pomraning (15) obtained by applying Noether's theorem to the diffusion equation. They integrate Eq. 5.67 over the volume of the reactor to define an "energy" of the diffusion process as

$$E(t) = \iiint_V \mathcal{H}\, d\vec{r} + \int_{t_0}^{t} dt \oint_S \vec{Q} \cdot d\vec{S} \tag{5.68}$$

in analogy to classical mechanics. Tavel, et al. obtained their result from an infinitesimal translation in the time coordinate which agrees with the interpretation of the vector $\vec{Q}$ as an energy flow vector for the process.

The calculation of the components of $\vec{V}$ gives the result

$$\sum_{i=1}^{3} V_i = -\sum_{i=1}^{3} \sum_{\mu=1}^{n} \frac{\partial \mathcal{L}}{\partial \phi} \frac{\partial \phi_\mu}{\partial x_i} = \frac{1}{2v} [\phi^* \nabla \phi - \phi \nabla \phi^*] \tag{5.69}$$

The equations analogous to Eq. 4.35 can be written in a simple form by using the dyadic notation (33), i.e.,

$$\overrightarrow{\overrightarrow{\Pi}} \cdot \vec{\nabla} + \frac{\partial \vec{V}}{\partial \tau} = 0 \tag{5.70}$$

This dyadic is referred to in mechanics as the stress dyadic and is made up of components corresponding to the upper left array in the $\mathfrak{B}$ tensor. Equation 5.70 expresses a condition on the neutron field when $\mathcal{H}$ does not depend explicitly on the coordinates which implies constant coefficients. The vector $\vec{V}$ is seen to be the same as the vector $\vec{J}$ introduced in the discussion of the continuity equation. The relationship given in Eq. 5.70 does not appear to have much use in connection with the diffusion equation because of the difficulty in making physical interpretations of the terms involved.

Relationship of Hamilton-Jacobi Theory to Other Techniques

The action integral

The action integral has been defined as the Hamilton integral expressed as a function of tis limits, i.e.,

$$S = \int_{\tau_1}^{\tau_2} \mathcal{L} \, d\tau \tag{5.71}$$

There are two ways to visualize the motion as determined by an action principle of this type. That is, the natural motion of any dynamical system can be found if two events are known to occur during the course of the motion. Then the variation of the integral in Eq. 5.71 between the known events must be stationary for small variations about the actual path of the

motion. For some types of problems, this interpretation of the motion is unsatisfactory. This is the case when the solution of the equations of motion is to be obtained from knowledge of some initial configuration. The form of the canonical equations suggests that they require only the initial data to be known.

If the variation in the action is considered as due to a small variation in the upper bound of Eq. 5.71, the expression for δS becomes

$$\delta S = \int_{t_0}^{T+\delta t} \iiint \mathcal{L}\, dx\, dt - \int_{t_0}^{T} \iiint \mathcal{L}\, dx\, dt = \left[\mathcal{L} - \sum_{\mu=1}^{n} \pi_\mu \dot{\phi}_\mu\right]\Big|_{t=T} \delta t \tag{5.72}$$

where the origin of the terms has been discussed previously. Taking the limit as δt goes to zero gives the Hamilton-Jacobi equation. The difference in the value of the action due to the change in the field component at the upper bound is

$$\lim_{\delta t \to 0} \frac{S(T+\delta t, \phi_\mu) - S(T, \phi_\mu)}{\delta t} = \frac{\partial S}{\partial t}\Big|_{t=T} = \left[\mathcal{L} - \sum \pi_\mu \frac{\partial \phi_\mu}{\partial x_\mu}\right]\Big|_{t=T} \tag{5.73}$$

In the limit as $\delta\phi$ goes to zero, the relation of S to the momentum at the upper bound is obtained.

$$\lim_{\delta \phi_\mu \to 0} \frac{S(T, \phi_\mu + \delta\phi) - S(T, \phi_\mu)}{\delta \phi} = \pi_\mu(T)\, \delta\phi\Big|_{t=T} \tag{5.74}$$

From this derivation, the momenta (adjoint variables in the Hamiltonian formulation of the diffusion equation) are the terms that express the sensitivity of S to changes in the end conditions. This change of the action was for the progression of time. The action integral can also be used to define the

perturbation from one Lagrangian density to another. The change in the action then becomes

$$S' = \int_{t_0}^{T} \iiint \mathcal{L}\, d\vec{r}\, dt + \lambda \int_{t_0}^{T} \iiint \mathcal{L}'\, d\vec{r}\, dt = S_0 + \lambda S_1 \qquad (5.75)$$

where the parameter λ is a coupling parameter between the unperturbed and the perturbed situations. Note that the fixed time limits are now imposed. This allows the variation of the action to be written for a variation in the coupling parameter, i.e.,

$$\delta S' = S_0 + (\lambda + \delta\lambda) S' - (S_0 + \lambda S_1) = \delta\lambda S_1 \qquad (5.76)$$

where the S_0 refers to the unpreturbed action. The more general case of a perturbation under time evolution can be considered as a combination of the previously discussed cases. That is consider the variation of the action in the form

$$\bar{S} = \int_{t_0}^{T+\delta t} \iiint \mathcal{L}\, d\vec{r}\, dt + \lambda \int_{t_0}^{T+\delta t} \iiint \mathcal{L}'\, d\vec{r}\, dt \qquad (5.77)$$

This can be seen to be the sum of the variation due to the time evolution plus the variation due to the perturbation. Thus the result

$$\delta \bar{S} = \delta_t \bar{S} + \delta\lambda \bar{S}_1 \qquad (5.78)$$

The usual approach to solve this type of problem is to solve the unperturbed case first and then determine the perturbed motion from the unperturbed. In solving the time-dependent diffusion equation, the mixing of the space and time perturbation is possible due to the manner in which control

rods are moved. However, taking the system as a whole, when the spatial boundaries are fixed and the coefficients are constant, the solution to the equations is separable. The time-dependent motion of a control rod would change the relative relationship to the internal boundaries of the reactor. This would in general result in nonseparable solutions to the equations during the transit of the rod motion, and would affect to some degree the transient portion of the solution after rod motion has ceased. Thus perturbations made to a reactor so as not to violate the assumptions of separability are often of an unrealistic nature. For example, a sudden step change in the Hamiltonian of a reactor system can be expressed as the change between two conservative systems, i.e., the Hamiltonian is not an explicit function of space and time in both the perturbed and unperturbed cases.

The problem is to relate the solution of the unperturbed problem to the solution to the perturbed problem in terms of some operational procedure. In the usual modal approach to space-time problems, the initial or unperturbed solution is expressed in terms of modes (generally known space functions) which are generally derived from some type of eigenvalue problem. For example, consider the diffusion equation written in operator form as

$$\mathcal{M}_o \, \phi_o(\vec{r},t) = \dot{\phi}_o = 0 \qquad (5.79)$$

The solution to this problem can be expressed in terms of the eigenvectors of the operator $\mathcal{M}_o$ as

$$\phi_0(\vec{r}) = \sum_{n=0}^{\infty} C_n \phi_{0n}(\vec{r}) \tag{5.80}$$

where the C_n are constants to be determined from the initial condition. The perturbed problem can be written as

$$\frac{\partial \phi}{\partial t} = (M_0 + M_1)\phi \tag{5.81}$$

with the solution expressed in terms of the eigenvectors of the unperturbed operator as

$$\phi(\vec{r},t) = \sum_{n=0}^{\infty} q_n(t)\, \phi_{0n}(\vec{r}) \tag{5.82}$$

where the q_n are unknown time coefficients. The Hamilton's integral can be used to determine the q_n by substituting the assumed solutions into the Lagrangian density for the governing equation and finding the conditions that make the integral stationary with respect to variations of the unknown time coefficients. This is the way that the variational procedure is usually used as a computational tool. It requires the use of certain trial functions for the spatial portion of the solution. The assumptions are made that separability occurs for each mode. This is based on the form of the infinite series solution to problems that posses eigenvalue type expansions. The action integral solves the Hamilton-Jacobi equation for the principle function from which the solution to the equations of motion can be obtained

Relationship to evolution operator method

The variation of the action integral consists of two parts, namely a variation due to the time coordinate and a

variation in the field components due to the variation in the coordinate. The temporal portion is

$$\delta S = \mathcal{H} \delta t \tag{5.83}$$

which is the same form obtained when considering the infinitesimal transformations. This leads to the representation of the variation in the canonical variables in terms of δS as

$$\delta \phi_\mu = -\frac{\partial \delta S}{\partial \pi_\mu} \tag{5.84}$$

$$\delta \pi_\mu = \frac{\partial (\delta S)}{\partial \phi_\mu} \tag{5.85}$$

which follow from Eqs. 4.11 and 4.12.

Now consider an arbitrary dynamical quantity which is a function of the canonical variables.

$$F = F(t, \phi_\mu, \pi_\mu) \tag{5.86}$$

The variation of F due to the infinitesimal changes in the canonical variables is

$$\delta F = \sum_{\mu=1}^{n} \left[\frac{\partial (\delta S)}{\partial \phi_\mu} \frac{\partial F}{\partial \pi_\mu} - \frac{\partial (\delta S)}{\partial \pi_\mu} \frac{\partial F}{\partial \phi_\mu} \right] \tag{5.87}$$

where the variation δ is to be distinguished from the change due to the explicit dependence denoted by the usual partial differential sign. Thus the total differential of F is

$$dF = \delta F + \partial F \tag{5.88}$$

This total differential can also be expressed in terms of a Poisson bracket as

$$dF = \partial F + [F, H] \tag{5.89}$$

which illustrates the relationship already established between S and $\mathcal{H}$.

The perturbation of a system can be expressed in terms of the variation of S as discussed in Eq. 5.75. The variation in the coupling parameter λ causes a change in the canonical variables, i.e.,

$$\phi_{\mu(\lambda+\delta\lambda)} = \phi_{\mu(\lambda)} + \delta_\lambda \phi_\mu \tag{5.90}$$

$$\pi_{\mu(\lambda+\delta\lambda)} = \pi_{\mu(\lambda)} + \delta_\lambda \pi_\mu \tag{5.91}$$

where the increments represent changes in ϕ_μ and π_μ when λ is changed to $\lambda+\delta\lambda$ during the fixed time interval t to t_0. Then from the infinitesimal transformation relations, these equations become

$$\delta_\lambda \phi_\mu = -\delta\lambda \frac{\partial S_1}{\partial \pi_\mu} \tag{5.92}$$

$$\delta_\lambda \pi_\mu = \delta\lambda \frac{\partial S_1}{\partial \phi_\mu} \tag{5.93}$$

The change in F due to the change in λ is

$$\frac{\delta_\lambda F}{\delta\lambda} = \sum_{\mu=1}^{n} \left[\frac{\partial S_{1(\lambda)}}{\partial \phi_{\mu(\lambda)}} \frac{\partial F_{(\lambda)}}{\partial \pi_{\mu(\lambda)}} - \frac{\partial S_{1(\lambda)}}{\partial \pi_{\mu(\lambda)}} \frac{\partial F_{(\lambda)}}{\partial \phi_{\mu(\lambda)}} \right] \tag{5.94}$$

When $\delta\lambda$ is approximately zero, this variation can be expressed in terms of the unperturbed variables as

$$\left.\frac{\delta F}{\delta\lambda}\right|_{\lambda=0} = \sum_{\mu=1}^{n} \left[\frac{\partial S_{1(0)}}{\partial \phi_{\mu(0)}} \frac{\partial F_{(0)}}{\partial \pi_{\mu(0)}} - \frac{\partial S_{1(0)}}{\partial \pi_{\mu(0)}} \frac{\partial F_{(0)}}{\partial \phi_{\mu(0)}} \right] \tag{5.95}$$

If F is expanded in terms of a Taylor's series about the unperturbed variables, the following result is obtained.

$$F(t, \phi_\mu, \pi_\mu)_{\lambda=1} = F(t, \phi_{\mu(0)}, \pi_{\mu(0)}) + \lambda \left.\frac{\delta_\lambda F_\lambda}{\delta\lambda}\right|_{\lambda=0} + \frac{1}{2!}\lambda^2 \frac{\delta_\lambda^2 F_\lambda}{\delta^2\lambda} + \cdots \tag{5.96}$$

Now with respect to this expansion, the so-called evolution operator can be defined through the operational relationship

$$F(t,\phi_u,\pi_u)_{\lambda=1} = \mathcal{E}_1(t)\,F(t,\phi_{u(0)},\pi_{u(0)}) \qquad (5.97)$$

The goal is to relate the operator $\mathcal{E}_1$ to the action or the Hamiltonian. Note that the evolution operator for the perturbation problem relates the value of F in terms of the unperturbed variables at a given time t. The operator can also be expanded in a Taylor's series as

$$\mathcal{E}_1(t) = \mathcal{E}_0(t) + \frac{\delta\mathcal{E}_\lambda}{\delta\lambda}\Big|_{\lambda=0} + \frac{1}{2!}\frac{\delta^2\mathcal{E}_\lambda}{\delta\lambda^2}\Big|_{\lambda=0} + \cdots \qquad (5.98)$$

where $\mathcal{E}_0$ is the unperturbed operator. One can also associate an operator with the expression in Eq. 5.94. That is define

$$\Pi'_\lambda \triangleq \sum_{u=1}^{n}\left[\frac{\partial S_{1(\lambda)}}{\partial\phi_{u(\lambda)}}\frac{\partial}{\partial\pi_{u(\lambda)}} - \frac{\partial S_{1(\lambda)}}{\partial\pi_{u(\lambda)}}\frac{\partial}{\partial\phi_{u(\lambda)}}\right] \qquad (5.99)$$

where S_1 refers to the perturbed action. Turley (1) defines a similiar operator, derived from the Poisson bracket as (see Appendix B)

$$\Sigma'_\lambda \triangleq \sum_{u=1}^{n}\left[\frac{\partial\mathcal{H}'_{(\lambda)}}{\partial\pi_{u(\lambda)}}\frac{\partial}{\partial\phi_{u(\lambda)}} - \frac{\partial\mathcal{H}'_{(\lambda)}}{\partial\phi_{u(\lambda)}}\frac{\partial}{\partial\pi_{u(\lambda)}}\right] \qquad (5.100)$$

Another operator can also be defined in terms of the perturbed Lagrangian as

$$U'_\lambda \triangleq \sum_{u=1}^{n}\left[\frac{\partial\mathcal{L}'}{\partial\phi_{u(\lambda)}}\frac{\partial}{\partial\pi_{u(\lambda)}} - \frac{\partial\mathcal{L}'}{\partial\pi_{u(\lambda)}}\frac{\partial}{\partial\phi_{u(\lambda)}}\right] \qquad (5.101)$$

However, by the definition of the action S, this operator is related to Π'_λ by

$$\Pi'_\lambda = \int_{t_0}^{t} U'_\lambda\,dt \qquad (5.102)$$

which is also the relationship between Π_λ' and Ω_λ' since the perturbed Lagrangian and the perturbed Hamiltonian are the same when the perturbation is not directly made to the time derivative terms. Thus it is seen that the action operator is the integral of the operator that appears in Turley's work, and expressed as a function of the time at the upper limit of the action integral.

The relationship can be carried further by finding an equivalent expression for the evolution operator $\mathcal{E}_\lambda$. The first term in the Taylor's series of Eq. 5.96 becomes

$$\frac{\delta F_{(\lambda)}}{\delta \lambda} = \Pi_\lambda' F_{(\lambda)} \tag{5.103}$$

Differentiating Eq. 5.97 and comparing terms with Eq. 5.103 gives the result

$$\frac{\delta \mathcal{E}_\lambda}{\delta \lambda}\Big|_{\lambda=1} = \Pi_\lambda' \mathcal{E}_\lambda \tag{5.104}$$

The second term in the Taylor's series for $\mathcal{E}_\lambda$ becomes

$$\frac{\delta^2 \mathcal{E}_\lambda}{\delta \lambda^2} = \frac{\delta \Pi_\lambda'}{\delta \lambda} \mathcal{E}_\lambda + \Pi_\lambda' \frac{\delta \mathcal{E}_\lambda}{\delta \lambda} \tag{5.105}$$

Feynman (42) and Garrido (43) have shown that

$$\frac{\delta \Pi_\lambda'}{\delta \lambda} = \int_{t_0}^{t_1} dt' \left[\Pi_\lambda'(t'), U_\lambda'(t') \right] \tag{5.106}$$

which allows Eq. 5.105 to be rewritten as

$$\frac{\delta^2 \mathcal{E}_\lambda}{\delta \lambda^2} = \left\{ \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \, U_\lambda'(t'') U_\lambda'(t') + \int_{t_0}^{t} \int_{t'}^{t} dt'' \, U_\lambda'(t') U_\lambda'(t'') \right\} \mathcal{E}_\lambda \tag{5.107}$$

The general term in the series is

$$\frac{\delta^n \mathcal{E}_\lambda}{\delta \lambda^n} = \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' \cdots \int_{t_0}^{t} dt^{(n)} \left\{ U_\lambda'(t') \cdots U_\lambda'(t^{(n)}) \right\}_- \mathcal{E}_\lambda \tag{5.108}$$

where the symbol $\{\ \}_-$ denotes a time ordering process for the evaluation of the operational integrals (42). The expression for the evolution operator then can be written symbolically as

$$\mathcal{E}_{\lambda=1} = \left\{ e^{\int_{t_0}^{t} U'_{\lambda=0}(t')\,dt'} \right\}_- \mathcal{E}_{\lambda=0} \tag{5.109}$$

This is essentially equivalent to the result that Turley obtained (see Appendix B) if the relationship between iterated integrals given by Hildebrand (44) is used.

$$\int_{t_0}^{t}\cdots\int_{t_0}^{t} f(t)\,dt\cdots dt = n!\int_{t_0}^{t}\int_{t_0}^{t_1}\cdots\int_{t_0}^{t_n} f(t)\,dt_1\,dt_2\cdots dt_n \tag{5.110}$$

Relationship to Lie series

As a starting point consider the transformation of the canonical variables as given by

$$\Pi_\mu = [\pi_\mu] = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} D^n \pi_\mu \tag{5.111}$$

$$\Phi_\mu = [\phi_\mu] = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} D^n \phi_\mu \tag{5.112}$$

where α is a parameter and D is an operator of the form

$$D = \sum_{\mu=1}^{n} \xi_\mu \frac{\partial}{\partial \phi_\mu} + \sum_{\mu=1}^{n} \eta_\mu \frac{\partial}{\partial \pi_\mu} \tag{5.113}$$

This operator follows from a consideration of a general Taylor's series expansion of the new canonical variables about the old, i.e.,

$$\Pi_\mu = \pi_\mu + \alpha \left.\frac{d\pi_\mu}{d\alpha}\right|_{\alpha=0} + \frac{\alpha^2}{2!} \left.\frac{d^2\pi_\mu}{d\alpha^2}\right|_{\alpha=0} + \cdots \quad (5.114)$$

$$\Phi_\mu = \phi_\mu + \alpha \left.\frac{d\phi_\mu}{d\alpha}\right|_{\alpha=0} + \frac{\alpha^2}{2!} \left.\frac{d^2\phi_\mu}{d\alpha^2}\right|_{\alpha=0} + \cdots \quad (5.115)$$

The functions ξ_μ and η_μ are seen to be functions that help generate the transformation along the path of the motion. Later these functions will be explicitly related to the solution of the Hamilton-Jacobi equation but for the time being the infinitesimal canonical transformation serves to define them.

$$\Pi_\mu = \pi_\mu + \alpha \xi_\mu \quad (5.116)$$

$$\Phi_\mu = \phi_\mu + \alpha \eta_\mu \quad (5.117)$$

A general dynamical quantity F can be expressed in terms of the new canonical variables through the use of the operator D as

$$F(\Pi_\mu, \Phi_\mu) = F([\pi_\mu],[\phi_\mu]) = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} D^n F(\phi_\mu, \pi_\mu) \quad (5.118)$$

Now consider the expression used in considering the canonical transformations between old and new variables.

$$\sum_{\mu=1}^{n} \pi_\mu \delta\phi_\mu - \mathcal{H}\delta t - \sum_{\mu=1}^{n} \Pi_\mu \delta\Phi_\mu + \mathcal{K}\delta t = \delta S \quad (5.119)$$

If the expression of the transformation in Eqs. 5.111 and 5.112 are substituted into this equation together with the following expansion of S

$$S = \sum_{n=0}^{\infty} \alpha_n S_n \quad (5.120)$$

then the result is

$$\sum_{\mu=1}^{n} \pi_\mu \delta\phi_\mu - \mathcal{H}\delta t = \sum_{n=1}^{\infty} [\pi_\mu + \alpha\xi_\mu + \frac{\alpha^2}{2!} D\xi_\mu + \cdots][\delta\phi_\mu + \alpha\delta\eta_\mu + \cdots] - \quad (5.121)$$
$$- \mathcal{K}\delta t + \delta \sum_{n=1}^{\infty} \alpha^n S_n$$

If the new Hamiltonian is expressed in terms of a Taylor's series in the old variables, then the relationship defined in Eq. 5.118 can be used to express the new Hamiltonian in terms of the old, i.e.,

$$\mathcal{K}(t, \Phi_\mu, \Pi_\mu) = \mathcal{H}(t, \phi_\mu, \pi_\mu) + \alpha D\mathcal{H} + \frac{1}{2!}\alpha^2 D^2\mathcal{H} + \cdots \quad (5.122)$$

From this equation, a form of successive approximation to the Hamilton-Jacobi equation can be obtained. Comparison of powers of α gives that $S_0=0$ and that the expression for S_1 is

$$\delta S_1 = \sum_{\mu=1}^{n} \xi_\mu \delta\phi_\mu + \sum_{\mu=1}^{n} \pi_\mu \delta\eta_\mu - D\mathcal{H}\delta t \quad (5.123)$$

Now define W as

$$W = \sum_{\mu=1}^{n} \pi_\mu \eta_\mu - S_1 \quad (5.124)$$

and its variation as

$$\delta W = \sum_{\mu=1}^{n} (\delta\pi_\mu \eta_\mu + \pi_\mu \delta\eta_\mu) - \delta S_1 \quad (5.125)$$

Then Eq. 5.123 becomes

$$\sum_{\mu=1}^{n} \xi_\mu \delta\phi_\mu - \sum_{\mu=1}^{n} \eta_\mu \delta\pi_\mu = D\mathcal{H}\delta t - \delta W \quad (5.126)$$

If the variation of W is computed based on its functional dependence, then a comparison of the result with Eq. 5.125 yields the equations

$$\frac{\partial W}{\partial t} = D\mathcal{H} \quad (5.127)$$

$$\xi_\mu = -\frac{\partial W}{\partial \phi_\mu} \quad (5.128)$$

$$\eta_\mu = \frac{\partial W}{\partial \pi_\mu} \quad (5.129)$$

from which the expression for D now becomes

$$D = \sum_{\mu=1}^{n} \left(\frac{\partial W}{\partial \pi_\mu} \frac{\partial}{\partial \phi_\mu} - \frac{\partial W}{\partial \phi_\mu} \frac{\partial}{\partial \pi_\mu} \right) \tag{5.130}$$

The remaining terms of the expansion for S can be expressed in terms of successive operations by the D operator. The transformation equations can be written in terms of W as

$$\Pi_\mu = \pi_\mu - \alpha \frac{\partial W}{\partial \phi_\mu} + \frac{\alpha^2}{2!} D \frac{\partial W}{\partial \phi_\mu} - \cdots \tag{5.131}$$

$$\bar{\Phi}_\mu = \phi_\mu + \alpha \frac{\partial W}{\partial \pi_\mu} + \frac{\alpha^2}{2!} D \frac{\partial W}{\partial \pi_\mu} + \cdots \tag{5.132}$$

The operator D is of the same form as that considered in the Lie series. This is expected since the transformation used is essentially the same form that Lie originally considered in his work on continuous transformations (45). A brief presentation of the Lie series is given in Appendix C. The specialization of the operator to the form in Eq. 5.130 is a particular case of the operator corresponding to the evolution of the system. The relationship to the evolution operator technique is apparent. The parameter α can stand for the time increments or be used as a perturbation parameter.

Convergence properties of the Lie series are considered by Gröbner (46) and also the possibility of analytic continuation. These topics are beyond the scope of this study.

Relationship to Laplace transforms

The Laplace transformed diffusion equation can be written as

$$D \nabla^2 \bar{\Phi}_s(\vec{x}, s) + A \bar{\Phi}_s(\vec{x}, s) = \frac{s}{v} \bar{\Phi}_s(\vec{x}, s) - \phi(0) \tag{5.133}$$

The solution to this equation can be expressed formally in terms of the inverse operator.

$$\bar{\Phi}_s(\vec{x},s) = -(D\nabla^2 + A - s)^{-1}\phi(0) = -(M-s)^{-1}\phi(0) \tag{5.134}$$

or upon expanding the inverse as a series,

$$\bar{\Phi}_s(\vec{x},s) = (I + sM^{-1} + s^2M^{-2} + \cdots)M^{-1}\phi(0) \tag{5.135}$$

the Neumann series results which gives rise to the following set of equations

$$\left.\begin{aligned} M\psi_1 + \phi(0) &= 0 \\ M\psi_2 - \psi_1 &= 0 \\ &\vdots \\ M\psi_n - \psi_{n-1} &= 0 \end{aligned}\right\} \tag{5.136}$$

as given by Hoshino et al. (47), where ψ_1 is the steady state solution. Equation 5.135 can then be written as

$$\bar{\Phi}_s(\vec{x},s) = (I + sM^{-1})^{-1}\psi_1 \tag{5.137}$$

which is analogous to a Taylor's series expansion about the origin of the s-plane. Inversion yields the familiar exponential type solution.

$$\phi(\vec{x},t) = e^{tM}\phi(\vec{x},0) \tag{5.138}$$

From Eq. 5.133, a Hamiltonian can be defined for the transformed equaion by treating s as a parameter and considering the momenta to be defined in terms of the spatial derivatives, i.e.,

$$\mathcal{H} = -D(\nabla\bar{\Phi}_s)^2 + (A - v^{-1}s)\bar{\Phi}_s^2 \tag{5.139}$$

The problem has been reduced in dimension which is the usual result from application of the Laplace transform to partial differential equations. The investigation of Hamiltonian

mechanics on transformed domains is an area that has received little published attention. The dynamics should follow in a similiar manner to ordinary dynamics, with the motion now being considered as a transformation between states with different s parameters. This would seem to indicate a parallel to the perturbation process with an appropiate action integral as discussed in the previous subsection. Much more work needs to be done in laying the mathematical foundation for this theory.

Solution of Example Problems in Reactor Theory by the Hamilton-Jacobi Equation

One-dimensional slab reactor

The diffusion equation for the one-dimensional time independent slab reactor is

$$\frac{d}{dx} D \frac{d}{dx} \phi(x) + A\phi(x) = 0 \tag{5.140}$$

where $A = [\nu\Sigma_f - \Sigma_a]$. The Lagrangian for this equation is

$$\mathcal{L} = \frac{D}{2}\left(\frac{d\phi}{dx}\right)^2 - \frac{A}{2}\phi^2 \tag{5.141}$$

due to the selfadjointness of the equation under consideration. The momenta for the problem are defined through the spatial derivatives as

$$\pi = \frac{\partial \mathcal{L}}{\partial \phi_x} = D\frac{d\phi}{dx} \tag{5.142}$$

and the Hamiltonian becomes

$$\mathcal{H} = \frac{1}{2D}\pi^2 + \frac{A}{2}\phi^2 \tag{5.143}$$

A check on the canonical equations reveals that this is a correct Hamiltonian. The Hamilton-Jacobi equation for Eq. 5.140 is then

$$\frac{\partial S}{\partial x} + \frac{1}{2D}\left(\frac{\partial S}{\partial \phi}\right)^2 + \frac{A}{2}\phi^2 = 0 \tag{5.144}$$

To solve this equation, the function S is assumed to be separable into the form

$$S = W(\phi, \pi) - \alpha x \tag{5.145}$$

where α is some constant which is determined from the initial conditions on the problem. This type of solution implies that $\mathcal{H}$ is not an explicit function of x as is the case for constant coefficients. The Hamilton-Jacobi equation reduces to

$$\frac{1}{2D}\left(\frac{\partial W}{\partial \phi}\right)^2 + \frac{A}{2}\phi^2 = \alpha = \mathcal{H}\left(\phi, \frac{\partial W}{\partial \phi}\right) \tag{5.146}$$

under the assumed solution. This can be solved for $\frac{\partial W}{\partial \phi}$ as

$$\frac{\partial W}{\partial \phi} = \sqrt{2D\left(\alpha - \frac{A}{2}\phi^2\right)} \tag{5.147}$$

Integration gives the result

$$W = \int_{\phi(x=0)}^{\phi(x)} \sqrt{AD}\,\sqrt{\frac{2\alpha}{A} - \phi^2}\,d\phi \tag{5.148}$$

where the limits have been taken as $\phi(x)$ and $\phi(x=0)$. From the transformation equations, the momenta can be written as

$$\pi(x) = \frac{\partial S}{\partial \phi(x)} = \sqrt{AD}\,\sqrt{\left(\frac{2\alpha}{A} - \phi^2\right)} \tag{5.149}$$

$$\beta = -\frac{\partial S}{\partial \alpha} = -\sqrt{\frac{D}{A}}\int_{\phi(0)}^{\phi}\left[\frac{2\alpha}{A} - \phi^2\right]^{-1/2} d\phi + X \tag{5.150}$$

If β is analogous to the x=0 value of the flux, Eq. 5.149 gives the result

$$\pi(x=0) = \frac{\partial S}{\partial \phi(0)} = \sqrt{2\alpha D} \tag{5.151}$$

or solving for α

$$\alpha = \frac{\pi^2(x=0)}{2D} \tag{5.152}$$

which is the value of the Hamiltonian. Therefore, $\frac{\partial S}{\partial \alpha}$ is proportional to β and the corresponding coordinate must be x=0, i.e., $\beta = 0$. This result could have also been obtained by solving Eq. 5.150 for ϕ,

$$\phi\Big/_{\phi(0)}^{\phi(x)} = \sqrt{\frac{2\alpha}{A}} \sin \sqrt{\frac{A}{D}}\,(\beta + x) \tag{5.153}$$

Since the flux is required to go to zero at the extrapolated boundaries of the slab, the conditions on the flux are that $\phi(0)=0$ and $\phi(a)=0$. The first condition forces the requirement that $\beta = 0$, and the second maintains that $\sqrt{A/D} = \frac{\pi}{a}$. Then the solution $\phi(x)$ can be written as

$$\phi(x) = \sqrt{\frac{2\alpha}{A}} \sin \frac{\pi}{a} x = \sqrt{\frac{2H}{A}} \sin \frac{\pi}{a} x \tag{5.154}$$

which is the familiar form obtained by ordinary methods.

The coefficient of Eq. 5.154 is related to the Hamiltonian which is constant irregardless of the point of evaluation. For example,

$$\mathcal{H} = \frac{1}{2D}\pi^2 + \frac{A}{2}\phi^2 = \frac{1}{2D}\left[\frac{\pi}{a} D \sqrt{\frac{2\alpha}{A}} \cos \frac{\pi}{a} x\right]^2 +$$

$$+ \frac{A}{2}\left[\sqrt{\frac{2\alpha}{A}} \sin \frac{\pi}{a} x\right]^2 = \alpha \tag{5.155}$$

Also the fact that this is a conservative type system is shown

by evaluating the action integral between x=0 and x=a,

$$S = \int_0^q \mathcal{L}\, d\chi = \alpha \int_0^a \cos\frac{2\pi}{a}\chi\, dx = 0 \qquad (5.156)$$

which indicates that the problem is periodic with a period of a units since the action integral vanishes over this interval. This becomes an obvious conclusion when the form of the original equation is compared to that for the harmonic oscillator.

The expression for S can now be written as

$$S = \sqrt{AD}\int \sqrt{\frac{2\alpha}{A} - \frac{2\alpha}{A}\sin^2\frac{\pi}{a}x}\, d\phi - \alpha x \qquad (5.157)$$

and simple algebra shows that this is indeed the integral of the Lagrangian density. The usefulness of knowing S can be deduced from Eq. 5.148 since the solution given in Eq. 5.154 followed directly from the transformation relationships and the initial conditions.

Space-time problem

The time-dependent diffusion equation and its adjoint were written in Eqs. 5.1 and 5.2 along with the Hamiltonian density

$$\mathcal{H} = -v D \nabla\phi \cdot \nabla\pi + v A \phi \pi \qquad (5.158)$$

and the Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} - v D \nabla\phi \cdot \nabla\frac{\partial S}{\partial \phi} + v A \phi \frac{\partial S}{\partial \phi} = 0 \qquad (5.159)$$

If the assumption of constant coefficients is made, the solution to the Hamilton-Jacobi equation can be assumed to be

separable, i.e.,

$$S(t,\phi,\alpha) = W(\phi,\pi) - f(\alpha)t \tag{5.160}$$

where f(α) is some function of the new coordinate α, which is independent of time. Substitution of Eq. 5.160 into Eq. 5.159 yields the result

$$-vD\nabla\phi\cdot\nabla\frac{\partial W}{\partial\phi} + vA\phi\frac{\partial W}{\partial\phi} = f(\alpha) \tag{5.161}$$

and also the condition

$$\mathcal{H}\left(t,\phi,\frac{\partial S}{\partial\phi}\right) = f(\alpha) \tag{5.162}$$

so that $\mathcal{H}$ is independent of time. Integrating Eq. 5.161 over all space and using the vector identity

$$\nabla\cdot\frac{\partial W}{\partial\phi}\nabla\phi = \nabla\frac{\partial W}{\partial\phi}\cdot\nabla\phi + \frac{\partial W}{\partial\phi}\nabla^2\phi \tag{5.163}$$

results in the expression

$$\iiint\left(vD\frac{\partial W}{\partial\phi}\nabla^2\phi + vA\phi\frac{\partial W}{\partial\phi}\right)dV = \iiint f(\alpha)\,dV \tag{5.164}$$

which implies the relation between integrands.

$$\frac{\partial W}{\partial\phi}\left[vD\nabla^2\phi + vA\phi\right] = f(\alpha) \tag{5.165}$$

The quantity in the brackets can be formally divided out of the left hand side of Eq. 5.165 when it is not identically zero. This gives the expression

$$\frac{\partial W}{\partial\phi} = \frac{f(\alpha)}{\left[vD\nabla^2\phi + vA\phi\right]} \tag{5.166}$$

The denominator is observed to be just the spatial part of the diffusion equation. In the normal approach to modal

type problems, the denominator of Eq. 5.166 is assumed to satisfy an eigenvalue equation of the form

$$M\phi_n = [v\mathcal{D}\nabla^2 + v\Sigma_A]\phi_n = \omega_n \phi_n \tag{5.167}$$

where the ω_n are the eigenvalues of the operator M and the ϕ_n are the eigenfunctions. Equation 5.166 becomes

$$\frac{\partial W}{\partial \phi} = \sum_{n=1}^{\infty}{}' \frac{f(\alpha)}{\omega_n \phi_n} \tag{5.168}$$

which can be integrated directly to give

$$W = \int \sum_{n=1}^{\infty}{}' \frac{f(\alpha)}{\omega_n \phi_n}\, d\phi_n = \sum_{n=1}^{\infty}{}' \frac{f(\alpha)}{\omega_n} \ln \phi_n + \text{constant} \tag{5.169}$$

Then S becomes

$$S = \sum_{n=1}^{\infty}{}' \frac{f(\alpha)}{\omega_n} [\ln \phi] - f(\alpha)t \tag{5.170}$$

To obtain the solutions to the diffusion equation from S, the transformation equations are computed.

$$\pi(t) = \frac{\partial S}{\partial \phi(t)} = \frac{\partial W}{\partial \phi} = \sum_{n=1}^{\infty}{}' \frac{f(\alpha)}{\omega_n} \frac{1}{\phi_n} \tag{5.171}$$

$$\phi(0) = \frac{\partial S}{\partial \pi(0)} = \frac{\partial S}{\partial f(\alpha)} = \sum_{n=1}^{\infty}{}' \frac{\ln \phi_n}{\omega_n} - t = f(\beta) \tag{5.172}$$

From Eq. 5.171, the combination $\pi\phi$ is seen to be independent of time, and from Eq. 5.172 the solution is

$$\phi = \sum_{n=1}^{\infty}{}' e^{\omega_n (f(\beta)+t)} + \text{constant} \tag{5.173}$$

If initially the flux has the solution $\phi = \phi_0$, then Eq. 5.173 becomes

$$\phi(\vec{x},t) = \sum_{n=1}^{\infty}{}' \phi_n(\vec{x},0)\, e^{\omega_n t} \tag{5.174}$$

which is the same result as obtained from the original equations by separation of variables.

DISCUSSION AND SUMMARY

The basic goal of this study has been to extend the Hamiltonian formalism to reactor theory in a general manner. The means of obtaining this goal was a systematic exploration of the general development followed by a specific application to the equations of reactor theory and reactor dynamics. This served to illustrate the overall picture as well as the particular application to a specific equation. The introduction of the Hamilton-Jacobi equation was seen to serve as a bridge between the abstract formulation and the physical reality of natural phenomena. The main accomplishments of this study are listed below.

1. The general development of the Hamilton-Jacobi equation through the Lagrangian and Hamiltonian formulations of a general field concept.

2. An illustration of the relationship between the various forms of the solution of the Hamilton-Jacobi equation and quantities such as the components of the stress-energy-momentum tensor and the derivation of terms leading to Noether's theorem.

3. Derivation of the Hamiltonian density function for several forms of equations used in reactor theory. These include the time-dependent diffusion equation, point reactor kinetics equations, telegrapher's equation, and the diffusion equation with delayed neutrons.

4. Discussion of a continuity equation occuring from the diffusion equation, and the derivation of the components analogous to the stress tensor for the diffusion equation.

5. The illustration of the relationship of the action integral and the Hamilton-Jacobi equation to the evolution operator through the development of a closely related operator method. The relationship to the Lie series was made through the consideration of a continuous transformation of the canonical equations.

6. The solution of two sample problems from reactor theory using the Hamilton-Jacobi equation. The results were shown to be the same as obtained from other methods.

SUGGESTIONS FOR FUTURE STUDY

In the course of preforming the research presented in this dissertation, several possibilities for future work were revealed. These are listed below together with a brief discussion.

1. The use of a variational principle for dissipative problems that possess no inertia type terms is somewhat awkward to handle. This type of situation occurs when considering the diffusion equation. The use of the dual space defined by the adjoint formulation is needed to formulate the Lagrangian and the Hamiltonian. A possible way to reformulate the basic problem is through the use of the "spinor" concept that is used in quantum mechanics. This can be thought of as a two-dimensional complex space which corresponds to the four-dimensional space-time. For example, when the field is a spinor, linearity in the field derivatives occurs and this is compensated for by terms similiar in form to that used in constructing the Lagrangian for the time-dependent diffusion equation. This leads to the speculation that the dual of flux and adjoint field components may be formulated in terms of spinor components.

2. The Hamilton-Jacobi theory has a natural extension to the optimal control problem for dynamical systems. This is due to the formulation of control problems as variational problems. Snow (48) has considered this relationship for cer-

tain general optimal control problems. He illustrates that when the addition of the control vector to the problem and the condition for determining the control vector is the minimization of a functional, then the solution of the corresponding Hamilton-Jacobi equation gives the optimal control. He also derives the Hamilton-Jacobi equation from the Pontyagin maximum principle. Wang (49) illustrates the derivation of the Hamilton-Jacobi equation for distributed parameter systems by the use of dynamic programming and the principle of optimality. The usefulness of the Hamilton-Jacobi equation and the Hamiltonian formulism in the optimal control of nuclear reactors and reactor systems has not been considered. This would also add to the range of the Hamiltonian concept as a basic formulation for the theory of reactor dynamics.

3. An investigation of the use of some of the special functions and polynomials as an aid in solving the Hamilton-Jacobi equation. For example, the so-called heat polynomials are the fundamental solution to the heat equation which is very similiar to the diffusion equation. These polynomials satisfy certain transformations and biorthogonality relations with their Appell transforms which could proved to be useful in their manipulation. Also some consideration should be given to a general class of polynomials which are basically power series expansions in several variables. For example, the expansion of

$$(1-zx)^{-b}(1-zy)^{-b'}$$

leads to the definition of the polynomial in two variables

$$R_n(b,b';x,y) = \frac{n!}{(b+b',n)} \sum_{m=0}^{n} \frac{(b,m)(b',m+n)}{m!\,(n-m)!} x^m y^{n-m}$$

Hence, the investigation of various forms of the special functions through polynomials or functional relationships may be the basis for a standard procedure for solving the Hamilton-Jacobi equation and hence the equations of motion.

4. Investigation of the use of the Hamiltonian formulation in connection with Laplace transforms as a means for solving space-time problems.

5. Investigations of more complex problems then were solved in this study by using the Hamilton-Jacobi equation. This would require some form of approximation, possibly based on the operator approaches that were mentioned in this study.

BIBLIOGRAPHY

1. Turley, Richard Eyring. Perturbation Theory Applied to a Variational Analogy between Reactor Theory and Classical Mechanics. Unpublished Ph.D. thesis. Library, Iowa State University, Ames, Iowa. 1966.

2. Selengut, D. S. Variational Analysis of Multidimensional Systems. U.S. Atomic Energy Commission Report HW-59126 Hanford Works, Richland, Washington . 1958.

3. Lewins, Jeffery. Variational Representation in Reactor Physics Derived from a Physical Principle. Nuclear Science and Engineering 8: 95-104. 1960.

4. Pomraning, G. C. and Clark, M., Jr. The Variational Method Applied to the Monoenergetic Boltzmann Equation. Part 1. Nuclear Science and Engineering 16: 147-154. 1963.

5. Kaplan, S., Marlow, O. J., and Bewick, J. Application of Synthesis Techniques to Problems Involving Time Dependence. Nuclear Science and Engineering 18: 163-176. 1964.

6. Lewins, Jeffery. Time-Dependent Variational Principles for Nonconservative Systems. Nuclear Science and Engineering 20: 517-520. 1964.

7. Becker, Martin. On the Inclusion of Boundary Terms in Time-Dependent Synthesis Techniques. Nuclear Science and Engineering 22: 385-386. 1965.

8. Pomraning, G. C. A Variational Description of Dissipative Processes. Journal of Nuclear Energy 20: 617-634. 1966.

9. Henry, A. F. Few-Group Approximation Based on a Variational Principle. Nuclear Science and Engineering 27: 493-510. 1967.

10. Pomraning, G. C. A Derivation of Variational Principles for Inhomogeneous Equations. Nuclear Science and Engineering 29: 220-236. 1967.

11. Dickson, Paul Wesley, Jr. A Study of the Variational Principles of Nuclear Reactor Physics. Unpublished Ph.D. thesis. Library, North Carolina State College, Raleigh, North Carolina. 1962.

12. Kaplan, S. An Analogy between the Variational Principles of Reactor Theory and Those of Classical Mechanics. Nuclear Science and Engineering 23: 234-237. 1965.

13. Clancy, B. E. and Tavel, M. An Analogy between Time-Dependent Diffusion Theory and Classical Mechanics. Nuclear Science and Engineering 28: 105-110. 1967.

14. Kaplan, S. and Davis, James A. Canonical and Involutory Transformations of the Variational Problems of Transport Theory. Nuclear Science and Engineering 28: 166-176.

15. Tavel, M. A., Clancy, B. E., and Pomraning G. C. Use of Noether's Theorem in Reactor Physics. Nuclear Science and Engineering 29: 58-66. 1967.

16. Goldstein, Herbert. Classical Mechanics. Addison-Wesley Publishing Co., Inc., Reading, Massachusetts. 1950.

17. Lanzcos, Cornelius. The Variational Principles of Mechanics. 3rd edition. University of Toronto Press, Toronto, Canada. 1966.

18. Moiseiwitsch, B. L. Variational Principles. Interscience Publishers, New York, New York. 1966.

19. Corben, H. C. and Stehle, Philip. Classical Mechanics. 2nd edition. John Wiley and Sons, Inc., New York, New York. 1960.

20. Leech, J. W. Classical Mechanics. 2nd edition. Methuen and Co., Ltd., London, England. 1965.

21. Mercier, André. Analytical and Canonical Formulism in Physics. North-Holland Publishing Co., Amsterdam, Holland. 1959.

22. Ter Harr, D. Elements of Hamiltonian Mechanics. 2nd edition. North-Holland Publishing Co., Amsterdam, Holland. 1964.

23. Rzewuski, Jan. Field Theory. Part 1. Classical Theory. Panstwowe Wydawnictwo Naukowe, Warsaw, Poland. 1958.

24. Hamilton, William R. The Mathematical Papers of Sir William Rowan Hamilton. Vol. 2. Dynamics. Edited by A. W. Conway and A. J. McConnell. Cambridge Press, Cambridge, England. 1940.

25. Synge, John L. and Griffith, Byron A. Principles of Mechanics. 3rd edition. McGraw-Hill Book Co., Inc., New York, New York. 1959.

26. Flanders, Harley. Differential Forms. Academic Press, New York, New York. 1963.

27. Pars, L. A. A Treatise on Analytical Dynamics. John Wiley and Sons, Inc., New York, New York. 1965.

28. Caratheodory, C. Calculus of Variations and Partial Differential Equations of the First Order. Parts 1 and 2. Translated by R. B. Dean and J. J. Brandstatter. Holden-Day, Inc., San Francisco, California. 1965.

29. Rund, Hanno. The Hamilton-Jacobi Theory in the Calculus of Variations. D. Van Nostrand Co., Ltd., London, England. 1966.

30. Courant, R. and Hilbert, D. Methods of Mathematical Physics. Volumes 1 and 2. Interscience Publishers, Inc., New York, New York. 1953.

31. Whittaker, E. T. A Treatise on the Analytical Dynamics of Particles and Rigid Bodies. 4th edition. Dover Publications, New York, New York. 1944.

32. DeWitt, Bryce S. Dynamical Theory of Groups and Fields. Gordon and Breach, New York, New York. 1965.

33. Morse, Philip M. and Feshbach, Herman. Methods of Theoretical Physics. Parts 1 and 2. McGraw-Hill Book Co., Inc., New York, New York. 1953.

34. Gel'fand, I. M. and Fomin, S. V. Calculus of Variations. Translated and edited by R. A. Silverman. Prentice-Hall, Inc., Englewood Cliffs, New Jersey. 1963.

35. Glasstone, Samuel and Edlund, Milton C. The Elements of Nuclear Reactor Theory. D. Van Nostrand Co., Inc., Princeton, New Jersey. 1952.

36. Henry, A. F. The Application of Reactor Kinetics to the Analysis of Experiments. Nuclear Science and Engineering 3: 52-70. 1958.

37. Kaplan, S. The Property of Finality and the Analysis of Problems in Reactor Space-Time Kinetics by Various Modal Expansions. Nuclear Science and Engineering 9: 357-361. 1961.

38. Ash, Milton. Nuclear Reactor Kinetics. McGraw-Hill Book Co., New York, New York. 1965.

39. Weinberg, A. M. and Wigner, Eugene P. The Physical Theory of Neutron Chain Reactors. The University of Chicago Press, Chicago, Illinois. 1958.

40. Isbin, H. S. Introductory Nuclear Reactor Theory. Reinhold Publishing Corp., New York, New York. 1963.

41. Ussachof, L. N. Equation for the Importance of Neutrons, Reactor Kinetics, and the Theory of Perturbations. United Nations International Conference on the Peaceful Uses of Atomic Energy Proceedings 1st, Vol. 5: 503-510. 1955.

42. Feynman, Richard P. An Operator Calculus Having Applications in Quantum Electrodynamics. Physical Review 84: 108-128. 1951.

43. Garrido, L. M. Action Principle for Classical Mechanics. Journal of Mathematical Analysis and Applications 3: 295-314. 1961.

44. Hildebrand, Francis B. Methods of Applied Mathematics. 2nd edition. Prentice-Hall, Inc., Englewood Cliffs, New Jersey. 1965.

45. Lie, Sophus. Theorie der Transformationsgruppen. Verlag und Druck Von B. G. Teubner, Berlin, Germany. 1930.

46. Gröbner, Wolfgang. Die Lie-Reihen und ihre Anwendungen. Ved Deutscher Verlag der Wissenschaften, Berlin, Germany. 1960.

47. Hoshino, T., Wakabayashi, J., and Hayashi, S. New Approximate Solution of Space- and Energy- Dependent Reactor Kinetics. Nuclear Science and Engineering 23: 170-182. 1965.

48. Snow, Donald R. Caratheodory-Hamilton-Jacobi Theory in Optimal Control. Journal of Mathematical Analysis and Applications 17: 99-118. 1967.

49. Wang, P. K. C. Control of Distributed Parameter Systems. Advances in Control Systems 1: 75-172. 1964.

50. Messiah, Albert. Quantum Mechanics. Volume 1. North-Holland Publishing Co., Amsterdam, Holland. 1958.

51. Garrido, L. M. Perturbations in Classical Mechanics. Physical Society of London Proceedings 76: 33-35. 1960.

52. Garrido, L. M. and Gascon, F. General Theory of Perturbations in Classical Mechanics. Physical Society of London Proceedings 81: 1115-1121. 1963.

53. Mennig, J. and Auerbach, T. The Application of Lie Series to Reactor Theory. Nuclear Science and Engineering 28: 159-165. 1967.

54. Cap, Ferdinand and Schett, Alois. Analytical Continuation for Calculating Multigroup-Multizone Eigenvalue Problems Using Lie Series. Nuclear Science and Engineering 26: 517-521. 1966.

ACKNOWLEDGMENTS

The author wishes to thank Dr. Glenn Murphy and Dr. Richard Danofsky for their assistance and encouraging interest during the course of this undertaking. Also the author gratefully acknowledges support by the Atomic Energy Commission by the award of a special fellowship in nuclear engineering, administered by Oak Ridge Associated Universities.

APPENDIX A

Nomenclature and Definitions

In this appendix, a brief discussion of the nomenclature used in the theory of general dynamical systems will be given followed by definitions used in discussing the equations from reactor theory.

General dynamical systems

Capital English or script letters have been used to denote functional quantities. The script has been reserved for functionals that in general have a density type definition. The script notation has been used for generating functions of a general nature with the generator of the Hamilton-Jacobi equation being always denoted by the traditional capital S. The field components have been referred always as ϕ_μ or its Greek capital Φ_μ and similiarly for the momenta π_μ^ω . The subscripts refer to the summation indices. The indices on the coordinates x_ω will always run from 1 to 4 unless otherwise noted. In the time-preferred case, the indices will run form 1 to 3 but the context will be clear when this is the case. The indices on the field components always runs from 1 to n, and the indices on the momenta are combinations of the coordinate and field component indices. All other symbols are defined when introduced, and are generally of a more specific nature.

Reactor systems

In considering reactor system, the asterisk will always be used to denote the adjoint variables. The symbol A has been used in this study to denote the combination of terms $[\nu\Sigma_f - \Sigma_a]$ or its multigroup equivalent. v denotes the neutron velocity or group velocity whichever applies. S_{ext} denotes external sources. D denotes the diffusion coefficient and Σ_a denotes the absorbtion cross section and $\nu\Sigma_f$ denotes the fission cross section times the neutron yield per fission. These terms become more involved when considering multigroup problems and one is referred to Glasstone and Edlund (35) for a more detailed definition of the terms that appear in the general diffusion equation.

For the reactor equations with xenon feedback, the f and s subscripts refer to the fast and slow groups. The subscripted λ's refer to decay constants and the subscripted γ's refer to the fission yields for the appropiate variables. The terms in the matrix M and R_0 in Eq. 5.43 are defined below. For more detail see Kaplan (37).

$$P_1 = [\lambda_X + \sigma_{Xf}\phi_{f0} + \sigma_{Xs}\phi_{s0}] \quad ; \quad P_2 = [\gamma_X \Sigma_{Ff} - \sigma_{Xf} X_0]$$

$$P_3 = [\gamma_X \Sigma_{Fs} - \sigma_{Xs} X_0] \quad ; \quad \mathcal{L}_f = [\nabla \cdot D_f \nabla - \Sigma_f - \sigma_{Xf} X_0 + \nu\Sigma_{Ff}]$$

$$\mathcal{L}_s = [\nabla \cdot D_s \nabla - \Sigma_s - \sigma_{Xs} X_0]$$

$$R_0 = \begin{pmatrix} 0 \\ X_0[\sigma_{Xf}\phi_{f0} + \sigma_{Xs}\phi_{s0}] \\ \nu_f X_0 \sigma_{Xf}\phi_{f0} \\ \nu_s X_0 \sigma_{Xs}\phi_{s0} \end{pmatrix}$$

APPENDIX B

Evolution Operator Method

This appendix is a brief presentation of the basic principles of the so-called evolution operator method. Chapter five illustrates the close relationship between this method and results obtained from perturbation theory based on the Hamilton-Jacobi equation. The similiarity to the infinitesimal canonical transformation relations should also be noted.

The evolution operator is a concept that has been used in quantum and statistical mechanics with much sucess. Messiah (50) gives a good account of the application to the Schrodinger equation and general quantum mechanical systems. Application to classical systems has been somewhat limited due to the fact that classical systems are not usually viewed from an operator approach. Many of the perturbation techniques are based on this type of approach. For example, the WKB method is used where the Schrodinger equation can be replaced by its classical limit except for certain regions about singular points. In fact, the classical limit of the Schrodinger equation is the Hamilton-Jacobi equation. This provides the impetus for considering classical analogs to methods and techniques usually reserved for quantum mechanical systems.

Recent papers by Garrido (43, 51) and Garrido and Gascon (52), and the thesis of Turley (1) provide the basis for the

following brief discription of the evolution operator technique as applied to classical systems.

In quantum mechanics, the evolution operator is defined for linear systems as the operator which carries one dynamical state into another in the course of time.

$$|\psi(t)\rangle = U(t,t_0)\,|\psi(t_0)\rangle \tag{B.1}$$

For a classical system, consider the Liouville operator (51) defined as

$$\Omega = \left(\frac{\partial H}{\partial p}\frac{\partial}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial}{\partial p}\right) \tag{B.2}$$

where H is the Hamiltonian and p and q are the canonically conjugate variables for this one-dimensional development. A functional F of these canonical variables

$$F = F[q(t), p(t), t] \tag{B.3}$$

yields the following expression for its total time derivative

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q}\frac{dq}{dt} + \frac{\partial F}{\partial p}\frac{dp}{dt} \tag{B.4}$$

By use of Hamilton's canonical equations for the system, i.e.,

$$\dot{q} = \frac{\partial H}{\partial p} \tag{B.5}$$

$$\dot{p} = -\frac{\partial H}{\partial q} \tag{B.6}$$

Eq. B.4 becomes

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial F}{\partial p}\frac{\partial H}{\partial q} \tag{B.7}$$

or using the definition of the Liouville operator

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \Omega F \tag{B.8}$$

Note the resemblance of the operator Ω to the Poisson bracket considered in Eq. 4.16. The commutator of Ω and F can be written as

$$[\Omega, F] = \Omega F - F\Omega \tag{B.9}$$

which becomes

$$[\Omega, F] = \frac{\partial H}{\partial p}\frac{\partial F}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial F}{\partial p} - F\frac{\partial H}{\partial p}\frac{\partial}{\partial q} + F\frac{\partial H}{\partial q}\frac{\partial}{\partial p} \tag{B.10}$$

by the definition of Ω. If the commutator (which is an operator) operates on the scalar unity, then the commutator of Eq. B.10 reduces to the Poisson bracket, i.e.,

$$[\Omega, F]_{com} = [H, F]_{P.B.} \tag{B.11}$$

where the notation of the brackets has been retained, but subscripts used to distinguish between terms.

If the functional F does not depend explicitly on t, the operator S(t) is defined by the following property

$$F[q(t), p(t)] = S(t) F[q_0, p_0] \tag{B.12}$$

where the subscripts denote values of q and p at t=0. This indicates that S(t) is the operator that generates the dynamical evolution of the system. The operator Ω likewise undergoes evolution by the operator S(t), i.e.,

$$\Omega[q(t), p(t), t] = S(t)\Omega[q_0, p_0, t] \tag{B.13}$$

Ω will be an explicit function of t because in general H will be.

If the total time derivative of F is now computed from eq. B.12, the result is

$$\frac{dF[t]}{dt} = \frac{dS}{dt} F[0] - S \frac{dF[0]}{dt} \tag{B.14}$$

If the previous result of Eq. B.8 is equated with Eq. B.14, the following expression is obtained.

$$\frac{dS}{dt} F[0] = [\Omega, F] \tag{B.15}$$

By Eq. B.12 and Eq. B.13, this expression can be written as

$$\frac{dS}{dt} F[0] = [S\Omega[0], SF[0]] \tag{B.16}$$

which results in the relation

$$\frac{dS}{dt} = S\Omega[q_0, p_0, t] \tag{B.17}$$

This can be solved, at least formally, for S(t) as

$$S = e^{\int_0^t \Omega[q_0, p_0, t']\,dt'} S_0 \tag{B.18}$$

or if Ω does not depend explicitly on t,

$$S = e^{t\Omega} S_0 \tag{B.19}$$

Instead of the differential expression of Eq. B.17, and integral equation could have been written from which to determine S(t), i.e.,

$$S = 1 + \int_0^t S(t')\Omega(t')\,dt' \tag{B.20}$$

A solution by successive approximation based on S_0 which must be unity from Eq. B.12, gives the result

$$S = 1 + \int_0^t \Omega[q_0, p_0, t']\,dt' + \int_0^t \int_0^{t_1} \Omega[t_1]\Omega[t_2]\,dt_1 dt_2 \tag{B.21}$$

APPENDIX C

Lie Series

In this appendix, a brief discussion of the basic properties of the Lie series is presented. Its usefulness in solving certain sets of differential equations makes them particularly attractive. The relationships to methods and expressions discussed in this study should be apparent.

The Lie series is a name given by Gröbner (46) to a series obtained from a continuous transformation used by Sophus Lie. It is a generalization of a Taylor's series in the sense that the series derived is based on the defining equations between the variables. It is a useful method for integrating autonomous and nonautonomous equations and certain form of partial differential equations. Its application to reactor problems has been limited to shielding and steady state reactor problems (53, 54).

The basis of the Lie series approach is the operator

$$D = \varphi_1(z)\frac{\partial}{\partial z_1} + \varphi_2(z)\frac{\partial}{\partial z_2} + \cdots + \varphi_n(z)\frac{\partial}{\partial z_n} \qquad (C.1)$$

where the functions $\varphi_i(z)$ are functions of the complex variables z_i, $(i = 1, 2, \ldots n)$. The notation used here is largely that of Grobner, but has been changed somewhat to facilitate the comparison and extension to work in the main text. However, the general consideration of complex variables will be retained in order that the full mathematical nature of the

theory may be revealed. The application of the operator e^{tD} to the analytic function f(z) yields the Lie series,

$$e^{tD} f(z) = \sum_{\nu=0}^{\infty} \frac{t^\nu}{\nu!} D^\nu f(z) \tag{C.2}$$

which converges as a power series in t. Some of properties of D and e^{tD} are expressed in the following equations.

$$D^0 f(z) = f(z) \tag{C.3}$$

$$D^\nu f(z) = D^{\nu-1}(Df(z)) \tag{C.4}$$

$$D^\nu [f_1(z) + f_2(z)] = D^\nu f_1(z) + D^\nu f_2(z) \tag{C.5}$$

$$D [f_1(z) f_2(z)] = f_2(z) Df_1(z) + f_1(z) Df_2(z) \tag{C.6}$$

$$D^\nu [f_1(z) f_2(z)] = \sum_{\alpha=0}^{\nu} \binom{\nu}{\alpha} [D^\alpha f_1(z)][D^{\nu-\alpha} f_2(z)] \tag{C.7}$$

$$e^{tD}[c_1 f_1(z) + \cdots + c_m f_m(z)] = c_1 e^{tD} f_1(z) + \cdots + c_m e^{tD} f_m(z) \tag{C.8}$$

$$e^{tD}[f_1(z) \cdots f_m(z)] = [e^{tD} f_1(z)] \cdots [e^{tD} f_m(z)] \tag{C.9}$$

To determine the differential equations that the Lie series satisfy, it is desirable to introduce the following function

$$X_i = \varphi_i(z; t) = e^{tD} z_i \qquad (i = 1, 2, \cdots n) \tag{C.10}$$

which represents the Lie series within a region of analyticity of the operator D in the neighborhood of t=0. If for t=0, the function X_i is denoted by

$$(X_i)_{t=0} = \varphi_i(z; 0) = z_i \qquad (i = 1, 2, \cdots n) \tag{C.11}$$

Then and function F(X) can be written as

$$F(X) = \sum_{\nu=0}^{\infty} \frac{t^\nu}{\nu!} D^\nu F(z) \tag{C.12}$$

or in a symbolic notation

$$F(e^{tD}\underline{z}) = e^{tD}F(\underline{z}) \tag{C.13}$$

If the partial derivative of Eq. C.10 with respect to t is taken, the following differential equation results,

$$\frac{\partial X_i}{\partial t} = e^{tD}(D z_i) \qquad (i=1,2,\cdots n) \tag{C.14}$$

or more simply as

$$\frac{\partial X_i}{\partial t} = \varphi_i(\underline{X}) \qquad (i=1,2,\cdots n) \tag{C.15}$$

where

$$\varphi_i(\underline{X}) = e^{tD}\varphi_i(\underline{z}) = e^{tD}(D z_i) \tag{C.16}$$

Note that when D reduces to the total differential d/dt, the Lie series reduces to the familiar Taylor's series, i.e.,

$$\left.\begin{aligned} \underline{X} &= e^{tD}\underline{z} = \underline{z} + t \\ F(\underline{z}+t) &= \sum_{\nu=0}^{\infty} \frac{t^\nu}{\nu!} F^{(\nu)}(\underline{z}) \end{aligned}\right\} \tag{C.17}$$

for the expression of a function about the point $\{z_i\}$.

From the previous discussion, the solution to equations of the type as Eq. C.15 are seen to posses the solution of a Lie series about some initial point. Equations of this type are common in the state variable form of linear system theory and the Hamiltonian form of mechanical systems. Equations without the explicit t dependence of $\varphi(\alpha)$ are usually called autonomous. The results can be extended to nonautonomous systems be adding a new state variable $X_0 = t$. Then the system equations are

$$\frac{dX_0}{dt} = 1 \tag{C.18}$$

and

$$\frac{dX_i}{dt} = \varphi_i(X, X_0) \qquad (i=1,2,\cdots n) \qquad (C.19)$$

and the solution is the Lie series form with D now modified as

$$D = \frac{\partial}{\partial z_0} + \varphi_1(z; z_0)\frac{\partial}{\partial z_1} + \cdots + \varphi_n(z, z_0)\frac{\partial}{\partial z_n} \qquad (C.20)$$

where z_0 denotes the initial value of X_0. The solution to Eqs. C.18 and C.19 becomes

$$X_j = \left(e^{\tau D} z_j\right)\Big|_{z_0=0} \qquad (j=0,1,2,\cdots n) \qquad (C.21)$$

Then any function F(X;t) can be expressed in terms of the initial values of X_i by the Lie series

$$F(X;t) = \left(e^{\tau D} F(z,\gamma)\Big|_{\gamma=0}\right) = \sum_{\nu=0}^{\infty} \frac{\tau^\nu}{\nu!}\left(D^\nu F(z,\gamma)\Big|_{\gamma=0}\right) \qquad (C.22)$$

where z_0 has been replaced by γ.

A multi-dimensional form of the Lie series operator can be defined as

$$D_m = \varphi_{m1}(z)\frac{\partial}{\partial z_1} + \cdots + \varphi_{mn}(z)\frac{\partial}{\partial z_n} \qquad (m=1,2\cdots s) \qquad (C.23)$$

Then the corresponding form of the Lie series can be expressed by operating with D_i on the function f(z).

$$e^{\tau_1 D_1 + \cdots + \tau_s D_s} f(z) = \sum_{\nu=0}^{\infty} \frac{1}{\nu!}\left[\tau_1 D_1 + \tau_2 D_2 + \cdots + \tau_s D_s\right]^{(\nu)} f(z) \qquad (C.24)$$

In a manner similiar to the one dimensional case, the function

$$X_\kappa = \varphi_\kappa(z;t) = e^{\tau_1 D_1 + \cdots + \tau_s D_s} z_\kappa \qquad (C.25)$$

can be defined, and the function of X_k can be written as

$$F(X) = e^{\xi_1 D_1 + \cdots + \xi_s D_s} F(z) \tag{C.26}$$

This development can be visualized more easily by considering the special case where

$$D_j = \frac{\partial}{\partial z_j} \qquad (j = 1, 2, \cdots n) \tag{C.27}$$

which gives rise to the multidimensional form of the Taylor's series since

$$X_k = e^{\xi_1 D_1 + \cdots + \xi_s D_s} z_k \qquad (k = 1, 2, \cdots n) \tag{C.28}$$

and

$$F(z_1+\xi_1, \cdots z_n+\xi_n) = \sum{}' \frac{1}{\nu!} \left[\xi_1 \frac{\partial}{\partial z_1} + \cdots + \xi_n \frac{\partial}{\partial z_n}\right]^{(\nu)} F(z_1 \cdots z_n) \tag{C.29}$$

or

$$F(z_1+\xi_1, \cdots z_n+\xi_n) = \sum_{\nu_1=0}^{\infty} \cdots \sum_{\nu_n=0}^{\infty} \frac{\xi_1^{\nu_1} \cdots \xi_n^{\nu_n}}{\nu_1! \cdots \nu_n!} \frac{\partial^{\nu_1+\nu_2+\cdots\nu_n}}{\partial z_1^{\nu_1} \cdots \partial z_n^{\nu_n}} F(z) \tag{C.30}$$

The operator D_j posses some interesting properties that have some similiarity and relationship to properties of the infinitesimal transformation and bracket relations considered in chapter four. Consider what Grobner calls the "Jacobischen Klammersymbole",

$$[D_j, D_k] = D_j D_k - D_k D_j \tag{C.31}$$

This will be translated as Jacobi bracket and referred to as such. This can be written more explicitly as

$$[D_j, D_k] = \sum\sum \left\{ \varphi_{ji} \frac{\partial \varphi_{ki}}{\partial z_i} \frac{\partial}{\partial z_k} - \varphi_{ki} \frac{\partial \varphi_{ji}}{\partial z_i} \frac{\partial}{\partial z_k} + (\varphi_{ji} \varphi_{ki} - \varphi_{ki} \varphi_{ji}) \cdot \frac{\partial^2}{\partial z_i \partial z_k} \right\} \tag{C.32}$$

from the definition of D_i. If the coefficients φ_{ji} and φ_{ki} commute, then Eq. C.32 becomes

$$[D_j, D_k] = \sum_{i=1}^{n} \left[\sum_{l=1}^{n} \left(\varphi_{jl} \frac{\partial \varphi_{ki}}{\partial x_l} - \varphi_{kl} \frac{\partial \varphi_{ji}}{\partial x_l} \right) \right] \frac{\partial}{\partial x_i} \qquad (C.33)$$

The Jacobi bracket has the antisymmetric property,

$$[D_j, D_k] = -[D_k, D_j] \qquad (C.34)$$

commutes with itself when i=j, and exhibits a distributive property.

$$[D_j, D_k + D_l] = [D_j, D_k] + [D_j, D_l] \qquad (C.35)$$

The Jacobi bracket can also be shown to satisfy the relation

$$[[D_1, D_2], D_3] + [[D_2, D_3], D_1] + [[D_3, D_1], D_2] = 0 \qquad (C.36)$$

generally referred to as Jacobi's identity.

A general system of partial differential equation of the form

$$\frac{\partial X_i}{\partial t_k} = \varphi_{ki}(X, t) \qquad \begin{matrix} (i = 1, 2, \cdots n) \\ (k = 1, 2 \cdots s) \end{matrix} \qquad (C.37)$$

with the initial conditions,

$$(X_i)_{t_1 = t_2 = \cdots t_s = 0} = x_i \qquad (i = 1, 2 \cdots n) \qquad (C.38)$$

has a solution that can be expressed in Lie series form as

$$X_i = (e^{\tau_1 D_1 + \cdots + \tau_m D_m} x_i)_{\tau_1 = \tau_2 = \cdots \tau_s = 0} \qquad (C.39)$$

or

$$= \sum_{\nu=0}^{\infty} \frac{1}{\nu!} \left[(\tau_1 D_1 + \cdots + \tau_s D_s)^{(\nu)} x_i \right]_{\tau_1 = \tau_2 = \cdots = \tau_s = 0} \qquad (C.40)$$

where D_k is the modified Lie operator

$$D_k = \frac{\partial}{\partial \tau_k} + \varphi_{k1}(x; \tau) \frac{\partial}{\partial x_1} + \cdots + \varphi_{kn}(x; \tau) \frac{\partial}{\partial x_n} \qquad (C.41)$$

and the functions φ_{ki} are to be analytic in the variables $\{X_i\}$ and $\{t_k\}$ and satisfy the integrability condition,

$$\frac{\partial \varphi_{ki}}{\partial t_l} + \sum_{j=1}^{n} \varphi_{lj} \frac{\partial \varphi_{ki}}{\partial x_j} = \frac{\partial \varphi_{li}}{\partial t_k} + \sum_{j=1}^{n} \varphi_{kj} \frac{\partial \varphi_{li}}{\partial x_j} \qquad (C.42)$$

Because of this requirement, the commutator between operators D_k and D_l takes the form

$$D_k D_l = D_l D_k \qquad (C.43)$$

In analogy to the one dimensional case, an arbitrary function F(X;t) can be defined through a Lie series as

$$F(x,t) = \left(e^{\tau_1 D_1 + \cdots + \tau_s D_s} F(z;\tau)\right)_{\tau_1=\tau_2=\cdots=\tau_s=0} \qquad (C.44)$$