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A PEDESTRIAN'S GUIDE TO LIE TRANSFORMS: A NEW APPROACH TO PERTURBATION THEORY IN CLASSICAL MECHANICS

Robert G. Littlejohn

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A PEDESTRIAN'S GUIDE TO LIE TRANSFORMS:

A NEW APPROACH TO PERTURBATION THEORY IN CLASSICAL MECHANICS*

Robert G. Littlejohn

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

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ABSTRACT

Lie transforms are developed as a practical tool for perturbation theory in classical mechanics. The spirit of the presentation is pedagogical. In order to define the general context of Lie transform perturbation methods, an extensive discussion is given of traditional perturbation methods in Hamiltonian and other systems, with an emphasis on averaging techniques.

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1. Introduction

This paper concerns perturbation theory in classical mechanics and especially the use of Lie transforms in the Hamiltonian subset thereof. The characteristic feature of the Lie transform method in perturbation theory is the exploitation of the group structure of the set of canonical transformations. In the Lie transform method, Lie operators are used to generate canonical transformations, so that canonical transformations are in effect parametrized by their Lie generators. This parametrization turns out to provide a compact notation for the transformations themselves as well as for the various formulas which naturally arise in perturbation theory.

The use of Lie transforms as a practical computational tool has only come about in the last ten years or so. The tardiness of the discovery of this application of Lie groups might seem surprising, since classical mechanics is an old subject, and the basic theory of Lie groups has been in existence since the late nineteenth century. Actually, there have been a number of workers throughout the years who have come close to discovering the Lie transform method. In one of the earliest papers on quantum mechanics, Heisenberg, Born and Jordan[1] developed a perturbation theory for quantum mechanics which is similar in spirit to the classical theory presented here. These authors failed to make the necessary changes to transcribe their theory into classical mechanics, perhaps in part because they did not know how to effect that transcription. The first use of the Lie transform method in classical mechanics was made by Hori,[2] a worker in celestial mechanics, and his ideas were developed and extended by Deprit,[3] Dewar,[4] and others.

The object of this paper is to make the Lie transform method as accessible

as possible to those with a minimum of experience with classical perturbation theory, group theory, etc. Therefore the theory will not be developed in its most abstract form, and general formulas will not be given; but some idea of the general theory will be indicated from place to place. For a more rigorous and complete presentation of Lie transforms, the work of Cary[5] may be consulted.

The level of knowledge of Hamiltonian mechanics required for this paper is that of a graduate level course in classical mechanics. For the less experienced reader, a section on Hamiltonian mechanics has been included which can serve as a reminder or a reference for certain basic, well-known facts. Nevertheless, there is no pretense that this survey is complete. In the development of Lie transforms, a few theorems of Hamiltonian mechanics are required which are not so well-known. These will be developed and proved as they are needed.

2. Ordinary Differential Equations In Classical Mechanics

In this section we discuss some mathematical properties of ordinary differential equations which are relevant to classical mechanics, and especially those properties which will be needed for later developments in this paper. We begin by emphasizing the fruitfulness of thinking in terms of first order differential equations. A phase plane analysis is given of a differential equation arising in a physical context in order to show the power of the phase space concept. We next define autonomous and non-autonomous systems, and discuss the differences. Then we establish the connection between systems of ordinary differential equations and families of mappings of phase space onto itself. Finally, we discuss constants of integration, and their use as a means of solving differential equations.

A central mathematical problem of classical mechanics is the solution of systems of ordinary differential equations. If these equations are derived from Newton's laws or from a Lagrangian formulation of mechanics, then they will typically be second order differential equations in the independent variable, which is time. On the other hand, the mathematical theory of differential equations is best developed around systems which are first order in the independent variable. There is no loss of generality in such a development, since any system of differential equations of any order can be easily transformed into another system of first order equations. In physical applications, the change from a system of second order differential equations to a system of first order equations most often corresponds to a change of interpretational emphasis from configuration space to phase space.

The phase space in question may be the familiar phase space of Hamiltonian mechanics, or it may be something somewhat more general, as the following example will show.

As an example to illustrate the great conceptual utility of phase space, we consider the motion of a body falling near the earth's surface, subject to a frictional drag due to the atmosphere. In order to make a simple model of this physical system, we assume that the motion is purely in the vertical direction, and that the force of friction is proportional to the velocity. We let x represent the height of the body above the ground, and we let m, k and g represent respectively the mass of the body, the proportionality constant in the friction law, and the acceleration of gravity. Then Newton's laws give the following differential equation for the motion:

$$m\ddot{x} + K\dot{x} + mg = 0 \tag{2.1}$$

Although this equation is easily solved in closed form, we wish instead to analyze it in phase space to gain information of a qualitative nature about the solution.

The configuration space implied by (2.1) is one-dimensional. We may transform (2.1) into a pair of coupled, first order differential equations via the substitution

$$v = \dot{x} \tag{2.2}$$

which gives for the transformed set

$$\left.\begin{aligned} \dot{x} &= v \\ \dot{v} &= -\frac{K}{m}v - g \end{aligned}\right\} \tag{2.3}$$

The two-dimensional (x,v) space in which the solution to (2.3) evolves may be considered to be a kind of generalized phase space. By "generalized" we mean that there is no necessary connection with Hamiltonian mechanics; the phase space in question is nothing more than a compound configuration-velocity space.

A number of properties stem from the fact that the system (2.3) consists of first order equations. We note that a complete set of initial conditions for the system (2.3) consists of a point (x_o,v_o) in phase space. It does not matter at what time the initial conditions are given, since the right-hand sides of equations (2.3) are independent of time. Thus, there is a unique trajectory passing through every point in phase space. This property is not shared by configuration space, where many trajectories will pass through a given point. One can use this property of phase space to assign a vector to each point, indicating the direction of the trajectory passing through that point and, by its magnitude, the rate of the flow along the trajectory. In other words, a set of first order differential equations such as (2.3) can be used to define a vector field in phase space, representing the flow generated by the equations.

The flow field of the set (2.3) is shown graphically in Fig. 1. In this figure, the flow vectors have all been normalized to a standard length, so that the vector field shows only the direction of the flow, not its magnitude.

In order to emphasize the value of the phase space concept, we note the following properties of the system (2.3) which can be seen from Fig. 1. First, the invariance of the flow field with respect to translations in the x coordinate is obvious. This fact can be used to construct a constant of

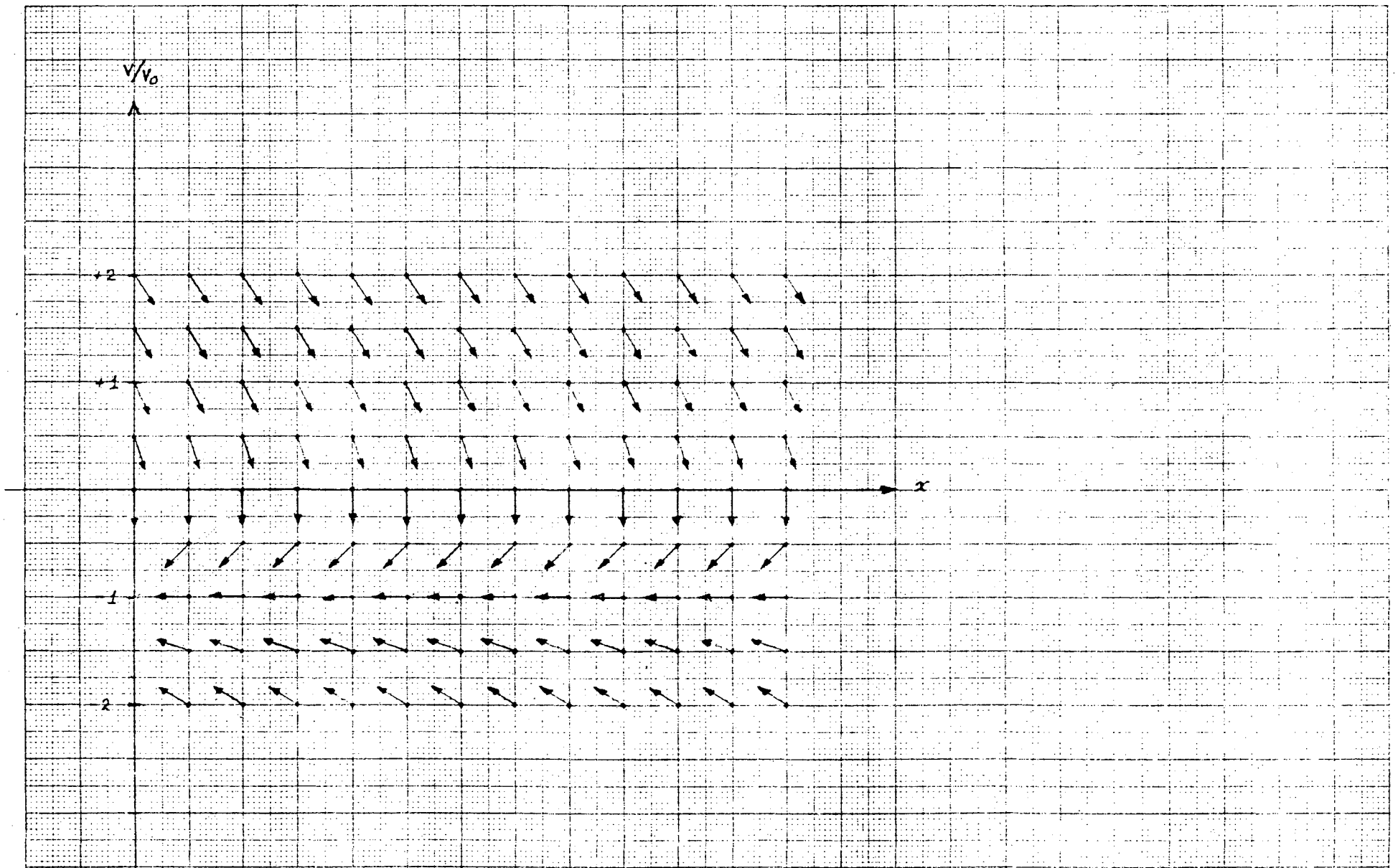

FIG. 1. PHASE FLOW FOR DIFFERENTIAL EQUATIONS (2.3)

integration. Next, we see that there is a limiting velocity v_o, given by

$$v_o = \frac{mg}{K} \tag{2.4}$$

No matter what the initial conditions, all trajectories evolve so that the velocity approaches $-v_0$ as $t \to \infty$. This is the terminal velocity for fall in the atmosphere. A body falling with $v > -v_0$ is accelerated downward, while one falling with $v < -v_0$ is accelerated upward, i.e. its fall is braked by the atmosphere. Finally, we note that the shape of the actual trajectories can be filled in by eye by looking at the flow field. Although it happens that (2.3) can be solved in closed form, it is easy to imagine slight modifications to (2.3) which would result in a system that could not be easily solved. The plot of the phase flow, however, would hardly be any more difficult to generate or interpret.

We return now to the more general problem of an arbitrary set of ordinary differential equations. It is easy to see that by some simple substitution, analogous to (2.2), the set can be transformed into a system of first order equations which describe a flow in a generalized phase space of some finite dimensionality. We denote the dimensionality of the phase space by D, and we let $\underset{\sim}{z}$ be an D-vector which represents a point in that space. The flow field will be a D-dimensional vector field, which we denote by $\underset{\sim}{F}(\underset{\sim}{z},t)$; in general, it will depend explicitly on the time. The equations of motion will take on the following very general form:

$$\dot{\underset{\sim}{z}} = \underset{\sim}{F}(\underset{\sim}{z}, t) \tag{2.5}$$

In the case that the functions $\underset{\sim}{F}$ are independent of time, the set (2.5) is said to be <u>autonomous</u>. (In Hamiltonian mechanics, an autonomous set

corresponds to a conservative system.) For an autonomous set of differential equations, there is a unique trajectory passing through every point of phase space, as in the example just given above. Furthermore, different trajectories never intersect one another, although a given trajectory may close on itself, in the form of a smooth, simply connected loop.* For a non-autonomous set, none of these properties hold, since the flow field changes as time progresses. In a later section we shall use non-autonomous Hamiltonian equations of motion to generate canonical transformations.

It is frequently useful to associate the system (2.5) with a family of mappings of phase space onto itself. To make this correspondence, consider some initial time t_0 and some initial point in phase space $\underset{\sim}{z} = \underset{\sim}{z}_0$ (an initial condition). At a later time t_1 the phase point $\underset{\sim}{z}$ will have evolved along a trajectory to a new position $\underset{\sim}{z} = \underset{\sim}{z}_1$. If the initial point $\underset{\sim}{z}_0$ is now regarded as a variable which ranges over all of phase space, then we have associated with the set (2.5) and the two times t_0 and t_1 a certain mapping of phase space onto itself, which we denote by $M(t_0,t_1)$. To illustrate the action of this mapping we write

$$\underset{\sim}{z}_1 = M(t_0, t_1)\, \underset{\sim}{z}_0 \tag{2.6}$$

This mapping can be regarded as a time evolution operator.

For an autonomous system of differential equations, the associated mapping of phase space onto itself $M(t_0,t_1)$ depends only on the time difference $\tau = t_1 - t_0$. Furthermore, the set of all such mappings for all possible time differences τ forms a one-parameter Lie group, in which τ may be chosen as

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*These two statements depend on certain continuity and differentiability requirements on the functions $\underset{\sim}{F}$. These requirements almost always hold for systems of physical interest, except possibly at singular points such as the origin in the Kepler problem.

the parameter. The group multiplication law is expressed by

$$M(\tau_1)\,M(\tau_2) = M(\tau_1 + \tau_2) \tag{2.7}$$

This result is intuitively obvious; in a later section, a similar line of reasoning will be followed in the development of direct canonical transformations.

Let us now consider the actual solution of a system of differential equations such as (2.5). Of course, the general solution for arbitrary functions $\underset{\sim}{F}$ cannot be written down, but the general form will be

$$\underset{\sim}{z} = \underset{\sim}{Y}(\underset{\sim}{a}, t) \tag{2.8}$$

In this expression the vector $\underset{\sim}{a}$ represents the D constants of integration which necessarily appear in the general solution, and $\underset{\sim}{Y}$ is a vector function which causes the differential equations to be satisfied. The constants of integration may be the initial conditions $\underset{\sim}{z}_0$ at some time t_0, or they may be other quantities of interest, such as the energy, momentum, etc.

It is often useful to consider the inverse of (2.8). Regarding the time t as a parameter, (2.8) can be inverted, giving the D quantities $\underset{\sim}{a}$ as functions of the D quantities $\underset{\sim}{z}$. The result is a relation of the form

$$\underset{\sim}{a} = \underset{\sim}{A}(\underset{\sim}{z}, t) \tag{2.9}$$

This expression shows that the constants of integration can be regarded as time-dependent phase functions. Alternatively, we can interpret (2.9) as a time-dependent change of variables, taking $\underset{\sim}{z}$ into $\underset{\sim}{a}$, and taking the set of differential equations (2.5) into the new set

$$\dot{\underset{\sim}{a}} = 0 \tag{2.10}$$

Of course, it is trivial to solve the new set (2.10).

Clearly, finding the transformation of variables (2.9) is equivalent to solving the original system of equations. Indeed, the whole of Hamilton-Jacobi theory is built around this idea, that differential equations can be solved by finding the right coordinate transformation. This philosophy will be further developed in the next section, where we discuss Hamiltonian mechanics.

3. An Overview of Hamiltonian Mechanics

In this section we review some standard results of Hamiltonian mechanics, and we introduce some notation which, while not quite standard, will be useful for later work. The review of Hamiltonian mechanics presented here is not intended to be complete; it is only included in order to enhance the continuity of the presentation of this paper. In particular, we only state, and do not prove, certain well-known theorems. For a more thorough discussion of Hamiltonian mechanics, the standard references[6,7,8] on classical mechanics may be consulted.

In the last section we used the term "phase space" to mean a compound configuration-velocity space, or, more loosely, any space in which the evolution of a system of first order differential equations takes place. In the context of Hamiltonian mechanics, the term phase space has a more restricted meaning, which we now proceed to elaborate upon.

Hamiltonian phase space always has an even number of dimensions, which we denote by 2N. The quantity N is called the number of degrees of freedom. A point in phase space is represented by a 2N-vector $\underset{\sim}{z}$. It is customary to divide the 2N components of $\underset{\sim}{z}$ into N components, called the q's, and N more components, called the p's. The q's and p's can be regarded as two N-vectors, $\underset{\sim}{q}$ and $\underset{\sim}{p}$. The convention we shall adopt for the decomposition of $\underset{\sim}{z}$ into $\underset{\sim}{q}$ and $\underset{\sim}{p}$ is as follows:

$$\begin{aligned} \underset{\sim}{z} &= (z_1,\ldots,z_N,z_{N+1},\ldots,z_{2N}) \\ &= (q_1,\ldots,q_N,p_1,\ldots,p_N) \\ &= (\underset{\sim}{q},\underset{\sim}{p}) \end{aligned} \tag{3.1}$$

The q's are called generalized coordinates and the p's generalized momenta. We shall often call the z's, including both the q's and p's, simply "coordinates", meaning coordinates in phase space.

In Hamiltonian mechanics, the equations of motion for the coordinates $\underset{\sim}{z}$ or $(\underset{\sim}{q},\underset{\sim}{p})$ take on a special form. The equations of motion are derivable from a certain scalar function on phase space, the Hamiltonian, denoted by $H(\underset{\sim}{q},\underset{\sim}{p},t)$. In general, the Hamiltonian will be time-dependent. The equations of motion are given by

$$\begin{aligned} \dot{\underset{\sim}{q}} &= \frac{\partial H}{\partial \underset{\sim}{p}} \\ \dot{\underset{\sim}{p}} &= -\frac{\partial H}{\partial \underset{\sim}{q}} \end{aligned} \tag{3.2}$$

These equations are a special case of (2.5), in that the functions $\underset{\sim}{F}$ appearing there can be written in terms of the derivatives of the scalar H. This is a strong restriction on the form of the functions $\underset{\sim}{F}$, and gives rise to numerous properties of Hamiltonian systems which are not shared by more general sets of differential equations. In view of these properties, flow fields $\underset{\sim}{F}$ which have the form of the right hand side in (3.2) are called Hamiltonian flows.

It is customary to derive the Hamiltonian equations of motion (3.2) by proceeding from a Lagrangian through the Legendre transformation. Here they have simply been posited, in effect as a definition of a special case of systems of first order differential equations. This has been done for several reasons. First, it is assumed that the customary procedure is familiar. Next, we wish here to emphasize the connection between Hamiltonian mechanics

and the theory of ordinary differential equations, as outlined in the last section. And finally, we want to play down the interpretation of the q's as physical coordinates and the p's as physical momenta, since canonical transformations will in general mix the q's and p's in such a way as to make this interpretation no longer valid.

It is often convenient to employ the symbol $\underset{\sim}{z}$ for a point in phase space, instead of the more usual $(\underset{\sim}{q},\underset{\sim}{p})$. Not only does this notation treat the q's and p's on an equal footing, thereby giving rise to more compact formulas, but it also clarifies the connection with the theory presented in section 2. Nevertheless, the usual $(\underset{\sim}{q},\underset{\sim}{p})$ notation is sometimes more transparent, and in this paper we shall use the two notations interchangeably. In this section, we will present the standard theorems of Hamiltonian mechanics in both the $(\underset{\sim}{q},\underset{\sim}{p})$ notation and the $\underset{\sim}{z}$ notation.

We begin with the equations of motion, (3.2). To rewrite these in the $\underset{\sim}{z}$ notation, it is convenient to introduce a certain 2Nx2N matrix $\underset{\approx}{\gamma}$, which is defined by its partition into four NxN matrices:

$$\underset{\approx}{\gamma} = \left[\begin{array}{c|c} 0 & I \\ \hline -I & 0 \end{array}\right] \tag{3.3}$$

Using the matrix $\underset{\approx}{\gamma}$, (3.2) can be rewritten as follows:

$$\dot{\underset{\sim}{z}} = \underset{\approx}{\gamma} \cdot \frac{\partial H}{\partial \underset{\sim}{z}} \tag{3.4a}$$

In component form, this is

$$\dot{z}_i = \sum_{j=1}^{2N} \gamma_{ij} \frac{\partial H}{\partial z_j} \tag{3.4b}$$

The following properties of $\underset{\approx}{\gamma}$ are important to note. First, the components of $\underset{\approx}{\gamma}$ are real constants. Second, $\underset{\approx}{\gamma}$ is antisymmetric:

$$\gamma_{ij} = -\gamma_{ji} \tag{3.5a}$$

And finally, $\underset{\approx}{\gamma}$ is orthogonal:

$$\sum_{i=1}^{2N} \gamma_{ij}\,\gamma_{ik} = \delta_{jk} \tag{3.5b}$$

Equations (3.2) or (3.4) are special uses of the Poisson Bracket. In $(\underset{\sim}{q},\underset{\sim}{p})$ notation, the Poisson Bracket is defined as follows. Given any two phase functions* $A(\underset{\sim}{q},\underset{\sim}{p},t)$ and $B(\underset{\sim}{q},\underset{\sim}{p},t)$, the Poisson Bracket of these two functions, written $\{A,B\}$, is another phase function, given by

$$\{A,B\} = \sum_{i=1}^{N}\left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i}\right) \tag{3.6a}$$

In $\underset{\sim}{z}$ notation, the definition of the Poisson Bracket reads

$$\{A,B\} = \frac{\partial A}{\partial \underset{\sim}{z}}\cdot\underset{\approx}{\gamma}\cdot\frac{\partial B}{\partial \underset{\sim}{z}} \tag{3.6b}$$

or, in component form,

$$\{A,B\} = \sum_{i,j=1}^{2N} \frac{\partial A}{\partial z_i}\,\gamma_{ij}\,\frac{\partial B}{\partial z_j} \tag{3.6c}$$

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*By "phase function" we mean a real-valued function on phase space, which may depend additionally on time. For functions of physical interest, the term "dynamical variable" is virtually synonymous.

Using the Poisson Bracket notation, the equations of motion (3.4) can be compactly written as follows:

$$\dot{\underset{\sim}{\xi}} = \{\underset{\sim}{\xi}, H\} \tag{3.7}$$

The Poisson Bracket has the following important properties.* For any phase functions A, B, C and for any real numbers λ, μ we have, first, the linearity of the Poisson Bracket in its two operands:

$$\{\lambda A+\mu B,C\} = \lambda\{A,C\} + \mu\{B,C\} \tag{3.8a}$$

$$\{A,\lambda B+\mu C\} = \lambda\{A,B\} + \mu\{A,C\} \tag{3.8b}$$

Next, the Poisson Bracket is anti-symmetric in its two operands:

$$\{A,B\} = -\{B,A\} \tag{3.8c}$$

Finally, it obeys the Jacobi identity:

$$\{A,\{B,C\}\} + \{B,\{C,A\}\} + \{C,\{A,B\}\} = 0 \tag{3.8d}$$

We now introduce an alternative notation for the Poisson Bracket, which will be of great use when we discuss the development of direct canonical transformations in terms of their associated Lie generators. Since the Poisson Bracket {A,B} is linear in the second operand B, it may be regarded as a linear operator, specified by A, which takes the phase function B into the new phase function {A,B}. We denote the operator by L_A, and write

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*The properties (3.8) are exactly the properties required to classify the set of all phase functions as a Lie algebra,[9] with the Poisson Bracket acting as the Lie product. The corresponding Lie group is the group of canonical transformations.

$$L_A B = \{A,B\} \tag{3.9a}$$

or

$$L_A = \{A, \ \} \tag{3.9b}$$

The symbol L is a mnemonic for "Lie"; the L operators are elements of a Lie algebra. To illustrate the use of the L operators, we transcribe properties (3.8) into the alternative notation. First, the linearity property:

$$L_{(\lambda A+\mu B)} = \lambda L_A + \mu L_B \tag{3.10a}$$

$$L_A(\lambda B+\mu C) = \lambda L_A B + \mu L_A C \tag{3.10b}$$

Next, anti-symmetry:

$$L_A B = -L_B A \tag{3.10c}$$

Finally, the Jacobi identity:

$$[L_A, L_B] = L_{\{A,B\}} \tag{3.10d}$$

In (3.10d) the square brackets represent the usual commutator of two linear operators.

We now recall some facts about canonical transformations, and develop upon them. A coordinate transformation of the form

$$\begin{aligned} \underset{\sim}{q}' &= \underset{\sim}{q}'(\underset{\sim}{q},\underset{\sim}{p},t) \\ \underset{\sim}{p}' &= \underset{\sim}{p}'(\underset{\sim}{q},\underset{\sim}{p},t) \end{aligned} \tag{3.11}$$

is said to be a canonical transformation, by definition, if the following relations hold:

$$\left.\begin{aligned} \{q_i', q_j'\} &= \{p_i', p_j'\} = 0 \\ \{q_i', p_j'\} &= -\{p_i', q_j'\} = \delta_{ij} \end{aligned}\right\} \quad (i,j = 1,\ldots,N) \tag{3.12}$$

This definition is transcribed into $\underset{\sim}{z}$ notation as follows. The transformation

$$\underset{\sim}{z}' = \underset{\sim}{z}'(\underset{\sim}{z},t) \tag{3.13}$$

is canonical if

$$\{z_i', z_j'\} = \gamma_{ij} \qquad (i,j = 1,\ldots,2N) \tag{3.14a}$$

i.e., if

$$\sum_{\substack{k,l\\=1}}^{2N} \frac{\partial z_i'}{\partial z_k} \gamma_{kl} \frac{\partial z_j'}{\partial z_l} = \gamma_{ij} \tag{3.14b}$$

Canonical transformations have the following properties. First, the Jacobian of a canonical transformation is unity:

$$\det\left[\frac{\partial \underset{\sim}{z}'}{\partial \underset{\sim}{z}}\right] = 1 \tag{3.15}$$

This fact is of use in transforming density functions in phase space to a new set of canonical coordinates, since it implies $d\underset{\sim}{z} = d\underset{\sim}{z}'$. It also means that every canonical transformation has an inverse. Concerning the inverse we have another property:* the inverse of a canonical transformation is also a canonical transformation, i.e. if (3.14b) holds, then we have

$$\sum_{\substack{k,l\\=1}}^{2N} \frac{\partial z_i}{\partial z_k'} \gamma_{kl} \frac{\partial z_j}{\partial z_l'} = \gamma_{ij} \tag{3.16}$$

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*This property and the next one are required in the proof that the set of canonical transformations forms a group.

Finally, we have the important property that the product of two canonical transformations is another canonical transformation. That is, if $\underset{\sim}{z} \to \underset{\sim}{z}'$ and $\underset{\sim}{z}' \to \underset{\sim}{z}''$ are canonical transformations, then so is $\underset{\sim}{z} \to \underset{\sim}{z}''$.

Canonical transformations and the Poisson Bracket operation are closely connected. We note here one important relation between the two, namely, the invariance of the Poisson Bracket with respect to canonical transformations. By this we mean that if $\underset{\sim}{z} \to \underset{\sim}{z}'$ is a canonical transformation, then

$$\{A,B\} = \frac{\partial A}{\partial \underset{\sim}{z}} \cdot \underset{\approx}{\gamma} \cdot \frac{\partial B}{\partial \underset{\sim}{z}} = \frac{\partial A}{\partial \underset{\sim}{z}'} \cdot \underset{\approx}{\gamma} \cdot \frac{\partial B}{\partial \underset{\sim}{z}'} \tag{3.17}$$

Thus the value of a Poisson Bracket expression is independent of the set of canonical variables which are used to compute the derivatives appearing therein.

The importance of canonical transformations lies in the following theorem. We consider a Hamiltonian $H(\underset{\sim}{z},t)$, and a possibly time-dependent coordinate transformation $\underset{\sim}{z} \to \underset{\sim}{z}'$. Due to the time evolution of the coordinates $\underset{\sim}{z}$ engendered by $H(\underset{\sim}{z},t)$ through the equations (3.4), there will be a corresponding time evolution of the new coordinates $\underset{\sim}{z}'$. The theorem in question states that there will exist a function $K(\underset{\sim}{z}',t)$ such that

$$\dot{z}'_i = \sum_{j=1}^{2N} \gamma_{ij} \frac{\partial K}{\partial z'_j} \tag{3.18}$$

if and only if the transformation $\underset{\sim}{z} \to \underset{\sim}{z}'$ is canonical.* In other words, it is only under canonical transformations that the form of the Hamiltonian

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*Strictly speaking, for this theorem to be true as stated, the definition of canonical transformation (3.14) should be modified by replacing γ_{ij} on the right hand side by $c\gamma_{ij}$, where c is any non-zero constant. See references 7 and 8.

equations of motion is preserved.

Although this theorem ensures the existence of a new Hamiltonian K under a canonical transformation, it does not say how to find the functional form of K, given H and the transformation in question. In the special case of a time-independent transformation, however, the answer is simple: the old and new Hamiltonians are numerically equal, i.e.

$$K(\underset{\sim}{z}',t) = K(\underset{\sim}{z}'(\underset{\sim}{z}),t) = H(\underset{\sim}{z},t) \tag{3.19}$$

The case of a time-dependent transformation will be postponed for a moment.

Consider now the question of how to generate canonical transformations, which are so important in Hamiltonian mechanics. The standard method is to use mixed-variable generating functions, as we shall call them in this paper. There are 2^N types of these functions,[10] although we shall concentrate on only one type, the one called F_2 by Goldstein.[11] This generating function is a function $S(\underset{\sim}{q},\underset{\sim}{p}',t)$ of the old coordinates and new momenta, and possibly the time, and it generates a canonical transformation via the prescription

$$\left.\begin{aligned} \underset{\sim}{p} &= \frac{\partial S}{\partial \underset{\sim}{q}} \\ \underset{\sim}{q}' &= \frac{\partial S}{\partial \underset{\sim}{p}'} \end{aligned}\right\} \tag{3.20}$$

Note that the relations (3.20) express the old momenta and the new coordinates as functions of the new momenta and old coordinates. When the relations (3.20) are solved so as to express new variables strictly in terms of old variables, as in (3.11), or <u>vice versa</u>, then the result is always a canonical

transformation.

We give here a very simple example of a mixed variable generating function, namely

$$S(\underset{\sim}{q},\underset{\sim}{p}') = \underset{\sim}{q}\cdot\underset{\sim}{p}' \tag{3.21}$$

It is trivial to show that this function generates the identity transformation.

If the canonical transformation generated by (3.20) is time-dependent, it is possible to express the new Hamiltonian $K(\underset{\sim}{q}',\underset{\sim}{p}',t)$ in terms of the old Hamiltonian $H(\underset{\sim}{q},\underset{\sim}{p},t)$ and the generating function S. The relation is

$$K(\underset{\sim}{q}',\underset{\sim}{p}',t) = H(\underset{\sim}{q},\underset{\sim}{p},t) + \frac{\partial}{\partial t} S(\underset{\sim}{q},\underset{\sim}{p}',t) \tag{3.22}$$

Note that old and new variables are mixed throughout this expression. This formula generalizes (3.19) to the case of time-dependent transformations.

We have called the function S appearing in (3.20) a "mixed variable" generating function, because it mixes old and new variables. This terminology is not standard, but is used here to distinguish this type of generating functions from Lie generating functions, to which we devote a later section of this paper.

We turn now to a discussion of Hamilton-Jacobi theory.[12] In this paper it will never be necessary to solve the Hamilton-Jacobi equation, because the required solutions will either be obvious from inspection or else they will be standard and well-known. Nevertheless, from the standpoint of understanding the basic principles involved in our presentation of perturbation theory, Hamilton-Jacobi theory is very helpful. Therefore the following material, if not already familiar, can be regarded as primarily of enrichment value.

In section 2 we discussed the idea that a system of differential equations could be solved by finding a coordinate transformation, such as (2.8) or (2.9), in which the new coordinates are all constants in time. In the context of Hamiltonian mechanics the same idea can be employed, although now the coordinate transformation must be a canonical transformation. It is in fact always possible, at least formally, to find a canonical transformation $(\underset{\sim}{q},\underset{\sim}{p}) \to (\underset{\sim}{q}',\underset{\sim}{p}')$ in which the old variables evolve according to some given Hamiltonian $H(\underset{\sim}{q},\underset{\sim}{p},t)$ and in which the new variables are all constants. The mixed variable generating function $S(\underset{\sim}{q},\underset{\sim}{p}',t)$ for this canonical transformation satisfies a certain partial differential equation, the Hamilton-Jacobi equation:

$$H\left(\underset{\sim}{q}, \frac{\partial S}{\partial \underset{\sim}{q}}, t\right) + \frac{\partial S}{\partial t} = 0 \tag{3.23}$$

The canonical transformation generated by S gives, for the new Hamiltonian K,

$$K(\underset{\sim}{q}', \underset{\sim}{p}', t) = 0 \tag{3.24}$$

From this it follows that the new variables $(\underset{\sim}{q}',\underset{\sim}{p}')$ are all constants in time. The generating function S which satisfies (3.23) is called "Hamilton's Principal Function".

In the case of Hamiltonians $H(\underset{\sim}{q},\underset{\sim}{p})$ which are independent of time there is a slight modification of the procedure outlined above which is often useful. Instead of seeking a transformation $(\underset{\sim}{q},\underset{\sim}{p}) \to (\underset{\sim}{q}',\underset{\sim}{p}')$ such that the new Hamiltonian K vanishes, one seeks a transformation such that the new Hamiltonian K depends only on the new generalized momenta, and is independent of the new generalized coordinates:

$$K = K(\underset{\sim}{p}') \tag{3.25}$$

This form for K ensures that the new generalized momenta $\underset{\sim}{p}'$ are constants of the motion, and that the new generalized coordinates $\underset{\sim}{q}'$ evolve linearly in time:

$$\underset{\sim}{q}'(t) = \frac{\partial K}{\partial \underset{\sim}{p}'} t + \underset{\sim}{q}'(0) \tag{3.26}$$

The generating function $W(\underset{\sim}{q},\underset{\sim}{p}')$ for this transformation is called "Hamilton's Characteristic Function", and it satisfies

$$H\left(\underset{\sim}{q}, \frac{\partial W}{\partial \underset{\sim}{q}}\right) = K(\underset{\sim}{p}') \tag{3.27}$$

The relationship between (3.27) and (3.23) is very similar to the relationship between the time-independent and time-dependent Schrödinger equations, respectively. For this reason we will call (3.27) the time-independent Hamilton-Jacobi equation, although this terminology seems not to be standard.

Since the new momenta $\underset{\sim}{p}'$ are constants of the motion, any functions of the $\underset{\sim}{p}'$ will also be constants. Therefore there is great arbitrariness in the choice of the $\underset{\sim}{p}'$, since any invertible functions $\underset{\sim}{p}'' = \underset{\sim}{p}''(\underset{\sim}{p}')$ can serve equally well as new momenta. This arbitrariness is reflected in the fact that the functional form of the new Hamiltonian $K(\underset{\sim}{p}')$ in (3.27) is unspecified. One can, in fact, choose this functional form virtually at will. One possible choice is to let K be equal to one of the new momenta, say p_1'.

For periodic or multiply periodic systems, however, it is common to choose the new momenta $\underset{\sim}{p}'$ to be the so-called action variables $\underset{\sim}{J}$. The action variables are defined by

$$J_i = \frac{1}{2\pi} \oint p_i \, dq_i \tag{3.28}$$

where the (q_i, p_i) are one pair of original coordinates in $H(\underset{\sim}{q}, \underset{\sim}{p})$. In order that the J_i given by (3.28) be constants of the motion, it is necessary that the Hamilton-Jacobi equation (3.27) be separable in the coordinates $(\underset{\sim}{q}, \underset{\sim}{p})$. In practice, this does not constitute a restriction on the use of action variables $\underset{\sim}{J}$ as new momenta, because the Hamilton-Jacobi equation is only solvable in the case that it is separable. Since the new momenta are specified by (3.28), the functional form of $K = K(\underset{\sim}{J})$ will also be specified. This specification will be unique unless there is more than one set of coordinates $(\underset{\sim}{q}, \underset{\sim}{p})$ in which the Hamilton-Jacobi equation is separable.

The new generalized coordinates $\underset{\sim}{q}'$ which are conjugate to $\underset{\sim}{J}$ are called angle variables, and are denoted by $\underset{\sim}{\theta}$. Thus the coordinate transformation generated by $W(\underset{\sim}{q}, \underset{\sim}{J})$, the solution to (3.27), takes the form $(\underset{\sim}{q}, \underset{\sim}{p}) \rightarrow (\underset{\sim}{\theta}, \underset{\sim}{J})$. The new variables are colledtively called "action-angle variables".

We will now give, without a detailed derivation, the action-angle transformation for the harmonic oscillator. This is done partly to illustrate some features of Hamilton-Jacobi theory, and partly because the harmonic oscillator will enter into examples later on. We begin with the harmonic oscillator Hamiltonian in the form

$$H(q,p) = \frac{1}{2}(p^2 + \omega^2 q^2) \tag{3.29}$$

The action variable J for this system is

$$J = \frac{1}{2\pi} \oint p\,dq = \frac{1}{2\omega}(p^2 + \omega^2 q^2) = \frac{H(q,p)}{\omega} \tag{3.30}$$

Hence, the new Hamiltonian has the form

$$K = \omega J \tag{3.31}$$

Then, the time-independent Hamilton-Jacobi equation for the generating function W(q,J) reads as follows:

$$\frac{1}{2}\left[\omega^2 q^2 + \left(\frac{\partial W}{\partial q}\right)^2\right] = \omega J \tag{3.32}$$

Finally, the solution W to this equation yields the following canonical transformation, the action-angle transformation:

$$\left.\begin{aligned} q &= \sqrt{\frac{2J}{\omega}}\ \sin\theta \\ p &= \sqrt{2\omega J}\ \cos\theta \end{aligned}\right\} \tag{3.33}$$

Evidently, solving the Hamilton-Jacobi equation (3.23) or its time-independent form (3.27) is equivalent to solving the original set of equations, (3.2). In practice, however, the Hamilton-Jacobi equation can be solved only in those cases where the original system (3.2) can be solved. Nevertheless, this does not mean that the Hamilton-Jacobi equation is useless, as will be shown in later sections.

4. An Overview of Non-Hamiltonian Perturbation Theory

There are very few dynamical systems in classical mechanics which can be solved in closed form in terms of well-known functions. Therefore for most problems it is necessary to develop the solution as some kind of infinite series, of which several types will be investigated here.

In this section we will discuss systems of ordinary differential equations without reference to Hamiltonian mechanics. Although the thrust of this paper is directed at Hamiltonian systems, there are several reasons to include the more general case in the discussion. First, there are many examples in the literature of perturbation methods applied to systems of differential equations, without using any Hamiltonian formalism. Often these systems are, in fact, derivable from a Hamiltonian, i.e. they represent Hamiltonian flows in phase space, but the authors have simply chosen not to use Hamiltonian methods. And sometimes the equations cannot be derived from a Hamiltonian. Second, a treatment of general systems helps clarify some of the steps taken in Hamiltonian systems, such as the introduction of action-angle variables. And third, a general system of differential equations is, after all, more general than the special case of Hamiltonian systems.

We begin this section with a discussion of infinite series developed in powers of time, and point out the drawbacks of such a development. Then we turn to power series in a small parameter ε, describing an expansion about a solvable problem. We discuss at length the desirability of subjecting systems of differential equations to a preparatory transformation, analogous to an action-angle transformation in Hamiltonian mechanics, before

performing any perturbation expansions. This transformation is illustrated by the example of the pendulum. Next we describe the method of successive approximations, and actually carry it out for the pendulum system. We discuss in detail a short-cut through the method of successive approximations, called the method of averaging, which is frequently used in practice. Finally, we discuss secular terms and their significance.

Let us consider solving a set of differential equations by developing a power series in time. We begin with (2.5), which we reproduce here:

$$\dot{z}_i = F_i(\underset{\sim}{z}, t) \tag{4.1}$$

This equation can be differentiated with respect to time, and by substituting (4.1) into the result, we can obtain $\ddot{\underset{\sim}{z}}$ as a function of $\underset{\sim}{z}$ and t only:

$$\begin{aligned} \ddot{z}_i &= \frac{\partial F_i}{\partial t} + \sum_{j=1}^{D} \dot{z}_j \frac{\partial F_i}{\partial z_j} \\ &= \frac{\partial F_i}{\partial t} + \sum_{j=1}^{D} F_j \frac{\partial F_i}{\partial z_j} \end{aligned} \tag{4.2}$$

Repeating this process, the third derivative $\dddot{\underset{\sim}{z}}$ can similarly be expressed as a function of $\underset{\sim}{z}$ and t only:

$$\begin{aligned} \dddot{z}_i = \frac{\partial^2 F_i}{\partial t^2} &+ \sum_{j=1}^{D} \left(\frac{\partial F_j}{\partial t} \frac{\partial F_i}{\partial z_j} + 2 F_j \frac{\partial^2 F_i}{\partial z_j \partial t} \right) \\ &+ \sum_{\substack{j,k \\ =1}}^{D} \left(F_k \frac{\partial F_j}{\partial z_k} \frac{\partial F_i}{\partial z_j} + F_j F_k \frac{\partial^2 F_i}{\partial z_j \partial z_k} \right) \end{aligned} \tag{4.3}$$

Clearly, this process can be continued to any order, and hence the derivatives $d^n\underset{\sim}{z}/dt^n$ for all n can be expressed as functions of $\underset{\sim}{z}$ and t.

If we are now given some initial conditions, say $\underset{\sim}{z} = \underset{\sim}{z}_0$ at $t = t_0$, then equations (4.1) to (4.3) and their generalizations allow us to compute $\dot{\underset{\sim}{z}}(t_0)$, $\ddot{\underset{\sim}{z}}(t_0)$, etc., and hence to develop $\underset{\sim}{z}(t)$ in powers of $t-t_0$:

$$\underset{\sim}{z}(t) = \underset{\sim}{z}(t_0) + (t-t_0)\,\dot{\underset{\sim}{z}}(t_0) + \frac{(t-t_0)^2}{2!}\,\ddot{\underset{\sim}{z}}(t_0) + \cdots \tag{4.4}$$

Thus we have a solution of the original set of differential equations (4.1) for some time interval centered around $t = t_0$.

In practice, the solution (4.4) is not completely useless, but it is a last resort. Even in cases where (4.4) has a large circle of convergence, its practical computational value is almost always restricted to very short time intervals. It is possible to use (4.4) and a large number of short time intervals to span a large time interval, and this is in fact what is done, with various modifications in the name of efficiency, in almost every algorithm for the numerical integration of differential equations. But the fact remains that developments such as (4.4) are best suited for the production of tables of numbers, and not for gaining analytic insight into the true solution.

In theoretical applications, power series developments such as (4.4) are sometimes very useful. For example, if a power series converges on some interval, then it uniquely defines an analytic function. Thus power series are useful in existence and uniqueness proofs. In this paper, we will use an expansion almost identical to (4.4) in our development of direct canonical transformations, and it is for this reason that we have discussed series

solutions of this type.

For many physical systems it is possible to develop other forms of infinite expansions which offer great improvements over the form (4.4). These are physical systems which are "close", in some sense, to a system which is solvable in closed form. The differential equations representing such systems will generally have the form

$$\dot{\underset{\sim}{z}} = \underset{\sim}{F}(\underset{\sim}{z},t,\varepsilon) \tag{4.5}$$

where ε is a small parameter, and where the system

$$\dot{\underset{\sim}{z}} = \underset{\sim}{F}(\underset{\sim}{z},t,0) \tag{4.6}$$

is solvable. Systems which cannot be put into the form (4.5) are usually relegated to numerical study.

For the remainder of this section we will restrict the form (4.5) in several important ways. First, we assume that the flow functions $\underset{\sim}{F}$ are independent of time, i.e. that the system of differential equations is autonomous. Next, we make the mild assumption that $\underset{\sim}{F}$ can be expanded in a power series in ε, which we write as follows:

$$\dot{\underset{\sim}{z}} = \underset{\sim}{F}(\underset{\sim}{z},\epsilon) = \underset{\sim}{F}_0(\underset{\sim}{z}) + \epsilon\,\underset{\sim}{F}_1(\underset{\sim}{z}) + \epsilon^2\,\underset{\sim}{F}_2(\underset{\sim}{z}) + \dots \tag{4.7}$$

The term $\underset{\sim}{F}_0$ taken alone generates the unperturbed trajectories, for which we assume the solution is known. Finally, we assume that the unperturbed motion is periodic. This is the most important assumption we make.

We impose these restrictions because our main purpose in discussing non-Hamiltonian perturbation theory is illustrative. In spite of these restrictions, however, the class of systems we shall study in the remainder

of this section is very common in practice, and many important features of perturbation theory are illustrated by it. Certain generalizations, such as to systems whose unperturbed motion is multiply periodic (e.g. the solar system), are relatively easy to effect. For these we refer the reader to the literature.[14]

It is useful to form a geometrical picture, due to Kruskal,[13] of the class of systems we shall be studying. We denote the dimensionality of phase space by D, so that $\underset{\sim}{z}$ is a D-vector. Since we are assuming that the unperturbed motion is periodic, the unperturbed trajectories will be closed loops, one of which passes through every point of phase space. It is easy to see that it will take D-1 quantities to specify an unperturbed loop, and one quantity to specify a point on a particular loop. The latter quantity can be chosen to be an angle-like variable with period 2π; this quantity evolves monotonically in time under the action of the unperturbed system. The D-1 quantities which identify a particular loop are all constants of the unperturbed motion. We do not assume that the motion around the loops is uniform, in any sense, or that the period of the motion is the same from one loop to another.

When carrying out a perturbation expansion it is best to use a set of coordinates which is "natural" to the unperturbed system. For the class of systems we are considering here, the natural set of coordinates is descriptive in a rather obvious way of the unperturbed loops. We denote some choice of the D-1 quantities which identify the unperturbed loops by $\underset{\sim}{y}$, which is a (D-1)-vector. In addition, we denote the angle-like variable specifying a position on a particular loop by θ. Altogether, the unperturbed loops allow us to define a certain coordinate transformation, $\underset{\sim}{z} \rightarrow (\underset{\sim}{y},\theta)$, which prepares the system of differential equations for a perturbation analysis. We will call this transformation the "preparatory transformation"; in

Hamiltonian mechanics, its analog is the action-angle transformation for the unperturbed system.

When the preparatory transformation is applied to the system (4.7), the equations of motion take on the following form:*

$$\left.\begin{aligned} \dot{\underset{\sim}{y}} &= \epsilon\, \underset{\sim}{G}_1(\underset{\sim}{y},\theta) + \epsilon^2\, \underset{\sim}{G}_2(\underset{\sim}{y},\theta) + \dots \\ \dot{\theta} &= \Phi_0(\underset{\sim}{y}) + \epsilon\, \Phi_1(\underset{\sim}{y},\theta) + \epsilon^2\, \Phi_2(\underset{\sim}{y},\theta) + \dots \end{aligned}\right\} \qquad (4.8)$$

Here the functions $\underset{\sim}{G}_1$, $\underset{\sim}{G}_2$, etc., are (D-1)-vectors. Note that there is no term $\underset{\sim}{G}_0$, since the D-1 quantities $\underset{\sim}{y}$ are all constants of the unperturbed motion. In terms of the variables $(\underset{\sim}{y},\theta)$, the unperturbed motion consists of an evolution in θ only. Later we shall give an example of the preparatory transformation; for the time being we simply note that it can be obtained in closed form, since the unperturbed system is assumed to be solvable.

Now we consider, on general topological grounds, the effects of the perturbing terms $\underset{\sim}{G}_1$, Φ_1, etc., in (4.8). Generally, there are two possibilities. It may happen that the perturbing terms will distort and change the frequency of the unperturbed loops, but will not break them. That is , it may happen that the true perturbed motion is periodic like the unperturbed motion. This is shown schematically as Case A in Fig. 2. Alternatively, the perturbing terms may break the loops, converting them into helices. In this case one has "drifts", since one can consider the true, perturbed motion as consisting of a slow drift of the unperturbed loops through phase space. This case is shown as case B in Fig. 2.

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*In general, the term in Φ_0 will depend on θ as well as $\underset{\sim}{y}$, but this dependence can always be transformed away. See Ref. 13.

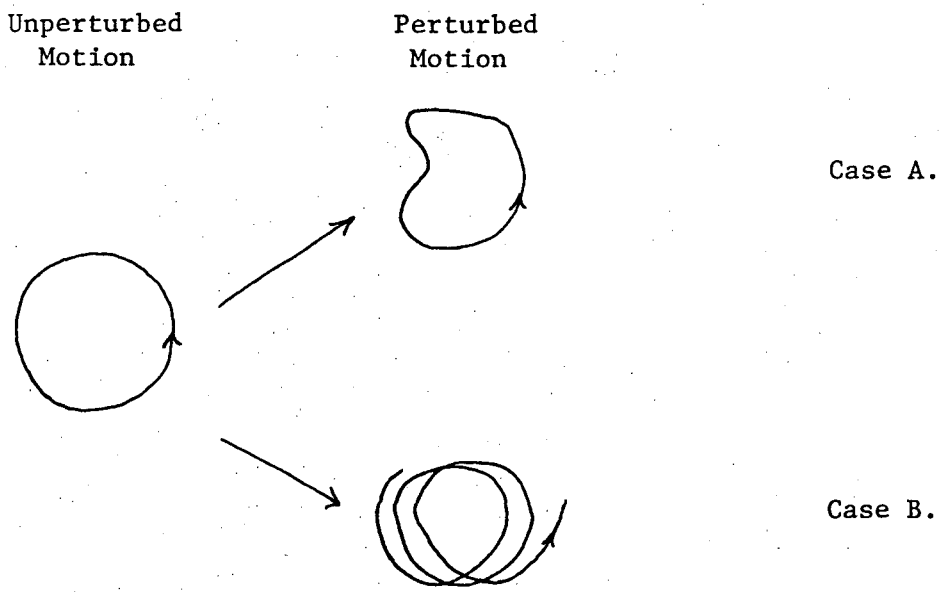

FIG. 2. THE EFFECTS OF PERTURBATIONS ON PERIODIC MOTION.

Let us now take an example of a system of the type described above and subject it to a preparatory transformation of the form $\underset{\sim}{z} \rightarrow (\underset{\sim}{y}, \theta)$. We choose for our example the pendulum, first, because it is a simple example of a non-linear oscillator, and second, because it has remarkably wide applications.

We set up the pendulum problem as follows. Fig. 3 defines the variable x, which is the angle the pendulum shaft, assumed to be massless, makes with its lower equilibrium position. Letting m, R and g represent the mass of the pendulum bob, the length of the shaft and the acceleration of gravity, respectively, we can immediately write down the kinetic and potential energies of the system:

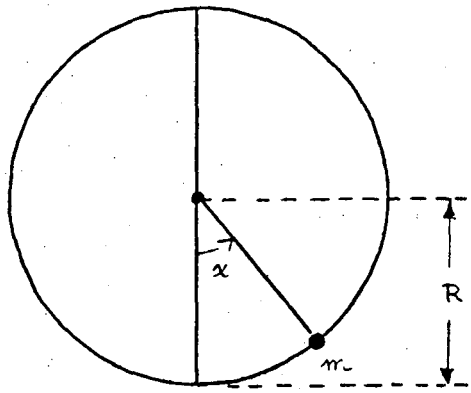

FIG. 3. PENDULUM VARIABLES.

$$\left.\begin{aligned} T &= \tfrac{1}{2} m R^2 \dot{x}^2 \\ V(x) &= mgR(1-\cos x) \end{aligned}\right\} \tag{4.9}$$

By using, for example, the Euler-Lagrange equations, we get for the equation of motion

$$\ddot{x} = -\omega_0^2 \sin x \tag{4.10}$$

where

$$\omega_0 = \sqrt{\frac{g}{R}} \tag{4.11}$$

is the frequency of small oscillations.

Equation (4.10) can be brought into the form (4.7) as follows.

First we define $v = \dot{x}$, in order to transform (4.10) into a coupled set of first order differential equations:

$$\left.\begin{aligned} \dot{x} &= v \\ \dot{v} &= -\omega_0^2 \sin x \end{aligned}\right\} \tag{4.12}$$

Next, we choose to consider only small oscillations, and to treat the effects of finite amplitude as a perturbation. (We exclude the case of amplitudes which are so large that the pendulum swings over the top.) To do this, we consider x to be a small quantity, and expand out the sin function in powers of x:

$$\left.\begin{aligned} \dot{x} &= v \\ \dot{v} &= -\omega_0^2 \left(x - \tfrac{1}{6} x^3 + \tfrac{1}{120} x^5 - \dots \right) \end{aligned}\right\} \tag{4.13}$$

Finally, we artificially introduce a parameter ε into (4.13), in order to remind ourselves which quantities are to be considered small. We do this in the following way:

$$\left.\begin{aligned} \dot{x} &= v \\ \dot{v} &= -\omega_0^2 x + \frac{\varepsilon}{6} \omega_0^2 x^3 - \frac{\varepsilon^2}{120} \omega_0^2 x^5 + \dots \end{aligned}\right\} \tag{4.14}$$

Evidently, every power of ε corresponds to two powers of x, i.e. $\varepsilon = O(x^2)$. Since ε is just a formal device for keeping track of the relative magnitude of terms, it can be set to unity at the completion of a perturbation expansion. Such an artificial introduction of a smallness parameter is common in perturbation theory.

The system (4.14) is now in the form indicated by (4.7). The vector $\underset{\sim}{z}$

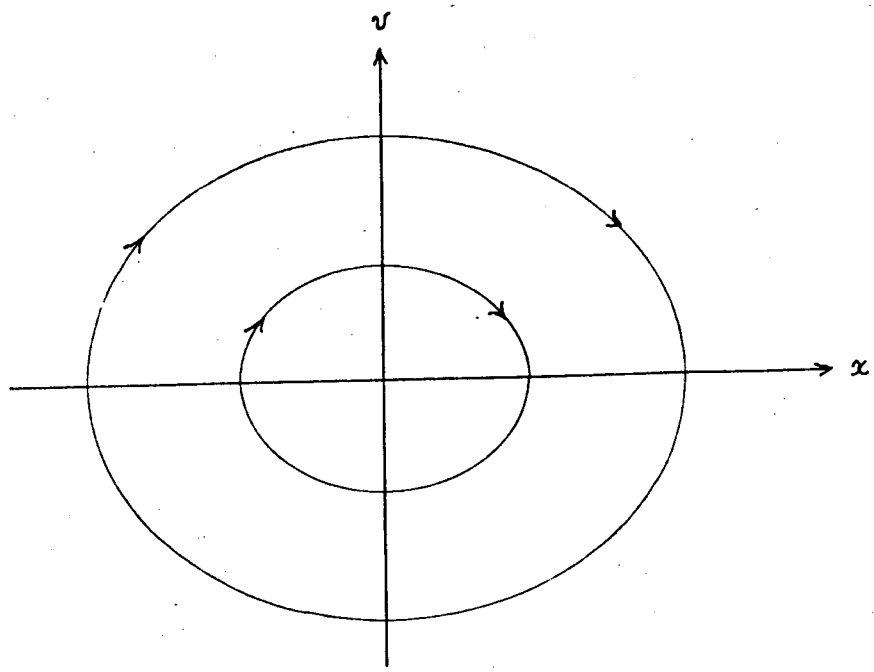

FIG. 4. UNPERTURBED TRAJECTORIES FOR SYSTEM (4.14).

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corresponds to the components (x,v); phase space is 2-dimensional. We next want to consider the transformation of the system (4.14)into the form indicated by (4.8). To do this, we first require a proof that the unperturbed system is periodic.

This proof is easy. The unperturbed system is a harmonic oscillator:

$$\left.\begin{aligned} \dot{x} &= v \\ \dot{v} &= -\omega_0^2 x \end{aligned}\right\} \tag{4.15}$$

The general solution to this is

$$\left.\begin{aligned} x &= A \sin(\omega_0 t + \phi) \\ v &= \omega_0 A \cos(\omega_0 t + \phi) \end{aligned}\right\} \tag{4.16}$$

where A (the amplitude) and ϕ (the initial phase) are constants of integration. The unperturbed motion is certainly periodic, and the loops in phase space

which represent the unperturbed trajectories are ellipses centered about the origin, as shown in Fig. 4. A given trajectory in phase space, i.e. a given ellipse, is specified by the quantity A, and the quantity $\omega_0 t+\phi$ specifies the location of a phase point on that trajectory.

We now consider the transformation $\underset{\sim}{z} = (x,v) \rightarrow (\underset{\sim}{y},\theta)$. Since $\underset{\sim}{z}$ is 2-dimensional, the vector $\underset{\sim}{y}$ will be 1-dimensional, i.e. a scalar. According to the discussion above, the quantity y must specify the unperturbed loop, and θ must specify the position along that loop. From the solution developed for the unperturbed system in the previous paragraph, it should be more than evident that we want to identify y with the amplitude* A and θ with the quantity $\omega_0 t+\phi_0$. Accordingly, we take as our transformation $(x,v) \rightarrow (A,\theta)$ the following:

$$\left.\begin{aligned} x &= A \sin\theta \\ v &= A\omega_0 \cos\theta \end{aligned}\right\} \tag{4.17}$$

When this is substituted into (4.14) there results the following system:

$$\left.\begin{aligned} \dot{A} &= \frac{\epsilon}{6}\omega_0^2 A^3 \sin^3\theta\cos\theta - \frac{\epsilon^2}{120}\omega_0^2 A^5 \sin^5\theta\cos\theta + \cdots && (4.18a) \\ \dot{\theta} &= \omega_0 - \frac{\epsilon}{6}\omega_0 A^2 \sin^4\theta + \frac{\epsilon^2}{120}\omega_0 A^4 \sin^6\theta - \cdots && (4.18b) \end{aligned}\right\}$$

Clearly, (4.18) is in the form indicated by (4.8), as required.

Let us now consider an actual perturbative solution to a system such as (4.8). In so doing, it is not our purpose to present a complete perturbation theory, free of pitfalls, for periodic systems of differential equations. Such theories exist; they are associated especially with the names Krylov, Bogoliubov,[15] Mitropolski,[16] and Kruskal.[13] Instead, we want to develop a rather naive perturbation method, which will illustrate certain typical qualitative results

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*Actually, any function of the amplitude A would serve equally well. C.f. the action-angle transformation, (3.33), where the action $J = \omega A^2/2$.

and give us a quantitative basis with which to compare further work. We will begin with the specific example of the pendulum.

Let us return to (4.18), where we left the pendulum problem. It simplifies later work to expand the trigonometric functions appearing there in terms of multiple angles, i.e. a Fourier series, and having done so we obtain

$$\dot{A} = \frac{\epsilon}{48}\omega_0^2 A^3\left(2\sin 2\theta - \sin 4\theta\right) - \frac{\epsilon^2}{3840}\omega_0^2 A^5\left(5\sin 2\theta - 4\sin 4\theta + \sin 6\theta\right) + O(\epsilon^3) \tag{4.19a}$$

$$\dot{\theta} = \omega_0 - \frac{\epsilon}{48}\omega_0 A^2\left(3 - 4\cos 2\theta + \cos 4\theta\right) + \frac{\epsilon^2}{3840}\omega_0 A^4\left(10 - 15\cos 2\theta + 6\cos 4\theta - \cos 6\theta\right) + O(\epsilon^3) \tag{4.19b}$$

It will be observed that the $O(\varepsilon^2)$ terms are complicated. For the time being we will focus our attention only on the terms through $O(\varepsilon)$, and the $O(\varepsilon^2)$ terms will simply be included for later reference.

The system (4.19) possesses a solution $A(t)$, $\theta(t)$, which we seek as a power series expansion in ε. To do this we posit the following ansatz:

$$\left.\begin{aligned} A(t) &= A_0(t) + \epsilon A_1(t) + \epsilon^2 A_2(t) + \dots \\ \theta(t) &= \theta_0(t) + \epsilon\theta_1(t) + \epsilon^2\theta_2(t) + \dots \end{aligned}\right\} \tag{4.20}$$

The subscripts on the right hand side of (4.20) represent the order of the terms. Note in particular that the symbols A_0 and θ_0 are meant to represent functions of time, and not initial conditions. The expressions (4.20) are to be substituted into (4.19), all functions of (A,θ) are to be expanded out as power series in ε, and then terms are collected, order by order. When this is done, there results, first at order zero, the following set:

$$\left.\begin{aligned} \dot{A}_0 &= 0 \\ \dot{\theta}_0 &= \omega_0 \end{aligned}\right\} \tag{4.21a}$$

At order one:*

$$\left.\begin{aligned} \dot{A}_1 &= \frac{1}{48}\,\omega_0^2 A_0^3 \left(2\sin 2\theta_0 - \sin 4\theta_0\right) \\ \dot{\theta}_1 &= -\frac{1}{48}\,\omega_0 A_0^2 \left(3 - 4\cos 2\theta_0 + \cos 4\theta_0\right) \end{aligned}\right\} \tag{4.21b}$$

And at order two:

$$\dot{A}_2 = \frac{1}{48}\,\omega_0^2 \left[3A_0^2 A_1 \left(2\sin 2\theta_0 - \sin 4\theta_0\right) + 4A_0^3\theta_1 \left(\cos 2\theta_0 - \cos 4\theta_0\right)\right]$$

$$-\frac{1}{3840}\,\omega_0^4 A_0^5 \left(5\sin 2\theta_0 - 4\sin 4\theta_0 + \sin 6\theta_0\right)$$

$$\dot{\theta}_2 = -\frac{1}{48}\,\omega_0 \left[2A_0 A_1 \left(3 - 4\cos 2\theta_0 + \cos 4\theta_0\right) + 4A_0^2\theta_1 \left(2\sin 2\theta_0 - \sin 4\theta_0\right)\right]$$

$$+\frac{1}{3840}\,\omega_0 A_0^4 \left(10 - 15\cos 2\theta_0 + 6\cos 4\theta_0 - \cos 6\theta_0\right) \tag{4.21c}$$

Note that the system (4.21) forms a hierarchy, in which the derivatives of (A_n, θ_n) at any order are expressed purely in terms of (A_n, θ_n) at lower orders. Thus it is possible to solve for the functions (A_n, θ_n) order by order, in an iterative process.

Let us carry out this solution through first order. At order zero we have

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*In this paper "order zero" will mean the term in ε^0, i.e. the term which is $O(1)$. Likewise, "order one" will mean $O(\varepsilon^1)$, etc.

$$\left.\begin{aligned} A_0(t) &= C_0 \qquad (4.22a)\\ \theta_0(t) &= \omega_0 t + \phi_0 \qquad (4.22b)\end{aligned}\right\}$$

where C_0 and ϕ_0 are constants of integration. Of course, this solution is that of the unperturbed system, the simple harmonic oscillator. We now substitute (4.22) into (4.21b) to get

$$\left.\begin{aligned} \dot{A}_1 &= \frac{\omega_0^2}{48} C_0^3 \left[2 \sin 2(\omega_0 t + \phi_0) - \sin 4(\omega_0 t + \phi_0)\right]\\ \dot{\theta}_1 &= -\frac{\omega_0}{48} C_0^2 \left[3 - 4\cos 2(\omega_0 t + \phi_0) + \cos 4(\omega_0 t + \phi_0)\right]\end{aligned}\right\} \qquad (4.23)$$

These can be immediately integrated to give

$$\left.\begin{aligned} A_1(t) &= C_1 + \frac{\omega_0 C_0^3}{192}\left[-4\cos 2(\omega_0 t + \phi_0) + \cos 4(\omega_0 t + \phi_0)\right]\\ \theta_1(t) &= \phi_1 - \frac{C_0^2}{192}\left[12\omega_0 t - 8\sin 2(\omega_0 t + \phi_0) + \sin 4(\omega_0 t + \phi_0)\right]\end{aligned}\right\} \qquad (4.24)$$

where C_1 and ϕ_1 are new constants of integration.* Evidently, this process can be carried to any order; for example, to get the second order solutions, we would substitute (4.24) and (4.22) into (4.21c) and then integrate. Due to the substitution of lower order solutions into higher order equations, the procedure outlined here is sometimes called "the method of successive approximations."

We have in equations (4.24) a quantitative expression of the first order effects of finite amplitude in the pendulum. Let us examine these equations

*It can be shown that all the constants which appear in this order-by-order integration are dependent on only two constants, as required by the original system (4.19).

to see what they imply physically.

First we look at the expression for A_1. The term C_1 will combine with the term C_0 in (4.22a)to give $C_0+\varepsilon C_1$, which we may call C', another constant. The only other terms in (4.24a) are oscillatory in time. Therefore, through first order, we can write, for the time evolution of the quantity A,

$$A(t) = C' + \varepsilon(\text{oscillatory terms}) + O(\varepsilon^2) \tag{4.25}$$

We see that the effect of the perturbation on the quantity A, which is a constant of the unperturbed motion, is simply to introduce small amplitude oscillations, and that the time average of the amplitude A is a constant even in the presence of the perturbation. This tells us that the pendulum system is of the type called Case A in Fig. 2.

Actually, on physical grounds, we can expect the pendulum to be of the Case A type, without doing any mathematics. Even for finite amplitudes, the pendulum system is periodic, because it swings between two turning points. This means that the true trajectories in phase space must be closed loops, and hence the quantity A, which is defined in terms of the unperturbed loops, can never deviate very far from its unperturbed value. In particular, the true trajectories cannot be inward or outward going spirals, nor can they be loops which drift off.

In fact, the periodicity of the pendulum system, even for finite amplitudes, is a reflection of the fact that there is a time-independent constant of the true motion, whose contours are the true trajectories in phase space. This constant is, of course, the energy, and it would appear naturally in a Hamiltonian formulation of the pendulum problem. For the time being we are deliberately ignoring Hamiltonian mechanics, and as a result we have "missed"

the energy constant.

We can, however, imagine a slight modification to the pendulum problem for which no energy constant would exist, and for which Hamiltonian mechanics would be useless. Suppose that the pendulum experienced a small frictional force, so that the swings were gradually slowing down. If we were to treat the frictional force as an additional perturbation, we would find that there would be another term in the expression for A(t), (4.25), which would represent a monotonic decrease in the amplitude. The trajectories in phase space of the true motion would be spirals slowly winding toward the origin, and we would have an example of the type of system called Case B in Fig. 2.

Next, let us look at (4.24b), the equation for $\theta_1(t)$, and interpret it. The constant ϕ_1 can be combined with the constant ϕ_0 to give a new constant $\phi' = \phi_0 + \epsilon\phi_1$, just as was done for the constants C_0 and C_1. In addition to the term ϕ_1, there are oscillatory terms, similar to those in the expression for A_1. Finally, there is a term which is linear in time. Altogether, we can write for the time evolution of θ,

$$\theta(t) = \phi' + \omega_0\left(1 - \frac{\epsilon C_0^2}{16}\right)t + \epsilon\left(\text{oscillatory terms}\right) + O(\epsilon^2) \qquad (4.26)$$

The effects of the perturbation on the quantity θ are thus twofold. First, there are small amplitude oscillations which are introduced; their time average vanishes, and for the long-term qualitative behaviour of the system they are unimportant. Second, the angle θ no longer evolves, even on the average, at the frequency ω_0, but at a slightly reduced frequency, given by

$$\omega = \omega_0 \left(1 - \epsilon \frac{C_0^2}{16} \right) + O(\epsilon^2) \tag{4.27}$$

By referring to (4.22a), we see that the true frequency ω is dependent on the amplitude A, and that large amplitude oscillations are slower than small ones:

$$\omega = \omega_0 \left(1 - \epsilon \frac{A^2}{16} \right) + O(\epsilon^2) \tag{4.28}$$

A frequency shift of this type is often an important qualitative effect; for example, it implies phase mixing in an ensemble of systems.

We have not meant to be cavalier in our dismissal of the oscillatory terms in (4.24). Certainly, if one wants to find the position of the system at a particular moment in time, these terms cannot be ignored. But for many problems, one is not interested in oscillatory terms, but rather only in the long-term behaviour of the system, such as frequency shifts or drifts of loops in phase space. The problem of the adiabatic motion of a charged particle (the guiding center problem) provides a good physical picture of this point of view. Typically, one does not care about all the "little wiggles" in the particle's motion, but only about where the particle will drift to after some long period of time.

In such cases, there is a shortcut through the method of successive approximations, as we have developed it for the pendulum problem, which leads directly to the long-term behaviour of a system and bypasses all the oscillatory terms, as well as most of the algebra. This shortcut is called "the method of averaging", and it is described here because of its great intuitive appeal and because of its frequent occurrence in the literature.

To illustrate the method of averaging, we return to the set (4.19), and

look only at the terms through $O(\varepsilon)$. The prescription we follow is to take the $O(\varepsilon)$ expressions and simply throw away all oscillatory terms. The result is

$$\left.\begin{aligned} \dot{A} &= 0 \\ \dot{\theta} &= \omega_0\left(1 - \epsilon\frac{A^2}{16}\right) \end{aligned}\right\} \tag{4.29}$$

These equations contain all the essentials of the long-term behaviour of the pendulum system, which we discussed above, but they omit the oscillatory terms.

Let us now look at the method of averaging in the context of the general system (4.8). We ignore the terms of second and higher order, and focus only on the first order terms, $\underset{\sim}{G}_1(\underset{\sim}{y},\theta)$ and $\Phi_1(\underset{\sim}{y},\theta)$. As we did with the pendulum problem, we expand the perturbing terms $\underset{\sim}{G}_1$ and Φ_1 in a Fourier series in θ, which we may express as follows:

$$\left.\begin{aligned} \underset{\sim}{G}_1(\underset{\sim}{y},\theta) &= \sum_{n=-\infty}^{+\infty} \underset{\sim}{G}_{1n}(\underset{\sim}{y})\, e^{in\theta} \\ \Phi_1(\underset{\sim}{y},\theta) &= \sum_{n=-\infty}^{+\infty} \Phi_{1n}(\underset{\sim}{y})\, e^{in\theta} \end{aligned}\right\} \tag{4.30}$$

Then the averaging procedure is effected by throwing away all the terms in the series (4.30) except the ones corresponding to $n = 0$. The result will be

$$\left.\begin{aligned} \dot{\underset{\sim}{y}} &= \epsilon\, \underset{\sim}{G}_{10}(\underset{\sim}{y}) \\ \dot{\theta} &= \Phi_0(\underset{\sim}{y}) + \epsilon\, \Phi_{10}(\underset{\sim}{y}) \end{aligned}\right\} \tag{4.31}$$

We call (4.31) "the averaged equations".

Clearly, in order to apply the averaging procedure it is not necessary to compute the Fourier coefficients $\underset{\sim}{G}_{1n}(\underset{\sim}{y})$, $\Phi_{1n}(\underset{\sim}{y})$ for $n \neq 0$; only the $n=0$ coefficients are needed. These coefficients are given by

$$\left.\begin{aligned} \underset{\sim}{G}_{10}(\underset{\sim}{y}) &= \frac{1}{2\pi}\int_0^{2\pi} \underset{\sim}{G}_1(\underset{\sim}{y},\theta)\,d\theta \\ \Phi_{10}(\underset{\sim}{y}) &= \frac{1}{2\pi}\int_0^{2\pi} \Phi_1(\underset{\sim}{y},\theta)\,d\theta \end{aligned}\right\} \tag{4.32}$$

It is evident that the left hand sides of these equations are the average with respect to θ of the perturbing terms, and it is due to this circumstance that the method of averaging derives its name.

The averaging operation, which is equivalent to the selection of the n=0 Fourier coefficient, is of such frequent occurrence in this kind of work that we present here a special notation for it. Given any function $f(\theta)$, we define the averaged function, $\bar{f}$, as follows:

$$\bar{f} = \frac{1}{2\pi}\int_0^{2\pi} f(\theta)\,d\theta \tag{4.33}$$

The averaged function $\bar{f}$ is independent of θ. Note that the averaging operator, which we are denoting by an overbar, is a linear operator. It is also frequently convenient to have a notation for the complementary linear operator, which selects out the purely oscillatory terms. We denote this operator with an over-tilde, and define it by

$$\tilde{f}(\theta) = f(\theta) - \bar{f} \tag{4.34}$$

In terms of this new notation, we can rewrite the averaged equations (4.31) as follows:

$$\left.\begin{aligned} \dot{\underset{\sim}{y}} &= \epsilon\,\overline{\underset{\sim}{G}_1}(\underset{\sim}{y}) \\ \dot{\theta} &= \Phi_0(\underset{\sim}{y}) + \epsilon\,\overline{\Phi_1}(\underset{\sim}{y}) \end{aligned}\right\} \tag{4.35}$$

Geometrically speaking, the first D-1 of the averaged equations (4.35) represent the drifts or distortions of the phase space loops in an approximate sense, the approximation involved being the neglect of small amplitude oscillations. And the last of the averaged equations (4.35), the one in θ, gives the average rate of rotation around these loops, in the same approximation.

The intuitive appeal of the method of averaging comes from the fact that if one simply neglects all the oscillatory terms in the perturbing functions, then the resulting equations give the correct time evolution, apart from oscillatory terms, at least to first order in ε. We have shown this property explicitly in the case of the pendulum system, but it holds for the general system (4.8) and (4.35) as well. It is on the basis of this intuitive appeal that the method of averaging is frequently used in the literature, without rigorous justification.

Lest the method appear too obvious, however, we note the important fact that the method of averaging, as we have presented it, does not in general work beyond first order. That is, if one takes the original system (4.8), and averages both the $O(\varepsilon)$ and $O(\varepsilon^2)$ terms, the resulting set of averaged equations will not correctly describe the averaged time evolution through $O(\varepsilon^2)$. Another way of stating this is to say that the process of averaging and that of solving for the time evolution only commute through first order.

Let us now return to the pendulum problem as an example of the method of successive approximations, and consider the solution to second order. To effect this solution we must take (4.21c), substitute into it the expressions (4.22) and (4.24), and then integrate. A simple inspection of these equations immediately shows one important characteristic of the second order

results: they are very complicated. This complexity is reason in itself for finding a better method of effecting perturbation expansions than the method of successive approximations. As we shall see, there is a better method, at least for Hamiltonian systems; it is the Lie transform method.

For the time being, however, we want to focus on certain features of the second order terms without going through all the mathematical details. We consider the expression for $\dot{A}_2$ in (4.21c), and concentrate on the terms involving θ_1. From (4.24b) we see that θ_1 contains terms proportional to time, and thus $\dot{A}_2$ will contain terms proportional to

$$t \cos 2(\omega_0 t + \phi_0)$$

and others similar to it. When these are integrated, there will result terms like

$$t \sin 2(\omega_0 t + \phi_0)$$

Such terms are called <u>secular terms</u>, meaning that they are unbounded in time, and their appearance at second order constitutes a major shortcoming of the method of successive approximations.

To see why secular terms are a problem, let us write out, schematically, the solution A(t) through $O(\varepsilon^2)$, as we did above in (4.25) through $O(\varepsilon)$. We will have

$$\begin{aligned} A(t) = \; & A_0 + \varepsilon(\text{oscillatory terms}) \\ & + \varepsilon^2(\text{oscillatory terms}) \\ & + \varepsilon^2 t(\text{oscillatory terms}) + O(\varepsilon^3) \end{aligned} \tag{4.38}$$

Taken at face value, the secular terms at $O(\varepsilon^2)$ seem to say that the true trajectory in phase space experiences perturbative distortions, taking it away from the unperturbed trajectory, which grow in time until there is a total disruption of any resemblance to the unperturbed trajectory. And yet we argued above on physical grounds, appealing to conservation of energy for both the unperturbed and perturbed systems, that the function A(t) could never evolve very far from A_0, its constant, unperturbed value. Hence we seem to have a paradox.

The resolution to the paradox is that (4.38) is good only for limited amounts of time.* In particular, as soon as times t have been reached which are $O(1/\varepsilon)$, then the $O(\varepsilon^2)$ secular terms in (4.38) become comparable in magnitude to the $O(\varepsilon)$ terms, and the entire series expansion in ε becomes computationally useless. On the other hand, if series can be developed which are free from secular terms, then the ε ordering is good for all times, no matter how large.

The Hamiltonian methods which we describe in following sections allow for the easy development of series which are free from secular terms at all orders. Our purpose here has been to demonstrate how secular terms may arise in some perturbation approaches, and why they are a problem. Therefore we will not dwell on means of getting rid of them in a non-Hamiltonian theory.

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*When we write $A(t) = A_0 + \varepsilon A_1(t) + O(\varepsilon^2)$, we mean that there exists some number $M > 0$ such that

$$\lim_{\epsilon \to 0} \left| \frac{A(t) - A_0 - \epsilon A_1}{\epsilon^2} \right| < M$$

In general, the quantity M will depend on the value of t chosen. If we say that the ordering is uniform, we mean that there exists some $M = M_0$ good for all values of t, or, what is the same thing, that the function M(t) is bounded. The ordering (4.38) is, by these definitions, not uniform in the ε^2 terms.

This concludes our discussion of non-Hamiltonian perturbation theory. The ideas outlined in this section were largely developed by astronomers during the eighteenth and nineteenth centuries. Newton used what is essentially the method of averaging in his study of the effects of solar perturbations on the moon's orbit, and he obtained expressions for the average rate of drift of the line of nodes of the moon's orbit along the ecliptic. A precise calculation of this sort is essential for the accurate prediction of eclipses. The method of successive approximations was used by Lagrange and Laplace in their study of the celestial mechanics of the solar system. These and later workers were especially troubled by the appearance of secular terms, since they wished to determine whether the solar system is stable for indefinite periods of time. This concern gave impetus to a study of means of eliminating secular terms, and such means were found by Poincaré[17] at the end of the nineteenth century. We shall study Poincaré's method in the next section; essentially, it involves a kind of frequency renormalization.

In addition to the problem of secular terms, there was another difficulty which troubled workers in celestial mechanics during the nineteenth century. This latter difficulty is the so-called problem of small divisors. We have not discussed this problem in this section, because it makes its appearance only when the unperturbed system is multiply periodic, a case we have not considered. The problem of small divisors derives essentially from the effects of resonances between the different oscillators of the unperturbed system. In recent years there has been important progress in understanding this problem, and in connecting it with studies in statistical mechanics and other fields.

5. Hamiltonian Perturbation Theory: Traditional Methods

Hamiltonian systems deserve special attention, both from a physical and from a mathematical point of view. Hamiltonian flows in phase space are associated with a remarkable structure of mathematical properties, some of which were discussed in section 3. Physically speaking, Hamiltonian systems are in some sense fundamental, even though not every dynamical system can be represented by a Hamiltonian. For example, one aspect of the fundamental nature of Hamiltonian systems is that only such systems can be quantized.

From the point of view of practical perturbation calculations, Hamiltonian systems offer the important advantage that the equations of motion are contained implicitly in the Hamiltonian, which is a scalar function. This is in contrast to general systems of differential equations, such as (2.5), where the flow functions form a D-vector in a D-dimensional phase space. Hence, roughly speaking, manipulations on a Hamiltonian system will involve D times less labor than equivalent manipulations on an explicit set of differential equations. (For a Hamiltonian system of N degrees of freedom, D = 2N.) In addition, variable transformations in Hamiltonian mechanics, i.e. canonical transformations, are specified by a scalar function, which is the generating function. This may be the mixed variable generating function, discussed in section 3, or it may be the Lie generating function, to be discussed in a later section. For a general system of differential equations, a coordinate transformation must be explicitly specified, in the form of a vector-valued function.

We begin this section by discussing the preparatory transformation for Hamiltonian systems, and we relate this transformation to Hamilton-Jacobi

theory. Next we consider the method of averaging for several different classes of Hamiltonian systems. The method of averaging and Hamilton-Jacobi theory are then used to motivate the method of Poincaré and Von Zeipel, which is discussed at length. Finally, we point out some of the drawbacks of the Poincaré-Von Zeipel method, and we indicate how these drawbacks are alleviated by the Lie transform method.

As a starting point for our study of perturbation theory in Hamiltonian mechanics we consider Hamiltonians of the following form:

$$H(\underset{\sim}{z},t,\varepsilon) = H_0(\underset{\sim}{z},t) + \varepsilon H_1(\underset{\sim}{z},t) + \varepsilon^2 H_2(\underset{\sim}{z},t) + \ldots \tag{5.1}$$

We assume that the system described by H_0, the unperturbed system, is solvable in closed form. It follows that the Hamilton-Jacobi equation for the unperturbed system is also solvable.

In the examples to be considered in this paper, H_0 will be independent of time. In this case, which is very common in practice, the solution to the time-independent Hamilton-Jacobi equation for the unperturbed system yields a time-independent canonical transformation $\underset{\sim}{z} = (\underset{\sim}{q},\underset{\sim}{p}) \rightarrow \underset{\sim}{z}' = (\underset{\sim}{q}',\underset{\sim}{p}')$, such that H_0 depends on the momenta $\underset{\sim}{p}'$ alone. Thus, in terms of the variables $\underset{\sim}{z}'$, the Hamiltonian may be written

$$H(\underset{\sim}{z}',t,\varepsilon) = H_0(\underset{\sim}{p}') + \varepsilon H_1(\underset{\sim}{q}',\underset{\sim}{p}',t) + \varepsilon^2 H_2(\underset{\sim}{q}',\underset{\sim}{p}',t) + \ldots \tag{5.2}$$

If the unperturbed system is periodic or multiply periodic, then the variables $\underset{\sim}{z}'$ may be chosen to be the action-angle variables, represented by $(\underset{\sim}{\theta},\underset{\sim}{J})$. Restating (5.2) in terms of action-angle variables, we have

$$H(\underset{\sim}{\theta},\underset{\sim}{J},t,\varepsilon) = H_0(\underset{\sim}{J}) + \varepsilon H_1(\underset{\sim}{\theta},\underset{\sim}{J},t) + \varepsilon^2 H_2(\underset{\sim}{\theta},\underset{\sim}{J},t) + \ldots \tag{5.3}$$

In (5.2) or (5.3) the momenta $\underset{\sim}{p}'$ or the action variables $\underset{\sim}{J}$, respectively, are constants of the unperturbed motion.

By solving the Hamilton-Jacobi equation for the unperturbed system we find a set of variables, denoted by $\underset{\sim}{z}'$ in (5.2), which is "natural" to the unperturbed system. As a practical matter, finding the canonical transformation $\underset{\sim}{z} \to \underset{\sim}{z}'$ is the first step in any Hamiltonian perturbation analysis. It will be recognized that this transformation is the analog, for Hamiltonian systems, of the preparatory transformation discussed in section 4. This transformation may also be regarded in another light, namely as the first (order zero) step in a perturbative solution to the Hamilton-Jacobi equation for the full, perturbed Hamiltonian. More will be said about this point of view later.

To illustrate the preparatory transformation in Hamiltonian mechanics, we will use the example of the pendulum, which was discussed in section 4. Returning to (4.9), it is a simple matter to find the Lagrangian and thence the Hamiltonian. Setting the moment of inertia $mR^2 = 1$ for convenience, we have

$$H(x,p) = \tfrac{1}{2}p^2 + \omega_0^2(1 - \cos x) \tag{5.4}$$

Here the symbol x stands for the generalized coordinate q. As we did in section 4, we consider small oscillations, i.e. small x, and accordingly we expand the cos function in powers of x. In addition, we artificially introduce a parameter of smallness ε, exactly as we did in section 4. The resulting Hamiltonian is

$$H(x,p) = \tfrac{1}{2}(p^2 + \omega_0^2 x^2) - \frac{\epsilon}{24}\omega_0^2 x^4 + \frac{\epsilon^2}{720}\omega_0^2 x^6 - \dots \tag{5.5}$$

In (5.5) the unperturbed Hamiltonian represents a harmonic oscillator, as expected. To effect the preparatory transformation we need to solve the Hamilton-Jacobi equation for the harmonic oscillator. This solution has already been given in section 3, in the form of a transformation $(q,p) \to (\theta,J)$ to action-angle variables. Using (3.33) it is simple to transform the Hamiltonian (5.5) so that it appears in the form indicated by (5.3). The result is

$$H(\theta,J) = \omega_0 J - \frac{\epsilon}{6} J^2 \sin^4\theta + \frac{\epsilon^2}{90}\frac{J^3}{\omega_0}\sin^6\theta - \dots \tag{5.6}$$

For future reference, we write (5.6) in an alternate form, by expanding the perturbing terms in Fourier series in θ. This gives

$$\begin{aligned} H(\theta,J) = \; & \omega_0 J \\ & - \frac{\epsilon}{48} J^2 \left(3 - 4\cos 2\theta + \cos 4\theta\right) \\ & + \frac{\epsilon^2}{2880}\frac{J^3}{\omega_0}\left(10 - 15\cos 2\theta + 6\cos 4\theta - \cos 6\theta\right) \\ & + O(\epsilon^3) \end{aligned} \tag{5.7}$$

As another example of the preparatory transformation, let us consider the pendulum problem from another point of view. Instead of considering small oscillations about the equilibrium position, let us consider pendulum motion for which the kinetic energy dominates the potential energy, i.e. motion consisting of high speed, nearly free rotations completely around the circle shown in Fig. 3. In this case we may consider the unperturbed system to consist of free rotations, and we may treat the effects of gravity as a perturbation. Then it is appropriate to take the entire potential

energy term in (5.4) as a perturbation, and to introduce a smallness parameter ε as follows:

$$H = \frac{1}{2} p^2 + \epsilon \omega_0^2 (1 - \cos x) \tag{5.8}$$

It is easy to see that the unperturbed Hamiltonian in (5.8) represents free rotations.

From the point of view of the preparatory transformation, we see that there is no work to do on (5.8), since it is already in the form indicated by (5.2). The Hamiltonians (5.7) and (5.8) represent the pendulum in two limits, the former being the small energy limit, and the latter, the large energy limit. Of course, when $\varepsilon = 1$, the two Hamiltonians are numerically equal. In both these limits, the pendulum system has been prepared for a perturbation analysis.

We now take up the method of averaging, which is a simple form of first order perturbation theory, with Hamiltonian systems. We begin by considering special cases, and then extend the results to more general cases.

First we investigate systems of one degree of freedom, which are time-independent and periodic in their unperturbed motion. Due to the periodicity of the unperturbed system, there exist action-angle variables (θ,J) for the unperturbed system, and in terms of these variables the Hamiltonian takes the form

$$H(\theta,J) = H_0(J) + \varepsilon H_1(\theta,J) + \varepsilon^2 H_2(\theta,J) + \ldots \tag{5.9}$$

The variables (θ,J) are scalars, because the system has one degree of freedom.

The pendulum system in both its limits (5.7) and (5.8)* falls into this class.

In section 4 we showed that the process of throwing away oscillatory terms commutes with the process of solving the differential equations, at least through first order. For Hamiltonian systems, the only modification to this rule is that we throw away oscillatory terms, not in the equations of motion, but rather in the perturbing Hamiltonian H_1. The result will be "the averaged Hamiltonian", which we denote by the symbol K. According to the rule,

$$K(J) = H_0(J) + \varepsilon\overline{H}_1(J) + O(\varepsilon^2) \tag{5.10}$$

Note that, due to the averaging, the new Hamiltonian K is independent of θ. This means that the averaged equations of motion are trivial to solve, since the action J is a constant of the averaged motion.

We will illustrate the method of averaging with the pendulum system. In the low energy limit, the Hamiltonian (5.7) averages into

$$K = \omega_0 J - \frac{\epsilon}{16} J^2 \tag{5.11}$$

The equations of motion generated by this Hamiltonian are

$$\left.\begin{aligned} \dot{\theta} &= \omega_0 - \frac{\epsilon J}{8} \\ \dot{J} &= 0 \end{aligned}\right\} \tag{5.12}$$

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*In the large energy limit, the unperturbed system is periodic because of the topological properties of the x coordinate. I.e., the variable x appearing in (5.8) is really an angle (see Fig. 3), and has a period of 2π. The variables (x,p) in (5.8) are action-angle variables, and could perhaps more suggestively be written (θ,J).

By using equation (3.33) the action J and the amplitude A may be related to one another:

$$J = \frac{1}{2}\omega_0 A^2 \tag{5.13}$$

Hence it may be seen that (5.12) and (4.29) are equivalent, and that the results of our non-Hamiltonian treatment are recovered.

In the large energy limit, the Hamiltonian (5.8) averages into

$$K(p) = \frac{1}{2}p^2 + \epsilon\omega_0^2 \tag{5.14}$$

In this limit, the perturbing term has no effect, at first order, on the averaged equations. This follows since the $O(\varepsilon)$ term in (5.14) is a constant, and has no effect on the equations of motion. Later we will see that the perturbing term does have an effect at second order, the so-called ponderomotive force.

Now we take up the case of systems of N degrees of freedom, which are acted upon by a time-dependent perturbation. We assume that the perturbation is periodic in time with frequency ω. The Hamiltonian for such a system, after the preparatory transformation has been applied, has the form

$$H(\underset{\sim}{q}, \underset{\sim}{p}, t) = H_0(\underset{\sim}{p}) + \epsilon H_1(\underset{\sim}{q}, \underset{\sim}{p}, t) + O(\epsilon^2) \tag{5.15}$$

The assumption of periodicity allows us to expand H_1 in a Fourier series in $e^{i\omega t}$:

$$H_1(\underset{\sim}{q}, \underset{\sim}{p}, t) = \sum_n H_{1n}(\underset{\sim}{q}, \underset{\sim}{p})\, e^{in\omega t} \tag{5.16}$$

The Fourier coefficients H_{1n} are given by

$$H_{1n}(\underset{\sim}{q},\underset{\sim}{p}) = \frac{\omega}{2\pi}\int_0^{\frac{2\pi}{\omega}} dt\; e^{-in\omega t}\, H_1(\underset{\sim}{q},\underset{\sim}{p},t) \tag{5.17}$$

As an example of such a system we may consider a particle which is free except for the effects of a small amplitude electrostatic wave:

$$H(\underset{\sim}{x},\underset{\sim}{p},t) = \tfrac{1}{2}\underset{\sim}{p}^2 + \epsilon e \phi_0 \cos(\underset{\sim}{k}\cdot\underset{\sim}{x} - \omega t) \tag{5.18}$$

This system has 3 degrees of freedom; $\underset{\sim}{x}$, $\underset{\sim}{p}$ are 3-vectors in Cartesian coordinates. The similarity of this example to the large energy limit of the pendulum should be noted.

When a system such as (5.15) is solved by successive approximations or other perturbation methods, there result in the solution terms proportional to $e^{in\omega t}$. If one is not interested in these oscillatory terms, one can average the Hamiltonian first and then solve the equations of motion. The result will be the same as the solution to the exact, i.e. unaveraged, Hamiltonian, apart from oscillatory terms in $e^{in\omega t}$, at least through first order in ε. The averaging operation in this case is defined somewhat differently than in (4.33); here we want to select out the n = 0 Fourier coefficient in (5.16), so we define the averaging operator by

$$\overline{f}(\underset{\sim}{q},\underset{\sim}{p}) = \frac{\omega}{2\pi}\int_0^{\frac{2\pi}{\omega}} dt\; f(\underset{\sim}{q},\underset{\sim}{p},t) \tag{5.19}$$

With this definition of the averaging operator, we can write the averaged Hamiltonian K corresponding to (5.15) as follows:

$$K(\underset{\sim}{q},\underset{\sim}{p}) = H_0(\underset{\sim}{p}) + \varepsilon\overline{H_1}(\underset{\sim}{q},\underset{\sim}{p}) + O(\varepsilon^2) \tag{5.20}$$

It is easy to see, in the example (5.18), that the average of the perturbing term vanishes.

In practice, a system such as (5.15) often arises in a physical context in which the explicit time dependence of the Hamiltonian is in some sense "fast", while the implicit time dependence of the variables q,p is "slow". For example, (5.18) might represent a slow particle in a high frequency wave. Consequently, the averaging procedure we have described here is often used to get first order results in situations where there are two time scales.

A slight variation on Hamiltonians such as (5.15) is the case of time-independent Hamiltonians in which one of the (q,p) conjugate coordinate pairs is periodic and "fast", in comparison to the other degrees of freedom. In this case it would be appropriate to average with respect to the fast variables alone. Actually, it can be shown that this case encompasses both the previous two cases considered, (5.9) and (5.15).

Finally, let us consider systems which are time-independent and multiply periodic in their unperturbed motion. Furthermore, let us assume that the different oscillators of the unperturbed system all have comparable frequencies, so that there are no fast and slow time scales. The solar system is a good example of such a dynamical system, if the perturbing terms are taken to be the interplanetary gravitational potentials. Such a system can be written in terms of action-angle variables as

$$H(\underset{\sim}{\theta},\underset{\sim}{J}) = H_0(\underset{\sim}{J}) + \varepsilon H_1(\underset{\sim}{\theta},\underset{\sim}{J}) + \varepsilon^2 H_2(\underset{\sim}{\theta},\underset{\sim}{J}) + \ldots \tag{5.21}$$

In this case it is appropriate to expand the perturbing terms in a multiple Fourier series. For example, for H_1 we may write

$$H_1(\underset{\sim}{\theta},\underset{\sim}{J}) = \sum_{\underset{\sim}{n}} H_{1,\underset{\sim}{n}}(\underset{\sim}{J})\, e^{i\underset{\sim}{n}\cdot\underset{\sim}{\theta}} \tag{5.22}$$

In (5.22) $\underset{\sim}{n}$ is an N-vector of integers, for a Hamiltonian with N degrees of freedom, and the sum is taken over all such vectors of integers. The averaging is effected by selecting the $\underset{\sim}{n} = 0$ (by which we mean $\underset{\sim}{n} = (0,0, \ldots ,0)$) component in the Fourier series, as shown here for an arbitrary periodic function $f(\underset{\sim}{\theta})$:

$$\bar{f} = \frac{1}{(2\pi)^N} \int_0^{2\pi} d\theta_1 \ldots \int_0^{2\pi} d\theta_N \; f(\underset{\sim}{\theta}) \tag{5.23}$$

Then we have, for the averaged Hamiltonian K,

$$K(\underset{\sim}{J}) = H_0(\underset{\sim}{J}) + \varepsilon\overline{H}_1(\underset{\sim}{J}) + O(\varepsilon^2) \tag{5.24}$$

Note that the averaging procedure has removed the $\underset{\sim}{\theta}$ dependence of the Hamiltonian, so that all the actions $\underset{\sim}{J}$ are constants of the averaged motion.

There are many other possibilities for the averaging process, e.g. systems with some fast variables and some slow, or systems with three time scales, etc. In each case an averaging operator is defined on the basis of the approximation desired, and in each case the results are good through first order in ε. The pattern should by now be well established.

We will now use the Hamiltonian (5.21) and its averaged correspondent (5.24) in order to motivate the perturbation method of Poincaré and Von Zeipel. We recall that the canonical transformation generated by the solution to the Hamilton-Jacobi equation has the property that the new Hamiltonian depends only on the new momenta. In our Hamiltonian (5.24), the order zero term (the unperturbed Hamiltonian) depends only on the momenta because of the preparatory transformation, which is derived from the solution to the

Hamilton-Jacobi equation for the unperturbed system. We have already noted that finding the preparatory transformation is equivalent to the order zero step in a perturbative solution to the Hamilton-Jacobi equation for the full, perturbed system. Now we observe, in the averaged Hamiltonian (5.24), that the $O(\varepsilon)$ term also depends only on the generalized momenta. This suggests that the method of averaging is somehow connected with the $O(\varepsilon)$ solution of the Hamilton-Jacobi equation for the full, perturbed system.

The method of averaging has so far been presented as an approximation scheme, in the sense that selected terms are thrown away, both in the Hamiltonian and in the solution. In accordance with the philosophy of the Hamilton-Jacobi equation, however, we ask if the results of the averaging procedure can be achieved by a canonical transformation. That is, we want to see if instead of being thrown away, the terms in question can be transformed away. If so, then we will have found a transformation such that the new Hamiltonian is independent of the generalized coordinates, and this transformation must be generated by a solution to the Hamilton-Jacobi equation for the full, perturbed system.

The idea of eliminating the dependence of terms in the Hamiltonian on the generalized coordinates by means of a canonical transformation is an essential ingredient in the perturbation method of Poincaré and Von Zeipel. We shall develop this method on systems of the form (5.21), i.e. systems which are time-independent and multiply periodic in their unperturbed motion. At the end of this development, we will comment on the application of the Poincaré-Von Zeipel method to other classes of systems.

Following the idea of transforming terms away, we want to consider the application of a canonical transformation $(\underset{\sim}{\theta},\underset{\sim}{J}) \to (\underset{\sim}{\theta}',\underset{\sim}{J}')$ to the Hamiltonian

(5.21), such that the new Hamiltonian K depends only on the momenta $\underset{\sim}{J}'$. Since the unperturbed Hamiltonian H_0 is already a function of $\underset{\sim}{J}$ alone, we expect this canonical transformation to be the identity transformation plus corrections at first and higher orders. That is, we assume that the transformation has the form

$$\begin{aligned} \underset{\sim}{\theta}(\underset{\sim}{\theta}',\underset{\sim}{J}') &= \underset{\sim}{\theta}' + \varepsilon\underset{\sim}{\Theta}_1(\underset{\sim}{\theta}',\underset{\sim}{J}') + \varepsilon^2\underset{\sim}{\Theta}_2(\underset{\sim}{\theta}',\underset{\sim}{J}') + \ldots \\ \underset{\sim}{J}(\underset{\sim}{\theta}',\underset{\sim}{J}') &= \underset{\sim}{J}' + \varepsilon\underset{\sim}{J}_1(\underset{\sim}{\theta}',\underset{\sim}{J}') + \varepsilon^2\underset{\sim}{J}_2(\underset{\sim}{\theta}',\underset{\sim}{J}') + \ldots \end{aligned} \tag{5.25}$$

Here we have chosen to express the old variables $(\underset{\sim}{\theta},\underset{\sim}{J})$ as functions of the new variables $(\underset{\sim}{\theta}',\underset{\sim}{J}')$. The functions $\underset{\sim}{\Theta}_1$, $\underset{\sim}{J}_1$, $\underset{\sim}{\Theta}_2$, $\underset{\sim}{J}_2$, etc., of the new variables, are to be chosen so that the transformation is canonical and so that the new Hamiltonian K is independent of $\underset{\sim}{\theta}'$. We will call a transformation such as (5.25) a <u>near-identity</u> transformation, because the order zero terms represent the identity transformation.

In the perturbation method of Poincaré and Von Zeipel, the transformation (5.25) is generated by a mixed variable generating function, which we take to be a function of the old generalized coordinates $\underset{\sim}{\theta}$ and the new generalized momenta $\underset{\sim}{J}'$, and which we denote by $F(\underset{\sim}{\theta},\underset{\sim}{J}')$. This generating function is expanded in a power series in ε, and the order zero term (see equation (3.21)) is chosen so as to generate the identity transformation:

$$F(\underset{\sim}{\theta},\underset{\sim}{J}') = \underset{\sim}{\theta}\cdot\underset{\sim}{J}' + \varepsilon F_1(\underset{\sim}{\theta},\underset{\sim}{J}') + \varepsilon^2 F_2(\underset{\sim}{\theta},\underset{\sim}{J}') + \ldots \tag{5.26}$$

Writing out the canonical transformation generated by this function, we have

$$\underset{\sim}{\theta}' = \underset{\sim}{\theta} + \epsilon\,\frac{\partial F_1}{\partial \underset{\sim}{J}'}(\underset{\sim}{\theta},\underset{\sim}{J}') + \epsilon^2\,\frac{\partial F_2}{\partial \underset{\sim}{J}'}(\underset{\sim}{\theta},\underset{\sim}{J}') + \ldots \tag{5.27a}$$

$$\underset{\sim}{J} = \underset{\sim}{J}' + \epsilon\,\frac{\partial F_1}{\partial \underset{\sim}{\theta}}(\underset{\sim}{\theta},\underset{\sim}{J}') + \epsilon^2\,\frac{\partial F_2}{\partial \underset{\sim}{\theta}}(\underset{\sim}{\theta},\underset{\sim}{J}') + \ldots \tag{5.27b}$$

In terms of the undetermined functions F_1, F_2, etc., the transformation (5.27) is a completely general near-identity canonical transformation.

We would now like to compare (5.25) and (5.27) in order to determine the functions $\underset{\sim}{\Theta}_1$, $\underset{\sim}{J}_1$, etc., in terms of the derivatives of F_1, etc. This determination is not immediate, because (5.25) expresses the old variables solely in terms of the new variables, whereas (5.27) mixes old and new variables on both sides of both equations. Hence it is necessary to "disentangle" (5.27) to express old variables purely as a function of new variables.

The disentangling is not difficult if only carried through first order. Since the old and new variables are equal to one another with $O(\varepsilon)$ corrections, they may be freely interchanged in the $O(\varepsilon)$ terms if errors at $O(\varepsilon^2)$ are being ignored. By replacing $\underset{\sim}{\theta}$ by $\underset{\sim}{\theta}'$ in the $O(\varepsilon)$ terms and solving (5.27a) for the old variables as functions of the new, we have

$$\underset{\sim}{\theta} = \underset{\sim}{\theta}' - \epsilon \frac{\partial F_1}{\partial \underset{\sim}{J}'}(\underset{\sim}{\theta}', \underset{\sim}{J}') + O(\epsilon^2) \tag{5.28a}$$

$$\underset{\sim}{J} = \underset{\sim}{J}' + \epsilon \frac{\partial F_1}{\partial \underset{\sim}{\theta}'}(\underset{\sim}{\theta}', \underset{\sim}{J}') + O(\epsilon^2) \tag{5.28b}$$

This can be directly compared to (5.25).

We may now substitute (5.28) into (5.21) to determine the new Hamiltonian K. (Since the transformation is time-independent, the old and new Hamiltonians are numerically equal to one another. See (3.19) and (3.22).) Expanding the result to first order in ε, we have

$$\begin{aligned} K(\underset{\sim}{\theta}', \underset{\sim}{J}') &= H(\underset{\sim}{\theta}, \underset{\sim}{J}) \\ &= H_0(\underset{\sim}{J}') \\ &\quad + \epsilon \left[H_1(\underset{\sim}{\theta}', \underset{\sim}{J}') + \frac{\partial H_0(\underset{\sim}{J}')}{\partial \underset{\sim}{J}'} \cdot \frac{\partial F_1(\underset{\sim}{\theta}', \underset{\sim}{J}')}{\partial \underset{\sim}{\theta}'} \right] \\ &\quad + O(\epsilon^2) \end{aligned} \tag{5.29}$$

It is convenient to write the new Hamiltonian K also as a power series in ε:

$$K(\underset{\sim}{\theta}',\underset{\sim}{J}') = K_0(\underset{\sim}{J}') + \varepsilon K_1(\underset{\sim}{\theta}',\underset{\sim}{J}') + \varepsilon^2 K_2(\underset{\sim}{\theta}',\underset{\sim}{J}') + \ldots \tag{5.30}$$

We then collect terms in (5.29) in powers of ε, and we get a hierarchy of equations, of which the first two are

$$K_0(\underset{\sim}{J}') = H_0(\underset{\sim}{J}') \tag{5.31a}$$

$$K_1(\underset{\sim}{\theta}',\underset{\sim}{J}') = H_1(\underset{\sim}{\theta}',\underset{\sim}{J}') + \frac{\partial H_0(\underset{\sim}{J}')}{\partial \underset{\sim}{J}'} \cdot \frac{\partial F_1(\underset{\sim}{\theta}',\underset{\sim}{J}')}{\partial \underset{\sim}{\theta}'} \tag{5.31b}$$

We are now in a position to choose the function F_1, and hence the functions $\underset{\sim}{\Theta}_1$, $\underset{\sim}{J}_1$, so as to make K independent of $\underset{\sim}{\theta}'$. By examining (5.31a), we see that K_0 is (as expected) already independent of $\underset{\sim}{\theta}'$. As for K_1, we examine (5.31b), and we see that if K_1 is to be independent of $\underset{\sim}{\theta}'$, then the term containing $\frac{\partial F_1}{\partial \underset{\sim}{\theta}'}$ must cancel the $\underset{\sim}{\theta}'$ dependence of H_1. Accordingly, we break H_1 into its averaged and oscillatory parts, and write

$$K_1(\underset{\sim}{J}') = \overline{H_1}(\underset{\sim}{J}') + \widetilde{H}_1(\underset{\sim}{\theta}',\underset{\sim}{J}') + \frac{\partial H_0(\underset{\sim}{J}')}{\partial \underset{\sim}{J}'} \cdot \frac{\partial F_1(\underset{\sim}{\theta}',\underset{\sim}{J}')}{\partial \underset{\sim}{\theta}'} \tag{5.32}$$

This suggests that we find a function F_1 such that

$$\frac{\partial H_0(\underset{\sim}{J}')}{\partial \underset{\sim}{J}'} \cdot \frac{\partial F_1(\underset{\sim}{\theta}',\underset{\sim}{J}')}{\partial \underset{\sim}{\theta}'} = -\widetilde{H}_1(\underset{\sim}{\theta}',\underset{\sim}{J}') \tag{5.33}$$

If such an F_1 can be found, then

$$K_1(\underset{\sim}{J}') = \overline{H_1}(\underset{\sim}{J}') \tag{5.34}$$

This result is satisfying, because it gives for K_1 simply the average of H_1, and it makes K identical to the averaged Hamiltonian shown in (5.24), at least through $O(\varepsilon)$.

Now we examine (5.33) to try to find a solution for F_1. It may be seen that (5.33) is a first order, linear, partial differential equation for F_1. Appendix A summarizes the theory of such differential equations, and shows that (5.33) does, indeed, always have a solution. For the time being we can simply solve (5.33) by inspection.

To do this, we define the vector $\underset{\sim}{\omega}_0(\underset{\sim}{J})$ as the frequency vector of the unperturbed oscillators, i.e. the vector $\dot{\underset{\sim}{\theta}}$ as determined by the unperturbed Hamiltonian H_0:

$$\underset{\sim}{\omega}_0(\underset{\sim}{J}) = \frac{\partial H_0(\underset{\sim}{J})}{\partial \underset{\sim}{J}} \tag{5.35}$$

For the term $\tilde{H}_1$, we use the Fourier expansion (5.22), the definition of the averaging operator, (5.23), and the definition of the complementary operator, (4.34), to write

$$\tilde{H}_1(\underset{\sim}{\theta}', \underset{\sim}{J}') = \sum_{\underset{\sim}{n} \neq 0} H_{1,\underset{\sim}{n}}(\underset{\sim}{J}')\, e^{i\underset{\sim}{n}\cdot\underset{\sim}{\theta}'} \tag{5.36}$$

Then the equation (5.33) can be written

$$\underset{\sim}{\omega}_0(\underset{\sim}{J}') \cdot \frac{\partial F_1(\underset{\sim}{\theta}', \underset{\sim}{J}')}{\partial \underset{\sim}{\theta}'} = -\sum_{\underset{\sim}{n} \neq 0} H_{1,\underset{\sim}{n}}(\underset{\sim}{J}')\, e^{i\underset{\sim}{n}\cdot\underset{\sim}{\theta}'} \tag{5.37}$$

It is then easy to see that a solution F_1 to (5.37) is given by

$$F_1(\underset{\sim}{\theta}', \underset{\sim}{J}') = \sum_{\underset{\sim}{n} \neq 0} i\, \frac{H_{1,\underset{\sim}{n}}(\underset{\sim}{J}')\, e^{i\underset{\sim}{n}\cdot\underset{\sim}{\theta}'}}{\underset{\sim}{n} \cdot \underset{\sim}{\omega}_0(\underset{\sim}{J}')} \tag{5.38}$$

In (5.38) it is necessary to assume that the denominator does not vanish, which is equivalent to assuming that there are no "first-order resonances" among the unperturbed oscillators.

Through $O(\varepsilon)$, we have accomplished what we wanted. A canonical transformation has been found, via the generator given in (5.38), which eliminates the $\underset{\sim}{\theta}$ dependence of the Hamiltonian. In fact, the process we have just described for the $O(\varepsilon)$ term can be carried to any order, and it yields a new Hamiltonian K which is independent of $\underset{\sim}{\theta}'$ to all orders. This Hamiltonian is often called the "averaged Hamiltonian", since it agrees with the results of the method of averaging at first order. In effect, the Poincaré-Von Zeipel method allows the definition of the averaged Hamiltonian to be extended to arbitrary order. Corresponding to this terminology, the Poincaré-Von Zeipel method is sometimes called the "generalized method of averaging", or simply "the method of averaging", without any qualification.

Now suppose we want to find the explicit functions of time, $\underset{\sim}{\theta}(t)$, $\underset{\sim}{J}(t)$, which are the solutions to (5.21). The first step is to find the time evolution of the variables $\underset{\sim}{\theta}'$, $\underset{\sim}{J}'$. This is easy, since the averaged Hamiltonian K depends only on the momenta $\underset{\sim}{J}'$:

$$K(\underset{\sim}{J}') = K_0(\underset{\sim}{J}') + \varepsilon K_1(\underset{\sim}{J}') + \ldots \tag{5.39}$$

This means that the momenta $\underset{\sim}{J}'$ are all constants of the motion:

$$\dot{\underset{\sim}{J}}' = -\frac{\partial K}{\partial \underset{\sim}{\theta}} = 0 \tag{5.40}$$

As for the angles $\underset{\sim}{\theta}'$, they evolve linearly in time, with a frequency which we may call $\underset{\sim}{\omega}$:

$$\dot{\underset{\sim}{\theta}}' = \underset{\sim}{\omega}(\underset{\sim}{J}') = \frac{\partial K(\underset{\sim}{J}')}{\partial \underset{\sim}{J}'} \tag{5.41}$$

It may be observed that if ω is expanded in a power series in ε, then

the first (order zero) term is the frequency $\underset{\sim}{\omega}_0$, defined in (5.35) in terms of the unperturbed Hamiltonian:

$$\underset{\sim}{\omega}(\underset{\sim}{J}') = \underset{\sim}{\omega}_0(\underset{\sim}{J}') + \epsilon \frac{\partial K_1(\underset{\sim}{J}')}{\partial \underset{\sim}{J}'} + \dots \tag{5.42}$$

The explicit solutions to (5.40) and (5.41) are

$$\underset{\sim}{J}'(t) = \text{constant} \tag{5.43a}$$

$$\underset{\sim}{\theta}'(t) = \underset{\sim}{\omega}(\underset{\sim}{J}')t + \underset{\sim}{\theta}_0' \tag{5.43b}$$

where $\underset{\sim}{\theta}_0'$ is a set of initial conditions.

After we have the functions $\underset{\sim}{\theta}'(t)$, $\underset{\sim}{J}'(t)$, we can use the transformation (5.28) in order to find the functions $\underset{\sim}{\theta}(t)$, $\underset{\sim}{J}(t)$. So far we have not actually written out the transformation equations. Rather we have simply found their generating function, given by (5.38). On substituting the generating function into (5.28) we get the following, explicit form for the transformation:

$$\underset{\sim}{\theta} = \underset{\sim}{\theta}' - \epsilon \sum_{\underset{\sim}{n} \neq 0}' i \frac{\partial}{\partial \underset{\sim}{J}'} \left(\frac{H_{1,\underset{\sim}{n}}(\underset{\sim}{J}')}{\underset{\sim}{n} \cdot \underset{\sim}{\omega}_0(\underset{\sim}{J}')} \right) e^{i\underset{\sim}{n}\cdot\underset{\sim}{\theta}'} + O(\epsilon^2) \tag{5.44a}$$

$$\underset{\sim}{J} = \underset{\sim}{J}' - \epsilon \sum_{\underset{\sim}{n} \neq 0}' \underset{\sim}{n} \frac{H_{1,\underset{\sim}{n}}(\underset{\sim}{J}')}{\underset{\sim}{n} \cdot \underset{\sim}{\omega}_0(\underset{\sim}{J}')} e^{i\underset{\sim}{n}\cdot\underset{\sim}{\theta}'} + O(\epsilon^2) \tag{5.44b}$$

It is then trivial to substitute $\underset{\sim}{\theta}'(t)$, $\underset{\sim}{J}'(t)$ into (5.44) to get $\underset{\sim}{\theta}(t)$, $\underset{\sim}{J}(t)$.

Let us carry out the Poincaré-Von Zeipel perturbation method through first order for the pendulum system in the low energy limit, as given by (5.6) or (5.7). This example has only one degree of freedom, so all the N-vectors appearing in the equations (5.25) to (5.44) become scalars. It

is a simple matter to specialize all these equations to the pendulum problem; let us begin with (5.31), which becomes

$$K_0(J') = \omega_0 J' \tag{5.45a}$$

$$K_1(J',\theta') = -\frac{J'^2}{48}(3 - 4\cos 2\theta' + \cos 4\theta') + \omega_0 \frac{\partial F_1(\theta',J')}{\partial\theta'} \tag{5.45b}$$

We choose F_1 to cancel the oscillatory part of (5.45b). This choice gives the following partial differential equation for F_1:

$$\omega_0 \frac{\partial F_1(\theta',J')}{\partial\theta'} = \frac{J'^2}{48}\left(-4\cos 2\theta' + \cos 4\theta'\right) \tag{5.46}$$

This equation corresponds to (5.37) in the general case, and upon integration it yields

$$F_1(\theta',J') = \frac{1}{192}\frac{J'^2}{\omega_0}\left(-8\sin 2\theta' + \sin 4\theta'\right) \tag{5.47}$$

For the new Hamiltonian K we have

$$K(J') = \omega_0 J' - \frac{\epsilon}{16} J'^2 + O(\epsilon^2) \tag{5.48}$$

which agrees with (5.11), obtained by the method of averaging. The solution to the equations of motion of the averaged Hamiltonian are

$$\begin{aligned} J' &= \text{constant} \\ \theta' &= \omega t + \theta_0' \end{aligned} \tag{5.49}$$

where θ_0' is a constant of integration and where ω is the true frequency, given by

$$\omega = \omega_0 - \frac{\epsilon}{8} J' + O(\epsilon^2) \tag{5.50}$$

Finally, the transformation $(\theta,J) \to (\theta',J')$ can be explicitly determined using F_1 and equations (5.44) or (5.28). These give

$$\theta = \theta' - \frac{\epsilon}{96}\frac{J'}{\omega_0}\left(-8\sin 2\theta' + \sin 4\theta'\right) + O(\epsilon^2) \tag{5.51a}$$

$$J = J' + \frac{\epsilon}{48}\frac{J'^2}{\omega_0}\left(-4\cos 2\theta' + \cos 4\theta'\right) + O(\epsilon^2) \tag{5.51b}$$

It is relatively straightforward to compare this work on the pendulum system to the results of the method of successive approximations, given in section 4, and to show that they are equivalent. There are important differences in form, however, relating to frequency renormalization and secular terms. These will be discussed later, after we have Lie transforms at our disposal.

The essence of the perturbation method of Poincaré and Von Zeipel is the use of near-identity canonical transformations, generated by mixed variable generating functions, to eliminate the dependence of a Hamiltonian on one or more variables or classes of terms. We have illustrated this method for systems whose unperturbed motion is multiply periodic, and shown how to eliminate the dependence of the Hamiltonian on the angles $\underset{\sim}{\theta}$. The method is flexible, however, and can be used with other classes of systems. For example, in the case of time-dependent systems such as (5.15), it is possible to choose the transformation so that the new Hamiltonian K is independent of time. Or, with systems with some fast variables and some slow variables, it may be desirable to choose the transformation so that the dependence on the fast generalized coordinates is eliminated. All these goals can be achieved with the method.

We have discussed the Poincaré-Von Zeipel method because it illustrates

many of the features of the Lie transform method in a more familiar context, and because it is the traditional perturbation method for Hamiltonian systems. We have illustrated the method only to first order, however, because to go to higher order would take us too far astray from our main goal, which is the Lie transform method. Since we have not developed higher order perturbations, it has not been possible to give a complete discussion of the problem of secular terms. Such a discussion will come later.

Before moving on to the Lie transform technique, we will point out some of the difficulties from which the Poincaré-Von Zeipel method suffers, difficulties which are remedied by the Lie technique. The foremost difficulty of the Poincaré-Von Zeipel method arises from the use of mixed variable generating functions, and it is in this respect that the Lie method is characteristically different. The use of mixed variable generating functions means that the new and old variables must be disentangled before the new Hamiltonian can be found. We have succeeded above in disentangling our transformation to first order. To higher orders, the disentangling process is very complicated and laborious, and gives rise to formulas of no apparent symmetry or structure. A related problem is that it is frequently desirable to have not only the canonical transformation, such as (5.44), but also its inverse, and then one must either invert a power series or else perform the disentangling in the reverse order. In the Lie method, canonical transformations are generated without mixing old and new variables, thereby completely bypassing the disentangling process. Furthermore, in the Lie transform technique both the canonical transformations generated and their inverses are expressed in terms of Poisson brackets, which represent

Lie products in the Lie algebra of the group of canonical transformations. This allows not only for a simple and clear relation between canonical transformations and their inverses, but also gives rise to a compact and powerful notation for expressions between variables and functions. We turn now to a description of the generation of canonical transformations with Lie generators.

6. Near-Identity Canonical Transformations and Their Lie Generators

In this section we develop formulas relating canonical transformations, expressed as a power series, to their Lie generators. We begin this section by establishing some notational conventions concerning functions on phase space and transformation operators on those functions. Then we prove an important theorem which connects Hamiltonian flows to canonical transformations. Finally, we use this theorem to write canonical transformation operators in terms of their associated Lie operators.

There is a certain notational problem which arises in work with near-identity transformations, canonical or otherwise, which sometimes causes confusion. Although this problem is essentially trivial, it can, unless properly dealt with, consume a distracting amount of attention. Therefore we will discuss the problem and establish certain notational conventions before proceeding with the development of near-identity canonical transformations.

The source of the problem can be traced to certain ambiguous aspects of the notation commonly used by physicists for functions and values of functions. In the common parlance of physicists, the word "function", especially when applied to physically meaningful quantities, has a meaning which roughly corresponds to the <u>name of a value</u>. Consider, for example, the electrostatic potential Φ in 3-dimensional space. If a certain point of space is described both by its Cartesian coordinates (x,y,z) and by its spherical coordinates (r,θ,ϕ), then it would be common for a physicist to write $\Phi(x,y,z) = \Phi(r,\theta,\phi)$, meaning that the value of the potential is the same no matter how the points of space are labeled. Similarly, in

Hamiltonian mechanics, when we perform a time-independent canonical transformation $\underset{\sim}{z} \to \underset{\sim}{z}'$, the old and new Hamiltonians are numerically equal to one another, and it would be common for a physicist to write $H(\underset{\sim}{z}) = H(\underset{\sim}{z}')$. This transformation law has the same meaning as the equality of electrostatic potentials written above. Operationally, it means the following. First we find the old coordinates $\underset{\sim}{z}$ as functions of the new coordinates $\underset{\sim}{z}'$, giving the functions $\underset{\sim}{z}(\underset{\sim}{z}')$. These are then substituted into $H(\underset{\sim}{z})$ to eliminate $\underset{\sim}{z}$ in favor of $\underset{\sim}{z}'$. The result is what is called $H(\underset{\sim}{z}')$.

The intuitive picture behind the physicist's notation for functions is that the values of a function, whether it be the electrostatic potential or the Hamiltonian, are attached to points of space, which are viewed as geometrical entities. In a sense, geometrical points are considered to form the independent variable of functions, and the coordinates (x,y,z) or (r,θ,ϕ), or $\underset{\sim}{z}$ or $\underset{\sim}{z}'$, are simply taken to be labels of points. Hence an equation such as $H(\underset{\sim}{z}) = H(\underset{\sim}{z}')$ has the import of the statement, "Let's relabel the points of phase space."

The physicist's notation for functions is often convenient and physically suggestive, but it is somewhat imprecise. Usually the level of imprecision is acceptable, but not always, as is the case with near-identity transformations.* The source of the imprecision is that whereas geometrical points may form the independent variable in conception, nevertheless n-tuples of numbers form the independent variable in notation.

This problem may be illustrated with a simple example drawn from

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*More generally, the problem occurs with families of transformations, especially groups, which are continuously connected with the identity transformation. A similar problem occurs with the study of rotation operators, especially in quantum mechanics. See Ref. 18.

Hamiltonian mechanics. Let us take the transformation law for Hamiltonians under a time-independent canonical transformation $\underset{\sim}{z} \to \underset{\sim}{z}'$:

$$H(\underset{\sim}{z}) = H(\underset{\sim}{z}') \tag{6.1}$$

Here the idea is that points of phase space, in a geometrical sense, form the independent variable of H. Now suppose the actual transformation is given by

$$\underset{\sim}{z}' = \underset{\sim}{z} + \underset{\sim}{a} \tag{6.2}$$

for some constant vector $\underset{\sim}{a}$. (This is, in fact, a canonical transformation.) Then substituting (6.2) into (6.1) gives

$$H(\underset{\sim}{z}) = H(\underset{\sim}{z}+\underset{\sim}{a}) \tag{6.3}$$

which, taken at face value, says that H is periodic with period $\underset{\sim}{a}$. This is, of course, nonsense.

The problem is that when we made the substitution, we were treating the independent variable of H, not as a set of geometrical points, but rather as n-tuples of numbers. The contradiction arose because we have used two interpretations of the independent variable in one breath, so to speak. Since we have here two points of view, which are in danger of being confused, it is important that we commit ourselves to one or the other, as convenient, and to be alert to the possibility of confusion.

In work with near-identity canonical transformations, it turns out to be most convenient to adopt the convention that the independent variables of phase functions are n-tuples (really 2N-tuples) of numbers. According

to this interpretation, equation (6.1) has the following meaning: There exist two 2N-tuples, $\underset{\sim}{z}$ and $\underset{\sim}{z}'$, for which the function H takes on the same value. Clearly, this meaning is not the intent of the transformation law. To state the transformation law according to our convention for interpretation of independent variables, we must use a different symbol for the new Hamiltonian, because it is a distinct function. In this regard, we may consider (3.19), which we reproduce here:

$$K(\underset{\sim}{z}') = K(\underset{\sim}{z}'(\underset{\sim}{z})) = H(\underset{\sim}{z}) \tag{6.4}$$

An important thing to observe is that the coordinate transformation $\underset{\sim}{z} \to \underset{\sim}{z}'$ has caused the function H to be transformed into a new and distinct function K.

Since we are treating the independent variables of phase functions as 2N-tuples of numbers, and not as geometrical points, we can no longer think of a function as the name of a value. Instead, it is better to keep in mind the precise mathematical definition of the word "function": A function is a mapping from one set to another. The former set is called the domain, and the image of the domain in the latter set is called the range. For phase functions, the domain is the set $\mathbb{R}^{2N}$; there may also be additional parameters, such as time. In this paper we use the word "function" in the mathematician's sense*, which may be succinctly contrasted with the physicist's use of the word by saying that a function is a <u>mapping</u>, and not a <u>value</u>.

In accordance with this usage, we shall strive, especially in this

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*The usual physicist's terminology is lurking in certain places, but never, it is hoped, where any confusion can arise.

section and the next, to carefully distinguish functions from the values of functions. For example, if H is a function, and $\underset{\sim}{z} \in \mathbb{R}^{2N}$, then $H(\underset{\sim}{z})$ is a value, i.e. a number. To be precise, a statement such as $H = H(\underset{\sim}{z})$ makes no sense; it is like equating apples and oranges. We have already violated this rule in (6.4), where we have treated $\underset{\sim}{z}'$ both as a 2N-tuple and also as a function. To be more precise, we can state the transformation law (6.4) as follows. If the function $\underset{\sim}{Z}$ is a canonical transformation, so that the image $\underset{\sim}{z}'$ of a point $\underset{\sim}{z}$ under the transformation is given by

$$\underset{\sim}{z}' = \underset{\sim}{Z}(\underset{\sim}{z}) \tag{6.5}$$

then the new Hamiltonian K is given in terms of the old Hamiltonian H by

$$K(\underset{\sim}{z}') = K(\underset{\sim}{Z}(\underset{\sim}{z})) = H(\underset{\sim}{z}) \tag{6.6}$$

We have in (6.6) an example of how relations among functions may be defined in terms of the values of functions. The simplest relation is that of equality. We say that two phase functions F and G are equal, i.e. F = G, if

$$F(\underset{\sim}{z}) = G(\underset{\sim}{z}) \tag{6.7}$$

for all $\underset{\sim}{z}$. Other operations among functions, such as addition, are defined in the obvious way. Note that in (6.6) it is not true that K = H; the loose statement that the old and new Hamiltonians are equal must be interpreted with caution.

It is important to observe that the symbol $\underset{\sim}{z}$ appearing in (6.7) is really a dummy; any other symbol for the phase space point would do as well. In this regard it is instructive to examine (5.31) and the

equations leading up to it. It may be seen that the variables $\underset{\sim}{\theta}'$, $\underset{\sim}{J}'$, while being written so as to indicate "new" variables, are really dummies. The set (5.31) could be rewritten as a set of relations among functions, as follows:

$$\begin{aligned} K_0 &= H_0 \\ K_1 &= H_1 + \frac{\partial H_0}{\partial \underset{\sim}{J}} \cdot \frac{\partial F_1}{\partial \underset{\sim}{\theta}'} \end{aligned} \tag{6.8}$$

In all the steps leading up to (5.31), functions were treated as if the independent variables were 2N-tuples of numbers, and not geometrical points. For example, $F_1(\underset{\sim}{\theta}',\underset{\sim}{J}')$ means $F_1(\underset{\sim}{\theta},\underset{\sim}{J}')$ evaluated at $\underset{\sim}{\theta}= \underset{\sim}{\theta}'$, and not $F_1(\underset{\sim}{\theta},\underset{\sim}{J}')$ re-expressed as a function of $\underset{\sim}{\theta}'$ through the relation (5.25).

Now we define a class of transformation operators, which are very useful in work with Lie series. We consider a near-identity transformation, given by $\underset{\sim}{z}' = \underset{\sim}{Z}(\underset{\sim}{z})$, and we associate with $\underset{\sim}{Z}$ a certain transformation operator, which we denote by T, which acts upon phase functions to give other phase functions. If F is a phase function, then we will represent the action of T upon F by TF, which we may call G. The operator T is defined by specifying its action upon all phase functions F, as follows. If G = TF, and T is associated with the near-identity transformation $\underset{\sim}{Z}$, then

$$G(\underset{\sim}{z}) = F(\underset{\sim}{Z}(\underset{\sim}{z})) \tag{6.9}$$

for all $\underset{\sim}{z}$. Another way to write this is

$$(TF)(\underset{\sim}{z}) = F(\underset{\sim}{Z}(\underset{\sim}{z})) \tag{6.10}$$

where the parentheses around TF mean that the operator T acts first on the function F, giving a new function, which is then evaluated at $\underset{\sim}{z}$.

Actually, since T acts on functions and not numbers, it makes no sense to evaluate first and operate with T second; nevertheless, the notation (6.10) leaves no room for confusion.

The right hand side of (6.10) has the form of the "composition" of the two functions F and Z, which is sometimes denoted in the mathematical literature by the symbol $\circ$. Thus we could write $TF = F \circ Z$. We shall not use this notation in this paper, but the importance of the composing operation should be noted. Composing two functions together to obtain a third can be used as a definition of the "multiplication" of two functions, and it is precisely this multiplication law which allows the set of all canonical transformations to be considered a group.*

We have in (6.6) an example where the T operator is useful. The transformation law for time-independent canonical transformations can be written

$$H = TK \tag{6.11}$$

This equation will be of use in the next section.

To follow our definition of the T operator perfectly rigorously, we can allow T to act only on functions, and not on numbers or phase points (i.e. 2N-tuples of numbers). Nevertheless, we are dealing with near-identity canonical transformations, and such transformations can be regarded as mappings of phase space onto itself. Hence it is sometimes convenient to think of T as the mapping itself, and to write

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*In this regard, it may be noted that the T operators form a linear representation of the group of canonical transformations. The "carrier space" of this representation, i.e. the linear vector space upon which the operators act, is the set of all phase functions.

$$\underset{\sim}{z}' = \underset{\sim}{Z}(\underset{\sim}{z}) = T\underset{\sim}{z} \tag{6.12}$$

This notation was used in (2.6), without elaboration.

To bring (6.12) into a form which is rigorously in accordance with the definition of T, we may introduce the identity function $\underset{\sim}{\mathcal{I}}$, which is defined in terms of its values as follows:

$$\underset{\sim}{\mathcal{I}}(\underset{\sim}{z}) = \underset{\sim}{z} \tag{6.13}$$

for all $\underset{\sim}{z}$. Then to be precise, we can write (6.12) as

$$T\underset{\sim}{\mathcal{I}} = \underset{\sim}{Z} \tag{6.14}$$

Although this usage may seem pedantic, it is useful in cases of confusion.

It is often useful to deal, not only with T, but also with its inverse. Now we change notation, and write $\underset{\sim}{Z}_f$ for what we have been calling $\underset{\sim}{Z}$, representing a canonical transformation. The subscript f stands for "forward"; we will write $\underset{\sim}{Z}_b$ for the inverse transformation, where b stands for "backward". Since the two transformations are inverses, we have

$$\underset{\sim}{Z}_f(\underset{\sim}{Z}_b(\underset{\sim}{z})) = \underset{\sim}{Z}_b(\underset{\sim}{Z}_f(\underset{\sim}{z})) = \underset{\sim}{z} \tag{6.15}$$

for all $\underset{\sim}{z}$. The transformation which is inverse to T, which we denote by T^{-1}, is defined by

$$(T^{-1}F)(\underset{\sim}{z}) = F(\underset{\sim}{Z}_b(\underset{\sim}{z})) \tag{6.16}$$

From this definition and from (6.15) it follows that

$$T^{-1}\,T = T\,T^{-1} = I \tag{6.17}$$

where I is the identity transformation.

Earlier in this paper, in section 3, we introduced certain operators which represent the operation of forming the Poisson bracket. These are the L operators, and their action upon a phase function produces another phase function. In this sense they are in the same family as the T operators, although they are defined quite differently. As we shall see, there is an intimate connection between the L operators and the T operators: the former are the Lie generators of the latter.

Now we state an important theorem, which will form the heart of our development of canonical transformations via their Lie generators. Suppose we have some Hamiltonian $H(\underset{\sim}{z},t)$, which we take to be time-dependent. We choose some pair of times $t = t_0$ and $t = t_1$, and we choose some initial conditions $\underset{\sim}{z} = \underset{\sim}{z}_0$ at $t = t_0$. Following the evolution of the phase point under the action of H, $\underset{\sim}{z}$ will move along a trajectory from $\underset{\sim}{z}_0$ at $t = t_0$ to a new point, which we will call $\underset{\sim}{z}_1$, at $t = t_1$. We now regard $\underset{\sim}{z}_0$ as a variable, and think of $\underset{\sim}{z}_1$ as being a function of $\underset{\sim}{z}_0$, parametrized by the two times t_0 and t_1. In accordance with our conventions for functions, we reserve the symbol $\underset{\sim}{z}_1$ for a value, and write $\underset{\sim}{Z}_f$ for the function:

$$\underset{\sim}{z}_1 = \underset{\sim}{Z}_f(\underset{\sim}{z}_0;t_0,t_1) \tag{6.18}$$

Although we are using the symbol $\underset{\sim}{Z}_f$, which was used in an earlier paragraph for a canonical transformation, we are here not assuming that $\underset{\sim}{Z}_f$ is canonical. This is, however, exactly the point of the theorem in question. The theorem states: For any Hamiltonian $H(\underset{\sim}{z},t)$ and for any pair of times t_0 and t_1, the transformation $\underset{\sim}{z}_0 \to \underset{\sim}{z}_1$, given by (6.18), is a canonical transformation. In other words, Hamiltonian flows in phase

space generate canonical transformations.

In order to prove this theorem, we first prove a weaker version, namely that the transformation (6.18) is canonical for infinitesimal time differences t_1-t_0. We set $\Delta t = t_1-t_0$, and assume that Δt is small. Then, by using the equations of motion (3.7) and a power series expansion in Δt, such as was developed in equation (4.4), we can write

$$\underset{\sim}{z}_1 = \underset{\sim}{z}_0 + \Delta t\{\underset{\sim}{z}_0, H(\underset{\sim}{z}_0, t_0)\} + O(\Delta t^2) \tag{6.19}$$

We prove that (6.19) is canonical by appealing directly to the definition, (3.14). Taking the variables $\underset{\sim}{z}_0$ as the variables with respect to which derivatives are formed in the Poisson brackets, we have

$$\begin{aligned}\{z_{1i}, z_{1j}\} = \{z_{0i}, z_{0j}\} \\ &+ \Delta t\{z_{0i}, \{z_{0j}, H(\underset{\sim}{z}_0, t_0)\}\} + \Delta t\{\{z_{0i}, H(\underset{\sim}{z}_0, t_0)\}, z_{0j}\} \\ &+ O(\Delta t^2)\end{aligned} \tag{6.20}$$

The first term gives γ_{ij}, and for the other two terms we can use the Jacobi identity (3.8d) to write

$$\begin{aligned}\{z_{1i}, z_{1j}\} &= \gamma_{ij} - \Delta t\{\gamma_{ij}, H(\underset{\sim}{z}_0, t_0)\} + O(\Delta t^2) \\ &= \gamma_{ij} + O(\Delta t^2)\end{aligned} \tag{6.21}$$

The term in Δt vanishes, since the γ_{ij} are constants. Hence the transformation (6.19) is canonical through $O(\Delta t)$.

Now let us consider finite time differences. We change notation a bit, and write t for t_1 and $\underset{\sim}{z}$ for $\underset{\sim}{z}_1$, and we will define τ by $\tau = t_1-t_0$. We do not assume that τ is small. Then (6.18) becomes

$$\underset{\sim}{z} = \underset{\sim}{Z}_f(\underset{\sim}{z}_0; t_0, t_0+\tau) \tag{6.22}$$

where $t = t_0+\tau$. Corresponding to this transformation we have an operator T, which we write as $T(t_0,t)$ or $T(t_0,t_0+\tau)$ to show the parametric dependence on the times. T may be thought of as an evolution operator or a propagator.

We consider some time t' intermediate between t_0 and $t = t_0+\tau$, i.e. $t_0<t'<t$. Then it is evident, by compounding two partial evolutions, that

$$T(t_0,t) = T(t',t)T(t_0,t') \tag{6.23}$$

Note the order of the factors; the right-most operator propagates the system from t_0 to t', and then the left-most operator propagates it from t' to t.

We can go further than this. Let us divide the time interval $\tau= t-t_0$ into a large number n of small time intervals of duration Δt:

$$\Delta t = \tau/n \tag{6.24}$$

We denote the k-th time value by t_k, given by

$$t_k = t_0 + k\Delta t, \qquad k = 1,\ldots,n \tag{6.25}$$

Then we have, in analogy to (6.23),

$$T(t_0,t) = T(t_{n-1},t)T(t_{n-2},t_{n-1}) \ldots T(t_1,t_2)T(t_0,t_1) \tag{6.26}$$

Now we let n become very large. According to (6.21), each of the factors in (6.26) is canonical with an error at worst of order Δt^2, i.e. $O(1/n^2)$. Since the product of any two canonical transformations is canonical, and since there are n factors in (6.26), the overall transformation is canonical with an error at worst of order 1/n. But n may be made arbitrarily large, so the whole transformation $T(t_0,t_0+\tau)$ is canonical.

This complete our proof of the theorem. The proof is not rigorous, but it conveys the right idea.

In perturbation theory we are interested in near-identity canonical transformations, and one of the virtues of the Lie transform method is its relative simplicity when dealing with higher order (i.e. second and beyond) perturbations. Therefore we will now carry out the expansion (6.19) through second order.

To be systematic about this, we follow the same steps as we did in deriving (4.4). We shuffle notation again, letting $\underset{\sim}{z}$ be a phase point at $t = t_0$, and $\underset{\sim}{z}'$ the new point at time t. We use this notation because we are thinking of a canonical transformation in the form $\underset{\sim}{z} \to \underset{\sim}{z}'$. Hence we will have

$$\underset{\sim}{z}' = \underset{\sim}{Z}_f(\underset{\sim}{z};t_0,t) \tag{6.27}$$

for the canonical transformation; we want to expand this in powers of $\tau = t-t_0$.

To do this we need the various derivatives of $\underset{\sim}{Z}_f$ with respect to t, evaluated at $t = t_0$. These derivatives we denote by $\dot{\underset{\sim}{z}}$, $\ddot{\underset{\sim}{z}}$, etc. The first derivative is given by the equations of motion:

$$\dot{\underset{\sim}{z}}(t) = -\{H(\underset{\sim}{z},t),\underset{\sim}{z}\} \tag{6.28}$$

Here we have reversed the order of the terms in the Poisson bracket for future notational convenience. The second derivative is obtained by differentiating (6.28):

$$\ddot{\underset{\sim}{z}}(t) = -\{\frac{\partial H}{\partial t}(\underset{\sim}{z},t),\underset{\sim}{z}\} + \{H(\underset{\sim}{z},t),\{H(\underset{\sim}{z},t),\underset{\sim}{z}\}\} \tag{6.29}$$

These two equations should be compared to (4.1) and (4.2).

We take these two equations, set $t=t_0$, and then substitute them into the Taylor series expansion,

$$\underset{\sim}{z}(t) = \underset{\sim}{z}(t_0) + \tau\dot{\underset{\sim}{z}}(t_0) + \frac{\tau^2}{2!}\ddot{\underset{\sim}{z}}(t_0) + O(\tau^3) \tag{6.30}$$

Here we are calling $\underset{\sim}{z}(t_0)$ simply $\underset{\sim}{z}$ and we are representing $\underset{\sim}{z}(t)$ by $\underset{\sim}{z}'$. Altogether this gives

$$\begin{aligned}\underset{\sim}{z}' = \; & \underset{\sim}{z} - \tau\{H(\underset{\sim}{z},t_0), \underset{\sim}{z}\} \\ & + \frac{\tau^2}{2!}\left[-\left\{\frac{\partial H}{\partial t}(\underset{\sim}{z},t_0), \underset{\sim}{z}\right\} + \{H(\underset{\sim}{z},t_0),\{H(\underset{\sim}{z},t_0), \underset{\sim}{z}\}\}\right] \\ & + O(\tau^3)\end{aligned} \tag{6.31}$$

According to the theorem above, the transformation (6.31) is canonical to all orders, for all functions $H(\underset{\sim}{z},t)$. It is clear that the process we have used to derive (6.31) can be carried to arbitrary order. Now we want to modify the notation in the expression (6.31) in various ways.

First, let us define a sequence of functions H_0, H_1, ..., etc., by expanding H itself about $t=t_0$:

$$H(\underset{\sim}{z},t) = \sum_{n=0}^{\infty} \tau^n H_n(\underset{\sim}{z}) \tag{6.32}$$

We have chosen to absorb the n! denominators into the definition of the H_n, so that

$$H_n(\underset{\sim}{z}) = \frac{1}{n!}\frac{\partial^n H}{\partial t^n}(\underset{\sim}{z},t_0) \tag{6.33}$$

Eliminating H in (6.31) in favor of the H_n gives

$$\begin{aligned} \underset{\sim}{z}' &= \underset{\sim}{z} - \tau\{H_0, \underset{\sim}{z}\} \\ &+ \frac{\tau^2}{2!}\left[-\{H_1, \underset{\sim}{z}\} + \{H_0, \{H_0, \underset{\sim}{z}\}\}\right] \\ &+ O(\tau^3) \end{aligned} \tag{6.34}$$

Next, we will use the L operators to rewrite the Poisson brackets appearing in (6.34). This gives

$$\begin{aligned} \underset{\sim}{z}' &= \underset{\sim}{z} - \tau L_{H_0} \underset{\sim}{z} \\ &+ \frac{\tau^2}{2!}\left[-L_{H_1} + L_{H_0}^2\right] \underset{\sim}{z} \\ &+ O(\tau^3) \end{aligned} \tag{6.35}$$

We note that if we write $\underset{\sim}{z}' = T\underset{\sim}{z}$, as in (6.12), then (6.35) can be written

$$T(t_0,t)\,\underset{\sim}{z} = \left[I - \tau L_{H_0} + \frac{\tau^2}{2!}\left(-L_{H_1} + L_{H_0}^2\right) + O(\tau^3)\right]\underset{\sim}{z} \tag{6.36}$$

As noted before, this equation should be regarded as describing the action of the operators T, L_{H_0}, L_{H_1}, etc., not on the coordinates $\underset{\sim}{z}$, but rather on the identity function $\underset{\sim}{\mathcal{I}}(\underset{\sim}{z})$.

Finally, we state without proof the fact that if (6.36) holds, as an equality between the actions of two operators on the identity function $\underset{\sim}{\mathcal{I}}$, then it holds for the actions of these operators on an arbitrary function. This means, by the definition of equality of operators, that the two operators are equal. Hence we may restate (6.36) in the following

form:

$$T(t_0,t) = I - \tau L_{H_0} + \frac{\tau^2}{2!}\left(-L_{H_1} + L_{H_0}^2\right) + O(\tau^3) \tag{6.37}$$

This result establishes the connection between canonical transformations T and their Lie generators L. Often we will call the function $H(\underset{\sim}{z},t)$, which on account of (6.33) implicitly contains all the functions $H_n(\underset{\sim}{z})$, the "Lie generator". Since H is a phase function, and since it generates canonical transformations, it is analogous to the mixed-variable generating functions which were used in section 5. In contrast to those functions, however, the Lie generator, through the Lie transform series (6.37), generates canonical transformations without mixing old and new variables.

The n-th order term in (6.37) gets more and more complicated as n gets large, although there does exist a simple algorithm for generating the n-th order term. In the case of time-independent Hamiltonians, however, it is easy to write down the general term. In this case, $H = H_0$, $\frac{\partial H}{\partial t} = 0$, and equations (6.28) and (6.29) generalize into

$$\frac{d^n \underset{\sim}{z}}{dt^n}(t) = (-1)^n \{H, \{H, \ldots \{H, \underset{\sim}{z}\}\} \ldots\} \tag{6.38}$$

where the Poisson bracket is iterated n times. Using this and following the steps leading to (6.37) gives an interesting result, in which we have set $t_0=0$ for convenience:

$$T(t) = \sum_{n=0}^{\infty} \frac{(-t)^n}{n!} L_H^n = \exp(-t L_H) \tag{6.39}$$

Using (6.39) it is possible to express, at least formally, the solution $\underset{\sim}{z}(t)$ to a time-independent Hamiltonian system in terms of

the initial conditions:

$$\underset{\sim}{z}(t) = \exp(-tL_H)\ \underset{\sim}{z}_0 \tag{6.40}$$

This result is not of much practical value for finding the function $\underset{\sim}{z}(t)$, since it is really nothing more than a Taylor series expansion of $\underset{\sim}{z}(t)$ in powers of time about t=0. But it does have theoretical interest. For example, it may be compared to its quantum mechanical analog, also for a time-independent Hamiltonian:

$$|\psi(t)\rangle = \exp(-itH)\ |\psi(0)\rangle \tag{6.41}$$

In general, the connection between classical and quantum mechanics is made much more clear by the introduction of the L and T operators, although we will not elaborate on this subject here.

Let us now return to the general case of a time-dependent Hamiltonian, and consider the issue of finding the inverse of the transformation $T(t_0,t)$ given in (6.37). From the basic meaning of the evolution operators it should be evident that

$$T(t_0,t)\ T(t,t_0) = I \tag{6.42}$$

so that

$$T^{-1}(t_0,t) = T(t,t_0) \tag{6.43}$$

Hence the inverse of $T(t_0,t)$ is obtained simply by swapping t_0 and t, which will cause τ to go into $-\tau$. Nevertheless, it is not possible to invert (6.37) simply by taking $\tau \to -\tau$, because the functions H_0, H_1, etc., defined in (6.33), depend implicitly on the time t_0.

If, however, we swap t and t_0 in (6.37), i.e. set $\tau \to -\tau$, and replace H_n by H'_n, where

$$H'_n(\underset{\sim}{z}) = \frac{1}{n!}\frac{\partial^n H}{\partial t^n}(\underset{\sim}{z},t) \tag{6.44}$$

then we will obtain $T(t,t_0)$. Carrying this out gives

$$\begin{aligned} T(t,t_0) &= T^{-1}(t_0,t) \\ &= I + \tau L_{H'_0} + \frac{\tau^2}{2}\left(-L_{H'_1} + L^2_{H'_0}\right) + O(\tau^3) \end{aligned} \tag{6.45}$$

This is not the most convenient form for $T^{-1}(t_0,t)$, since the forward transformation $T(t_0,t)$ is given in terms of one set of Lie operators, L_{H_0}, L_{H_1}, etc., whereas the inverse is expressed in terms of another set, $L_{H'_0}$, $L_{H'_1}$, etc. Therefore we choose to express $L_{H'_n}$ in terms of L_{H_n}, and to rewrite $T^{-1}(t_0,t)$ in terms of the latter operators.

To do this, we apply the definition of H'_n, (6.44), to (6.32). After a little algebra this gives

$$H'_n = \sum_{k=n}^{\infty} \binom{k}{n} \tau^{k-n} H_k \tag{6.46}$$

Writing this out explicitly for the first two orders, we have

$$\begin{aligned} H'_0 &= H_0 + \tau H_1 + O(\tau^2) \\ H'_1 &= H_1 + O(\tau) \end{aligned} \tag{6.47}$$

Substituting this back into (6.45) then gives

$$T^{-1}(t_0,t) = I + \tau L_{H_0} + \frac{\tau^2}{2!}\left(L_{H_1} + L^2_{H_0}\right) + O(\tau^3) \tag{6.48}$$

This is the desired form for the inverse of $T(t_0,t)$.

The transformation (6.37) and its inverse (6.48) are not intended for effecting series developments in powers of time. The drawbacks of such developments were pointed out in section 4. Rather, the purpose of developing the theory of Lie generators of canonical transformations has been to employ those transformations in perturbation theory.

In the next section we will illustrate the use of Lie transforms in perturbation theory. For now, however, we will simply comment on the change in the point of view, from canonical transformations resulting from the time evolution of a Hamiltonian system, to the "ε-evolution" associated with a Lie generator. This whole theory has been developed from the standpoint of the time evolution of a Hamiltonian system purely for suggestive value. There is no mathematical reason why t should be interpreted as time, or H as a Hamiltonian.

To effect the change in point of view, we will henceforth denote the Lie generator by the symbol w instead of H, and we will likewise replace t by ε. We consider w to be a function of ε, and we expand w about ε=0. This corresponds to setting $t_0=0$ in the results above, and to associating both t and τ with ε. We use this expansion to define a series of functions w_1, w_2, ... , similar to H_0, H_1, ... defined in (6.33). For future notational convenience, we shift the subscripts by 1, so that w_{n+1} corresponds to H_n. Thus we have the following expansion for $w(\varepsilon)$:

$$\begin{aligned} w(\epsilon) &= w_1 + \epsilon w_2 + \epsilon^2 w_3 + \dots \\ &= \sum_{n=0}^{\infty} \epsilon^n w_{n+1} \end{aligned} \tag{6.49}$$

Finally, we abbreviate the Lie operator L_{W_n} by writing simply L_n.

Using these conventions, we can easily transcribe the transformation operator (6.37) and its inverse (6.48) into the new notation:

$$T(\varepsilon) = I - \varepsilon L_1 + \frac{1}{2}\varepsilon^2(-L_2 + L_1^2) + O(\varepsilon^3) \tag{6.50}$$

$$T^{-1}(\varepsilon) = I + \varepsilon L_1 + \frac{1}{2}\varepsilon^2(L_2 + L_1^2) + O(\varepsilon^3) \tag{6.51}$$

In the next section we will apply these formulas to perturbation theory.

We state here a rule for finding T^{-1}, given T. First, we replace L_n wherever it appears by $-L_n$. Second, we invert the order of all non-commuting L operators. The L operators do not in general commute,* as may be seen from the Jacobi identity, (3.10d). The non-commutivity of the L operators first becomes an issue at third order, where terms such as L_1L_2 appear. This must be distinguished from L_2L_1.

In this section we have developed the theory of Lie generators in a relatively <u>ad hoc</u> way. A much more elegant derivation has been summarized by Cary[5], who centers his arguments around a certain differential equation in operator space. Cary's formulas, including a Lie generator equivalent of the Hamilton-Jacobi equation, are expressed in closed form, i.e. not as a power series in ε. We turn now to the application of the Lie series to perturbation theory.

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*For two phase functions A and B, L_A and L_B commute if and only if $\{A,B\}$ is a constant.

7. Hamiltonian Perturbation Theory With Lie Transforms

Many of the basic principles of Hamiltonian perturbation theory were discussed in section 5. The main difference between this section and that one is that here we shall effect near-identity canonical transformations with Lie transforms. Hence much of the discussion of the techniques surrounding Hamiltonian perturbation theory need not and will not be repeated.

Our first object is to study the application of near-identity canonical transformations to a Hamiltonian. We will begin with the case of time-independent transformations and later generalize our results to the time-dependent case. We obtain from this study a set of formulas in tabular form which can be used in perturbation theory. Then we apply these formulas to two examples.

Let us consider a time-independent Hamiltonian H and a time-independent near-identity canonical transformation $\underset{\sim}{z} \to \underset{\sim}{z}'$, given by the function $\underset{\sim}{Z}$:

$$\underset{\sim}{z}' = \underset{\sim}{Z}(\underset{\sim}{z}) \tag{7.1}$$

Associated with $\underset{\sim}{Z}$ is a transformation operator T according to (6.10), and by (6.11) we have

$$H = TK \tag{7.2}$$

where K is the new Hamiltonian.

Since we are usually interested in finding K, given H, we write (7.2) in the following form:

$$K = T^{-1}H \tag{7.3}$$

This equation is developed perturbatively, i.e. as a power series in ε,

as follows. First we expand both K and H in powers of ε, according to the rules

$$K = \sum_{n=0}^{\infty} \epsilon^n K_n \tag{7.4}$$

$$H = \sum_{n=0}^{\infty} \epsilon^n H_n \tag{7.5}$$

Next, we use (6.51) to expand T^{-1} in terms of the generators w_1, w_2, etc. Then, multiplying series together in (7.3) and collecting terms, order by order, gives a hierarchy of equations, which we tabulate here through $O(\varepsilon^2)$:

$$K_0 = H_0 \tag{7.6a}$$

$$K_1 = H_1 + L_1 H_0 \tag{7.6b}$$

$$K_2 = H_2 + L_1 H_1 + \frac{1}{2}(L_2 + L_1^2) H_0 \tag{7.6c}$$

The first equation, (7.6a), says that the old and new Hamiltonians are equal at order zero. This is not surprising.

The $O(\varepsilon)$ equation, (7.6b), is a partial differential equation for the Lie generator w_1 in terms of the known function H_1 and the function K_1, which is to be determined. To see this, note that the term $L_1 H_0$ can be written

$$L_1 H_0 = \{ w_1, H_0 \} = \frac{\partial w_1}{\partial \underset{\approx}{\xi}} \cdot \underset{\approx}{\gamma} \cdot \frac{\partial H_0}{\partial \underset{\approx}{\xi}} \tag{7.7}$$

In fact, since we are assuming that the transformation T, and hence the generators w_n, are independent of time, it may be seen that $L_1 H_0$ is nothing more than the total time derivative of w_1, taken with respect to the unperturbed Hamiltonian H_0. We will denote this time derivative

with the symbol D_0; for a general, time-dependent function $f(\underset{\sim}{z},t)$, we have, by definition,

$$D_0 f = \frac{\partial f}{\partial t} + \{f,H_0\} \tag{7.8}$$

Since w_1 does not depend explicitly on time, we can apply (7.8) to (7.6b) to get

$$D_0 w_1 = K_1 - H_1 \tag{7.9}$$

Equation (7.9) is a first-order, linear, partial differential equation for w_1. Appendix A summarizes the theory of such equations; for our purposes here we simply note that the solution w_1 can always be found, by the process of "integrating along unperturbed trajectories". Our ability to solve (7.9) for w_1 depends critically on our ability to solve the unperturbed system.

The importance of the D_0 operator is such that we wish to eliminate all Poisson brackets with H_0 and replace them with the D_0 notation. This step is only a matter of convenience, and the real reason for doing it will be seen later when we take up the case of time-dependent transformations. For the time being we may take the desirability of this step on faith, and rewrite (7.6) as follows:

$$K_0 = H_0 \tag{7.10a}$$

$$K_1 = H_1 + D_0 w_1 \tag{7.10b}$$

$$K_2 = H_2 + L_1 H_1 + \frac{1}{2}(D_0 w_2 + L_1 D_0 w_1) \tag{7.10c}$$

Finally, we take each equation at order n in the hierarchy, and use

equations of lower order to eliminate the terms in $D_0 w_k$ for $k < n$. We bring the term in $D_0 w_n$ to the left hand side. This gives

$$0 = K_0 - H_0 \tag{7.11a}$$

$$D_0 w_1 = K_1 - H_1 \tag{7.11b}$$

$$D_0 w_2 = 2(K_2 - H_2) - L_1(H_1 + K_1) \tag{7.11c}$$

The hierarchy is written in this form because we will want to regard the equations as inhomogeneous linear differential equations for the w_n, which will be solved in an iterative process.

Before applying these results to perturbation theory, let us extend them to the case of time-dependent canonical transformations. If the canonical transformation is expressed in terms of its mixed-variable generating function S, then the transformation law relating old and new Hamiltonians is given by (3.22), which is in contrast to (3.19) or (7.2) for time-independent transformations. Our object now is to develop a formula analogous to (3.22) for the Lie generator.

There are several strategies for doing this. One would be to express S in terms of w, and then use (3.22). The mixed-variable nature of S, however, makes this approach very awkward. A rather elegant method is given by Cary,[5] who works with an equation involving derivatives of the T operators with respect to both t and ε parameters. Here we shall take a more simple-minded approach, which is to imbed a time-dependent Hamiltonian system of N degrees of freedom in a time-independent, i.e. autonomous, Hamiltonian system of N+1 degrees of freedom. We shall call the latter system the "extended system". Since the extended system is

autonomous, we can use the formulas (7.11). We then examine what these formulas, for the extended system, imply for the original system.

The imbedding process we describe here is common in studies of differential equations, the object being to take a non-autonomous system and to make it autonomous by going to a phase space of larger dimensionality. We suppose that we have some Hamiltonian $H(\underset{\sim}{z},t)$ of N degrees of freedom, with $\underset{\sim}{z}$ representing $(q_1,\ldots q_N,p_1,\ldots,p_N)$. Then we consider a new phase space of N+1 degrees of freedom, whose coordinates $\underset{\sim}{\mathcal{Z}}$ are given by $(q_1,\ldots,q_N,t,p_1,\ldots,p_N,h)$. In the extended space, t does not represent time, but rather one of the coordinates; it is effectively q_{N+1}. Likewise, h is not a phase function, but rather a generalized momentum; it is effectively p_{N+1}. We will use script symbols, such as $\underset{\sim}{\mathcal{Z}}$, for quantities referring to the extended phase space.

We would like to find, in the extended phase space, a Hamiltonian $\mathcal{H}$ which gives autonomous equations of motion which are equivalent to the non-autonomous equations of motion generated by H in the original phase space. Such a Hamiltonian exists, and it may be taken to be

$$\mathcal{H}(\underset{\sim}{\mathcal{Z}}) = \mathcal{H}(\underset{\sim}{q},t,\underset{\sim}{p},h) = H(\underset{\sim}{q},\underset{\sim}{p},t) + h \tag{7.12}$$

The flow generated by $\mathcal{H}$ in the extended phase space will be characterized by a time-like parameter, which we call s. This whole construction is simply a mathematical artifice, so we need not attach any physical significance to s. The equations of motion generated by (7.12) are autonomous, because $\mathcal{H}$ has no explicit dependence on s. Hence the transformation formulas developed in this section can be applied to $\mathcal{H}$, if the operations are taken in the extended phase space.

First we write down the equations of motion resulting from $\mathcal{H}$ in the extended space. These are

$$\frac{d\underset{\sim}{q}}{ds} = \frac{\partial \mathcal{H}}{\partial \underset{\sim}{p}}(\underset{\sim}{z}) = \frac{\partial H}{\partial \underset{\sim}{p}}(\underset{\sim}{\xi},t) \tag{7.13a}$$

$$\frac{d\underset{\sim}{p}}{ds} = -\frac{\partial \mathcal{H}}{\partial \underset{\sim}{q}}(\underset{\sim}{z}) = -\frac{\partial H}{\partial \underset{\sim}{q}}(\underset{\sim}{\xi},t) \tag{7.13b}$$

$$\frac{dt}{ds} = \frac{\partial \mathcal{H}}{\partial h}(\underset{\sim}{z}) = 1 \tag{7.13c}$$

$$\frac{dh}{ds} = -\frac{\partial \mathcal{H}}{\partial t}(\underset{\sim}{z}) = -\frac{\partial H}{\partial t}(\underset{\sim}{\xi},t) \tag{7.13d}$$

From (7.13c) we have dt = ds, so (7.13a) and (7.13b) are the same equations of motion, with t as the independent variable, as the Hamiltonian H generates in the original phase space.

Now let us suppose that H is expanded as a power series in ε, as in (7.5). We allow each of the terms H_n, including H_0, to depend on time. We associate with this expansion a similar expansion of $\mathcal{H}$, by defining

$$\mathcal{H}_0(\underset{\sim}{z}) = H_0(\underset{\sim}{\xi},t) + h \tag{7.14a}$$

$$\mathcal{H}_n(\underset{\sim}{z}) = H_n(\underset{\sim}{\xi},t) \ , \quad n > 0 \tag{7.14b}$$

Hence, of all the $\mathcal{H}_n$, only $\mathcal{H}_0$ depends on the variable h.

This expansion allows us to apply a Lie transform to $\mathcal{H}$ and to obtain a new Hamiltonian $\mathcal{K}$ in the extended phase space. Let us be careful as to what this means. The Lie transform corresponds to a certain s-independent canonical transformation in the extended phase space, which we

denote by $\mathcal{T}$. Hence we will have

$$\mathcal{K} = \mathcal{T}^{-1}\mathcal{H} \tag{7.15}$$

This canonical transformation will take the variables $\underset{\sim}{\mathcal{Z}}$ into new variables $\underset{\sim}{\mathcal{Z}}'$, such that if the s-evolution of $\underset{\sim}{\mathcal{Z}}$ is given by $\mathcal{H}$, then the s-evolution of $\underset{\sim}{\mathcal{Z}}'$ is given by $\mathcal{K}$. The canonical transformation will correspond to a certain Lie generator, which will be a function of $\underset{\sim}{\mathcal{Z}}$ (and hence in general of t and h), and which will enter into the formulas (7.6) or their equivalents.

We will want to design the transformation $\mathcal{T}$ so that the variable t, which is a dynamical variable in the extended phase space, does not change under the transformation. To achieve this goal, we simply restrict ourselves to generators w which are independent of h. We do allow w to depend on $\underset{\sim}{z}$ and t, however. We do not use a script symbol for the Lie generator w, for although it is a function on the extended phase space, it can also be considered to be a time-dependent function on the original phase space.

To prove that if w is independent of h, then $\mathcal{T}$ does not change t, we must consider the Poisson bracket on the extended space. If we write $\{\ ,\ \}_{\underset{\sim}{\mathcal{Z}}}$ for the extended Poisson bracket, and simply $\{\ ,\ \}$ for the Poisson bracket in the original space, then we have, for any two functions $\mathcal{A}$ and $\mathcal{B}$ on the extended space,

$$\{\mathcal{A}, \mathcal{B}\}_{\underset{\sim}{\mathcal{Z}}} = \{\mathcal{A}, \mathcal{B}\} + \frac{\partial \mathcal{A}}{\partial t}\frac{\partial \mathcal{B}}{\partial h} - \frac{\partial \mathcal{A}}{\partial h}\frac{\partial \mathcal{B}}{\partial t} \tag{7.16}$$

Suppose now that $\mathcal{A}$ is some w_n, and independent of h, and that $\mathcal{B}$ is t. Then applying (7.16) gives

$$\{w_n, t\}_{\underset{\sim}{z}} = 0 \tag{7.17}$$

By examining (6.50), it is easy to see that

$$\mathcal{T} t = t \tag{7.18}$$

When we apply the Lie transform $\mathcal{T}$ to $\mathcal{H}$ to get the new Hamiltonian $\mathcal{K}$, we will be forming extended Poisson brackets between w_n and $\mathcal{H}_n$, as indicated by (7.6). However, of the $\mathcal{H}_n$, only $\mathcal{H}_0$ depends on h, and then in a very simple way; and w_n is independent of h. Therefore, by applying (7.16) to (7.14) we have

$$\{w_n, \mathcal{H}_0\}_{\underset{\sim}{z}} = \{w_n, H_0\} + \frac{\partial w_n}{\partial t} \tag{7.19a}$$

$$\{w_n, \mathcal{H}_m\}_{\underset{\sim}{z}} = \{w_n, \mathcal{H}_m\}, \quad m > 0 \tag{7.19b}$$

It should be noted that in (7.19a) we have the total time derivative of w_n, computed along unperturbed trajectories, including the term in $\frac{\partial w_n}{\partial t}$, for the case that w_n depends explicitly on the time.

The extended canonical transformation $\mathcal{T}$ will take the coordinates $\underset{\sim}{z}$ into new coordinates $\underset{\sim}{z}'$, which we may write as $(\underset{\sim}{q}', t', \underset{\sim}{p}', h')$ or $(\underset{\sim}{z}', t', h')$. It will also produce the new Hamiltonian $\mathcal{K}$, which will describe the s-evolution of the new coordinates $\underset{\sim}{z}'$, according to the equations of motion:

$$\frac{d\underset{\sim}{q}'}{ds} = + \frac{\partial \mathcal{K}}{\partial \underset{\sim}{p}'}(\underset{\sim}{z}') \tag{7.20a}$$

$$\frac{d\underset{\sim}{p}'}{ds} = - \frac{\partial \mathcal{K}}{\partial \underset{\sim}{q}'}(\underset{\sim}{z}') \tag{7.20b}$$

$$\frac{dt'}{ds} = + \frac{\partial \mathcal{K}}{\partial h'}(\underset{\sim}{z}') \tag{7.20c}$$

$$\frac{dh'}{ds} = - \frac{\partial \mathcal{K}}{\partial t'}(\underset{\sim}{z}') \tag{7.20d}$$

Let us consider (7.20c). Because of the restricted form we have chosen for the Lie generator w of $\mathcal{T}$, namely $\frac{\partial w}{\partial h} = 0$, we have t' = t. Also, from (7.13c) we had dt = ds. Therefore we have dt' = ds, and (7.20c) must give us

$$\frac{\partial \mathcal{K}}{\partial h'}(\underset{\sim}{z}') = 1 \tag{7.21}$$

or

$$\mathcal{K}(\underset{\sim}{z}') = h' + K(\underset{\sim}{\xi}', t') \tag{7.22}$$

for some function K. It may be guessed, although it remains to be proved, that K is the new Hamiltonian in the original phase space. This proof is, however, easy. We simply substitute (7.22) back into (7.20), to get

$$\frac{d\underset{\sim}{q}'}{ds} = \frac{\partial K}{\partial \underset{\sim}{p}'}(\underset{\sim}{\xi}', t') \tag{7.23a}$$

$$\frac{d\underset{\sim}{p}'}{ds} = -\frac{\partial K}{\partial \underset{\sim}{q}'}(\underset{\sim}{\xi}', t') \tag{7.23b}$$

$$\frac{dt'}{ds} = 1 \tag{7.23c}$$

$$\frac{dh'}{ds} = -\frac{\partial K}{\partial t'}(\underset{\sim}{\xi}', t') \tag{7.23d}$$

Equation (7.23c), when substituted into (7.23a) and (7.23b), shows that the variables $\underset{\sim}{q}', \underset{\sim}{p}'$ evolve according to the Hamiltonian equations of motion, with K as the Hamiltonian and t as the independent parameter. By definition, then, K is the new Hamiltonian in the original phase space.

Now we apply formulas (7.6) for $\mathcal{T}$ taking $\mathcal{H}$ into $\mathcal{K}$. We expand both $\mathcal{K}$ and K in a power series in ε, like (7.4), and, bearing in mind the form

(7.22), we get

$$\mathcal{K}_0(\underset{\sim}{\mathcal{Z}}) = K_0(\underset{\sim}{z},t) + h \tag{7.24a}$$

$$\mathcal{K}_n(\underset{\sim}{\mathcal{Z}}) = K_n(\underset{\sim}{z},t) \tag{7.24b}$$

Here we have dropped the primes on the variables $\underset{\sim}{\mathcal{Z}}$, $\underset{\sim}{z}$, t, h. The primed variables were used in the last two paragraphs to suggest "new variables", but they are really dummies. We do this because the hierarchy (7.6) is a set of relations among functions, not values.

First let us write out (7.6) for extended phase space operations. We translate the L operators into extended Poisson bracket notation. This gives

$$\mathcal{K}_0 = \mathcal{H}_0 \tag{7.25a}$$

$$\mathcal{K}_1 = \mathcal{H}_1 + \{w_1, \mathcal{H}_0\}_{\underset{\sim}{\mathcal{Z}}} \tag{7.25b}$$

$$\mathcal{K}_2 = \mathcal{H}_2 + \{w_1, \mathcal{H}_1\}_{\underset{\sim}{\mathcal{Z}}} + \tfrac{1}{2}\{w_2, \mathcal{H}_0\}_{\underset{\sim}{\mathcal{Z}}} + \tfrac{1}{2}\{w_1, \{w_1, \mathcal{H}_0\}_{\underset{\sim}{\mathcal{Z}}}\}_{\underset{\sim}{\mathcal{Z}}} \tag{7.25c}$$

Now we use (7.14), (7.19) and (7.24) to express this in terms of operations on the original phase space. This gives

$$K_0 = H_0 \tag{7.26a}$$

$$K_1 = H_1 + \{w_1, H_0\} + \frac{\partial w_1}{\partial t} \tag{7.26b}$$

$$K_2 = H_2 + \{w_1, H_1\} + \frac{1}{2}\{w_2, H_0\} + \frac{1}{2}\frac{\partial w_2}{\partial t} + \frac{1}{2}\{w_1, \{w_1, H_0\}\} + \frac{1}{2}\{w_1, \frac{\partial w_1}{\partial t}\} \tag{7.26c}$$

These equations are the generalization of (7.6) to the case of time-dependent canonical transformations.

As we did with (7.6), let us now rewrite (7.26) in a more usable form. To do this, we introduce again the operator D_0, representing time evolution as generated by H_0. Since the w_n now depend on time, we have terms in $\frac{\partial w_n}{\partial t}$, as is indicated by (7.8). That is, we write

$$D_0 w_n = \frac{\partial w_n}{\partial t} + \{w_n, H_0\} \tag{7.27}$$

Using this to eliminate $\frac{\partial w_n}{\partial t}$ in (7.26), we get

$$K_0 = H_0 \tag{7.28a}$$

$$K_1 = H_1 + D_0 w_1 \tag{7.28b}$$

$$K_2 = H_2 + \{w_1, H_1\} + \frac{1}{2} D_0 w_2 + \frac{1}{2} \{w_1, D_0 w_1\} \tag{7.28c}$$

It may be seen that these are exactly the same as equations (7.10), except that now D_0 has a more general meaning than it did before. From this it follows that the equations (7.11) are valid for time-dependent as well as time-independent canonical transformations, if only the operator D_0 is taken to represent the total time derivative along unperturbed orbits, as shown in (7.27). This fact remains true at all orders. Therefore it is the hierarchy (7.11) which we will use for perturbation theory, including time-dependent cases.

We comment on one final point concerning our procedure for dealing with time-dependent canonical transformations. To be complete, we need to show that the s-independent canonical transformation $\mathfrak{T}$ in the extended space, when restricted to the original phase space, produces a canonical transformation T in that space. This is easy to prove, although we shall not do so.

Let us now study the application of the Lie transform formulas (7.11)

with some examples. We remark that although the formulas (7.11) are valid for an arbitrary H, nevertheless they are generally useful in a practical sense only when H has been subjected to a preparatory transformation, so that H_0 depends only on the momenta $\underset{\sim}{p}$ or actions $\underset{\sim}{J}$ (for a periodic unperturbed system).

As an example of a time-independent system, let us analyze the low energy limit of the pendulum system. We return to (5.7), from which we tabulate the following:

$$H_0(\theta,J) = \omega_0 J \tag{7.29a}$$

$$H_1(\theta,J) = -\frac{1}{48} J^2(3 - 4\cos 2\theta + \cos 4\theta) \tag{7.29b}$$

$$H_2(\theta,J) = \frac{1}{2880}\frac{J^3}{\omega_0}(10 - 15\cos 2\theta + 6\cos 4\theta - \cos 6\theta) \tag{7.29c}$$

At order zero, using (7.11a), we have simply

$$K_0(J) = \omega_0 J \tag{7.30}$$

At order one, we use (7.11b). Given the explicit form of H_0, we write out the term $D_0 w_1$:

$$D_0 w_1 = \{w_1, H_0\} = \omega_0 \frac{\partial w_1}{\partial \theta} \tag{7.31}$$

Hence (7.11b) becomes the following differential equation for w_1:

$$\omega_0 \frac{\partial w_1}{\partial \theta} = K_1 - H_1 \tag{7.32}$$

This equation should be compared to (5.45b), which we solved without much comment. Here we want to elaborate upon the method of solution.

Equation (7.32) is a single equation in two unknowns, namely w_1 and

K_1. Therefore it has no unique solution. If we choose either w_1 or K_1, then (7.32) can be solved for the other, but some such choice must be made. This makes sense: different canonical transformations (specified by w_1) give rise to different new Hamiltonians.

In solving (5.45b) we had an equivalent latitude in our choice of solution, and there we took

$$K_1(J) = \overline{H_1}(J) = -\frac{J^2}{16} \tag{7.33}$$

This choice for K_1 certainly would allow us to solve (7.32) for w_1, and it has the agreeable consequence that it causes K_1 to be independent of θ, making the equations of motion generated by K easy to solve. Nevertheless, there are many ways to make K_1 independent of θ, the simplest of which is perhaps $K_1=0$. If we made this choice for K_1, we would, in effect, "transform away" the entire perturbing term, and not just its θ-dependent part.

To see why we do not want to take $K_1=0$, we may examine (7.32), and see what would happen if we did. The solution for w_1 would be

$$w_1(\theta, J) = \frac{1}{192}\frac{J^2}{\omega_0}\left(12\theta - 8\sin 2\theta + \sin 4\theta\right) \tag{7.34}$$

The problem with this solution is the term in 12θ. Since θ has an unbounded growth in time, this term is a secular term. When we use this form for w_1 in the transformation (6.50), and apply it to the old variables (θ,J) to find the new, the secular term in w_1 would cause secular terms to appear in the transformation. This is exactly the phenomenon we observed in the method of successive approximations, and its deleterious effects

on the convergence properties of the resulting power series have already been noted. In fact it may be shown that if we choose $K_n=0$ for all $n>0$, then the result is identical to the method of successive approximations.

Therefore in solving (7.32) we adopt a double criterion: first, K_1 must be independent of θ; and second, w_1 must be free of secular terms. The first requirement says that the term in $\frac{\partial w_1}{\partial \theta}$ in (7.32) must cancel all the θ dependence of H_1; and the second requirement says that $\frac{\partial w_1}{\partial \theta}$ must contain only terms which are oscillatory in θ, since otherwise, upon integration with respect to θ, there would result secular terms. This double criterion gives a unique choice for $\frac{\partial w_1}{\partial \theta}$ and K_1, which is most conveniently expressed in terms of the averaging operator and its complement, defined in (4.33) and (4.34):

$$\omega_0 \frac{\partial w_1}{\partial \theta} = -\widetilde{H}_1 \tag{7.35}$$

$$K_1 = \overline{H}_1 \tag{7.36}$$

It turns out that this criterion also gives a unique choice for w_n and K_n at all higher orders.

Examining (7.36), we have

$$K_1(J) = -\frac{J^2}{16} \tag{7.37}$$

and the results of the method of averaging appear once again. Not only that, but if we are not interested in the actual transformation, generated by w, but only in the averaged Hamiltonian K, then we need not even solve (7.35) for w_1. A similar property persists at all orders. In order to find K through order n, it is only necessary to know w through order n-1.

Nevertheless, it is easy enough to integrate (7.35) and actually obtain w_1:*

$$w_1(\theta, J) = \frac{1}{192}\frac{J^2}{\omega_0}\left(-8\sin 2\theta + \sin 4\theta\right) \tag{7.38}$$

Now let us carry the pendulum problem to second order. We examine (7.11c), and re-express the left-hand side in the form

$$\omega_0 \frac{\partial w_2}{\partial \theta} = 2(K_2 - H_2) - L_1(H_1 + K_1) \tag{7.39}$$

We break both H_1 and H_2 into their averaged and oscillatory parts, and we use (7.36) to rewrite this as

$$\omega_0 \frac{\partial w_2}{\partial \theta} = 2\left(K_2 - \overline{H}_2 - \tilde{H}_2\right) - 2\{w_1, \overline{H}_1\} - \{w_1, \tilde{H}_1\} \tag{7.40}$$

Like (7.32), this is a single equation for two unknowns, in this case, w_2 and K_2. Applying the criteria developed above, we want to absorb all the purely oscillatory terms into $\frac{\partial w_2}{\partial \theta}$, and leave the rest to define K_2. Considering the terms on the right-hand side of (7.40), the decomposition into averaged and oscillatory parts is obvious except for the last two terms, the Poisson brackets. Now, $\{w_1, \overline{H}_1\}$ is purely oscillatory, because w_1 is purely oscillatory and because $\overline{H}_1$ is purely averaged. That is, this term is linear in purely oscillatory quantities. The term $\{w_1, \tilde{H}_1\}$, however, is quadratic in purely oscillatory quantities, so it has an averaged as well as an oscillatory part. To see this, consider $\cos\theta$, which is purely oscillatory. Then consider $\cos^2\theta$, which has an oscillatory

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*A J-dependent constant of integration could be added to this result, but it would have no effect of importance except to make all the succeeding formulas unnecessarily complicated. Such a term corresponds to a shift in origin, as a function of J, of the "nice" phase in Kruskal's rings; see Ref. 13 for details. It is best to keep only purely oscillatory terms when integrating to get w_n.

part, namely $\frac{1}{2}\cos 2\theta$, and an averaged part, namely $\frac{1}{2}$. Therefore, on taking the average of (7.40), we have

$$0 = 2\left(K_2 - \overline{H}_2\right) - \overline{\{w_1, \tilde{H}_1\}} \tag{7.41}$$

which we can also write as

$$K_2 = \overline{H}_2 + \frac{1}{2}\overline{\{w_1, \tilde{H}_1\}} \tag{7.42}$$

Likewise, on taking the oscillatory part, we have

$$\omega_0 \frac{\partial w_2}{\partial \theta} = -2\tilde{H}_2 - 2\{w_1, \overline{H}_1\} - \widetilde{\{w_1, \tilde{H}_1\}} \tag{7.43}$$

To find the second order Hamiltonian K_2, we need to evaluate the right-hand side of (7.42). Note that, in addition to the average of H_2, K_2 contains an additional term. This term is responsible for preventing the method of averaging, as it was naively developed in sections 4 and 5, from being valid at second order. This term is a kind of non-linear effect, since it is quadratic in first order quantities. In fact, since it is the average of a term which is quadratic in first order quantities, it represents a zero frequency beat. To explicitly evaluate K_2, we first work out the Poisson bracket $\{w_1, \tilde{H}_1\}$; this requires a little algebra, which gives

$$\{w_1, \tilde{H}_1\} = -\frac{1}{1152}\frac{J^3}{\omega_0}\left(17 - 9\cos 2\theta + \cos 6\theta\right) \tag{7.44}$$

Substituting this into (7.42), we have

$$K_2(J) = -\frac{1}{256}\frac{J^3}{\omega_0} \tag{7.45}$$

Note that in order to find K_2, we needed w_1, but not w_2. Now (7.30), (7.37) and (7.45) can be combined to give

$$K(J) = \omega_0 J \left[1 - \frac{\epsilon}{16}\left(\frac{J}{\omega_0}\right) - \frac{\epsilon^2}{256}\left(\frac{J}{\omega_0}\right)^2 + O(\epsilon^3)\right] \tag{7.46}$$

From this it is easy to obtain the second order correction to the frequency:

$$\omega = \omega_0 \left[1 - \frac{\epsilon}{8}\left(\frac{J}{\omega_0}\right) - \frac{3\epsilon^2}{256}\left(\frac{J}{\omega_0}\right)^2 + O(\epsilon^3)\right] \tag{7.47}$$

The expansions (7.46) and (7.47) are actually convergent series for ε in some neighborhood of $\varepsilon=0$, and they are connected with certain elliptic integrals.

Now let us look at (7.43), the equation for w_2. Working out the right hand side gives

$$\omega_0 \frac{\partial w_2}{\partial \theta} = \frac{1}{1920}\frac{J^3}{\omega_0}\left(-35\cos 2\theta + 2\cos 4\theta + 3\cos 6\theta\right) \tag{7.48}$$

Upon integration, this yields

$$w_2(\theta, J) = \frac{1}{3840}\frac{J^3}{\omega_0^2}\left(-35\sin 2\theta + \sin 4\theta + \sin 6\theta\right) \tag{7.49}$$

This result, combined with (7.38), can be used to compute the canonical transformation $\underset{\sim}{z} \to \underset{\sim}{z}'$ explicitly. The results are not very illuminating, so we will not do this here. Nevertheless, it is worthwhile to note that if the explicit form of the transformation is not required, then it need not be worked out. This circumstance is a characteristic feature of Hamiltonian perturbation theory; it is not shared by non-Hamiltonian perturbation methods. Similarly, it may be noted that if a phase function (or perhaps a phase space density function, representing an ensemble) is to be transformed from the old to the new coordinates, then the Lie

operators in (6.50) or (6.51) can be applied directly to the function. It is, even in this case, not necessary to work out the transformation explicitly. This circumstance is a feature of the Lie transform method, and it is not shared by traditional Hamiltonian methods, such as the Poincaré-Von Zeipel method.

Although we have not worked out the transformation $\underset{\sim}{z} \to \underset{\sim}{z}'$, it is easy to see, from the fact that the w_n are purely oscillatory, that the transformation will have the form of a Fourier series in the angle θ or θ'. For example, if we express the old angle θ as a function of the new variables (θ',J'), as we show here in terms of the function Θ,

$$\theta = \theta' + \Theta(\theta',J') \tag{7.50}$$

then Θ will be a Fourier series in θ':

$$\Theta(\theta',J') = \sum_{n=-\infty}^{+\infty} \Theta_n(J')\, e^{in\theta'} \tag{7.51}$$

The Fourier coefficients Θ_n will be power series in ε, whose first few terms can be worked out using (7.38) and (7.49). We are guaranteed of a transformation of this form, since we have banished secular terms from the functions w_n. Since the angle θ' evolves linearly in time with a frequency ω, given by (7.47), we see that the solution $\theta(t)$ for the original angle variable is expanded in a Fourier series in time which employs the true frequency. The use of the true frequency ω in this expansion, rather than the unperturbed frequency ω_0, is the reason for referring to this perturbation method as a "frequency renormalization" technique.

We will now study a time-dependent system, and subject it to a perturbation analysis. The system we choose consists of a charged particle

which is free except for the effects of a small amplitude electrostatic wave. We let m and e be the mass and charge of the particle, and we let ϕ_0, k and ω be the amplitude, wave number, and frequency, respectively, of the wave. We treat this problem in one dimension, and we assume that the amplitude ϕ_0 is a constant. The Hamiltonian for this system can be written as

$$H(x,p,t) = \frac{1}{2m}p^2 + \epsilon e \phi_0 \cos(kx - \omega t) \tag{7.52}$$

A parameter of smallness ε has been introduced in (7.52) to indicate the perturbing term. This Hamiltonian gives the following sequence for H_n

$$H_0(x,p,t) = \frac{1}{2m}p^2 \tag{7.53a}$$

$$H_1(x,p,t) = e\phi_0 \cos(kx - \omega t) \tag{7.53b}$$

$$H_n = 0, \quad n > 1 \tag{7.53c}$$

Before applying the perturbation formulas (7.11), we must select a strategy for the perturbation analysis. In the previous example studied, the low energy limit of the pendulum, we chose the canonical transformation so that K would be independent of the generalized coordinate θ. Here we choose, in accordance with the averaging discussion in section 5, to eliminate the time dependence from K. In general, one would expect the resulting K to depend upon x, even after the time dependence is gone. Hence the new Hamiltonian K may well not be solvable, although it will certainly be simpler to deal with than H. It will turn out, however, for the Hamiltonian (7.53), that this general expectation is not borne out, and that when t is eliminated by the canonical transformation, then

x goes with it. For this reason, (7.53) is a very special case of time-dependent systems.

When we apply (7.11) to (7.53), we get, first, $K_0 = H_0$, as always. At order one we face, once again, the issue of determining criteria to make the choice for w_1 and K_1. The order one equation, from (7.11b), is

$$(D_0 w_1)(x,p,t) = K_1(x,p,t) - e\phi_0 \cos(kx - \omega t) \tag{7.54}$$

In order to make K_1 independent of t, the term in $D_0 w_1$ must cancel the time dependence on the right hand side. Since the perturbing term is periodic in time, we argue on analogy to the discussion surrounding (7.32), and we choose the term in $D_0 w_1$ to cancel the purely oscillatory part of the right hand side and no more. Thus w_1 itself will be purely oscillatory in time, and it will contain no secular terms. In this case the definition we choose for the averaging operator is given by (5.19). Note in particular that it ignores the coordinate x.

Applying these criteria, we get immediately from (7.54)

$$K_1 = 0 \tag{7.55}$$

This result was already noted in chapter 5. Intuitively, it is easy to see why the first order effects of the wave on the particle average to zero. As the particle moves with its velocity p/m and as the wave moves with its phase velocity ω/k, the particle will slide up and down the potential of the wave, first being accelerated as it goes downhill, and then being decelerated as it climbs uphill again. On the average, at least to first order, these two effects will cancel, and we get (7.55). This argument breaks down, however, if the particle is in resonance or

near resonance with the wave, a case we will consider later.

Now we consider the equation for w_1. Writing out $D_0 w_1$ according to (7.27), we have

$$D_0 w_1 = \frac{\partial w_1}{\partial t} + \frac{p}{m}\frac{\partial w_1}{\partial x} \tag{7.56}$$

Hence we need to solve the equation

$$\frac{\partial w_1}{\partial t}(x,p,t) + \frac{p}{m}\frac{\partial w_1}{\partial x}(x,p,t) = -e\phi_0 \cos(kx - \omega t) \tag{7.57}$$

The theory of equations of this type is given in Appendix A; the solution is easily found to be

$$w_1(x,p,t) = -\frac{e\phi_0}{\left(\frac{kp}{m} - \omega\right)} \sin(kx - \omega t) \tag{7.58}$$

As desired, w_1 is purely oscillatory in time.

Let us move on to the second order terms. Examining (7.11c) and using (7.55), we have

$$K_2 = \frac{1}{2}\overline{\{w_1, H_1\}} \tag{7.59}$$

and

$$D_0 w_2 = -\widetilde{\{w_1, H_1\}} \tag{7.60}$$

We will not solve (7.60), although it is easy to do so; instead we just work out K_2 using (7.53b) and (7.58):

$$K_2(p) = \frac{e^2 E_0^2}{4m\left(\frac{kp}{m} - \omega\right)^2} \tag{7.61}$$

where we have set $E_0 = k\phi_0$, representing the amplitude of the electric field. Altogether, then, we have for K,

$$K(p) = \frac{p^2}{2m} + \epsilon^2 \frac{e^2 E_0^2}{4m\left(\frac{kp}{m} - \omega\right)^2} + O(\epsilon^3) \tag{7.62}$$

The second order term is the "ponderomotive" term; as predicted above, it is not only independent of t, but also of x. There is an important generalization of the ponderomotive term which appears in certain applications. In our original Hamiltonian (7.52), the amplitude of the wave ϕ_0 was taken to be a constant. If instead this amplitude is taken to be a slowly varying function of x, which we may write as $\phi(\lambda x)$ for some $\lambda \ll 1$, then, in a certain approximation, the averaged Hamiltonian K becomes

$$K(x,p) = \frac{p^2}{2m} + \epsilon^2 \frac{e^2 \left(E(\lambda x)\right)^2}{4m\left(\frac{kp}{m} - \omega\right)^2} \tag{7.63}$$

Now the ponderomotive term does have a dependence on x, giving it the mathematical form of a potential energy. Hence this term is sometimes called the "ponderomotive potential". Its effect is to repel the particle, regardless of the sign of its charge, from regions of high field strength.

Consider now the denominators appearing in the expressions for w_1 and K_2. It is not hard to see that the quantity

$$\omega_D = \omega - kp/m \tag{7.64}$$

is the Doppler shifted frequency of the wave, as seen by the moving particle. Hence this denominator is small if the particle is nearly in resonance with the wave, and for exact resonance, the denominator vanishes. For a nearly resonant particle, we would expect the convergence of the series

(7.62) to be put in jeopardy, and this is, in fact, exactly the case.

The series (7.62) has a certain circle of convergence in ε space, centered about $\varepsilon=0$, and the radius of convergence is a function of ω_D, and hence of p. This radius of convergence goes to zero as ω_D goes to zero, as might be expected. An equivalent way of stating this is to say that for fixed ε (such as $\varepsilon=1$) there will be a region of phase space for which the series (7.62) does not converge. This region has the form of an interval surrounding the resonance value of the momentum, namely $p = m\omega/k$, and it is called the "trapping region". If the dynamics of the particle are to be understood in the trapping region, then another approximation scheme, apart from (7.52), must be used.

Many of the qualitative features of the Hamiltonian (7.52) can be understood by subjecting it to a certain closed-form canonical transformation. This transformation is generated by the following mixed-variable generating function:

$$S(x,p',t) = xp' + \frac{m\omega}{k}x - \frac{\omega t}{k}p' - \frac{m\omega^2}{2k^2}t \qquad (7.65)$$

When the Hamiltonian (7.52) is transformed by this canonical transformation, there results, apart from various constant factors, exactly the pendulum Hamiltonian. Physically, (7.65) corresponds to going to a frame of reference moving with the wave, and hence it causes the new Hamiltonian to be time-independent.

The phenomenon of resonances is a pervasive one with systems of more than one degree of freedom, or with time-dependent systems of one or more degrees of freedom. The convergence of the perturbative series is put very much in doubt by resonances, although the series may still be

computationally useful for long periods of time. In general, a near-resonance will mean, if not a complete invalidation of the series, then at least the presence of long-period terms whose amplitude is larger than would be expected according to the ε-ordering. For example, the planets Jupiter and Saturn are nearly in a 2-5 resonance, and associated with this near-resonance are large mutual perturbations with a period of about 1000 years.

Sometimes there may be several resonant regions of phase space. For example, a particle moving in the presence of two waves may be in resonance with one wave but not the other. In cases like this, it may be desirable to transform away the non-resonant terms, but to keep the resonant ones. The result will be a Hamiltonian K which still depends on time, but which has a simpler dependence than the original Hamiltonian. This case illustrates how Lie transforms can be used to achieve a variety of goals, depending on the circumstances.

Appendix A. Integrating Along Unperturbed Trajectories

In Hamiltonian perturbation theory we are often called upon to solve differential equations of the form

$$\frac{\partial f}{\partial t} + \{f, H_0\} = g \tag{A.1}$$

for the unknown function f. It is assumed that H_0 and g are given; the functions f and g may depend on time, but we assume that H_0 does not. (This latter assumption is not essential.) H_0 is the unperturbed Hamiltonian, and f usually represents a Lie generator. We are usually not interested in the general solution for f, but only in a particular solution with certain properties, such as the property of being purely oscillatory.

The equation (A.1) is a first order, linear, inhomogeneous partial differential equation for f. The theory of such equations is given in detail in Ref. 19; here we develop only those properties we need.

The left-hand side of (A.1) has the form of a convective derivative:

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{2N} \dot{z}_i \frac{\partial f}{\partial z_i} = g \tag{A.2}$$

where

$$\dot{z}_i = \{z_i, H_0\} \tag{A.3}$$

The solution to the partial differential equation (A.2) is conveniently expressed in terms of the solution to the system of ordinary differential equations (A.3). These ordinary differential equations are the equations of motion for the unperturbed Hamiltonian, which are solvable by hypothesis. These equations generate the unperturbed trajectories in phase space, which are called the <u>characteristics</u> of the partial differential equation (A.2).

Since the unperturbed system is solvable, it is possible to find the functions $\underset{\sim}{Z}_f$, representing the forward time evolution of the unperturbed system. These functions give $\underset{\sim}{z}$ as a function of t and the initial conditions $\underset{\sim}{z}_0$, which we assume are evaluated at t=0:

$$\underset{\sim}{z} = \underset{\sim}{Z}_f(\underset{\sim}{z}_0,t) \tag{A.4}$$

Likewise, it is possible to invert these functions and find the backwards evolution functions, $\underset{\sim}{Z}_b$:

$$\underset{\sim}{z}_0 = \underset{\sim}{Z}_b(\underset{\sim}{z},t) \tag{A.5}$$

To find the solution f to (A.1) or (A.2), the following prescription may be used. First, express the function g, assumed to be time-dependent, in terms of the variable t' and the initial conditions $\underset{\sim}{z}_0$, to give a new function G, as follows:

$$G(\underset{\sim}{z}_0,t') = g(\underset{\sim}{Z}_f(\underset{\sim}{z}_0,t'),t') \tag{A.6}$$

Second, integrate G with respect to t' with t'=t as an upper limit. The lower limit is unspecified, and may be taken in the sense of an indefinite integral. This gives a function F:

$$F(\underset{\sim}{z}_0,t) = \int^t dt'\, G(\underset{\sim}{z}_0,t') = \int^t dt'\, g(\underset{\sim}{Z}_f(\underset{\sim}{z}_0,t'),t') \tag{A.7}$$

The form of this integral suggests the expression, "integrating along unperturbed trajectories". Third and finally, use the functions $\underset{\sim}{Z}_b$, given in (A.5), to express the $\underset{\sim}{z}_0$ dependence of F in terms of $\underset{\sim}{z}$ and t. This gives

the solution f:

$$f(\underset{\sim}{z},t) = F(\underset{\sim}{Z}_b(\underset{\sim}{z},t),t) = \int^t dt'\, G(\underset{\sim}{Z}_b(\underset{\sim}{z},t),t')$$

$$= \int^t dt'\, g(\underset{\sim}{Z}_f(\underset{\sim}{Z}_b(\underset{\sim}{z},t),t'),t') \tag{A.8}$$

The last integral in (A.8) can be re-expressed in some other useful forms by compounding partial evolutions. This last step depends on the time-independence of H_0, and it gives

$$f(\underset{\sim}{z},t) = \int^t dt'\, g(\underset{\sim}{Z}_f(\underset{\sim}{z},t'-t),t')$$

$$= \int^0 d\tau\, g(\underset{\sim}{Z}_f(\underset{\sim}{z},\tau),t+\tau) \tag{A.9}$$

In the last integral we have set $\tau = t'-t$.

The fact that (A.9) or (A.8) satisfies (A.2) may be verified by direct substitution.

0 0 0 0 0 0 4 7 4 0 3

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Problems on Lie Transforms.

Problems 1 through 4 are designed as a review of some relevant features of Hamiltonian mechanics. If you are familiar enough with the material that these problems are trivial, then simply state "trivial".

1. Show that the product of two canonical transformations is canonical. Use the definition of canonical transformation in the form (3.14).

2. In deriving (6.29) from (6.28), the following theorem has been used. Given three phase functions A,B,C, evolving under a Hamiltonian H, such that A = {B,C}, then

$$\dot{A} = \{\dot{B},C\} + \{B,\dot{C}\}$$

The dot means total time derivative, e.g.

$$\dot{A} = \frac{\partial A}{\partial t} + \{A,H\}$$

Prove this theorem. Use only the algebra of the Poisson bracket, i.e. don't write things out in component form.

3. Take the harmonic oscillator Hamiltonian,

$$H = \frac{1}{2}(p^2 + \omega^2 q^2)$$

and solve for q(t), p(t) in terms of q_0, p_0 at t=0. Show that the transformation $(q_0,p_0) \rightarrow (q,p)$ is canonical for all values of t.

4. Solve equation (3.32) and show that a solution W generates (3.33). Don't worry about branches, i.e. signs of square roots.

5. Consider the non-relativistic motion of a particle of charge e and mass m in the following magnetic field:

$$\underset{\sim}{B} = (B_0 + \beta x)\ \hat{z}$$

where B_0 is a constant and β is a small quantity. Neglect the motion of the particle in the z-direction, i.e. treat the problem in the two perpendicular directions only.

Write down the Newton-Lorentz equations of motion for the particle in component form. Transform these equations to a set of first-order differential equations by means of the substitution $v_x = \dot{x}$, $v_y = \dot{y}$. Treat the terms containing β as a perturbation, and note that the unperturbed system is a set of linear equations, while the perturbation introduces a non-linearity. The unperturbed system is periodic (not only in configuration space, but also in phase space.) Observe that the system is in the form of equation (4.7).

The preparatory transformation for this system will bring it into the form of equation (4.8). Show that the following transformation will do this:

$$x = X + \frac{w}{\Omega_0} \cos \theta$$

$$y = Y - \frac{w}{\Omega_0} \sin \theta$$

$$v_x = -w \sin \theta$$

$$v_y = -w \cos \theta$$

where $\Omega_0 = eB_0/mc$. Observe that this transformation allows the solution to the unperturbed system to be written down immediately. Use this solution to give a physical interpretation of the new variables (X,Y,w,θ).

Finally, average the equations, to bring them into the form of equations (4.35). Interpret the results physically.

6. This problem is the same as problem 5, except that it uses Hamiltonian mechanics. Show that the following vector potential gives the same magnetic

field which was used in problem 5:

$$\underset{\sim}{A} = (B_0 x + \frac{1}{2}\beta x^2)\,\hat{y}$$

Use this vector potential in the standard Hamiltonian for non-relativistic charged particles in a magnetic field. Expand H in powers of β and ignore terms which are $O(\beta^2)$.

The Hamilton-Jacobi equation for the unperturbed Hamiltonian can be solved, and one such solution gives the following transformation:

$$x = \frac{1}{\sqrt{m\Omega_0}}\left(P + \sqrt{2J}\cos\theta\right)$$

$$y = \frac{1}{\sqrt{m\Omega_0}}\left(Q - \sqrt{2J}\sin\theta\right)$$

$$p_x = -\sqrt{2m\Omega_0 J}\,\sin\theta$$

$$p_y = \sqrt{m\Omega_0}\,P$$

The new canonical variables are (Q,P,θ,J). Show that this transformation is canonical by appealing to the definition (3.12). In doing this, it is easiest to compute the Poisson brackets of the old variables among themselves with respect to the new variables. Transform the Hamiltonian to the new variables, and solve the unperturbed system. Use this solution to give a physical interpretation of the variables (Q,P,θ,J).

Finally, average the perturbing term in the Hamiltonian, write down the averaged equations of motion, and interpret them.

This system is something of a hybrid, in the sense that one pair of canonical coordinates, the (θ,J) coordinates, represent periodic motion, while the other pair, the (Q,P) coordinates, may represent unbounded motion. Hence only the first pair are action-angle variables, and the Hamiltonian does not

fit the form of equation (5.21), although it is similar in spirit.

7. Carry out the expansion (6.50) to third order. Also, find the inverse (6.51) to third order by using the method in the notes. Show that it agrees with the rule on page 6.19. Multiply the two series together, keeping all terms through third order, and show that the result is the identity transformation.

8. Carry out (7.11) to third order. Don't worry about proving that it is valid for the time-dependent case. Save the results of problems 7 and 8. You may need them some day.

9. Consider the following Hamiltonian:

$$H = \frac{1}{2m} \underset{\sim}{p}^2 + \varepsilon e \phi(\underset{\sim}{x},t)$$

where

$$\phi(\underset{\sim}{x},t) = \tilde{\phi}(\lambda \underset{\sim}{x})\, e^{i(\underset{\sim}{k}\cdot\underset{\sim}{x} - \omega t)} + \text{c.c.}$$

This Hamiltonian differs from (7.52) in the following ways. First, it is 3-dimensional. Second, complex notation is used. The quantity $\tilde{\phi}$ may be complex, which allows for an arbitrary origin of phase for the wave. Third, the amplitude $\tilde{\phi}$ is not constant, but is rather a slowly varying function of $\underset{\sim}{x}$.

Both the dimensionless quantities ε and λ are small, but λ is to be considered much smaller than ε. We will expand results to order two in ε, but keep only order zero in λ. This means that we are examining one particular corner of parameter space.

Use Lie transforms to transform this Hamiltonian H into a new Hamiltonian K, which is to be independent of time. Since the form of the function $\tilde{\phi}$ is not specified, it is to be expected that K will also involve this unspecified

function, and hence not be solvable. It is, however, easier to interpret than H.

Begin by finding the Lie generator w_1. Use the rules of Appendix A to express w_1 as a semi-indefinite integral (i.e., the lower limit is indefinite) involving the unspecified function $\tilde{\phi}$. Show that an integration by parts will convert this integral into a power series in λ. Do this and keep only the term which is order zero in λ.

Then find K_1, K_2 and w_2. Use the expansion of the T operator, given in chapter 6, to express the old variables $\underset{\sim}{x},\underset{\sim}{p}$ in terms of the new variables $\underset{\sim}{x}',\underset{\sim}{p}'$, through $O(\varepsilon^2)$. Drop all terms of order λ. The new variables $\underset{\sim}{x}',\underset{\sim}{p}'$ are sometimes called "oscillation center" variables.

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