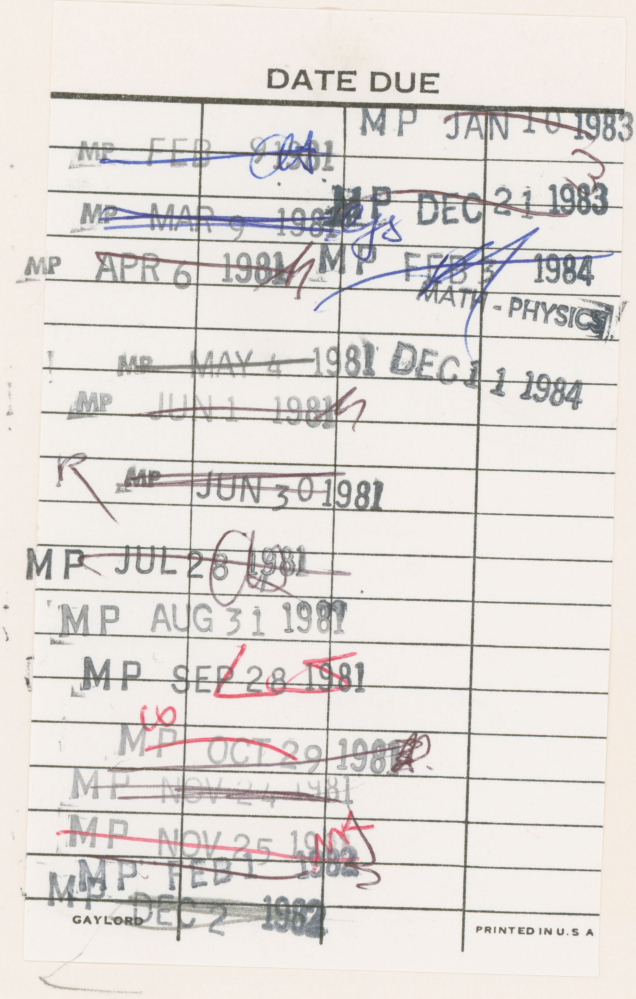
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SEMICLASSICAL QUANTIZATION
OF
NONSEPARABLE HAMILTONIAN SYSTEMS

by

Charles Jaffé

B.S., Antioch College, 1973

A thesis submitted to the Faculty of the Graduate School of the University of Colorado in partial fulfillment of the requirements of the degree of

Doctor of Philosophy

Committee on Chemical Physics

1979

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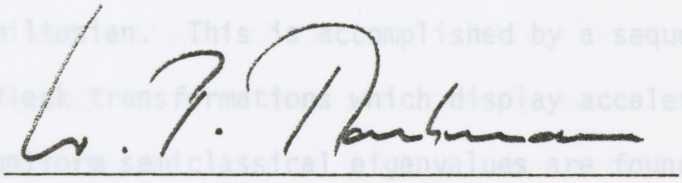
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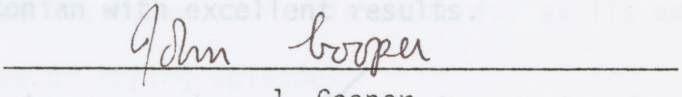
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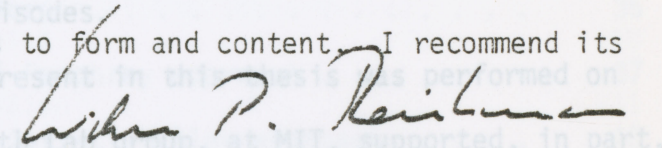
Semiclassical Quantization of Nonseparable Hamiltonian Systems

Thesis directed by Professor W. P. Reinhardt

Methods for the primitive and uniform semiclassical quantization of Nonseparable Hamiltonian Systems are developed. Integrable nonseparable Hamiltonians are transformed to angle-action variables by a sequence of Van Vleck transformations. This sequence of transformations displays accelerated convergence. The primitive semiclassical eigenvalues are found by evaluating the transformed Hamiltonian at the quantized values of the actions. For the nonintegrable problem, an integrable approximation is found by normalizing the Hamiltonian. This is accomplished by a sequence of Birkoff-Van Vleck transformations which display accelerate convergence. The uniform semiclassical eigenvalues are found by numerical evaluation of the uniform semiclassical quantization condition.

These methods have been applied to the degenerate Henon-Heiles Hamiltonian with excellent results.

This abstract is approved as to form and content. I recommend its publication.

Signed 

Faculty member in charge of dissertation

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INTRODUCTION

With the advent of lasers, chemistry has reached a turning point. It is now becoming possible to study the details of chemical reactions. An important question which arises is, when one prepares a molecule in a highly excited state, how does the energy migrate through the molecule. As an example, consider the following very simple model of ethane. Treat the methyl groups as rigid structures, then the two internal degrees of freedom are the vibration of the two methyl groups and their rotation with respect to each other. It is then possible to model the system by a Hamiltonian of the Henon-Heiles type which is treated later. The question now becomes, if one excites the rotational mode to a very high angular momentum state, can the energy migrate into the vibrational mode?

Answering questions of this nature by quantum mechanical methods often requires very large and troublesome calculations. However, since $\hbar$ is small compared to the physical quantities (of units $\hbar$) of the system, for highly excited molecules one might expect to be able to treat such questions by classical and semiclassical methods. This thesis discusses the semiclassical quantization of systems which resemble molecules.

Einstein, in his 1917 paper on quantization of classical Hamiltonian systems, notes that there exist two types of classical motion; type 1 is characterized by the fact that a trajectory is confined to an N-dimensional multipliconnected surface in 2N-dimensional phase space, which is topologically equivalent to a

torus, and type 2 is characterized by the classical motion filling a region of phase space of dimension larger than N. Einstein then proposes a set of quantization conditions for systems of the first type.

Several investigators have numerically implemented these quantization conditions for both zero order degenerate and nondegenerate Hamiltonian systems. In Chapter II of this thesis I developed an iterative method for the quantization of classical systems of the first type which displays accelerated convergence. The third chapter discusses the choice of the correct zero order variables in the case of near degenerate systems.

Until the present work, very little progress has been made on the problem of semiclassical quantization of systems characterized by motion of the second type. In Chapter IV systems of this nature are discussed. It is shown that such a system can be approximated by a system of the first type. The quantization is then straightforward.

CHAPTER I

PRELIMINARIES

A. CLASSICAL MECHANICS

The connection[1] between quantum mechanics and classical mechanics is most easily seen by comparing the Heisenberg formulation of quantum mechanics to Hamilton's formulation of classical mechanics. This formulation of classical mechanics is obtained from the standard Lagrangian formulation[2] by identifying the derivative of the Lagrangian with respect to the velocities as the canonical momenta. This in effect reduces the classical system of equations from a set of N second order differential equations to a set of 2N first order equations,

$$\frac{d\underset{\sim}{p}}{dt} = -\frac{\partial H(\underset{\sim}{p},\underset{\sim}{q})}{\partial \underset{\sim}{q}} = \{\underset{\sim}{p}, H\} \tag{1a}$$

$$\frac{d\underset{\sim}{q}}{dt} = \frac{\partial H(\underset{\sim}{p},\underset{\sim}{q})}{\partial \underset{\sim}{p}} = \{\underset{\sim}{q}, H\} \tag{1b}$$

where $\underset{\sim}{p}$ and $\underset{\sim}{q}$ are the conjugate canonical variables and $H(\underset{\sim}{p},\underset{\sim}{q})$ is the Hamiltonian function. When the Hamiltonian is explicitly time independent, which is assumed in all that follows, it can be shown[3] to be an integral of the motion and equal to the energy of the system.

---

*The brackets, $\{a,b\}$, are Poisson brackets and are defined as $\{a,b\} = \{\frac{\partial a}{\partial q}\frac{\partial b}{\partial p} - \frac{\partial a}{\partial p}\frac{\partial b}{\partial q}\}$.

1. Hamilton-Jacobi Theory and Angle-Action Variables

The classical solutions, i.e., trajectories, are found by integrating Eq. 1 to obtain the canonical variables as functions of time. One expects such solutions to contain 2N constants of integration. There are many different methods by which Eq. 1 can be integrated. Of these, the method of canonical transformations provides the closest approach[1] to quantum mechanical methods. The underlying idea of this approach is to transform the equations of motion, Eq. 1, into a form which can be immediately integrated. The choice of the new variables depends greatly upon the nature of the system. For the classical Hamiltonian systems which are of interest in this paper, that is, bound, conservative Hamiltonian systems, it is convenient to transform to a set of canonical variables such that the coordinates are ignorable.[4] The equations of motion then have the form,

$$\frac{d\underset{\sim}{P}}{dt} = 0 \tag{2a}$$

$$\frac{d\underset{\sim}{Q}}{dt} = -\frac{\partial H(\underset{\sim}{P})}{\partial \underset{\sim}{P}} \tag{2b}$$

It is not guaranteed that such a set of variables exist,[5] as will be discussed in more detail later in this section. The canonical momenta in Eq. 2 are constants and can be taken as N of the 2N constants of integration. Hamilton-Jacobi[6] theory provides a method of finding a canonical transformation to such a set of variables by providing a partial differential equation

$$H(\partial W(q,P)/\partial q, q) = E \tag{3}$$

for the generating function of the required transformation. W, which is called Hamilton's principal function, is, following Goldstein, a generating function of the F_2 type;[7] i.e., it is a function of the old coordinates and the new momenta. This function in general is multivalued. The equations of transformation are found by differentiating $W(\underset{\sim}{q},\underset{\sim}{P})$ with respect to its variables,

$$\underset{\sim}{p} = \partial W(q,\underset{\sim}{P})/\partial q \tag{4a}$$

$$\underset{\sim}{Q} = \partial W(q,\underset{\sim}{P})/\partial \underset{\sim}{P} \tag{4b}$$

Before discussing the solution of the Hamilton-Jacobi partial differential equation, it is necessary to define, in more detail, the properties of the new variables. The new coordinates, which are called angle variables, develop linearly in time. The motion of the system, that is, the old coordinates, are periodic functions of the angle variables. As a result the old coordinates and thus Hamilton's principal function, can be expressed as Fourier series. The periods of the angle variables will be taken to be 2π unless specifically stated otherwise. The new momenta, called action variables, are integrals of the motion, i.e., constants. In the 2N dimensional phase space defined by the old variables, the motion is confined to surfaces on which the actions are constant. The angle variables provide a coordinate system on this surface. These multipliconnected surfaces are called invariant tori. The multivaluedness

of Hamilton's principal function results from the fact that it has a value corresponding to each sheet of this multipliconnected surface (see Figure 1-1). An N dimensional invariant torus contains N closed paths, C_ℓ, which cannot be continuously deformed into each other or contracted into a single point without leaving the torus. The actions of a particular torus are given in terms of these paths

$$J_\ell = \frac{1}{2\pi} \oint_{C_\ell} \underset{\sim}{p} \cdot d\underset{\sim}{q} \tag{5}$$

for $\ell = 1,\ldots,N$. Integrating Eq. 3 to obtain Hamilton's principal function, then substituting this result into Eq. 4a, one obtains an integral for the angle variables,

$$\underset{\sim}{\psi} = \int^{\underset{\sim}{q}} \frac{\partial \underset{\sim}{p}(\underset{\sim}{q}, \underset{\sim}{P})}{\partial \underset{\sim}{P}} \cdot d\underset{\sim}{q} \tag{6}$$

To illustrate these ideas, consider the one-dimensional quartic oscillator. The Hamilton-Jacobi differential equation for this system is

$$E = \frac{1}{2}\left\{ \frac{\partial W(q,J)}{\partial q} \right\}^2 + \frac{1}{4} q^4 \tag{7}$$

This equation can be immediately integrated to obtain

$$W(q,J) = \int_q^{(4E)^{1/4}} \left(2E(J) - \tfrac{1}{2} q^4\right)^{1/2} dq \tag{8a}$$

$$= \{4E(J)\}^{3/4} F\left(\cos^{-1} q / \{4E(J)\}^{1/4} ; \tfrac{1}{2}\sqrt{2}\right) \tag{8b}$$

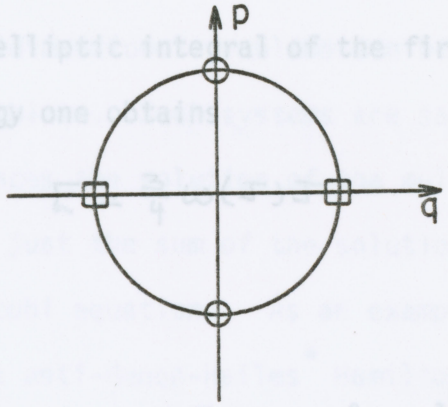


Figure 1-1. The Caustics of an Invariant Torus of a One Dimensional Oscillator. This figure shows a one-dimensional torus of an oscillator in two-dimensional phase space. Clearly the invariant torus is a multipliconnected surface composed of two sheets. Viewed from coordinate space these sheets are connected at the points marked by □, when viewed from momentum space the sheets are connected at the points marked by ○. These points, where the sheets join, are the caustics of the torus. A consequence of the multipliconnected nature of the invariant torus is that Hamilton's principal function is a multivalued function with one value for each sheet.

where $F(\alpha;k)$ is an elliptic integral of the first kind. The action is then found by integrating Eq. 5, giving

$$J = \{4E\}^{3/4}/3 \tag{9}$$

where we have chosen the period of the angle variable to be

$$\tau = 4K(\tfrac{1}{2}\sqrt{2}) . \tag{10}$$

K is the complete elliptic integral of the first kind.[8] Solving Eq. 9 for the energy one obtains

$$E = \tfrac{3}{4}\omega(J)J \tag{11}$$

where

$$\omega(J) = \frac{\partial E(J)}{\partial J} = \{3J\}^{1/3} \tag{12}$$

In order to find the parameterization of the torus, integrate Eq. 6

$$\varphi = \omega(J)\int_q^{(4E)^{1/4}} \frac{dq}{(2E(J)-\tfrac{1}{2}q^4)^{1/2}} = F\left(\cos^{-1}q/\{4E(J)\}^{1/4};\tfrac{1}{2}\sqrt{2}\right) \tag{13}$$

Inverting Eq. 13 and using Eq. 1b one obtains the old variables as functions of the new variables

$$q(J,\varphi) = \omega(J)\,cn\left(\varphi|\tfrac{1}{2}\sqrt{2}\right) \tag{14a}$$

$$p(J,\varphi) = -\omega^2(J)\,sn\left(\varphi|\tfrac{1}{2}\sqrt{2}\right)dn\left(\varphi|\tfrac{1}{2}\sqrt{2}\right) \tag{14b}$$

The functions cn, sn, and dn are Jacobi elliptic functions.[9] These equations together with the solutions of Eq. 2 give the time development of the system. It is clear from this example that, for one dimensional systems, angle-action variables exist. This results from the fact that the Hamiltonian is an integral of the motion.[3]

The integrability of one dimensional Hamiltonian systems, i.e., the existence of angle-action variables, is an important result. Many multidimensional problems can be reduced to a set of one dimensional problems. Such systems are said to be separable.[10] In these circumstances the solution of the multidimensional Hamilton-Jacobi equation is just the sum of the solutions of the one dimensional Hamilton-Jacobi equations. As an example of such a Hamilton system consider the anti-Henon-Heiles* Hamiltonian system,

$$E = \tfrac{1}{2}\{P_x^2 + x^2\} + \tfrac{1}{2}\{P_y^2 + y^2\} + \epsilon y\{x^2 + \tfrac{1}{3}y^2\} \qquad (15)$$

which differs from the Henon-Heiles Hamiltonian by a sign. This system is not separable in the present coordinates, however, a set of coordinates in which the system is separable can be found. The generating function of a transformation to such a set of variables is given by

$$W(x, y; P_x, P_y) = -\tfrac{1}{2}\sqrt{2}\left\{P_1(x+y) - P_2(x-y)\right\} \qquad (16)$$

---

*The Henon-Heiles Hamiltonian,[11] $H = \frac{1}{2}(P_x^2 + x^2) + \frac{1}{2}(P_y^2 + y^2) + \varepsilon yx^2 - \frac{\varepsilon}{3}y^3$, is an exceedingly famous problem originating in astrophysics. It is an example of a nonseparable, nonintegrable classical Hamiltonian. By changing the sign of the last term one obtains a separable, integrable classical Hamiltonian, hence we call this Hamiltonian the anti-Henon-Heiles Hamiltonian.

The transformed Hamiltonian is

$$E = E_1 + E_2 \tag{17a}$$

$$E_i = \tfrac{1}{2}(p_i^2 + q_i^2) - \tfrac{\epsilon}{3}\sqrt{2}\, q_i^3 \qquad \text{for } i = 1,2\ , \tag{17b}$$

which clearly is separable. The generating function of the transformation to angle-action variables can now be written as

$$W(q_1, q_2; J_1, J_2) = W_1(q_1, J_1) + W_2(q_2, J_2) \tag{18}$$

where

$$W_i(q_i, J_i) = \int^{q_i} \left\{ 2E_i(J_i) - q_i^2 + \tfrac{\epsilon}{2}\sqrt{2}\, q_i^3 \right\}^{1/2} dq \tag{19}$$

for i = 1,2.

The action and angle integrals can be evaluated, however, it is easier to find the parameterization of the torus by noting that the separated Hamiltonian can be written as

$$\left\{ \frac{dQ_i}{dt} \right\}^2 = 4Q_i^3 - g_2 Q_i - g_1 \tag{20}$$

where

$$\tau_i = \tfrac{1}{2}\left\{\frac{\epsilon}{3}\sqrt{2}\right\}^{1/2} t + \tau_{0_i} \tag{21a}$$

$$Q_i = q_i - \frac{1}{2\epsilon}\sqrt{2} \tag{21b}$$

$$g_1 = \frac{6\sqrt{2}}{\epsilon}\left\{\frac{1}{6\epsilon^2} - 2E_i\right\} \tag{21c}$$

$$g_2 = \frac{6}{\epsilon^2} \tag{21d}$$

for i = 1,2, and where

$$E = E_1 + E_2 \tag{22}$$

The solutions to this differential equation are Weierstrass elliptic functions[8]

$$Q_i(\tau_i) = \wp(\tau_i) \tag{23}$$

The parameterization of the torus is then given by

$$x = \tfrac{1}{2}\sqrt{2}\left\{\wp(\tau_2) - \wp(\tau_1)\right\} \tag{24a}$$

$$y = \tfrac{1}{2}\sqrt{2}\left\{\wp(\tau_2) + \wp(\tau_1)\right\} \tag{24b}$$

$$P_x = -\left\{\frac{3\sqrt{2}}{\epsilon}\right\}^{1/2}\left(\wp(\tau_1) - \wp(\tau_2)\right) \tag{24c}$$

$$P_y = -\left\{\frac{3\sqrt{2}}{\epsilon}\right\}^{1/2}\left(\wp(\tau_1) - \wp(\tau_2)\right) \tag{24d}$$

Not all integrable Hamiltonian systems are separable. The integration of the Hamilton-Jacobi equation in the nonseparable case is a formidable problem. Max Born[10] suggests solution by perturbative expansion of the Hamilton's principal function. Chapman, Garrett and Miller[11] have numerically implemented a procedure based on these ideas. In Chapter II a similar method is developed based upon a sequence of transformations, and displays properties of accelerated convergence. Percival[12] has developed a method of parameterizing the classical solutions of nonseparable systems which does not involve finding the solution of the Hamilton-Jacobi equations.

The question of uniqueness of the angle-action variables has been discussed at length by Born.[13] To summarize his results we note that this question can be treated in two parts. The first asks if the motion defines a unique invariant torus. The second asks if, for a given torus, the angle-action variables are unique. If the system is nondegenerate, that is, if the frequencies are not rationally related, then the motion is dense on the torus.[14] As a result a trajectory will define a unique torus. On the other hand, for degenerate systems a trajectory will not densely fill the torus;

but rather will densely fill a surface of lesser dimensionality. This surface can be thought of as the intersection of an infinite family of tori. In other words, a trajectory of a degenerate system will not define a unique torus, but a family of intersecting tori. The second question is, is there a unique coordinate system on a given torus? The answer is no, there is an infinite family of coordinate systems which are acceptable. These coordinate systems are related to each other by area preserving linear transformations (see Figure 1-2).

The discussion to this point has assumed the global existence of angle-action variables, i.e., that the system is integrable everywhere in phase space. As was noted earlier, this is not always the case.[5] The motion of a Hamiltonian system of this nature, in general, fills a volume of phase space of greater dimensionality than that of the invariant torus. We will call this motion irregular. Nonintegrability does not rule out the existence of invariant tori; Kolmogorov, Aronl'd, and Moser (KAM)[14] proved the existence of invariant tori for almost integrable systems. They showed that in regions of phase space surrounding periodic orbits there exist families of invariant tori, provided that the system is not degenerate and that the Hessian of the unperturbed system is not zero. We will call these regions of phase space the KAM regions. In KAM regions of phase space between the tori, there exists irregular motion (see Figure 1-3). Outside of the KAM regions, the invariant tori disappear, leaving only the irregular motion and periodic orbits.

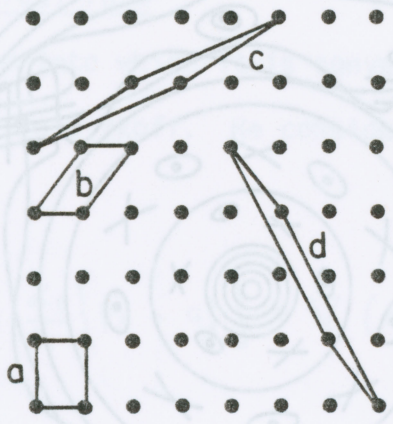


Figure 1-2. The Nonuniqueness of the Angle Variables. The periodic lattice shown above represents the angle space of a two-dimensional nondegenerate system. Each of the parallelograms a), b), c), and d) can be chosen to be the fundamental invariant torus. Then the rest of the angle space can be constructed by repeating this fundamental torus again and again (in crystallography the fundamental torus corresponds to the unit cell). a) represents the usual choice. All other possible choices can be found by area preserving integral linear transformations of a). The transformation for b) is $U_b = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$, for c) is $U_c = \begin{pmatrix} 1 & 2 \\ 1 & 3 \end{pmatrix}$ and for d) is $U_d = \begin{pmatrix} 1 & -1 \\ -2 & 3 \end{pmatrix}$. Since the determinant of these matrices are equal to ± 1, then transformations preserve the area of the torus.

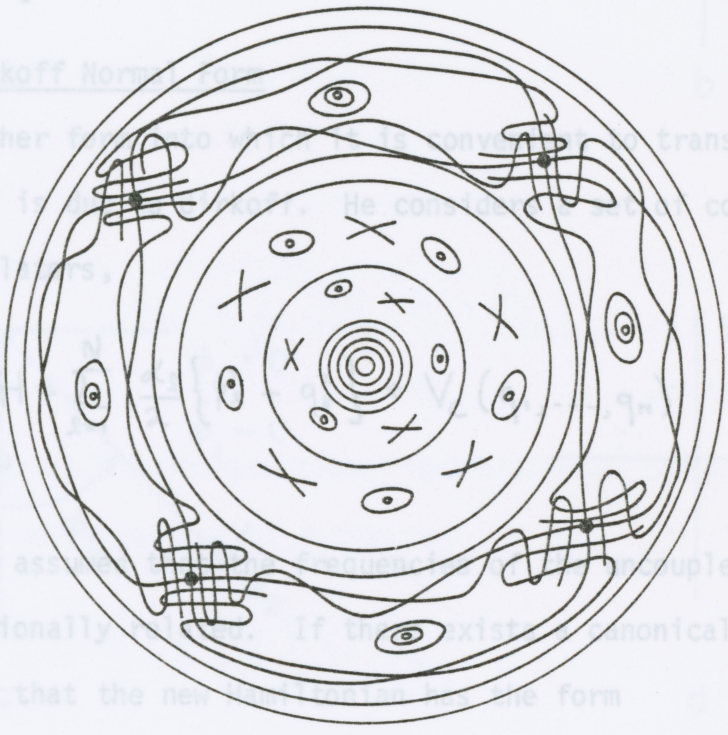


Figure 1-3. The Structure of Phase Space for Almost Integrable Systems. This figure, which has been redrawn from Ref. 14, shows the tori which surround a periodic orbit of an almost integrable system, that is, a nonintegrable system only slightly perturbed from an integrable problem. Characteristic of such problems is that in between the tori there exists motion which does not define a torus. For a detailed discussion of this behavior see Ref. 5.

An important device for the study of dynamical systems is the Poincaré surface of section.[14] It is most useful for two dimensional Hamiltonian systems (four dimensional phase space). The surface of section is constructed by plotting the points of intersection of the trajectory with the plane in phase space defined by $q_1 = 0$ and $p_1 > 0$ (see Figure 1-4).

2. The Birkoff Normal Form

Another form into which it is convenient to transform the Hamiltonian is due to Birkoff. He considers a set of coupled harmonic oscillators,

$$H = \sum_{\ell=1}^{N} \frac{\alpha_\ell}{2}\left\{p_\ell^2 + q_\ell^2\right\} + V_c(q_1, \ldots, q_N) \tag{25}$$

where it is assumed that the frequencies of the uncoupled problem are not rationally related. If there exists a canonical transformation such that the new Hamiltonian has the form

$$H = \sum_{\ell=1}^{N} \frac{\alpha_\ell}{2}\left\{P_\ell^2 + Q_\ell^2\right\} + V_c\left(\tfrac{1}{2}\left\{P_1^2 + Q_1^2\right\}, \ldots, \tfrac{1}{2}\left\{P_N^2 + Q_N^2\right\}\right) \tag{26}$$

then

$$\left\{\tfrac{1}{2}\left(P_\ell^2 + Q_\ell^2\right), H\right\} = 0 \tag{27}$$

that is,

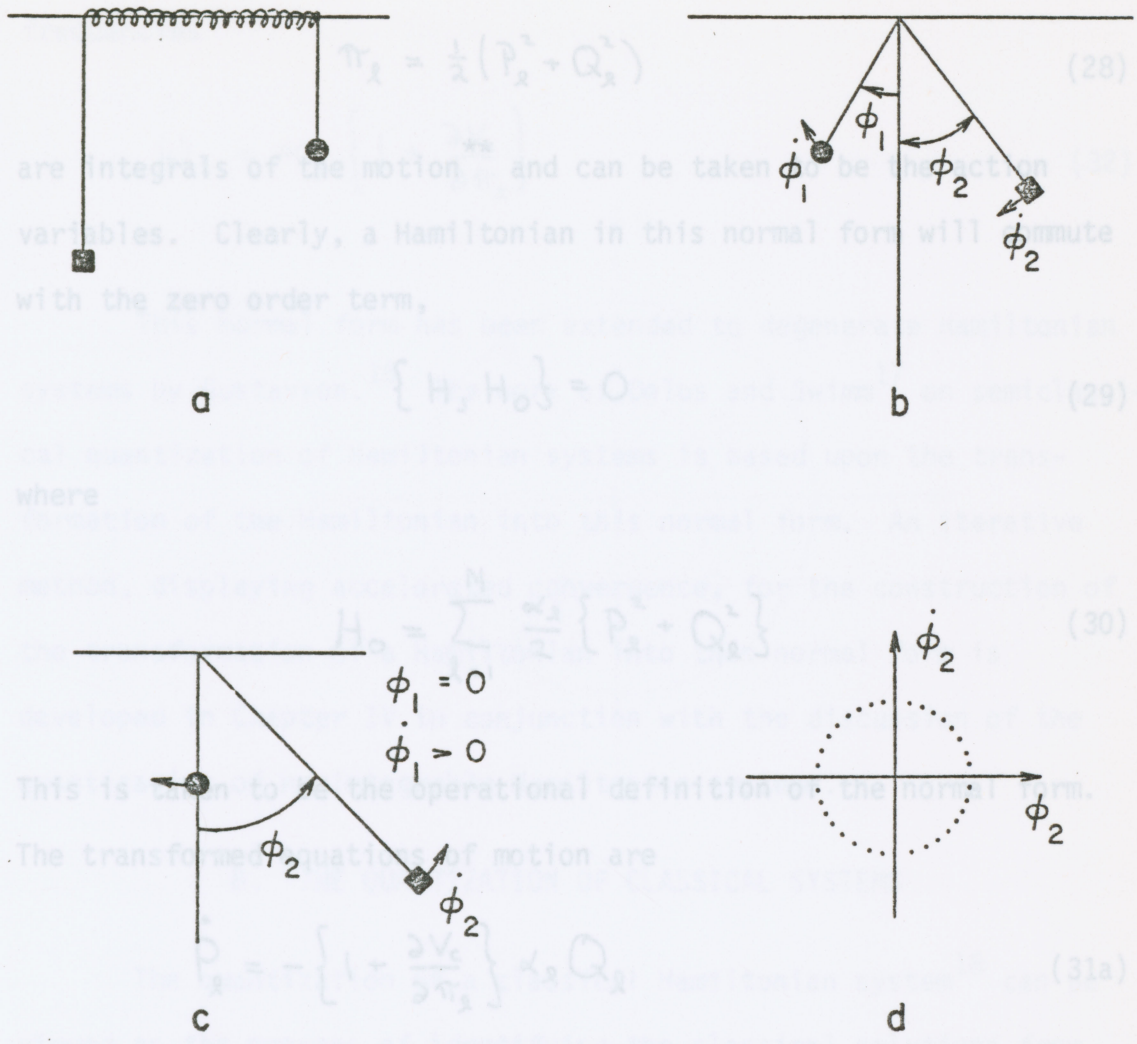


Figure 1-4. Construction of the Poincaré Surface of Section. Consider a system, shown in a), composed of two pendula, coupled in some unspecified manner. The phase space of this system is four dimensional. The canonical variables, shown in b), are the two angles of displacement, measured from the vertical, and the angular velocities of the pendula. The surface of section is given by the phase portrait, of the second pendulum when the first pendulum is vertical and swinging to the left as shown in c).

$$\pi_\ell = \tfrac{1}{2}\left(P_\ell^2 + Q_\ell^2\right) \tag{28}$$

are integrals of the motion** and can be taken to be the action variables. Clearly, a Hamiltonian in this normal form will commute with the zero order term,

$$\{H, H_0\} = 0 \tag{29}$$

where

$$H_0 = \sum_{\ell=1}^{N} \frac{\alpha_\ell}{2}\left\{P_\ell^2 + Q_\ell^2\right\} \tag{30}$$

This is taken to be the operational definition of the normal form. The transformed equations of motion are

$$\dot{P}_\ell = -\left\{1 + \frac{\partial V_c}{\partial \pi_\ell}\right\}\alpha_\ell Q_\ell \tag{31a}$$

$$\dot{Q}_\ell = \left\{1 + \frac{\partial V_c}{\partial \pi_\ell}\right\}\alpha_\ell P_\ell \tag{31b}$$

** To see that this is true expand Eq. 27,

$$\left\{\tfrac{1}{2}\left(P_\ell^2 + Q_\ell^2\right), H\right\} = -P_\ell \frac{dP_\ell}{dt} - Q_\ell \frac{dQ_\ell}{dt}$$

then substituting the equations of motion, Eq. 31, into this equation one obtains the desired result.

which we recognize as a set of uncoupled harmonic oscillators with frequencies

$$\omega_\ell = \alpha_\ell \left[1 + \frac{\partial V_c}{\partial \pi_\ell} \right] \tag{32}$$

This normal form has been extended to degenerate Hamiltonian systems by Gustavson.[16] The work of Delos and Swimm[17] on semiclassical quantization of Hamiltonian systems is based upon the transformation of the Hamiltonian into this normal form. An iterative method, displaying accelerated convergence, for the construction of the transformation of a Hamiltonian into this normal form is developed in Chapter IV in conjunction with the discussion of the quantization of nonintegrable Hamiltonian systems.

B. THE QUANTIZATION OF CLASSICAL SYSTEMS

The quantization of a classical Hamiltonian system[18] can be viewed as the process of identifying the classical solutions from which the semiclassical approximation of the wave function can be constructed. In the following discussion it is assumed that the classical system is (locally) integrable. The result of this assumption is that the classical solutions can be parameterized in terms of angle-action variables. This representation is useful in that it resolves the multivaluedness of the classical solutions (see Figure 1-5).

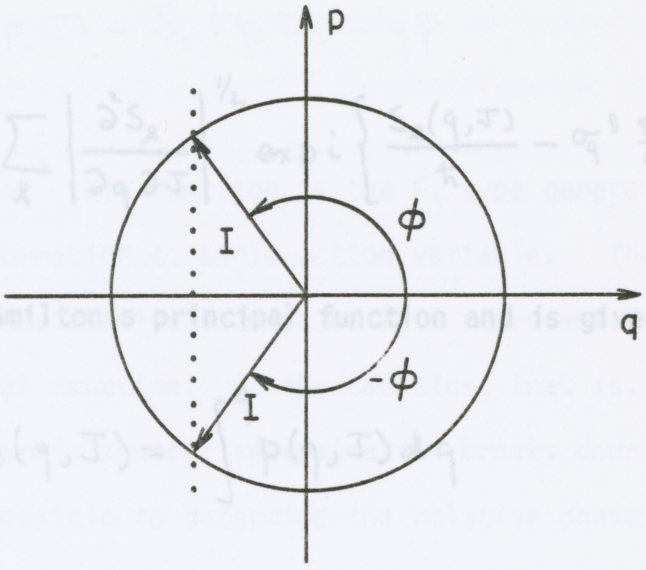


Figure 1-5. The Resolution of the Multivaluedness of the Classical Solution via use of Angle-Action Variables. Shown is an invariant torus of a one-dimensional harmonic oscillator, $E = \frac{1}{2}(P_1^2 + q_1^2)$, in its two-dimensional phase space. Corresponding to each value of q there are two values of p. This results in Hamilton's principal function being a multivalued function of the coordinate. Parameterizing this function in terms of angle-action variables resolves this multivaluedness, that is, one value of p and consequently of Hamilton's principal function corresponds to the angle variable having values between 0 and π and while the second value corresponds to values of the angle between $-\pi$ and 0.

1. The Primitive Semiclassical Quantization Conditions

The coordinate representation of the semiclassical wave function is defined to be equal to zero in the classically forbidden regions of coordinate space, and in the classically allowed regions to be

$$\Psi(q) \sim \sum_{\ell} \left| \frac{\partial^2 S_\ell}{\partial q \, \partial J} \right|^{1/2} \exp i \left\{ \frac{S_\ell(q,J)}{\hbar} - \sigma_q^{\ell} \frac{\pi}{4} \right\} \tag{33}$$

where $S(q,J)$ is Hamilton's principal function and is given by

$$S(q,J) = \int^{q} p(q,J) \, dq \tag{34}$$

The summation in Eq. 33 is over the multivaluedness of this function, that is, each of the multipliconnected sheets of the invariant torus contributes a term to the semiclassical wave function. It is this summation which is responsible for the quantum mechanical interference of the classical paths. One of the advantages of the Hamiltonian formulation of classical mechanics is that the canonical variables appear on an equal footing. As a result, one expects the momentum representation of the semiclassical wave function to have the same form. That is, it is equal to zero for the classically forbidden regions of momentum space, and is equal to

$$\Psi(p) \sim \sum_{k} \left| \frac{\partial^2 S_k}{\partial p \, \partial J} \right|^{1/2} \exp i \left\{ \frac{S_k(p,J)}{\hbar} - \sigma_p^{k} \frac{\pi}{4} \right\} \tag{35}$$

in the classically allowed regions. The function S(p,J) is the momentum representation of Hamilton's principal function and is given by

$$S_k(p,J) = S_\ell(q,J) - qp \tag{36}$$

Following Goldstein,[7] this function is the F_3 type generating function of the transformation to angle-action variables. The summation in Eq. 35 is over the multivaluedness of this representation of Hamilton's principal function. At the caustics, that is, the seams of the torus, the semiclassical approximation breaks down. As a result it is not possible to determine the relative phases of the different terms of either representation by matching them at the caustics. This difficulty in determining the relative phases can be overcome by recalling that the momentum representation is the Fourier transform of the coordinate representation of the semiclassical wave function,

$$\psi(p) = \int dq\, e^{-\frac{i}{\hbar}pq}\, \psi(q) \tag{37}$$

where the integral is evaluated in the stationary phase approximation. Substituting Eq. 33 and Eq. 35 into Eq. 37 one obtains

$$\sigma_p^k = \sigma_q^\ell - \mathrm{Sgn}(dp/dq) \tag{38}$$

From this relationship one can determine the phases of one

representation relative to the phases of the other representation (see Figure 1-6). As a direct result of the multipliconnected nature of the invariant torus, it is possible to determine the relative phases of one term with respect to another term in several different ways. Each of these corresponds to an independent path on the invariant torus. In order for the semiclassical wave function to be a well defined function the relative phase determined by each of these different paths must equal modulus 2π. This then gives the primitive semiclassical quantization conditions

$$\oint_{C_\ell} \underline{p} \cdot d\underline{q} = 2\pi\hbar\left(n_\ell + \frac{\alpha_\ell}{4}\right) \tag{39}$$

where α_ℓ, which is called Maslov's index, represents the phase loss at the caustics of the torus.[18]

2. Uniform Semiclassical Quantization Conditions[19]

In the case that the classically allowed region of either coordinate or momentum space is disjoint, the quantization conditions given above do not adequately describe the behavior of the quantum mechanical system; that is, the theory outlined above does not allow for such nonclassical phenomena as tunneling between the disjoint regions. Several investigators[20] have found that this nonclassical behavior can be described by analytic continuation of classical trajectories. This suggests that the invariant tori in the disjoint regions of phase space can be connected by analytic continuation of the angle variables. Such a continuation has the result of removing the restriction that the physical variables and

Hamilton's principal function be real valued functions of the angle variables. As an example consider the double well problem given by

$$E = \frac{1}{2}p^2 + \frac{1}{4}q^4 - \frac{\lambda}{2}q^2 \tag{40}$$

In a manner analogous to that used for the quartic oscillator in the previous section, one can find the parameterization of the torus, for $-\frac{\lambda^2}{2} \leq E \leq 0$

$$q = q_0(I)\, dn(\varphi | r) \tag{41a}$$

$$p = -\omega(I)\left[q_0^2(I) - q_i^2(I)\right] sn(\varphi|r)\, cn(\varphi|r) \tag{41b}$$

for $E > 0$

$$q = q_0(I)\, cn(\varphi|s) \tag{42a}$$

$$p = -\omega(I)\, q_0(I)\, sn(\varphi|s)\, dn(\varphi|s) \tag{42b}$$

where

$$q_0^2(I) = \lambda\left(1 + (1 + 4E/\lambda^2)^{1/2}\right) \tag{43a}$$

$$q_i^2(I) = \lambda\left(1 - (1 + 4E/\lambda^2)^{1/2}\right) \tag{43b}$$

$$r = 1/s = \left\{\frac{q_0^2 - q_i^2}{q_0^2}\right\}^{1/2} \tag{43c}$$

The transformed Hamiltonian

for $-\frac{\lambda^2}{4} \leq E \leq 0$ is

$$E = \frac{3}{4}\omega(I)I - \frac{\lambda^{3/2}}{4}\omega(I)\left\{2^{3/2}-3\right\} - \frac{\lambda^2}{4}, \tag{44a}$$

and for $E > 0$ is

$$E = \frac{3}{4}\omega(I)I - \frac{\lambda}{2}\omega(I)\left\{(2\lambda)^{1/2} - \omega(I)\right\} \tag{44b}$$

where the frequency of the classical motion

for $-\frac{\lambda^2}{4} \leq E \leq 0$ is

$$\omega(I) = (2\lambda)^{1/2}\cos\frac{1}{3}\left\{\cos^{-1}\left[\frac{3I}{(2\lambda)^{3/2}} - 1\right]\right\}, \tag{45a}$$

and for $E > 0$ is

$$\omega(I) = (2\lambda)^{1/2}\left\{\frac{3I}{(2\lambda)^{3/2}} - 1 + \frac{3}{4}\sqrt{2}\right\} \tag{45b}$$

In Eq. 41 and Eq. 42 sn, dn, and cn are Jacobi elliptic functions.[8] These functions are doubly periodic, the second period being complex. The fundamental period parallelograms for the cartesian canonical variables are given in Figures 1-7 and 1-8. These figures are a representation of the analytically continued torus. Motion along the real axis corresponds to the classical motion of the Hamiltonian

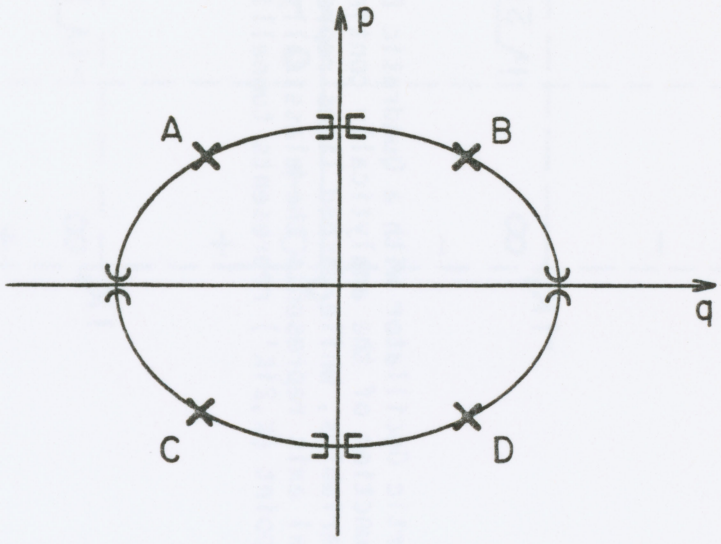
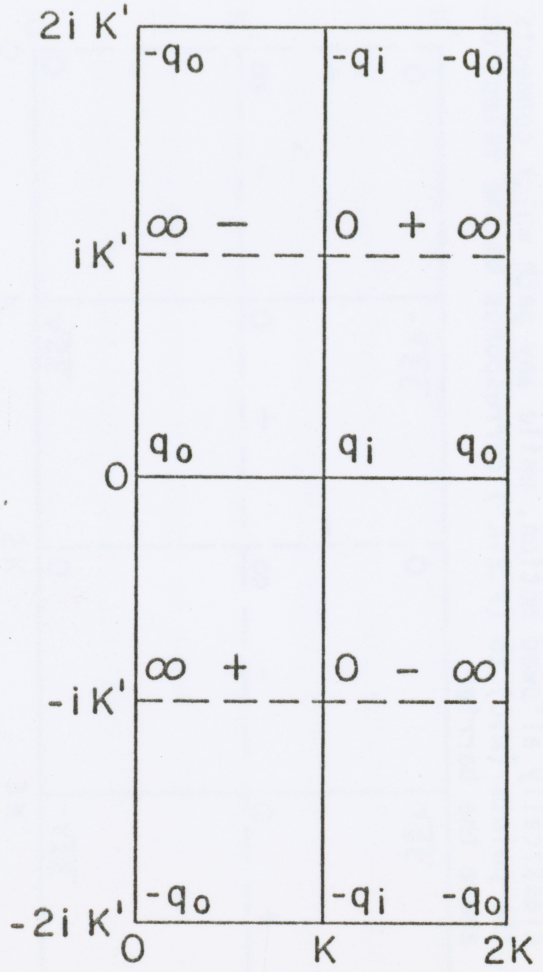
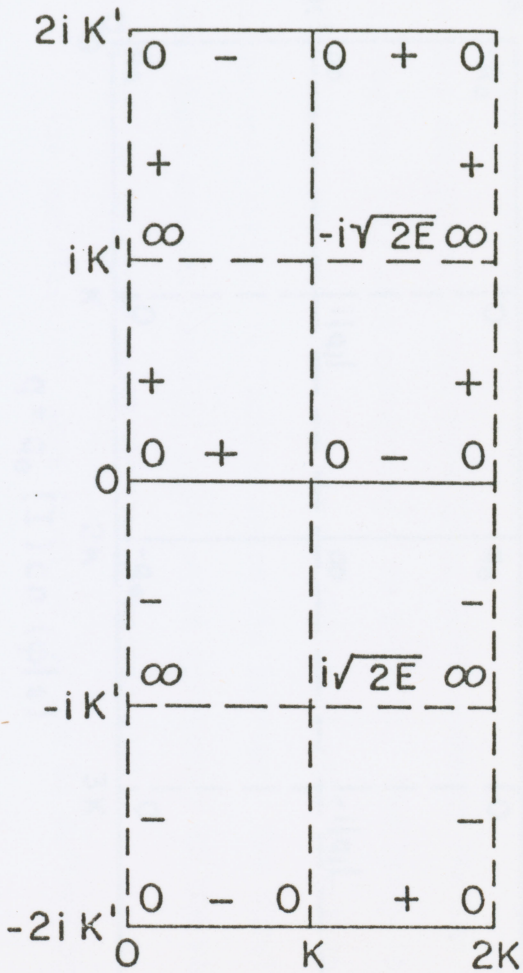


Figure 1-6. The Determination of the Relative Phases of the Terms of the Semiclassical Wave Function. Shown above is an invariant torus for a one dimensional oscillator in two-dimensional phase space. The coordinate representation of the semiclassical wave function has two terms, $\psi_q = \psi_U + \psi_L$, corresponding to the upper and lower halves of phase space respectively. The momentum representation of the semiclassical wave function also has two terms, $\psi_p = \psi_r + \psi_\ell$, in this case corresponding to the right and left halves of phase space. The phase of ψ_U can be determined relative to ψ_ℓ and ψ_r by Fourier transforming ψ_U at the points A and B respectively. In a similar manner one can determine the phase of ψ_L with respect to ψ_ℓ and ψ_r at the points C and D. Consequently, one can determine the phase of ψ_U relative to ψ_L by two independent paths. The requirement that these two determinations yield identical results, mod 2π, gives the primitive semiclassical quantization conditions.

Figure 1-7. The Analytically Continued Torus for the Quartic Oscillator with a Quadratic Barrier below the Barrier Height. Shown are the canonical variables as a function of the analytically continued angle variable. The solid lines represent real values of the variables, while dashed lines represent pure imaginary values of the variables. The path along the real axis represents the classically allowed motion, while any path connecting the point (K,0) to the point (K,2iK') represents tunnelling through the quadratic barrier.



$q = q_0(I)\,dn(\phi|r)$



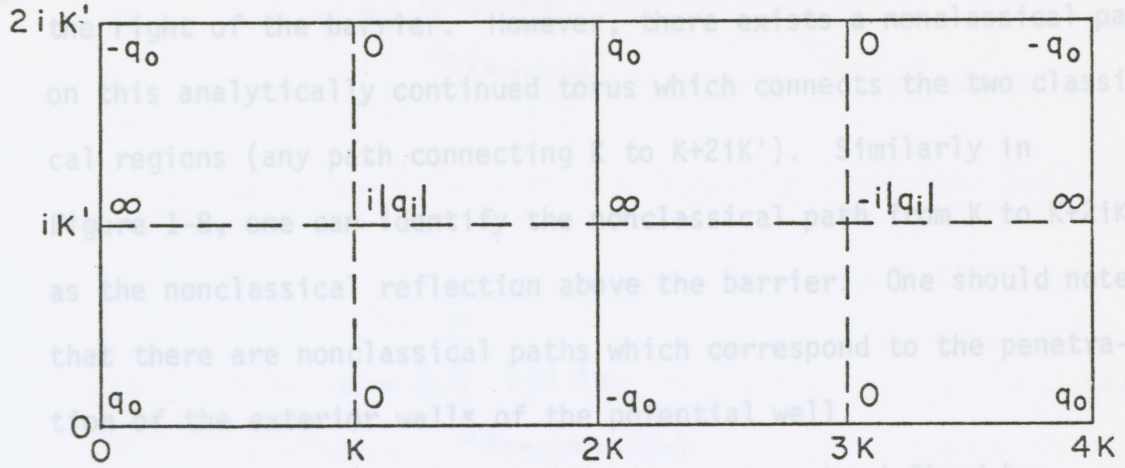
$p = -\omega(I)(q_0^2(I) - q_i^2(I))^{1/2}$

$cn(\phi|r)\,sn(\phi|r)$

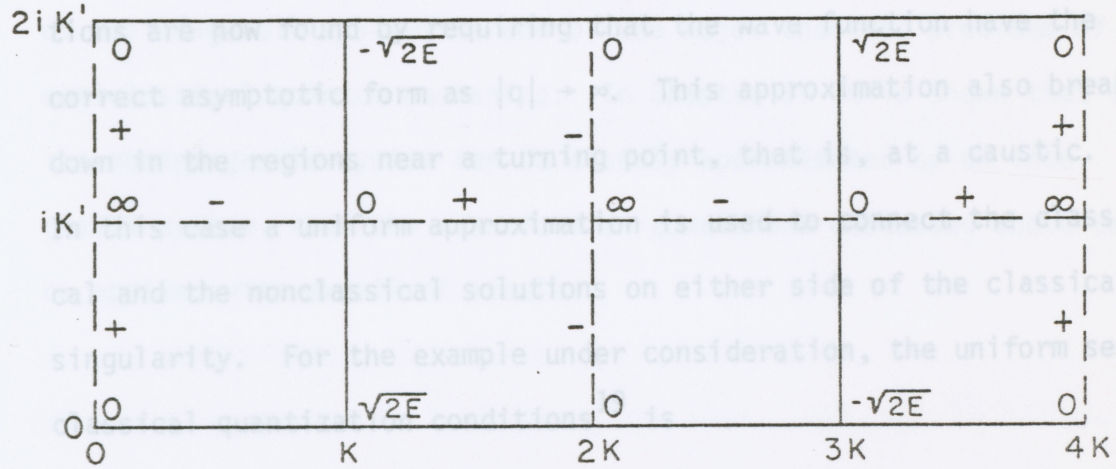
$$q = q_0(I)\,cn(\phi|s)$$

$$p = -\omega(I)\,q_0(I)\,sn(\phi|s)\,dn(\phi|s)$$

Figure 1-8. The Analytically Continued Torus for the Quartic Oscillator with a Quadratic Barrier above the Barrier Height. Shown are the canonical variables as a function of the analytically continued angle variable. The solid lines represent real values of the canonical variables, while the dashed lines represent pure imaginary values of these variables. The path along the real axis corresponds to the classically allowed motion, while any path which connects the points (K,0) to (K,2iK') corresponds to the relection above the barrier.



$$q = q_0\,(I)\,cn\,(\phi|s)$$



$$p = -\omega\,(I)\,q_0\,(I)\,sn\,(\phi|s)\,dn\,(\phi|s)$$

system. From Figure 1-7, one sees that for energies below the barrier height, the classical motion is confined in the region to the right of the barrier. However, there exists a nonclassical path on this analytically continued torus which connects the two classical regions (any path connecting K to K+2iK'). Similarly in Figure 1-8, one can identify the nonclassical path from K to K+2iK' as the nonclassical reflection above the barrier. One should note that there are nonclassical paths which correspond to the penetration of the exterior walls of the potential well.

The semiclassical wave function can now be defined by

$$\psi(q) \sim \sum_{\ell} \left| \frac{\partial^2 S_\ell}{\partial q \, \partial I} \right|^{1/2} \exp i \left\{ \frac{S_\ell(q, I)}{\hbar} - \sigma_q^\ell \frac{\pi}{4} \right\} \tag{46}$$

in both the classically allowed and classically forbidden regions of coordinate space. The uniform semiclassical quantization conditions are now found by requiring that the wave function have the correct asymptotic form as $|q| \to \infty$. This approximation also breaks down in the regions near a turning point, that is, at a caustic. In this case a uniform approximation is used to connect the classical and the nonclassical solutions on either side of the classical singularity. For the example under consideration, the uniform semiclassical quantization conditions[19] is

$$\left[1 + e^{-2\epsilon}\right]^{1/2} \cos(\alpha - \phi) = -e^{-\epsilon} \tag{47a}$$

where

$$\alpha = \oint_{\text{Classical}} p\, dq \tag{47b}$$

and

$$\epsilon = 2 \oint_{\text{Nonclassical}} |p|\, dq \tag{47c}$$

and

$$\phi = \arg \Gamma(i\epsilon + 1/2) - \epsilon \ln|\epsilon| + \epsilon \tag{47d}$$

The discussion to this point has assumed the integrability of the classical system. The problem of semiclassical quantization of nonintegrable systems is one of the major unsolved problems of semiclassical quantum mechanics. In Chapter IV it is shown that if the nonintegrable system can be closely approximated by an integrable system, then the quantization conditions discussed above can be applied with excellent results.

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CHAPTER II

SEMICLASSICAL QUANTIZATION VIA TRANSFORMATION TO ANGLE-ACTION VARIABLES

A. INTRODUCTION

This chapter discusses the semiclassical quantization of nonseparable, integrable Hamiltonian systems via a canonical transformation to angle-action variables. This problem has attracted the interest of many investigators[1-6] in the recent past. This interest stems from a paper of A. Einstein[7] in which he outlines a procedure for the quantization of an integrable system. Einstein noted that, for integrable systems, the classical trajectories are confined to invariant multipliconnected surfaces in phase space and these surfaces, called invariant tori, are characterized by a finite set of topologically independent closed paths. His procedure identifies the action integrals performed over these independent paths as the variables to be quantized. In retrospect, the work of Noid and Marcus (NM),[3a] and Chapman, Garrett, and Miller (CGM)[5] can be understood in terms of Einstein's analysis of nonseparable dynamics. The work of Percival and Pomphrey (PP),[4] on the other hand, is based explicitly upon the existence of the invariant tori. Marcus has effectively constructed representations of the invariant tori using trajectories, via use of Poincaré surface of section and numerical solutions of the equations of motion. While this avoids many of the computational problems encountered in the more abstract forms of classical mechanics, it does require a fairly large computational

effort for determining the semiclassical quantum states. The time independent methods developed by Percival and Pomphrey, and Chapman, Garrett, and Miller allows one to directly find the quantum states of interest via an iterative determination of the transformation to angle-action variables. However, these methods do not necessarily provide convergent computational techniques, particularly in the regions of phase space characterized by small divisors. These methods are also dependent upon one's ability to choose 'good' zero order variables.

This chapter presents an iterative method for the construction of the invariant tori, which has the advantage of yielding rapid convergence. This comes about as, in opposition to the methods of Percival and Pomphrey, and Chapman, Garrett, and Miller, the canonical transformation is actually carried out at each stage of the iterative process, resulting in accelerated convergence. This method will be called the Van Vleck method as it can be shown that this method is the classical limit of the Van Vleck transformation. Section B reviews the methods of Percival and Pomphrey, and Chapman, Garrett, and Miller and outlines the method reported here. The next section gives the details of the derivation and is followed by a discussion of the numerical procedure. In Section E the nondegenerate Henon-Heiles Hamiltonian system is presented as an example. The finial section is a discussion of the results of this chapter.

B. CLASSICAL MECHANICS AND THE CONSTRUCTION OF INVARIANT TORI

At the foundation of the methods of PP and CGM is the assumption that there exist angle-action variables.[9] Angle-action

variables[10,11] are a set of variables that have a specific time dependence, the action variables are constants of the motion,

$$\frac{d\underset{\sim}{I}}{dt} = -\frac{\partial H}{\partial \underset{\sim}{\theta}} = 0 \tag{1}$$

and the angle variables develop linearly in time,

$$\frac{d\underset{\sim}{\theta}}{dt} = \frac{\partial H}{\partial \underset{\sim}{I}} = \underset{\sim}{\omega}(\underset{\sim}{I}) \tag{2}$$

where the $\underset{\sim}{\omega}$ are the angular frequencies. If these variables do exist it is then possible to make a number of powerful statements[1,10,11]:

(a) The Hamiltonian function depends only upon the actions.

(b) There exists a canonical transformation from the physical variables to the angle-action variables, and as a result there exists a generating function from which one may derive this transformation.

(c) The physical coordinates, momenta and the generating function may be represented as Fourier series expansions in terms of the angle-action variables.

(d) The motion, as viewed in phase space, is confined to surfaces of constant action. These surfaces of constant action are the invariant tori, and the angle variables provide a coordinate system on the tori.

1. Percival-Pomphrey approach

Percival,[4] recognizing the time-independent nature of the problem, has rederived Hamilton's equations of motion in such a way as to remove the explicit time dependence in favor of the angle variables. Hamilton's equations, for an N dimensional system, then take the form

$$\underset{\sim}{\omega} \cdot \frac{\partial \underset{\sim}{p}}{\partial \underset{\sim}{\phi}} = -\frac{\partial H(\underset{\sim}{p}, \underset{\sim}{q})}{\partial \underset{\sim}{q}} \tag{3a}$$

$$\underset{\sim}{\omega} \cdot \frac{\partial \underset{\sim}{q}}{\partial \underset{\sim}{\phi}} = \frac{\partial H(\underset{\sim}{p}, \underset{\sim}{q})}{\partial \underset{\sim}{p}} \tag{3b}$$

where

$$\underset{\sim}{\omega} \cdot \frac{\partial}{\partial \underset{\sim}{\phi}} = \sum_{i=1}^{N} \omega_i \frac{\partial}{\partial \phi_i} \qquad \frac{\partial}{\partial \underset{\sim}{p}} = \left\{ \frac{\partial}{\partial p_1}, \ldots, \frac{\partial}{\partial p_N} \right\}$$

It should be recognized that Hamilton's equations in this form represent a time-independent formulation of classical mechanics, and that as a result the solutions of these equations, for specific values of action variables, will define the invariant tori.

Following PP, we consider systems of coupled harmonic oscillators having Hamiltonians of the following form

$$H = \sum_{i=1}^{N} \frac{1}{2} \left\{ p_i^2 + \lambda_i^2 q_i^2 \right\} + \epsilon V^c(q) \tag{4}$$

and make use of the fact that the coordinates and momenta can be expanded in Fourier series[10]

$$q(I,\phi) = \sum_{\vec{\ell}} q_{\vec{\ell}}(I)\, e^{i\vec{\ell}\cdot\vec{\phi}} \tag{5a}$$

$$p(I,\phi) = \sum_{\vec{\ell}} p_{\vec{\ell}}(I)\, e^{i\vec{\ell}\cdot\vec{\phi}} \tag{5b}$$

Substituting Eq. (5) into Eq. (3) and Fourier analyzing one obtains

$$i(\vec{\ell}\cdot\vec{\omega})\, q_{\vec{\ell}} = p_{\vec{\ell}} \tag{6a}$$

$$i(\vec{\ell}\cdot\vec{\omega})\, p_{\vec{\ell}} = f^{HO}_{\vec{\ell}} + \epsilon f^{c}_{\vec{\ell}} \tag{6b}$$

where

$$f^{HO}_{\vec{\ell}} = \left\{ -\lambda_1^2 q_{1\vec{\ell}}, \ldots, -\lambda_N^2 q_{N\vec{\ell}} \right\}$$

and

$$f^{c}_{\vec{\ell}} = \oint d\tau \left[-\frac{\partial V^c(q)}{\partial q} \right] e^{i\vec{\ell}\cdot\vec{\phi}} \qquad \oint(\,) = \left(\frac{1}{2\pi}\right)^N \int_0^{2\pi} d\phi_1 \cdots \int_0^{2\pi} d\phi_N$$

Eliminating $p_{\vec{\ell}}$ from Eqs. (6a) and (6b) gives

$$\left\{ \lambda_k^2 - (\vec{\ell}\cdot\vec{\omega})^2 \right\} q_{k\vec{\ell}} = \epsilon f^{c}_{k\vec{\ell}} \qquad k = 1, \ldots, N \tag{7}$$

This set of equations, together with the N action integrals, provides the basis of the PP iterative method. The solution of the uncoupled system (ε=0) is used as the zero order approximation. Using this approximate solution they find the zero order Fourier coefficient of the coupling force. The fundamental Fourier equations ($|\underset{\sim}{\ell}| = 1$) are then solved for the first-order frequencies

$$\omega_k^{(1)} = \lambda_k^2 - \varepsilon \frac{f_{k\,\underset{\sim}{\ell}}^{c\,(0)}}{q_{k\,\underset{\sim}{\ell}}^{(0)}} \qquad |\underset{\sim}{\ell}| = 1\,,\ k = 1,\ldots,N \tag{8}$$

and the rest of the set of Eq. (7) are solved for the new coordinate Fourier coefficients

$$q_{k\,\underset{\sim}{\ell}}^{(1)} = \frac{\varepsilon f_{k\,\underset{\sim}{\ell}}^{c\,(0)}}{\lambda_k^2 - (\underset{\sim}{\ell}\cdot\underset{\sim}{\omega}^{(1)})^2} \qquad |\underset{\sim}{\ell}| \neq 1\,,\ k = 1,\ldots,N \tag{9}$$

It is seen that this leaves the new fundamental ($|\underset{\sim}{\ell}| = 1$) Fourier coefficient of the coordinate undetermined. These coefficients are determined by requiring that the constant of motion have specific values, PP use the action for this purpose. It is in this step that boundary or initial conditions are imposed, in a manner analogous to determination of a coefficient in a quantum mechanical wave function by an overall normalization requirement.

Making the procedure explicit, the first order approximation has the form

$$\underset{\sim}{q}^{(1)}(\underset{\sim}{I},\underset{\sim}{\theta}) = \underset{\sim}{q}^{HO}(\underset{\sim}{I},\underset{\sim}{\theta}) + \epsilon \underset{\sim}{q}_1(\underset{\sim}{I},\underset{\sim}{\theta})$$

$$\underset{\sim}{p}^{(1)}(\underset{\sim}{I},\underset{\sim}{\theta}) = \underset{\sim}{p}^{HO}(\underset{\sim}{I},\underset{\sim}{\theta}) + \epsilon \underset{\sim}{p}_1(\underset{\sim}{I},\underset{\sim}{\theta}) \qquad (10)$$

This process may be repeated until the desired convergence is achieved. After the ℓth iteration the solution will be of the following form

$$\underset{\sim}{q}^{(\ell)} = \underset{\sim}{q}^{HO} + \sum_{m=1}^{\ell} \epsilon^m \underset{\sim}{q}_m \quad , \quad \underset{\sim}{p}^{(\ell)} = \underset{\sim}{p}^{HO} + \sum_{m=1}^{\ell} \epsilon^m \underset{\sim}{p}_m \qquad (11)$$

where $\underset{\sim}{q}^{HO}$, $\underset{\sim}{q}_n$, $\underset{\sim}{p}^{HO}$ and $\underset{\sim}{p}_n$ are Fourier series.

2. Chapman-Garrett-Miller approach

Following the method of Born, CGM couch their method in the language of canonical transformations,[10] without specific mention of invariant tori. They give an iterative method for determining the generating function for the transformation to angle-action variables. That this is equivalent to finding the parameterization of the torus is easily seen by noting that for specific values of the action the derivatives of the generating function define a (phase space) surface

$$\frac{\partial S(\underset{\sim}{q},\underset{\sim}{I})}{\partial \underset{\sim}{q}} = \underset{\sim}{p} \qquad \frac{\partial S(\underset{\sim}{q},\underset{\sim}{I})}{\partial \underset{\sim}{I}} = \underset{\sim}{\theta}$$

which is the invariant torus.

CGM consider Hamiltonian systems of the form

$$H = H_0(p,q) + \epsilon V^c(q) \tag{12}$$

where $H(p,q)$ is integrable via an analytically known transformation. This means that one can transform the Hamiltonian to

$$H = \omega \cdot I + \epsilon V^c(I,\theta) \tag{13}$$

where provided $\epsilon=0$ the variables I,θ are the angle-action variables for H. We will refer to variables of this nature as "angle-action like" variables. The advantage of transforming to these variables is that the "unperturbed" surfaces of constant I may be continuously deformed into the "perturbed" invariant torus. As a result the generating function corresponding to a transformation to angle-action variables has the form

$$S(\theta,I) = \theta \cdot I + \epsilon W(\theta,I) \tag{14}$$

where

$$W(\theta,I) = \sum_{l} W_l(I) e^{il\cdot\theta}$$

The $\underset{\sim}{\theta}$ are the old coordinates, the $\underset{\sim}{J}$ are the new momenta. The first term on the right gives rise to the identity transformation, as a result the second term modifies the surface of constant $\underset{\sim}{I}$. Obtaining $\underset{\sim}{I}$ by differentiating Eq. (14) with respect to $\underset{\sim}{\theta}$ and substituting this into Eq. (13), one obtains

$$E = \underset{\sim}{\omega}\cdot\underset{\sim}{J} + \epsilon\,\underset{\sim}{\omega}\cdot\frac{\partial W}{\partial \underset{\sim}{\theta}} + \epsilon\, V^c\left(\underset{\sim}{J} + \epsilon\frac{\partial W}{\partial \underset{\sim}{\theta}}, \underset{\sim}{\theta}\right) \tag{15}$$

Fourier analyzing this equation one finds

$$\underset{\sim}{\ell} = 0 \qquad E = \underset{\sim}{\omega}\cdot\underset{\sim}{J} + \epsilon V^c_{\underset{\sim}{0}} \tag{16a}$$

$$\underset{\sim}{\ell} \neq 0 \qquad 0 = i(\underset{\sim}{\ell}\cdot\underset{\sim}{\omega})W_{\underset{\sim}{\ell}} + V^c_{\underset{\sim}{\ell}} \tag{16b}$$

Equation (16b) is the basis of CGM iterative procedure.

Taking $S = \underset{\sim}{\theta}\cdot\underset{\sim}{J}$ as the zero order approximation to the generating function, CGM calculate the Fourier coefficient of the coupling potential. Then using Eq. (16b) they calculate the first-order generating function

$$W_{\underset{\sim}{\ell}} = \frac{V^{c(0)}_{\underset{\sim}{\ell}}}{i(\underset{\sim}{\ell}\cdot\underset{\sim}{\omega})} \tag{17}$$

and Eq. (16a) gives the first order energy. One difference between the PP and CGM methods is that PP find a new frequency at each step, while CGM, because their Fourier expansions are in terms of the zero-order "angle-like" variable, need not find a new frequency after each iteration. Both of these methods provide perturbative expansions, i.e., power series expansions in the coupling constant, for their respective representations of the invariant toris. It is a well-known result that such expansions, in classical mechanics, are not always convergent;[11] however, provided that one avoids regions of phase space characterized by small divisors and energies close to dissociation these methods provide useful and practical computational procedures.

3. Accelerated convergence approach

Our approach will be seen as closely related to the method of CGM. Whereas both PP and CGM attempt to find a single canonical transformation to angle-action variables, we will construct the overall transformation as a series of canonical transformations.

In order to see how this will work, consider a time-independent Hamiltonian system,

$$E = H_0(\underset{\sim}{J}) + \epsilon H'(\underset{\sim}{J}, \underset{\sim}{\theta}) \tag{18}$$

where H_0 represents an integrable system, and H' is a coupling term. The equations of motion for this system are

$$\underset{\sim}{\omega}(\underset{\sim}{I},\underset{\sim}{\theta}) = \dot{\underset{\sim}{I}} = \epsilon \frac{\partial H'}{\partial \underset{\sim}{\theta}} \tag{19}$$

$$\underset{\sim}{\omega}(\underset{\sim}{I},\underset{\sim}{\theta}) = \dot{\underset{\sim}{\theta}} = \frac{\partial H_0}{\partial \underset{\sim}{I}} + \epsilon \frac{\partial H'}{\partial \underset{\sim}{I}} \tag{20}$$

We now seek a canonical transformation which will eliminate the terms of order ϵ from the above equations. The Hamiltonian and equations of motion in the new variables will then have the form

$$H = H_0(\underset{\sim}{I}') + \epsilon^2 H'(\underset{\sim}{I}', \underset{\sim}{\theta}') \tag{21a}$$

$$\underset{\sim}{\omega}(\underset{\sim}{I}', \underset{\sim}{\theta}') = \dot{\underset{\sim}{I}}' = -\epsilon^2 \frac{\partial H'}{\partial \underset{\sim}{\theta}} \tag{21b}$$

$$\underset{\sim}{\omega}(\underset{\sim}{I}', \underset{\sim}{\theta}') = \dot{\underset{\sim}{\theta}} = \frac{\partial H_0}{\partial \underset{\sim}{I}'} + \epsilon^2 \frac{\partial H'}{\partial \underset{\sim}{I}'} \tag{21c}$$

By successive applications of such a transformation we can obtain a representation of the invariant torus as a series where the n^{th} term is of order ϵ^{2^n}. Such a series clearly is more likely to converge. In fact techniques similar to this have been shown to yield

convergent results and have been used to prove a number of theorems of classical mechanics including the KAM theorem.[12]

In the following section we will derive such a sequence of transformations.

C. DERIVATION OF THE CLASSICAL VAN VLECK CANONICAL TRANSFORMATIONS

Our goal is to construct a transformation from the physical variables to angle-action variables. This will be accomplished by constructing a series of consecutive canonical transformations, each one of which will bring the system closer to true angle-action variables.

We will assume a Hamiltonian of the form,

$$H = H_0(\underset{\sim}{p},\underset{\sim}{q}) + \epsilon V^c(\underset{\sim}{p},\underset{\sim}{q}) \tag{22}$$

where $H_0(\underset{\sim}{p},\underset{\sim}{q})$ represents an integrable system perturbed by the potential $V^c(\underset{\sim}{p},\underset{\sim}{q})$, ϵ being the coupling constant. We first transform the system into the angle-action variables of the uncoupled system. The Hamiltonian and the equations of motion are then

$$H = H_I(\underset{\sim}{I}) + \epsilon V^c(\underset{\sim}{I},\underset{\sim}{\varphi}) \tag{23a}$$

$$\underset{\sim}{\mu}^{(0)}(\underset{\sim}{I},\underset{\sim}{\varphi}) = \frac{d\underset{\sim}{I}}{dt} = -\epsilon \frac{\partial V^c(\underset{\sim}{I},\underset{\sim}{\varphi})}{\partial \underset{\sim}{\varphi}} \tag{23b}$$

$$\underset{\sim}{\omega}^{(0)}(\underset{\sim}{I},\underset{\sim}{\phi}) = \frac{d\underset{\sim}{\phi}}{dt} = \underset{\sim}{\omega}_I(\underset{\sim}{I}) + \epsilon \frac{\partial V^c(\underset{\sim}{I},\underset{\sim}{\phi})}{\partial \underset{\sim}{I}} \tag{23c}$$

where

$$V^c(\underset{\sim}{I},\underset{\sim}{\phi}) = \sum_{\underset{\sim}{\ell}\neq 0} V_{\underset{\sim}{\ell}}(\underset{\sim}{I})\, e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{\phi}}$$

and

$$\underset{\sim}{\omega}_I(\underset{\sim}{I}) = \frac{\partial H_I(\underset{\sim}{I})}{\partial \underset{\sim}{I}}$$

Examining these equations one sees that the variables $\underset{\sim}{J},\underset{\sim}{\phi}$ are angle-action "like" to order ϵ. This suggests that the next transformation should be to variables which are angle-action "like" to order ϵ^2. The Hamiltonian and the equations of motion will then be of the form

$$H = H_1(\underset{\sim}{I}^{(1)}) + \epsilon^2 V_1^c(\underset{\sim}{I}^{(1)}, \phi^{(1)}) \tag{24a}$$

$$\underset{\sim}{\omega}^{(1)}(\underset{\sim}{I}^{(1)}, \underset{\sim}{\phi}^{(1)}) = \frac{d\underset{\sim}{\phi}^{(1)}}{dt} = \underset{\sim}{\omega}_I(\underset{\sim}{I}^{(1)}) + \epsilon^2 \frac{\partial V_1^c(\underset{\sim}{I}^{(1)}, \underset{\sim}{\phi}^{(1)})}{\partial \underset{\sim}{I}^{(1)}} \tag{24b}$$

$$\underset{\sim}{\mathcal{H}}^{(1)}\left(\underset{\sim}{H}^{(1)}, \underset{\sim}{\phi}^{(1)}\right) = \frac{d\underset{\sim}{H}^{(1)}}{dt} = -\epsilon^2 \frac{\partial V_1^c\left(\underset{\sim}{H}^{(1)}, \underset{\sim}{\phi}^{(1)}\right)}{\partial \underset{\sim}{\phi}^{(1)}} \tag{24c}$$

It is seen that Eqs. (23) and (24) have the same form, and that as a result applying the same type of transformation to Eq. (24) should yield angle-action like variables to order ϵ^4. Clearly after n such transformations one obtains the following Hamiltonian and equations of motion,

$$H = H_n\left(\underset{\sim}{H}^{(n)}\right) + \epsilon^{2^n} V_n^c\left(\underset{\sim}{H}^{(n)}, \underset{\sim}{\phi}^{(n)}\right) \tag{25a}$$

$$\underset{\sim}{\mathcal{H}}^{(n)}\left(\underset{\sim}{H}^{(n)}, \underset{\sim}{\phi}^{(n)}\right) = \frac{d\underset{\sim}{H}^{(n)}}{dt} = -\epsilon^{2^n} \frac{\partial V_n^c\left(\underset{\sim}{H}^{(n)}, \underset{\sim}{\phi}^{(n)}\right)}{\partial \underset{\sim}{\phi}^{n}} \tag{25b}$$

$$\underset{\sim}{\omega}^{(n)}\left(\underset{\sim}{H}^{(n)}, \phi^{(n)}\right) = \frac{d\underset{\sim}{\phi}^{(n)}}{dt} = \underset{\sim}{\omega}_n\left(\underset{\sim}{H}^{(n)}\right) + \epsilon^{2^n} \frac{\partial V_n^c\left(\underset{\sim}{H}^{(n)}, \phi^{(n)}\right)}{\partial \underset{\sim}{H}^{(n)}} \tag{25c}$$

From these equations we see that after the n^{th} transformations the variables are angle-action "like" to order ϵ^{2^n}.

To implement this procedure we must construct the transformation of Eq. (23) to Eq. (24). Following CGM, we transform the Hamiltonian to angle-action "like" variables with the generating function

$$S_1(\underset{\sim}{\varphi}^{(0)}, \underset{\sim}{I}^{(1)}) = \underset{\sim}{\varphi}^{(0)} \cdot \underset{\sim}{I}^{(1)} + \epsilon W_1(\underset{\sim}{\varphi}^{(0)}, \underset{\sim}{I}^{(1)})$$

where

$$W_1(\underset{\sim}{\varphi}^{(0)}, \underset{\sim}{I}^{(1)}) = \sum_{\underset{\sim}{k} \neq 0} W_{\underset{\sim}{k}}^1(\underset{\sim}{I}^{(1)}) e^{i \underset{\sim}{k} \cdot \underset{\sim}{\varphi}^{(0)}} \tag{26}$$

Differentiating, one finds

$$\underset{\sim}{I}^{(0)} = \underset{\sim}{I}^{(1)} + \epsilon \sum_{\underset{\sim}{k} \neq 0} i \underset{\sim}{k} W'_{\underset{\sim}{k}}(\underset{\sim}{I}^{(1)}) e^{i \underset{\sim}{k} \cdot \underset{\sim}{\varphi}^{(0)}} \tag{27a}$$

$$\underset{\sim}{\varphi}^{(1)} = \underset{\sim}{\varphi}^{(0)} + \epsilon \sum_{\underset{\sim}{k} \neq 0} \frac{\partial W'_{\underset{\sim}{k}}(\underset{\sim}{I}^{(1)})}{\partial \underset{\sim}{I}^{(1)}} e^{i \underset{\sim}{k} \cdot \underset{\sim}{\varphi}^{(0)}} \tag{27b}$$

To obtain the equations of motion one differentiates Eq. (27) with respect to time, recalling that

$$\frac{d}{dt} = \underset{\sim}{\mu}^{(m)}(\underset{\sim}{I}^{(m)}, \underset{\sim}{\varphi}^{(m)}) \cdot \frac{\partial}{\partial \underset{\sim}{I}^{(m)}} + \underset{\sim}{\omega}^{(m)}(\underset{\sim}{I}^{(m)}, \underset{\sim}{\varphi}^{(m)}) \cdot \frac{\partial}{\partial \underset{\sim}{\varphi}^{(m)}}$$

this gives

$$\tilde{\mu}^{(0)}(\tilde{I}^{(0)},\tilde{\phi}^{(0)}) = \tilde{\mu}^{(1)}(\tilde{I}^{(1)},\tilde{\phi}^{(1)}) + i\epsilon \sum_{\tilde{k}\neq\tilde{0}} \tilde{k}\,\tilde{\mu}^{(1)}(\tilde{I}^{(1)},\tilde{\phi}^{(1)}) \cdot$$

$$\frac{\partial W_{\tilde{k}}'(\tilde{I}^{(1)})}{\partial \tilde{I}^{(1)}} e^{i\tilde{k}\cdot\tilde{\phi}^{(0)}} - \epsilon \sum_{\tilde{k}\neq\tilde{0}} \tilde{k}\left[\tilde{\omega}_0^{(0)}(\tilde{I}^{(0)},\tilde{\phi}^{(0)})\cdot\tilde{k}\right] W_{\tilde{k}}'(\tilde{I}^{(1)}) e^{i\tilde{k}\cdot\tilde{\phi}^{(0)}} \tag{28a}$$

$$\tilde{\omega}^{(1)}(\tilde{I}^{(1)},\tilde{\phi}^{(1)}) = \tilde{\omega}^{(0)}(\tilde{I}^{(0)},\tilde{\phi}^{(0)}) + \epsilon \sum_{\tilde{k}\neq\tilde{0}} \tilde{\mu}^{(1)}(\tilde{I}^{(1)},\tilde{\phi}^{(1)}) \cdot \frac{\partial}{\partial \tilde{I}^{(1)}} \tag{28b}$$

$$\times \left[\frac{\partial W_{\tilde{k}}'(\tilde{I}^{(1)})}{\partial \tilde{I}^{(1)}}\right] e^{i\tilde{k}\cdot\tilde{\phi}^{(0)}} + i\epsilon \sum_{\tilde{k}\neq\tilde{0}} \left[\tilde{k}\cdot\tilde{\omega}^{(0)}(\tilde{I}^{(0)},\tilde{\phi}^{(0)})\right] \frac{\partial W_{\tilde{k}}'(\tilde{I}^{(1)})}{\partial \tilde{I}^{(1)}} e^{i\tilde{k}\cdot\tilde{\phi}^{(0)}}$$

In order to determine the Fourier coefficient of the generating function one substitutes Eqs. (23) and (27) into Eq. (28). Taylor expanding about $\tilde{\phi}^{(0)}$ and $\tilde{J}^{(1)}$ and collecting terms of order ϵ, recalling that

$$\tilde{\omega}^{(0)} = \tilde{\omega}_0^{(0)} + \mathcal{O}(\epsilon) \quad , \quad \tilde{\omega}^{(1)} = \tilde{\omega}_0^{(1)} + \mathcal{O}(\epsilon^2) \tag{29a}$$

$$\tilde{\mu}^{(0)} = \mathcal{O}(\epsilon) \quad , \quad \tilde{\mu}^{(1)} = \mathcal{O}(\epsilon^2) \tag{29b}$$

(these are the conditions which give the desired transformation), then gives

$$-i\epsilon \sum_{\underset{\sim}{\ell}\neq 0} \underset{\sim}{\ell}\, V_{\underset{\sim}{\ell}}(\underset{\sim}{I}^{(1)})\, e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{\phi}^{(0)}}\Big|_{\underset{\sim}{I}^{(0)}=\underset{\sim}{I}^{(1)}}$$

$$= -\epsilon \sum_{\underset{\sim}{\ell}\neq 0} \underset{\sim}{\ell}\left[\underset{\sim}{\ell}\cdot\underset{\sim}{\omega}_0^{(0)}(\underset{\sim}{I}^{(0)})\right] W_{\underset{\sim}{\ell}}^{1}(\underset{\sim}{I}^{(1)})\, e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{\phi}^{(0)}}\Big|_{\underset{\sim}{I}^{(0)}=\underset{\sim}{I}^{(1)}} \quad (30a)$$

$$0 = \epsilon \sum_{\underset{\sim}{\ell}\neq 0} \frac{\partial V_{\underset{\sim}{\ell}}(\underset{\sim}{I}^{(0)})}{\partial \underset{\sim}{I}^{(0)}}\, e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{\phi}^{(0)}}\Big|_{\underset{\sim}{I}^{(0)}=\underset{\sim}{I}^{(1)}}$$

$$+ i\epsilon \sum_{\underset{\sim}{\ell}\neq 0} \left[\underset{\sim}{\ell}\cdot\underset{\sim}{\omega}_0^{(0)}(\underset{\sim}{I}^{(0)})\right] \frac{\partial W_{\underset{\sim}{\ell}}^{1}(\underset{\sim}{I}^{(1)})}{\partial \underset{\sim}{I}^{(1)}}\, e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{\phi}^{(0)}}\Big|_{\underset{\sim}{I}^{(0)}=\underset{\sim}{I}^{(1)}} \quad (30b)$$

Solving Eq. (30) for the Fourier coefficients of the generating function and their derivatives, one obtains

$$W_{\underset{\sim}{\ell}}^{1}(\underset{\sim}{I}^{(1)}) = -\frac{V_{\underset{\sim}{\ell}}^{(0)}(\underset{\sim}{I}^{(0)})}{i\left[\underset{\sim}{\ell}\cdot\underset{\sim}{\omega}_0^{(0)}(\underset{\sim}{I}^{(0)})\right]}\Bigg|_{\underset{\sim}{I}^{(0)}=\underset{\sim}{I}^{(1)}} \quad (31a)$$

$$\left.\frac{\partial W_{\underset{\sim}{\ell}}^{1}(\underset{\sim}{I}^{(1)})}{\partial \underset{\sim}{I}^{(1)}} = -\frac{\partial V_{\underset{\sim}{\ell}}^{(1)}(\underset{\sim}{I}^{(0)})/\partial \underset{\sim}{I}^{(0)}}{i\left[\underset{\sim}{\ell}\cdot\underset{\sim}{\omega}_{0}^{(0)}(\underset{\sim}{I}^{(0)})\right]}\right|_{\underset{\sim}{I}^{(0)}=\underset{\sim}{I}^{(1)}} \tag{31b}$$

These equations provide the generating function of the first transformation. Since the new Hamiltonian will be of the same form as the old Hamiltonian, except that the coupling constant is now ε^2, this transformation can be applied successively to obtain variables which are angle-action "like" to the desired order. The Fourier coefficient of the generating function of the n^{th} transformation are given, in terms of $(n-1)^{th}$ Hamiltonian, by

$$W_{\underset{\sim}{\ell}}^{n}(\underset{\sim}{I}^{(n)}) = -\left.\frac{V_{\underset{\sim}{\ell}}^{(n-1)}(\underset{\sim}{I}^{(n-1)})}{i\left[\underset{\sim}{\ell}\cdot\underset{\sim}{\omega}_{0}^{(n-1)}(\underset{\sim}{I}^{(n-1)})\right]}\right|_{\underset{\sim}{I}^{(n-1)}=\underset{\sim}{I}^{(n)}} \tag{32a}$$

$$\left.\frac{\partial W_{\underset{\sim}{\ell}}^{(n)}(\underset{\sim}{I}^{(n)})}{\partial \underset{\sim}{I}^{(n)}} = -\frac{\partial V_{\underset{\sim}{\ell}}^{(n-1)}(\underset{\sim}{I}^{(n-1)})/\partial \underset{\sim}{I}^{(n-1)}}{i\left[\underset{\sim}{\ell}\cdot\underset{\sim}{\omega}_{0}^{(n-1)}(\underset{\sim}{I}^{(n-1)})\right]}\right|_{\underset{\sim}{I}^{(n-1)}=\underset{\sim}{I}^{(n)}} \tag{32b}$$

Equations (32) together with Eq. (27) provide the required transformations.

The Van Vleck transformation can be described in terms of the CGM method in the following way: In order to obtain the Van Vleck transformation to angle-action variables one finds the first approximation to the CGM generating function. Then using this generating function the Hamiltonian is transformed into the new variables. This procedure is then repeated, that is, using the transformed Hamiltonian a new CGM generating function is found and then the Hamiltonian is again transformed into the new variables. This process is repeated until the desired convergence is achieved. Clearly if one requires a scheme with better convergence properties than those of the method reported here one need only use a higher order CGM generating function in place of the first order generating function. In Appendix A we show the relationship between the proposed transformation scheme, and the Van Vleck transformation in quantum mechanics.

D. THE NUMERICAL IMPLEMENTATION OF THE VAN VLECK CANONICAL TRANSFORMATION

In the previous section it was shown that the transformation to angle-action variables can be accomplished approximately to order $\varepsilon^{(2^n)}$, by a series of n classical Van Vleck canonical transformations. The numerical procedure used is outlined in this section. The process can be divided into three parts. Steps 1-3, determine the generating function for the transformation; Steps 4-6, transform the Hamiltonian from the old action "like" variables to the new action "like" variables; Steps 7-10, transform the Hamiltonian from the old angle "like" variables, to the new angle "like" variables. In Step 11 we test to

determine whether or not the desired degree of approximation has been achieved. The details of the inversion in Step 8 are given in Appendix B.

A fundamental difference between PP and CGM methods, and the Van Vleck method is that the Van Vleck method requires and yields more information about the structure of phase space. Thus PP and CGM treat the action "like" variables as parameters, here they must be treated as variables of the system. As a result, the different functions which arise in this method must be represented on a 2N-dimensional grid. N dimensions of this grid correspond to the N angle "like" variables, since these variables are periodic in nature, those N dimensions are represented by a finite Fourier expansion. (So far this is equivalent to the methods of PP and CGM.) The other N dimensions correspond to the action "like" variables. One must take great care in how one constructs the grid in these N dimensions.[13] This is a result of the fact that the functional $\underset{\sim}{J}$ dependence of the Fourier coefficients depends upon the form of the potential. For example, a one-dimensional quartic potential gives a power series in J, while a one-dimensional cubic potential gives a power series in $J^{1/2}$. It is found that if the grid is constructed in such a way as to give an accurate description of the Hamiltonian, following the zeroth order transformation, then the succeeding transformations are in general relatively independent of the grid parameters. The derivatives with respect to the action "like" variables are found by finite difference, and in turn the derivatives with respect to the angle "like" variables are obtained via the properties of the Fourier series.

Outline of the numerical procedure

For a N dimensional system

Input: Hamiltonian an 2N dimensional grid

$$H(\underset{\sim}{I}^{(o)}, \underset{\sim}{\phi}^{(o)}) \tag{A}$$

Step 1: Fourier analysis $H(\underset{\sim}{J}^{(0)}, \underset{\sim}{\phi}^{(0)})$

$$h_{\underset{\sim}{\ell}}(\underset{\sim}{I}^{(o)}) \tag{B}$$

$$\left[h_{\underset{\sim}{\ell}} = v_{\underset{\sim}{\ell}} \quad , h_{\underset{\sim}{0}} = H_{\underset{\sim}{0}} \right]$$

Step 2: Determine derivatives of Fourier coefficients of H

$$\frac{\partial h_{\underset{\sim}{\ell}}(\underset{\sim}{I}^{(o)})}{\partial \underset{\sim}{I}^{(o)}}$$

$$\frac{\partial h_{\underset{\sim}{0}}}{\partial \underset{\sim}{I}^{(o)}} = \underset{\sim}{\omega}^{(o)} \qquad \frac{\partial h_{\underset{\sim}{\ell}}}{\partial \underset{\sim}{I}^{(o)}} = \frac{\partial v_{\underset{\sim}{\ell}}}{\partial \underset{\sim}{I}^{(o)}} \tag{C}$$

Step 3: Using Eq. (32), (B), (C) construct Fourier representation of generating function.

$$S = \underset{\sim}{\phi}^{(0)} \cdot \underset{\sim}{I}^{(1)} + \epsilon W^{1}\left(\underset{\sim}{\phi}^{(0)}, \underset{\sim}{I}^{(1)}\right) \tag{D}$$

$$W^{1}\left(\underset{\sim}{\phi}^{(0)}, \underset{\sim}{I}^{(1)}\right) = \sum_{\underset{\sim}{l} \neq 0} W^{1}_{\underset{\sim}{l}}\left(\underset{\sim}{I}^{(1)}\right) e^{i \underset{\sim}{l} \cdot \phi^{(0)}}$$

Step 4: Differentiate (D) with respect to $\underset{\sim}{\phi}^{(0)}$ to obtain old action "like" variable as functions of old angle and new action "like" variables

$$\underset{\sim}{I}^{(0)} = \sum_{\underset{\sim}{l} \neq 0} \underset{\sim}{l} \, \hat{J}^{(0)}_{\underset{\sim}{l}}\left(\underset{\sim}{I}^{(1)}\right) e^{i \underset{\sim}{l} \cdot \underset{\sim}{\phi}^{(0)}} \tag{E}$$

Step 5: Fourier transforms (E) to obtain $J^{(0)}$ an 2N dimensional grid

$$\underset{\sim}{I}^{(0)}\left(\underset{\sim}{\phi}^{(0)}, \underset{\sim}{I}^{(1)}\right) \tag{F}$$

Step 6: By interpolation compute Hamiltonian and grid defined by (F) to give

$$H\left(\underset{\sim}{\phi}^{(0)}, \underset{\sim}{I}^{(1)}\right) \tag{G}$$

Step 7: Differentiate (D) with respect to $\underset{\sim}{J}^{(1)}$ to obtain new angle "like" variable as Fourier representation in the old angle and the new action "like" variable

$$\underset{\sim}{\phi}^{(1)} = \sum_{\underset{\sim}{\ell}} \underset{\sim}{a}_{\underset{\sim}{\ell}}^{(1)} (\underset{\sim}{J}^{(1)}) e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{\phi}^{(0)}} \tag{H}$$

Step 8: Invert (H) to obtain old angle "like" variable as a Fourier representation in the new angle-action "like" variables (see Appendix B).

$$\underset{\sim}{\phi}^{(0)} = \sum_{\underset{\sim}{\ell}} \underset{\sim}{a}_{\underset{\sim}{\ell}}^{+} (\underset{\sim}{J}^{(1)}) e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{\phi}^{(1)}} \tag{I}$$

Step 9: Fourier transformation (I) to obtain the old angle "like" variable on a 2N-dimensional grid

$$\underset{\sim}{\phi}^{(0)} (\underset{\sim}{J}^{(1)}, \underset{\sim}{\phi}^{(1)}) \tag{J}$$

Step 10: By interpolation of (G) compute the Hamiltonian on the grid defined by (J) to give

$$H(\underset{\sim}{J}^{(1)}, \underset{\sim}{\phi}^{(1)}) \tag{K}$$

Step 11: Check convergence, if desired level of convergence is achieved, exit, otherwise use (K) as input and repeated Steps 1-11.

E. NUMERICAL RESULTS

To test the procedure described in the previous section we have applied the Van Vleck method to two non-degenerate harmonic oscillators perturbed by potentials of the type,

$$V_1 = \epsilon x (y^2 + \eta x^2) \tag{33a}$$

and

$$V_2 = b x^2 y^2 \tag{33b}$$

Semiclassical quantum levels were calculated for V_1 and are compared with those of MN, PP, and CGM as well as with exact quantum results in Table I. It is seen that all of these semiclassical methods give essentially the same results which is to be expected as all of the methods converged well for the parameters chosen for V_1. To compare convergence properties of the various methods, the second coupling potential V_2 was used. This potential was chosen because it can be shown not to give rise to ergodic behavior, i.e., all of phase space consists of invariant tori. For this coupling potential there are two regions of phase space that cause difficulties for the PP and CGM methods: Regions characterized by energies near dissociation, and by near-degenerate frequencies. The results of the convergence study in both of these regions and in a region where the methods of PP and CGM converge are given in Table IIA, B, C.

Table I. Comparison of the semiclassical eigenvalues calculated by the NM, PP, CGM, and accelerated convergence (VV) methods, for the Hamiltonian, $H = 1/2\ p_x^2 + 1/2\ p_y^2 + 1/2\ \omega_x^2 x^2 + 1/2\ \omega_y^2 y^2 + \varepsilon x(y^2 + \eta x^2)$. The Quantum Mechanical (QM) results are also shown.

n_x	n_y	N.M.	P.P.	C.G.M.	V.V.	Q.M.
$\omega_x^2 = 0.29375$		$\omega_y^2 = 2.12581$		$\varepsilon = -0.1116$		$\eta = 0.08414$
0	0	0.9922	0.9920	0.9920	0.9920	0.9916
1	0	1.5164	1.5164	1.5164	1.5164	1.5159
2	0	2.0313	2.0313	2.0313	2.0314	2.0308
0	1	2.4198	2.4194	2.4194	2.4191	2.4188
$\omega_x^2 = 0.36$		$\omega_y^2 = 1.96$		$\varepsilon = -0.1$		$\eta = 0.1$
0	0	0.9942	0.9941	0.9941	0.9941	0.9939
1	0	1.5812	1.5812	1.5812	1.5812	1.5809
2	0	2.1616	2.1615	2.1615	2.1616	2.1612
$\omega_x^2 = 0.49$		$\omega_y^2 = 1.69$		$\varepsilon = -0.1$		$\eta = 0.1$
0	0	0.9954	0.9955	0.9955	0.9955	0.9955
1	0	1.6870	1.6870	1.6870	1.6870	1.6870
0	1	2.2985	2.2782	2.2782	2.2782	2.2781
2	0	2.3751	2.3750	2.3750	2.3751	2.3750
1	1	2.9588	2.9584	2.9584	2.4584	2.9583
0	2	3.5480	3.5480	3.5480	3.5481	3.5479
$\omega_x^2 = 0.81$		$\omega_y^2 = 1.21$		$\varepsilon = -0.08$		$\eta = 0.1$
0	0	0.9978	0.9978	0.9978	0.9978	0.9980
1	0	1.8944	1.8941	1.8941	1.8941	1.8944
0	1	2.0889	2.0890	2.0890	2.0890	2.0890
2	0	2.7900	2.7896	2.7896	2.7896	2.7899

Table IIA. Comparison of convergence of the PP, CGM and VV methods in a region of phase space characterized by good convergence. The Hamiltonian is $1/2\ (P_x^2 + x^2 + P_y^2 + ay^2) + bx^2y^2$, where $a = 0.7$, $b = -0.02$. The action considered is, $I_x = I_y = 2.5$, i.e., the $n_x = 2$, $n_y = 2$ quantum state. The standard deviation of the energy on the approximate torus is shown in each case. All methods converge to a useful accuracy, although the V.V. method is superior in higher order.

Iter.	P.P.	C.G.M.	V.V.
0	1.7×10^{-1}	1.7×10^{-1}	1.7×10^{-1}
1	1.6×10^{-2}	2.5×10^{-2}	1.1×10^{-2}
2	2.9×10^{-3}	5.2×10^{-3}	2.4×10^{-4}
3	1.0×10^{-3}	1.2×10^{-3}	1.3×10^{-7}
4	3.7×10^{-4}	3.2×10^{-4}	2.4×10^{-11}

Table IIB. Comparison of convergence of the PP, CGM and VV methods in a region of phase space characterized by small divisors (near-degeneracy). $a = 0.93$, $b = -0.02$, $I_x = I_y = 2.5$ for the Hamiltonian of Table IIA. Shown are the standard deviations of the energy on the approximate torus.

Iter.	P.P.	C.G.M.	V.V.
0	1.4×10^{-1}	1.4×10^{-1}	1.4×10^{-1}
1	4.5×10^{-2}	1.5×10^{-2}	1.7×10^{-2}
2	Blows Up	2.3×10^{-3}	2.2×10^{-3}
3	Blows Up	3.9×10^{-4}	1.1×10^{-4}
4	Blows Up	7.9×10^{-5}	1.1×10^{-6}
5	Blows Up	1.7×10^{-5}	1.6×10^{-11}

Table IIC. Comparison of convergence of the PP, CGM and VV methods in a region of phase space characterized by an energy near dissociation. $a = 0.05$, $b = -0.02$, $I_x = 3.5$, $I_y = 2.5$ for the Hamiltonian of Table IIA. Shown are the standard deviations of the energy on the approximate torus.

Iter.	P.P.	C.G.M.	V.V.
0	2.8×10^{-1}	2.8×10^{-1}	2.8×10^{-1}
1	4.3×10^{-2}	6.8×10^{-2}	3.8×10^{-2}
2	7.2×10^{-3}	2.5×10^{-2}	6.5×10^{-4}
3	2.7×10^{-3}	1.2×10^{-2}	1.1×10^{-6}
4	Blows Up	6.5×10^{-3}	4.8×10^{-11}

The standard deviation of the energy on the approximate torus is used as a measure of the convergence. Clearly the Van Vleck approach gives superior convergence in all three regions of phase space. In regions of phase space that are characterized by small divisors the convergence of the Van Vleck method is initially slower than in the other regions. However, it is seen that this behavior disappears after the third iteration.

F. DISCUSSION

This chapter has developed a method of transforming a non-separable, integrable Hamiltonian system into angle-action variables. Transformations of this nature are complicated by the occurrence of small divisors. These are analogous to resonant denominators in degenerate or near-degenerate perturbation theory. The terms of most classical expansions (e.g., those of classical perturbation

theory) have a factor of the form $\underset{\sim}{\omega} \cdot \underset{\sim}{n} = \omega_1 n_1 + \ldots + \omega_N n_N$ in their denominator, as for example $t_{\underset{\sim}{n}} = \frac{N_{\underset{\sim}{n}}}{\underset{\sim}{\omega} \cdot \underset{\sim}{n}}$. As a consequence, if the frequencies are rationally related there will be vectors $\underset{\sim}{n}$ such that $\underset{\sim}{\omega} \cdot \underset{\sim}{n}$ is nearly zero. As a result the convergence of such classical expansions is in question in regions of phase space which are characterized by rationally or near rationally related frequencies. Existence proofs, such as the proof of the K.A.M. theorem, are often extremely difficult due to the occurrence of these small divisors. The technique[12] of treating a canonical transformation as an infinite series of canonical transformations was developed to facilitate the proof of such theorems. The general philosophy of these methods is to find a sequence of canonical transformations such that the numerators of the new terms, appearing as a result of the k^{th} transformation, are smaller than the denominators, $N_{\underset{\sim}{n}} < \underset{\sim}{\omega} \cdot \underset{\sim}{n}$. It is clear that the method developed in this chapter belongs to this class of techniques. Note should be taken that this does not solve all of the problems which arise in the degenerate or near-degenerate case. As in quantum mechanics, what is desired are the 'correct' zero order solutions. This is a non-trivial problem, for which a general solution is not presently known. However, some progress can be made in systematizing the choice of zero order variables. This is the subject of the following chapter.

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CHAPTER III

SEMICLASSICAL QUANTIZATION OF ZERO ORDER DEGENERATE HAMILTONIAN SYSTEMS

A. INTRODUCTION

The success of the Van Vleck method of construction of invariant tori when the zero order integrable problem is degenerate depends upon one's ability to choose a "good" zero order approximation to the invariant torus. An analogous problem arises in quantum mechanics. Recall, that in the case of degenerate perturbation theory[1] the zero order wave functions are not uniquely determined, but may be chosen as arbitrary linear combinations of a set of orthogonal functions which are associated with the degenerate subspace. The usual program in degenerate perturbation theory is to find the correct linear combination of the zero order wave functions by requiring that the matrix elements which connect the degenerate states vanish. Consequently the terms in the perturbation expansion which contain resonant denominators are identically zero. Similarly, in the classical case, the zero order action like variables which define the zero order torus may be chosen as linear combinations of a set of integrals associated with the zero order integrable problem. Again the correct linear combination can be found by requiring that the terms in the classical perturbation expansion which contain small divisors vanish identically.

This chapter discusses a technique by which one can identify a good choice of zero order angle-action variables. This process

involves identifying an intermediate integrable problem between the zero order problem and the total system, that is, an integrable problem which contains the zero order problem, and at the same time is a closer approximation to the total Hamiltonian. If the determination of such an intermediate problem breaks the degeneracy of the zero order problem one can identify the correct zero order variables. This process is discussed in the next section and is used to find the correct zero order variables for the degenerate Henon-Heiles Hamiltonian system in Section C. Section D discusses the primitive semiclassical quantization of this system.

B. A PEDAGOGICAL EXAMPLE OF THE IDENTIFICATION OF ZERO ORDER VARIABLES

In Chapter II the transformation to angle-action variables was constructed as a sequence of canonical transformations.[2] The initial step of this process is to transform the Hamiltonian from the physical variables (see Section C, Chapter II) to the angle-action variables[3] of the uncoupled Hamiltonian system (see Section C, Chapter II). This immediately raises the question of the uniqueness of the angle-action variables of the uncoupled problem. One finds that if the zero order integrable problem is nondegenerate any set of zero order angle-action variables is acceptable. On the other hand, if the zero order integrable problem is degenerate, it does not define unique tori, and as a result the choice of zero order angle-action variables is not trivial. This is illustrated in this section by consideration of a simple pedagogical example.

Consider the Hamiltonian system

$$H = H_o + V \tag{1}$$

where

$$H_o = \frac{1}{2}\left\{P_x^2 + x^2\right\} + \frac{1}{2}\left\{P_y^2 + y^2\right\} \tag{2a}$$

$$V = -\epsilon x^2 y^2 \tag{2b}$$

The zero order integrable problem is chosen to be degenerate, i.e., the frequencies of the normal modes are equal. This Hamiltonian has six readily identifiable (low frequency) periodic orbits: two unstable periodic orbits along the x and y axes, and four stable periodic orbits, two precessing and two librating. The librating orbits lie on the axis x = y and x = -y. It is convenient to rotate the coordinate system so that these orbits are on the new x and y axes. Following such a rotation the Hamiltonian in the new coordinates is

$$H_o = \frac{1}{2}\left\{P_x^2 + X^2\right\} + \frac{1}{2}\left\{P_y^2 + Y^2\right\} \tag{3a}$$

$$V = -\frac{\epsilon}{4}\left\{X^2 - Y^2\right\}^2 \tag{3b}$$

Transforming to cartesian angle-action variables one finds

$$H_o = I_x + I_y \tag{4a}$$

$$V = -\frac{\epsilon}{8}\left\{3I_x^2 - 4I_xI_y + 3I_y^2\right\} \tag{4b}$$

$$+\frac{\epsilon}{2}I_x(I_x-I_y)\cos 2\theta_x - \frac{\epsilon}{8}I_x^2\cos 4\theta_x \tag{4c}$$

$$+\frac{\epsilon}{2}I_y(I_y-I_x)\cos 2\theta_y - \frac{\epsilon}{8}I_y^2\cos 4\theta_y \tag{4d}$$

$$+\frac{\epsilon}{4}I_xI_y\cos 2(\theta_x+\theta_y) \tag{4e}$$

$$+\frac{\epsilon}{4}I_xI_y\cos 2(\theta_x-\theta_y) \tag{4f}$$

Application of the Van Vleck method to the Hamiltonian in these variables will fail due to the occurrence of small divisors. To see why this happens construct the generating function of the first Van Vleck transformation,

$$S = I_x'\theta_x + I_y'\theta_y \tag{5}$$

$$-\frac{\epsilon}{4\omega_x}I_x'(I_x'-I_y')\sin 2\theta_x + \frac{\epsilon}{32\omega_x}I_x'^2\sin 4\theta_x \tag{5c}$$

$$-\frac{\epsilon}{4\omega_y}I_y'(I_y'-I_x')\sin 2\theta_y + \frac{\epsilon}{32\omega_y}I_y'^2\sin 4\theta_y \tag{5d}$$

$$-\frac{\epsilon}{8(\omega_x+\omega_y)}I_x'I_y'\sin 2(\theta_x+\theta_y) \tag{5e}$$

$$-\frac{\epsilon}{8(\omega_x-\omega_y)}I_x'I_y'\sin 2(\theta_x-\theta_y) \tag{5f}$$

The terms in this equation are labelled to correspond to Eq. 4, and the new variables are primed. Clearly the denominator in term f will be small since the zero order frequencies are equal, that is, term f in the Hamiltonian is in resonance with the zero order problem. In order to see how to overcome this problem it is useful to transform to the variables defined by

$$I_1 = I_x + I_y \qquad \Theta_x = \Theta_1 + \Theta_2 \tag{6a}$$

$$I_2 = I_x - I_y \qquad \Theta_y = \Theta_1 - \Theta_2 \tag{6b}$$

The period of Θ_1 is 2π and the period of Θ_2 is π. The transformed Hamiltonian is

$$H_0 = I_1 \tag{7a}$$

$$V = -\frac{\epsilon}{16}\left\{ I_1^2 + 5I_2^2 \right\} \tag{7b}$$

$$+\frac{\epsilon}{4}(I_1+I_2)I_2 \cos 2(\Theta_1+\Theta_2) - \frac{\epsilon}{32}(I_1+I_2)^2 \cos 4(\Theta_1+\Theta_2) \tag{7c}$$

$$+\frac{\epsilon}{4}(I_1-I_2)I_2 \cos 2(\Theta_1-\Theta_2) - \frac{\epsilon}{32}(I_1-I_2)^2 \cos 4(\Theta_1-\Theta_2) \tag{7d}$$

$$+\frac{\epsilon}{16}(I_1+I_2)(I_1-I_2)\cos 4\Theta_1 \tag{7e}$$

$$+\frac{\epsilon}{16}(I_1+I_2)(I_1-I_2)\cos 4\Theta_2 \tag{7f}$$

And the generating function is

$$S = I_1'\theta_1 + I_2'\theta_2 \tag{8}$$

$$-\frac{\epsilon}{8(\omega_1+\omega_2)}(I_1'+I_2')I_2'\sin 2(\theta_1+\theta_2)+\frac{\epsilon}{128(\omega_1+\omega_2)}(I_1'+I_2')^2\sin 4(\theta_1+\theta_2) \tag{8c}$$

$$+\frac{\epsilon}{8(\omega_1-\omega_2)}(I_1'-I_2')I_2'\sin 2(\theta_1-\theta_2)+\frac{\epsilon}{128(\omega_1-\omega_2)}(I_1'-I_2')^2\sin 4(\theta_1-\theta_2) \tag{8d}$$

$$-\frac{\epsilon}{32\omega_1}(I_1'+I_2')(I_1'-I_2')\sin 4\theta_1 \tag{8e}$$

$$-\frac{\epsilon}{32\omega_2}(I_1'+I_2')(I_1'-I_2')\sin 4\theta_2 \tag{8f}$$

where again the terms are labelled to correspond to Eq. 4, and the new variables are primed. Clearly, the resonant term will not cause problems if the numerator is smaller than the denominator. Consequently, these variables are good zero order variables for the region of phase space characterized by $I_1 \sim |I_2|$. By setting $I_1 = I_2$(or $-I_2$) one finds the central periodic orbits of these tori, and, hence, can identify this region of phase space to correspond to the two librating tori on the x and y axes. The question now arises as how to treat the region of phase space characterized by $I_1 >> |I_2|$. This region can be handled by transforming the Hamiltonian in such a manner that the resonant term becomes part of the new action variable. For the case in hand, such a transformation is given by

$$J_1 = I_1 \tag{9a}$$

$$J_2 = (I_1^2 - I_2^2)^{1/2} \sin 2\theta_2 \tag{9b}$$

The period of ψ_1 is 2π and of ψ_2 is π. The transformed Hamiltonian is then

$$H_0 = J_1 \tag{10a}$$

$$V = -\frac{\epsilon}{8}\left(2J_1^2 - J_2^2\right) \tag{10b}$$

$$+ \frac{\epsilon}{4}(J_1^2 - J_2^2)\cos^2 2\varphi_2 \tag{10c}$$

and other terms (10d)

It should be noted that a new resonant term appears. This term results in the Van Vleck method breaking down in the region where $J_1 >> J_2$, that is, in the region where $I_1 \sim I_2$. These variables are a set of good zero order variables when $J_1 \sim J_2$. Setting $J_1 = J_2$ (or $-J_2$) one finds the central periodic orbits of these tori and hence can identify this region of phase space as corresponding to the two precessing tori.

The identification of these zero order variables could also have been accomplished in the following manner. In general, the coupling potential can be partitioned into two parts,

$$V = V_n + V' . \tag{11}$$

The first part, V_n, comprises the terms of the coupling potential which depend only upon the action like variables and the terms which are in resonance with the zero order problem. In this case

$$V_n = V_n(\underset{\sim}{I}, \underset{\sim}{k}\cdot\underset{\sim}{\varphi}), \tag{12}$$

where $\underset{\sim}{k}$ is given by

$$\underset{\sim}{k}\cdot\frac{\partial H_0}{\partial \underset{\sim}{I}} = 0 .$$

This term is the component of the coupling potential which is normal to H,

$$\{V_n, H_0\} = 0 .$$

The second part, V', is the remainder of the coupling potential. Now consider the following integrable Hamiltonian

$$H = H_0 + V_n . \tag{13}$$

If the normal component of the coupling potential breaks the degeneracy of the zero order problem, then by examining the periodic motions of this new integrable Hamiltonian one can construct good sets of zero order variables for the tori surrounding the central periodic orbits of the total problem. On the other hand, if Eq. 13 is still degenerate then one must transform the Hamiltonian so that new normal terms which break the degeneracy appear. This can be achieved by the use of Birkoff-Gustavson transformations, and is the subject of the next section.

C. ZERO ORDER VARIABLES OF THE HENON-HEILES HAMILTONIAN

In the last section it was shown that, if the Hamiltonian can be partitioned into a nondegenerate, integrable problem plus a term which couples the modes of this integrable problem, then by examining the solutions of this intermediate problem one can find good sets of zero order angle-action variables. It is not always possible to partition this Hamiltonian in this manner. An example of this nature, the Henon-Heiles Hamiltonian system, is considered in this section. This system has been studied exhaustively for the past fifteen years.[4] It is of interest in many branches of science as an example of a simple nonlinear system which displays both regular and stochastic behavior.[5] Numerical experiments[7] have revealed that there is a critical energy above which there are macroscopic volumes of phase space which are filled by stochastic trajectories. One also finds that there exist several families of trajectories surrounding periodic orbits. Corresponding to each of these families there is a set of angle-action variables. In these K.A.M. regions of phase space, stochastic trajectories lie in between these tori. Of these families of tori, five persist well below the critical energy and dominate the large scale dynamical flows. Three of these families, the box tori, are related by rotations of $\frac{2\pi}{3}$ radians in coordinate space (see Figure 3-1). The other two families of tori are precessing tori, and are equivalent except that they have opposite senses of rotation (see Figure 3-2). Consequently, one need only consider one family of each type of tori. In addition to the five central periodic orbits of these tori below the critical energy there also exist three unstable periodic orbits (see Figure 3-3). Above the

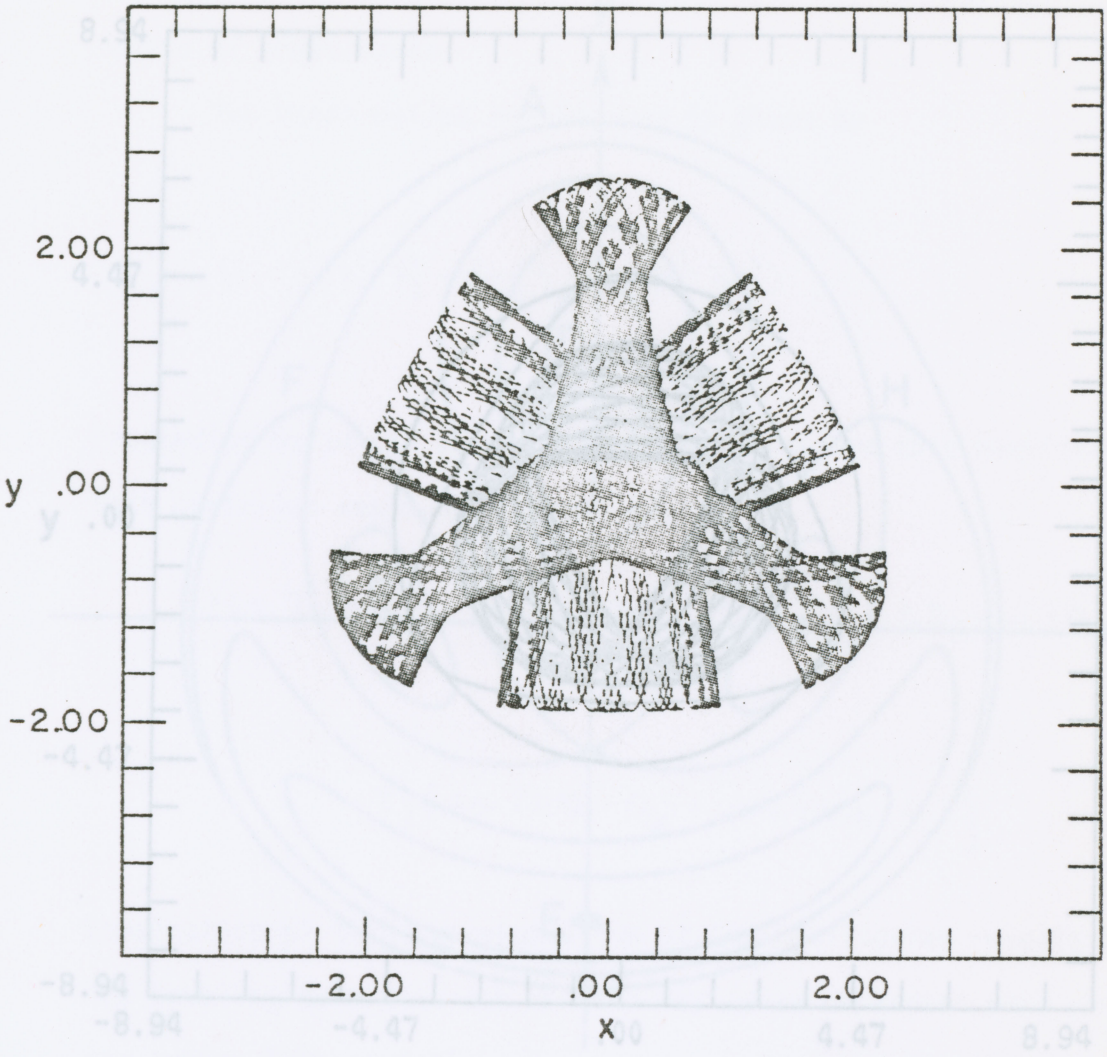


Figure 3-1. The Box Tori of the Henon-Heiles Hamiltonian System. The Henon-Heiles Hamiltonian system can be viewed as a threefold hindered rotor. The trajectories shown in this figure correspond to motion which does not have enough angular momentum to cross the dynamical barriers of the system. The C_{3v} symmetry of the Hamiltonian results with these three trajectories being symmetrical about the C_3 axis in coordinate space. Each of these trajectories represents disjoint tori, that is, disjoint classical trajectories. In Chapter IV it is shown that these disjoint tori can be connected by imaginary paths.

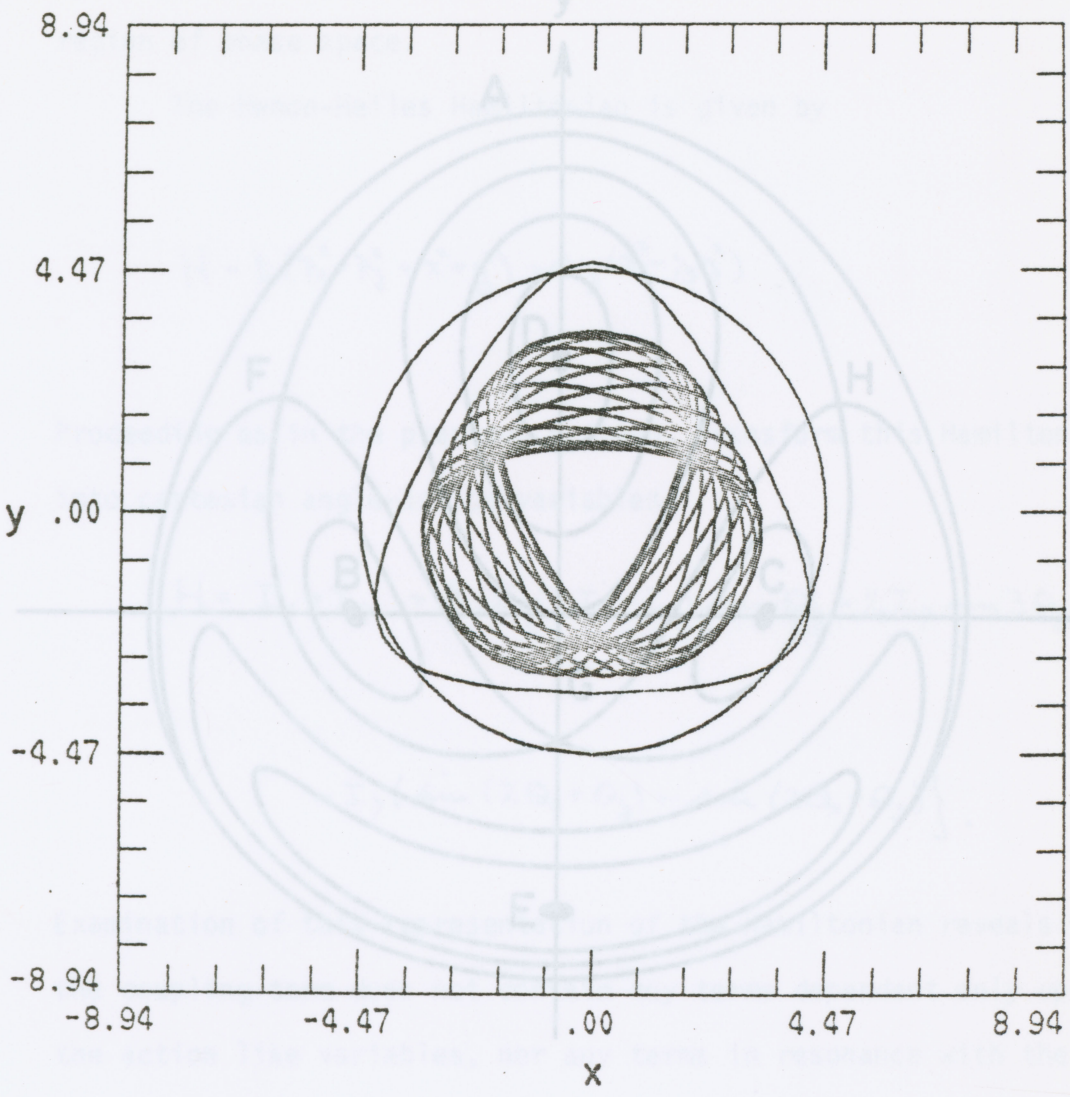


Figure 3-2. A Precessing Torus of the Henon-Heiles Hamiltonian System. The trajectory shown in this figure corresponds to the motion of a threefold hindered rotor which has enough angular momentum to cross the dynamical barriers. The C_{3v} symmetry of the Hamiltonian is clearly visible in this trajectory. In actuality there are two trajectories with this time independent configuration. They have opposite senses of rotation. In Chapter IV it is shown that these two disjoint precessing tori can be connected by imaginary paths which correspond to reflection above the dynamical barriers.

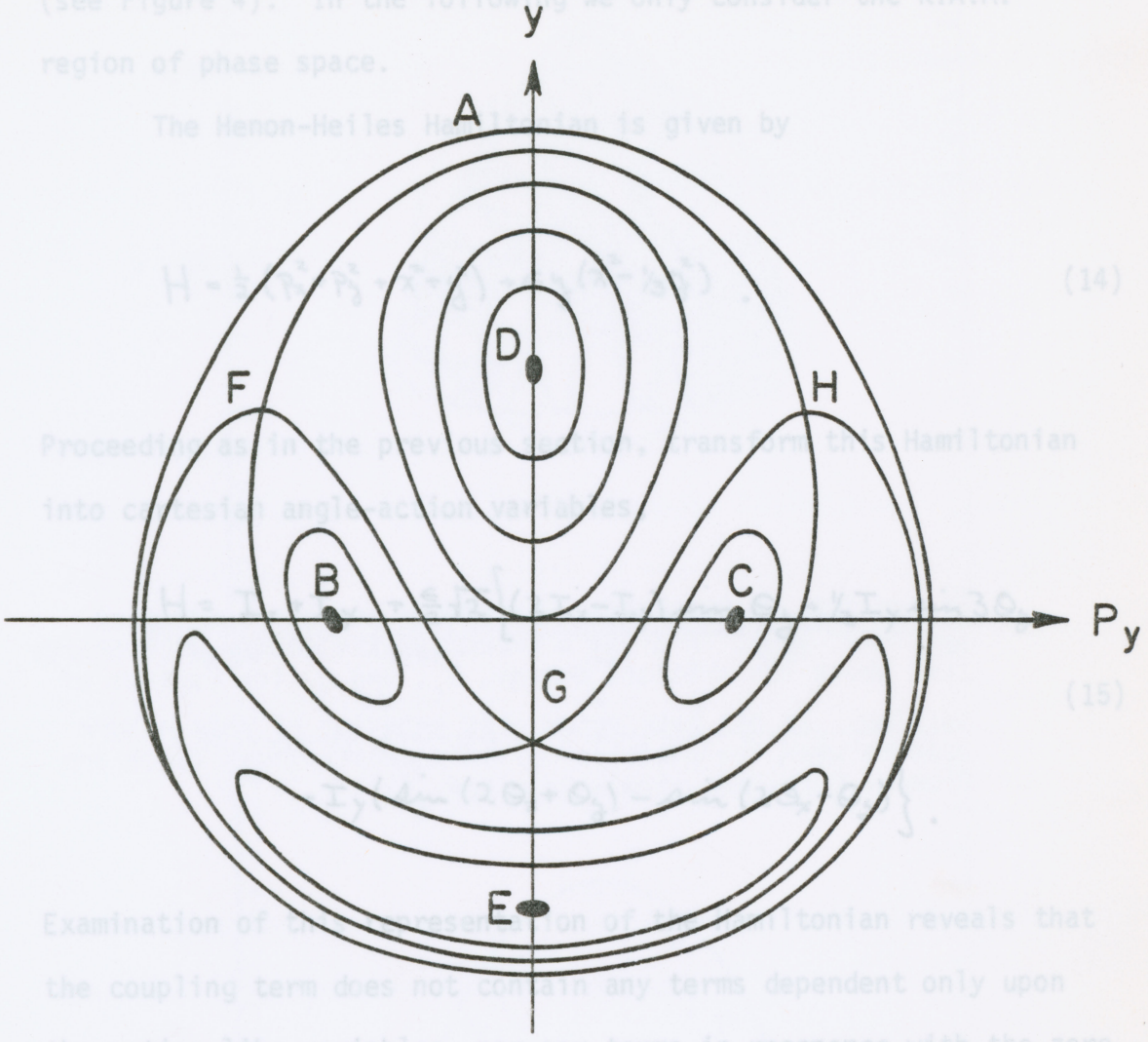


Figure 3-3. The Poincaré Surface of Section of the Henon-Heiles Hamiltonian. Shown in this figure are the surfaces of sections of several tori at half the dissociation energy. There are several different families of tori. The tori surrounding the points A, B, and C correspond to the box tori. The tori surrounding the points D and E are the precessing tori. The points F, G, and H correspond to three unstable periodic tori which oscillate in the saddle of the dynamical barrier. The first macroscopic stocastic behavior appears in the region around these unstable periodic orbits at an energy of about 8½.

critical energy the macroscopic volumes characterized by stochastic behavior first appear in the vicinity of these three unstable orbits (see Figure 4). In the following we only consider the K.A.M. region of phase space.

The Henon-Heiles Hamiltonian is given by

$$H = \tfrac{1}{2}(P_x^2 + P_y^2 + x^2 + y^2) + \epsilon y(x^2 - \tfrac{1}{3}y^2) \quad . \tag{14}$$

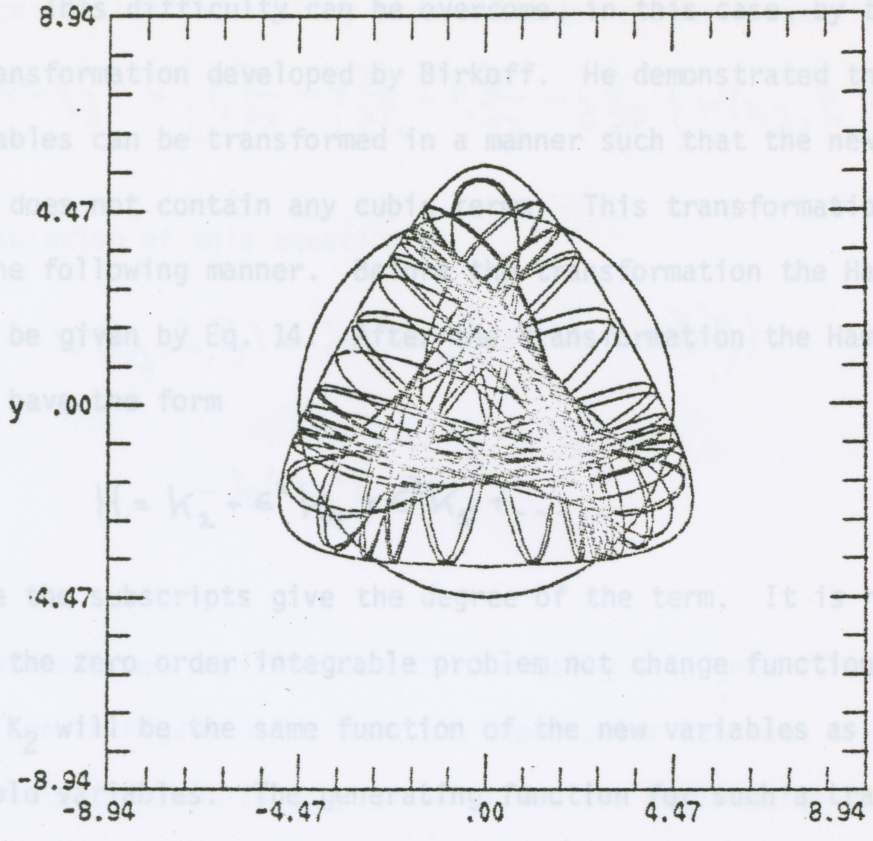
Proceeding as in the previous section, transform this Hamiltonian into cartesian angle-action variables,

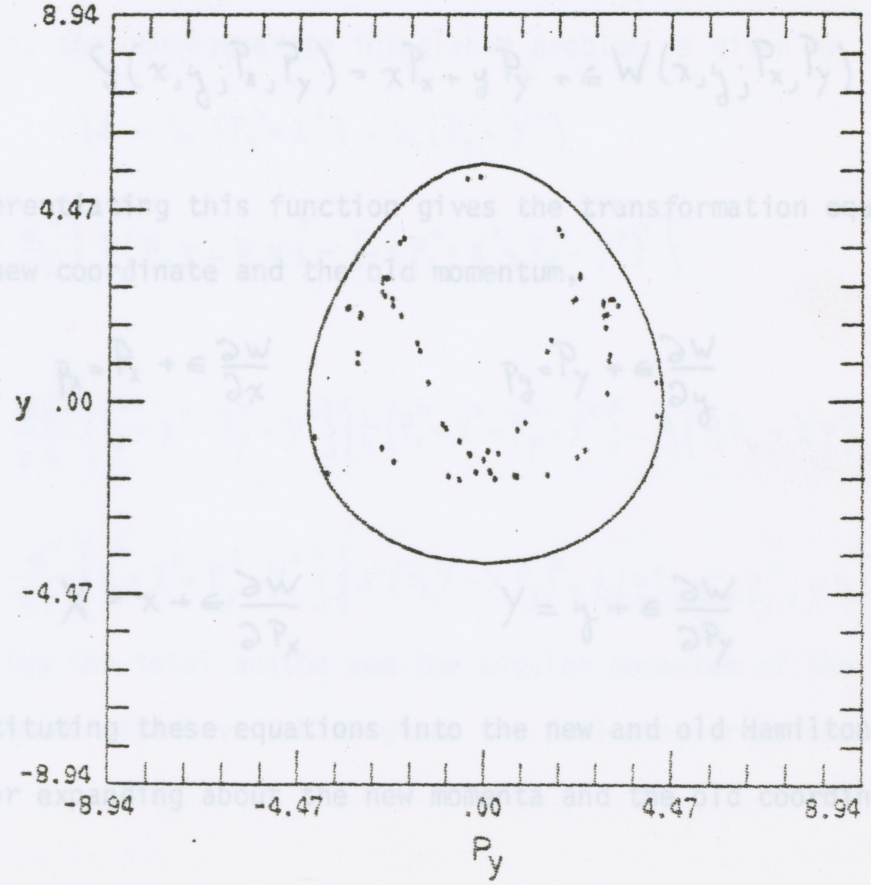
$$H = I_x + I_y + \frac{\epsilon}{2}\sqrt{2}\Big\{(2I_x - I_y)\sin\theta_y + \tfrac{1}{3}I_y \sin 3\theta_y - I_y(\sin(2\theta_x + \theta_y) - \sin(2\theta_x - \theta_y))\Big\} \quad . \tag{15}$$

Examination of this representation of the Hamiltonian reveals that the coupling term does not contain any terms dependent only upon the action like variables, nor any terms in resonance with the zero order problem. The latter observation, at first glance, suggests that the Van Vleck method will perhaps succeed. This is not the case. A consequence of the fact that the coupling potential does not contribute a term which is only a function of the action like variables is that the zero order degeneracy is not broken in these variables. As a result, if a resonant term appears in the subsequent iteration the Van Vleck method will fail.

8.94
4.47
.00
-4.47
-8.94
-8.94
-4.47
.00
4.47
8.94
y
P_y

Figure 3-4. A Stochastic Trajectory and its Surface of Section. Shown in a) is a stocastic trajectory with energy just above the critical energy, E_c, and b) its surface of section. It has been noted that behavior of this nature appears when the unstable periodic orbits first touch the Brummer-Duff-Toda circle (see Ref. 5).


8.94
4.47
y .00
-4.47
-8.94
-8.94
-4.47
.00
4.47
8.94
x


8.94
4.47
y .00
-4.47
-8.94
-8.94
-4.47
.00
4.47
8.94
P_y

This difficulty can be overcome, in this case, by the use of a transformation developed by Birkoff. He demonstrated that the variables can be transformed in a manner such that the new coupling term does not contain any cubic terms. This transformation is found in the following manner. Before the transformation the Hamiltonian will be given by Eq. 14. After the transformation the Hamiltonian will have the form

$$H = K_2 + \epsilon^2 K_4 + \epsilon^3 K_5 + \cdots \tag{16}$$

where the subscripts give the degree of the term. It is required that the zero order integrable problem not change functional form, thus K_2 will be the same function of the new variables as H_2 is of the old variables. The generating function for such a transformation will have the form

$$S(x, y, P_x, P_y) = xP_x + yP_y + \epsilon W(x, y, P_x, P_y) \tag{17}$$

Differentiating this function gives the transformation equations for the new coordinate and the old momentum,

$$p_x = P_x + \epsilon \frac{\partial W}{\partial x} \qquad p_y = P_y + \epsilon \frac{\partial W}{\partial y} \tag{18}$$

$$X = x + \epsilon \frac{\partial W}{\partial P_x} \qquad Y = y + \epsilon \frac{\partial W}{\partial P_y}$$

Substituting these equations into the new and old Hamiltonians, Taylor expanding about the new momenta and the old coordinates,

and collecting and setting terms of order ε equal, one finds

$$y(x^2-\tfrac{1}{3}y^2) = \left\{P_x\frac{\partial}{\partial x} - x\frac{\partial}{\partial P_x} + P_y\frac{\partial}{\partial y} - y\frac{\partial}{\partial P_y}\right\} W(x,y;P_x,P_y) \qquad (19)$$

The solution of this equation is

$$W(x,y;P_x,P_y) = \tfrac{1}{3}(2xyP_y + x^2P_y + 2P_x^2P_y) - \tfrac{1}{9}(3y^2P_y + 2P_y^3) \qquad (20)$$

The transformed Hamiltonian obtained using this generating function is given in Figure 3-5. Once the Hamiltonian has been transformed into this form, it is easy to partition the Hamiltonian into a non-degenerate, integrable system and a coupling term. To fourth order (in ε), the nondegenerate integrable problem is given by

$$H = \tfrac{1}{2}(P_x^2+X^2) + \tfrac{1}{2}(P_y^2+Y^2) + \frac{\epsilon^2}{12}\left\{7(P_xY-P_yX)^2 - \frac{5}{4}(P_x^2+X^2+P_y^2+Y^2)^2\right\} + \frac{7\epsilon^4}{36}\left\{P_x^2+X^2-P_y^2-Y^2\right\}\left\{\tfrac{1}{4}(P_x^2+X^2-P_y^2-Y^2)^2 - 3(P_xP_y+XY)^2\right\} - \frac{\epsilon^4}{81}\left\{P_x^2+X^2+P_y^2+Y^2\right\}\left\{5(P_xY-XP_y)^2 + \tfrac{1}{4}(P_x^2+X^2+P_y^2+Y^2)\right\} \qquad (21)$$

Choosing the total action and the angular momentum of the integrable problem as action variables gives the following transformation

$$X = \tfrac{1}{2}\sqrt{2}\left\{(J_1^2-J_2^2)^{1/2}\cos(\varphi_2+\varphi_1) + (J_1^2+J_2^2)^{1/2}\cos(\varphi_2-\varphi_1)\right\} \tag{22a}$$

$$Y = \tfrac{1}{2}\sqrt{2}\left\{(J_1^2-J_2^2)^{1/2}\sin(\varphi_2+\varphi_1) + (J_1^2+J_2^2)^{1/2}\sin(\varphi_2-\varphi_1)\right\} \tag{22b}$$

$$P_X = \tfrac{1}{2}\sqrt{2}\left\{-(J_1^2-J_2^2)^{1/2}\sin(\varphi_2+\varphi_1) + (J_1^2+J_2^2)^{1/2}\sin(\varphi_2-\varphi_1)\right\} \tag{22c}$$

$$P_Y = \tfrac{1}{2}\sqrt{2}\left\{(J_1^2-J_2^2)^{1/2}\cos(\varphi_2+\varphi_1) - (J_1^2+J_2^2)^{1/2}\cos(\varphi_2-\varphi_1)\right\}. \tag{22d}$$

The period of ϕ_1 is 2π and of ϕ_2 is π. The integrable problem then becomes

$$H = J_1 + \frac{\epsilon^2}{12}\left\{7J_2^2-5J_1^2\right\} - \frac{2\epsilon^4}{81}J_1^2(5J_2^2+J_1^2) - \frac{7\epsilon^4}{18}(J_1^2-J_2^2)^{3/2}\cos 6\varphi_2 . \tag{23}$$

These zero order variables provide good zero order tori if $J_1 \sim |J_2|$. When this condition is exact the resulting motion corresponds to the central periodic orbits of the precessing tori. A good set of variables for the box tori is found in an analogous manner. Consider the box tori on the y-axis. The central periodic orbit of this family of tori lies on the y-axis, consequently, one expects the action in the x-direction to be zero. This suggests the following transformation

$$X = (2(I_1 - I_2))^{1/2} \sin\theta_2 \qquad P_x = (2(I_1 - I_2))^{1/2} \cos\theta_2$$

$$Y = (2I_2)^{1/2} \sin(\theta_1 + \theta_2) \qquad P_y = (2I_2)^{1/2} \cos(\theta_1 + \theta_2) \tag{24}$$

The integrable problem in these coordinates is

$$H = I_1 + \frac{\epsilon^2}{12}\left\{28 I_1 (I_1 - I_2)\sin^2\theta_2 - 5 I_1^2\right\}$$

$$- \frac{7\epsilon^4}{18}(2I_1 - I_2)\left\{(2I_1 - I_2)^2 - I_1(I_1 - I_2)\cos^2\theta_2\right\} \tag{25}$$

$$- \frac{2\epsilon^4}{81} I_1^2 \left\{5(I_1 - I_2)\sin^2\theta_2 + I_1\right\}$$

Clearly, when $I_1 \sim |I_2|$, these variables provide good zero order tori for the box tori on the y-axis. The other two box tori can be treated by rotation of the coordinate system in Figure 3-5.

Once good sets of zero order variables have been identified, it is straightforward to apply the Van Vleck method to construct the invariant tori. The next section discusses the semiclassical quantization conditions and the subsequent quantization of the transformed Henon-Heiles Hamiltonian as given in Figure 3-5.

D. THE QUANTIZATION OF THE DEGENERATE HENON-HEILES HAMILTONIAN SYSTEM

Straightforward application of the primitive semiclassical quantization conditions[6] requires that the action variables of the

Figure 3-5. The Partially Normalized Henon-Heiles Hamiltonian. The Henon-Heiles Hamiltonian to order ε^6 following one Birkoff-Gustavson transformation. This transformation has the effect of eliminating the cubic terms. This Hamiltonian plus 55 terms of order ε^7 and 73 terms of order ε^8 was used to calculate the primitive semiclassical eigenvalues given in Table 3-1.

$$H = H_2 + \varepsilon^2 H_4 + \varepsilon^3 H_5 + \varepsilon^4 H_6 + \varepsilon^5 H_7 + \varepsilon^6 H_8 + \varepsilon^6 H_8 + \varepsilon^7 H_9 + \varepsilon^8 H_{10} + \cdots$$

$$H_2 = \frac{1}{2}\left(P_X^2+X^2\right) + \frac{1}{2}\left(P_Y^2+Y^2\right)$$

$$H_4 = \frac{1}{18}\left(-Y^4-2X^2Y^2+8P_X^2Y^2-16P_XP_YXY-X^4+8P_Y^2X^2-4P_Y^4-8P_X^2P_Y^2-4P_X^4\right)$$

$$H_5 = \frac{1}{27}\left(-2Y^5+4X^2Y^3-4P_Y^2Y^3+12P_X^2Y^3+16P_XP_YXY^2+6X^4Y\right.$$
$$\left.-20P_Y^2X^2Y-4P_X^2X^2Y+48P_X^2P_Y^2-16P_X^4Y+16P_XP_YX^3-48P_XP_Y^3X+16P_X^3P_YX\right)$$

$$H_6 = \frac{1}{81}\left(-7Y^6-3X^2Y^4-20P_Y^2Y^4+40P_X^2Y^4-48P_XP_YXY^3-33X^4Y^2\right.$$
$$+56P_Y^2X^2Y^2-16P_X^2X^2Y^2-12P_Y^4Y^2+24P_X^2P_Y^2Y^2-60P_X^4Y^2$$
$$-144P_XP_YX^3Y+192P_XP_Y^3XY-5X^6+28P_Y^2X^4-8P_X^2X^4$$
$$\left.-36P_Y^4X^2-120P_X^2P_Y^2X^2+12P_X^4X^2+144P_X^2P_Y^4-96P_X^4P_Y^2+16P_X^6\right)$$

$$H_7 = \frac{1}{243}\left\{-24Y^7+24X^2Y^5-84P_Y^2Y^5+140P_X^2Y^5+32P_XP_YXY^4+120X^4Y^3-88P_Y^2X^2Y^3-24P_X^2X^2Y^3\right.$$
$$-80P_Y^4Y^3+448P_X^2P_Y^2Y^3-240P_X^4Y^3+704P_XP_YX^3Y^2-544P_XP_Y^3XY^2+224P_X^3P_YXY^2+72X^6Y$$
$$-260P_Y^2X^4Y+92P_X^2X^4Y+176P_Y^4X^2Y+960P_X^2P_Y^2X^2Y+16P_X^4X^2Y-16P_Y^6Y-304P_X^2P_Y^4Y-176P_X^4P_Y^2Y$$
$$\left.+112P_X^6Y+160P_XP_YX^5-544P_XP_Y^3X^3+224P_X^3P_YX^3+320P_XP_Y^5X+256P_X^3P_Y^3X-64P_X^5P_YX\right\}$$

$$H_8 = \frac{1}{1458}\left\{-165Y^8+60X^2Y^6-672P_Y^2Y^6+1008P_X^2Y^6-480P_XP_YXY^5-750X^4Y^4-672P_Y^2X^2Y^4\right.$$
$$-528P_X^2X^2Y^4-840P_Y^4Y^4+2640P_X^2P_Y^2Y^4-1960P_X^4Y^4-4800P_XP_YX^3Y^3+1536P_XP_Y^3XY^3$$
$$+256P_X^3P_YXY^3-1060X^6Y^2-2592P_Y^2X^4Y^2-1008P_X^2X^4Y^2-912P_Y^4X^2Y^2-10080P_X^2P_Y^2X^2Y^2$$
$$+432P_X^4X^2Y^2-320P_Y^6Y^2+4480P_X^2P_Y^4Y^2-4160P_X^4P_Y^2Y^2+1280P_X^6Y^2-4320P_XP_YX^5Y+9728P_XP_Y^3X^3Y$$
$$-4352P_X^3P_YX^3Y-3200P_XP_Y^5XY-3840P_X^3P_Y^3XY-640P_X^5P_YXY-85X^8+480P_Y^2X^6-240P_X^2X^6$$
$$-776P_Y^4X^4-3120P_X^2P_Y^2X^4-104P_X^4X^4+320P_Y^6X^2+7040P_X^2P_Y^4X^2-3520P_X^4P_Y^2X^2$$
$$\left.-16P_Y^8-1216P_X^2P_Y^6-480P_X^4P_Y^4+576P_X^6P_Y^2-144P_X^8\right\}$$

precessing tori have the values,

$$J_1 = \frac{1}{2\pi}\oint_{C_1} \underline{p}\cdot d\underline{q} = \hbar(n+1)$$

$$J_2 = \frac{1}{2\pi}\oint_{C_2} \underline{p}\cdot d\underline{q} = \hbar l \qquad (26)$$

and that the action variables of the box tori have the values

$$I_1 = \frac{1}{2\pi}\oint_{C_3} \underline{p}\cdot d\underline{q} = \hbar(n+1)$$

$$I_2 = \frac{1}{2\pi}\oint_{C_4} \underline{p}\cdot d\underline{q} = \hbar(l+\tfrac{1}{2}) \qquad (27)$$

(see Figure 3-6 for definition of the paths of integration). It is found that quantization conditions give reasonable results for the precessing tori, but incorrect results for the box tori. In applying the conditions given in Eq. 27 to the box tori one is assuming that quantum tunneling is not an important effect. This is not the case for the Henon-Heiles Hamiltonian. The dynamical barriers which separate the box tori are not high (see Figure 3-7) and as a result tunneling through the barriers plays an important role in the quantum dynamics of the system.

Noid and Marcus[7] proposed the following ad hoc quantization conditions for the box tori,

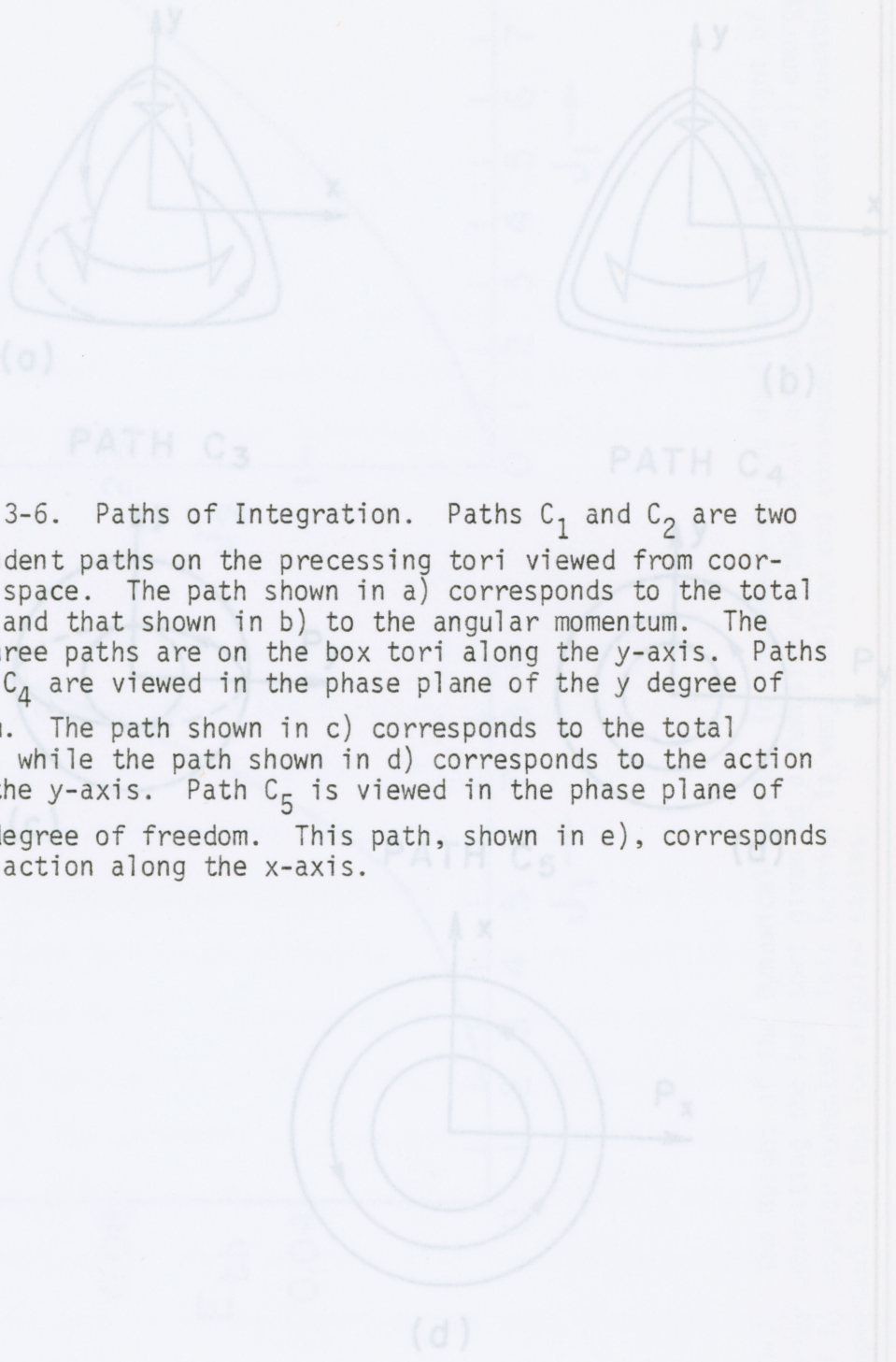
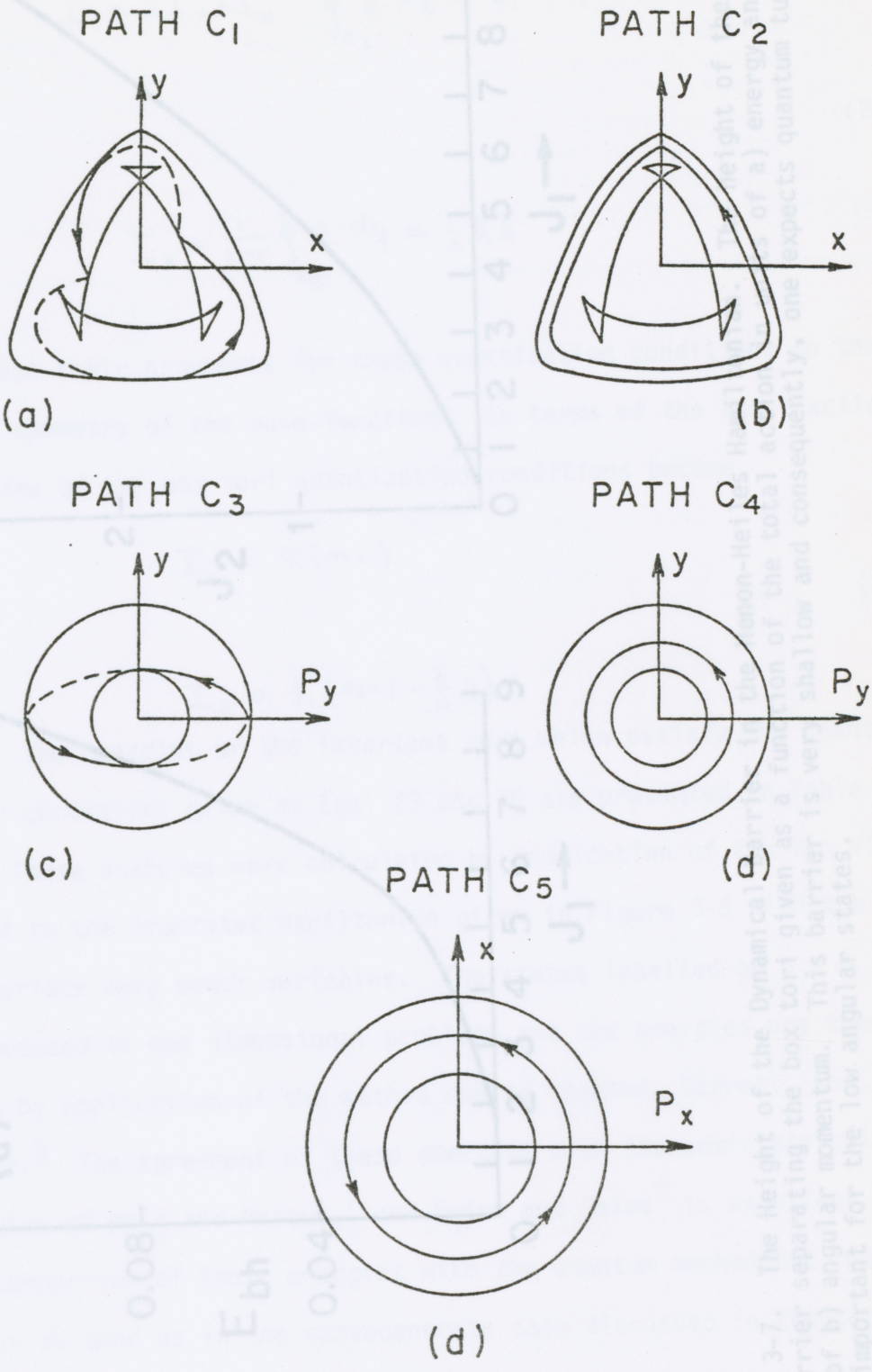


Figure 3-6. Paths of Integration. Paths C_1 and C_2 are two independent paths on the precessing tori viewed from coordinate space. The path shown in a) corresponds to the total action and that shown in b) to the angular momentum. The next three paths are on the box tori along the y-axis. Paths C_3 and C_4 are viewed in the phase plane of the y degree of freedom. The path shown in c) corresponds to the total action, while the path shown in d) corresponds to the action along the y-axis. Path C_5 is viewed in the phase plane of the x degree of freedom. This path, shown in e), corresponds to the action along the x-axis.


PATH C_1
y
x
(a)
PATH C_2
y
x
(b)
PATH C_3
y
P_y
(c)
PATH C_4
y
P_y
(d)
PATH C_5
x
P_x
(d)

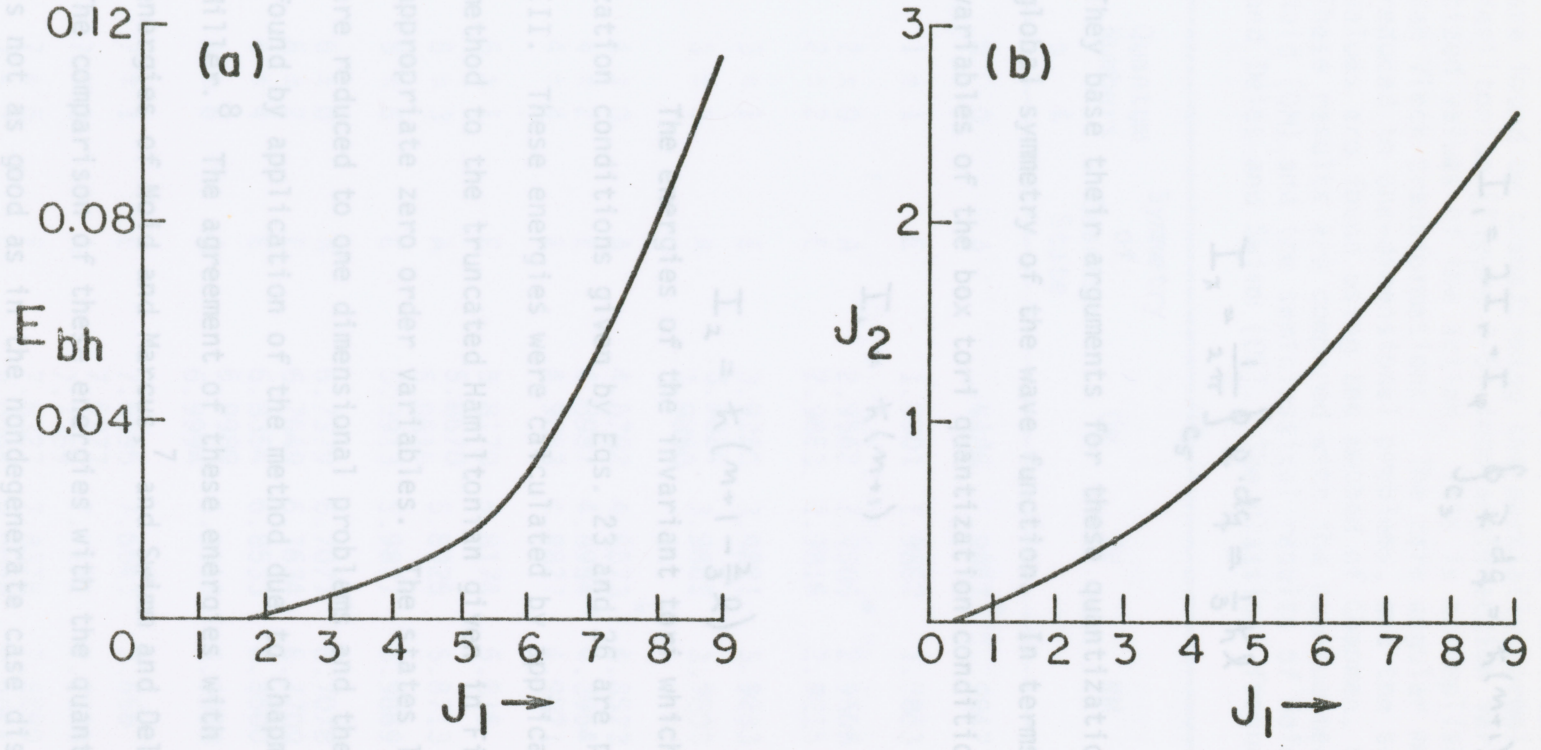


Figure 3-7. The Height of the Dynamical Barrier in the Henon-Heiles Hamiltonian. The height of the dynamical barrier separating the box tori given as a function of the total action in units of a) energy and in units of b) angular momentum. This barrier is very shallow and consequently, one expects quantum tunnelling to be important for the low angular states.

$$I_1 = 2I_r + I_\varphi \qquad \oint_{C_3} \vec{p}\cdot d\vec{q} = \hbar(n+1)$$

$$I_x = \frac{1}{2\pi}\oint_{C_5} \vec{p}\cdot d\vec{q} = \frac{1}{3}\hbar\ell \tag{28}$$

They base their arguments for these quantization conditions on the global symmetry of the wave function. In terms of the local action variables of the box tori quantization conditions become

$$I_1 = \hbar(n+1)$$

$$I_2 = \hbar\left(n+1-\frac{2}{3}\ell\right) \tag{29}$$

The energies of the invariant tori which satisfy the quantization conditions given by Eqs. 23 and 26 are presented in Table III. These energies were calculated by application of the Van Vleck method to the truncated Hamiltonian given in Figure 3-5 with the appropriate zero order variables. The states labelled by $\ell = 0$ are reduced to one dimensional problems and the energies are then found by application of the method due to Chapman, Garrett, and Miller.[8] The agreement of these energies with the semiclassical energies of Noid and Marcus,[7] and Swimm and Delos[9] is excellent. The comparison of these energies with the quantum mechanical results is not as good as in the nondegenerate case discussed in Chapter II. This can be attributed to the fact that the quantization conditions, while global in nature, do not include such effects as tunneling

Table III. The Primitive Semiclassical Eigenvalues of the Henon-Heiles Hamiltonian ($\varepsilon^2 = 1/80$). The semiclassical eigenvalues (VV) are found by transforming the partially normalized Henon-Heiles Hamiltonian (Figure 3-5) into angle-action variables for the quantized values of the action. This is accomplished via a sequence of Van Vleck transformations. The zero angular momentum states are reduced to one-dimensional problems, and the semiclassical eigenvalues are found using the method of Chapman, Garrett, and Miller. These results are compared with the quantum mechanical results of Noid (QM) and the semiclassical results of Noid and Marcus (NM), and Delos and Swimm (DS). The classical frequencies are also given.

Quantum Numbers n	ℓ	Symmetry of Quantum State	QM	VV	NM	DS	ω_1	ω_2
0	0	A	.9986	.9947*	.9947	.9947		
1	± 1	E	1.9901	1.9862	1.9863	1.9862	.979	.015
2	± 0	A	2.9562	2.9506*	2.9506	2.9506		
2	± 2	E	2.9853	2.9816	2.9815	2.9814	.968	.029
3	± 1	E	3.9260	3.9221	3.9233	3.9226	.957	.014
3	± 3	A	3.9824 3.9858	3.9805	3.9803	3.9801	.959	.043
4	± 0	A	4.8702	4.8573*	4.8573	4.8577		
4	± 2	E	4.8987	4.8954	4.8954	4.8954	.946	.030
4	± 4	E	4.9863	4.9827	4.9821	4.9821	.947	.057
5	± 1	E	5.8170	5.8174	5.816	---	.933	.024
5	± 3	A	5.8670 5.8815	5.8925	5.8713	5.8711	.934	.045
5	± 5	E	5.9913	5.9877	5.9869	5.9871	.937	.070
6	± 0	A	6.7379	6.7077*	6.7078	6.7078		
6	± 2	E	6.7649	6.7634	6.7709	6.7663	.922	.029
6	± 4	E	6.8354	6.8533	6.8500	6.8492	.924	.059
6	± 6	A	6.9989 6.9994	6.9948	6.9958	6.9951	.927	.081
7	± 1	E	7.6595	7.6541	7.655	---	.902	.041
7	± 3	A	7.6977 7.7369	7.7172	7.7178	7.7184	.910	.046
7	± 5	E	7.8327	7.8376	7.8289	7.8293	.913	.073
7	± 7	E	8.0094	8.0029	8.0054	8.005	.919	.089

Table III (continued)

Quantum Numbers n	ℓ	Symmetry of Quantum State	QM	VV	NM	DS	ω_1	ω_2
8	± 0	A	8.5541	8.4919*	8.4919	8.5003		
8	± 2**	E	8.5764	8.5940	---	---	.896	.040
8	± 4**	E	8.6779	8.6754	---	8.6717	.898	.062
8	± 6	A	8.8113 8.8152	8.8253	8.8083	8.8112	.903	.086
8	± 8	E	9.0217	9.0099	9.0151	9.0192	.915	.092

*These energies are calculated by the method of Chapman, Garrett, and Miller.

**Noid and Marcus identified these states as stochastic.

through or reflection above a barrier, effects which are apparently more important in the degenerate case than in the nondegenerate case considered. A surprising result is that in this manner one can calculate the energies of some low lying stocastic states; $n = 8$, $\ell \pm 2$ and $n = 8$, $\ell = \pm 4$ are examples. These states were found by Noid and Marcus[7] to be in the stochastic region of phase space. The reason that this method will work in these regions of phase space can be deduced from the work of Ford and Walker,[10] and Chirikov[11] on overlapping resonances. In the process of truncating the Hamiltonian, if one truncates one of the overlapping resonances then the motion will appear to become regular.

The next chapter follows up on these observations and presents the uniform quantization of the Henon-Heiles Hamiltonian in both the regular and stochastic regions of phase space.

References to Chapter III

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CHAPTER IV

THE UNIFORM SEMICLASSICAL QUANTIZATION OF NONINTEGRABLE HAMILTONIAN SYSTEMS

A. INTRODUCTION

The methods of quantizing classical Hamiltonian systems discussed to this point have their origins in old quantum theory,[1] and require the existence of invariant tori, at least locally. Little progress has been made on the problem of semiclassical quantization of classical Hamiltonian systems which display stochastic behavior. This chapter considers this problem.

The strategy we adopt is to find an integrable Hamiltonian system which closely approximates the nonintegrable problem. This is accomplished by partially transforming the Hamiltonian into a normal form such that the component of the Hamiltonian which is not in normal form is of high order in the coupling constant. The transformed Hamiltonian is then truncated leaving only the low order normal components. The useful normal form is a generalization of Birkoff's normal form.[2] The transformation process will be called the normalization of the classical Hamiltonian. Following this normalization and truncation of the classical Hamiltonian, it is, in general, possible to transform to angle-action 'like' variables which decouple the normal modes of the new integrable Hamiltonian, even in the degenerate case. This is an important result in that once the system is decoupled it is possible to carry out a uniform

semiclassical quantization[3] of the approximate integrable Hamiltonian in a straightforward manner.

The irregular motion of a nonintegrable system is discussed in the next section. In Section C Gustavson's extension[4] of Birkoff's normal form is discussed along with the Birkoff-Gustavson transformation to this normal form. A small modification of this transformation, which accelerates the convergence, is introduced in the following section. Section E describes the uniform semiclassical quantization of the Henon-Heiles Hamiltonian system. This is followed by a discussion.

B. IRREGULAR MOTION

Numerical experiments[5] reveal that phase space, in general, can be divided into two types of regions; regular regions characterized by the existence of invariant tori, and irregular regions characterized by stochastic trajectories. The irregular regions are associated, in a mathematically rigorous[6] manner, with the existence of homoclinic fixed points. In the following discussion it is sufficient to characterize the irregular motion in a more heuristic manner using Poincaré surfaces of section. Characterization of the irregular motion in this manner is most suitable for two dimensional problems. It is well known that if invariant tori exist, then a trajectory on a torus will intersect the surface of section on a smooth closed path (see Figure 4-1). If, on the other hand, one considers a trajectory in the irregular region of phase space, then the locus of intersection points with the surface of section will appear to fill a two-dimensional area (see Figure 4-2). This is a

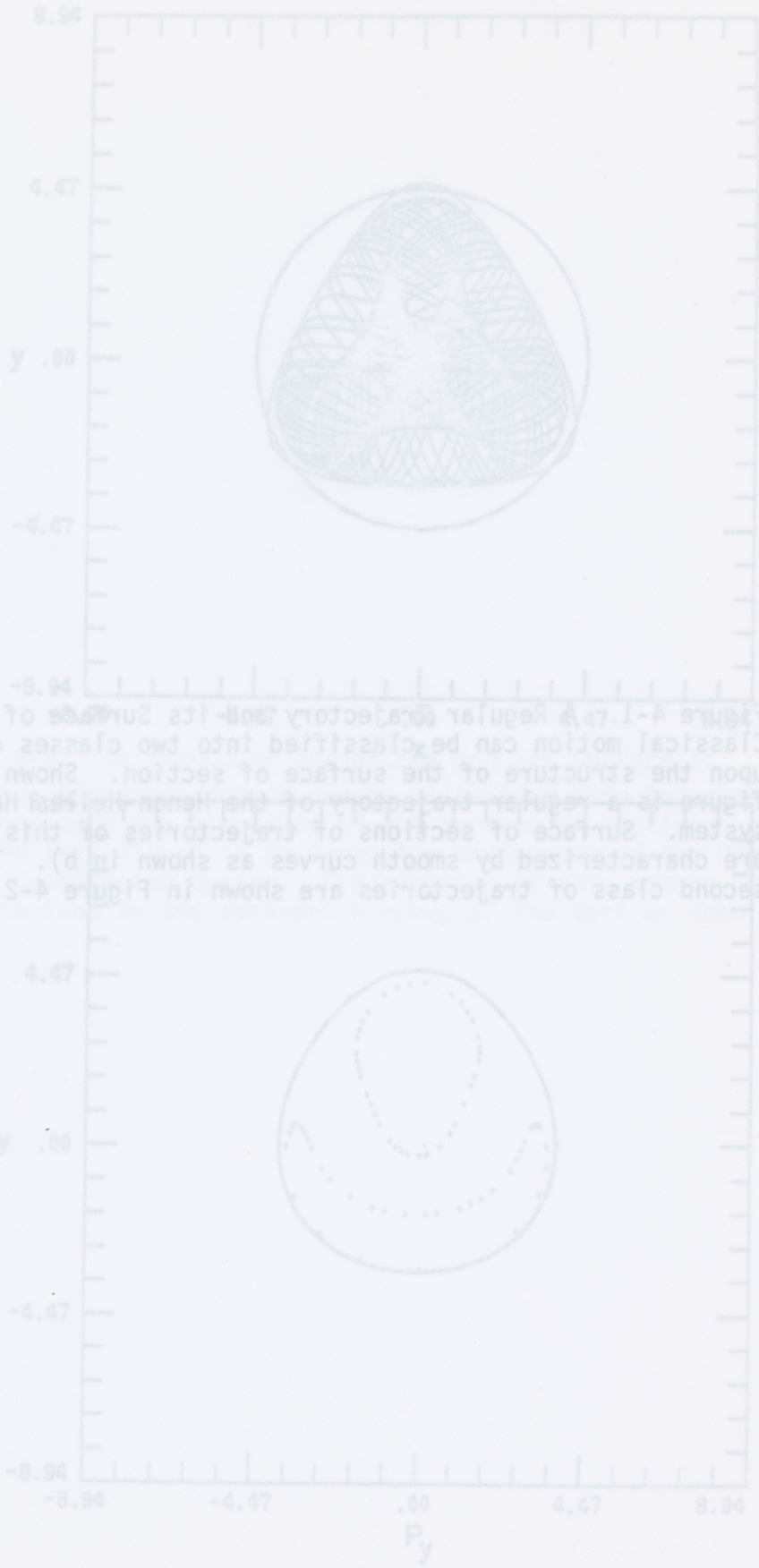
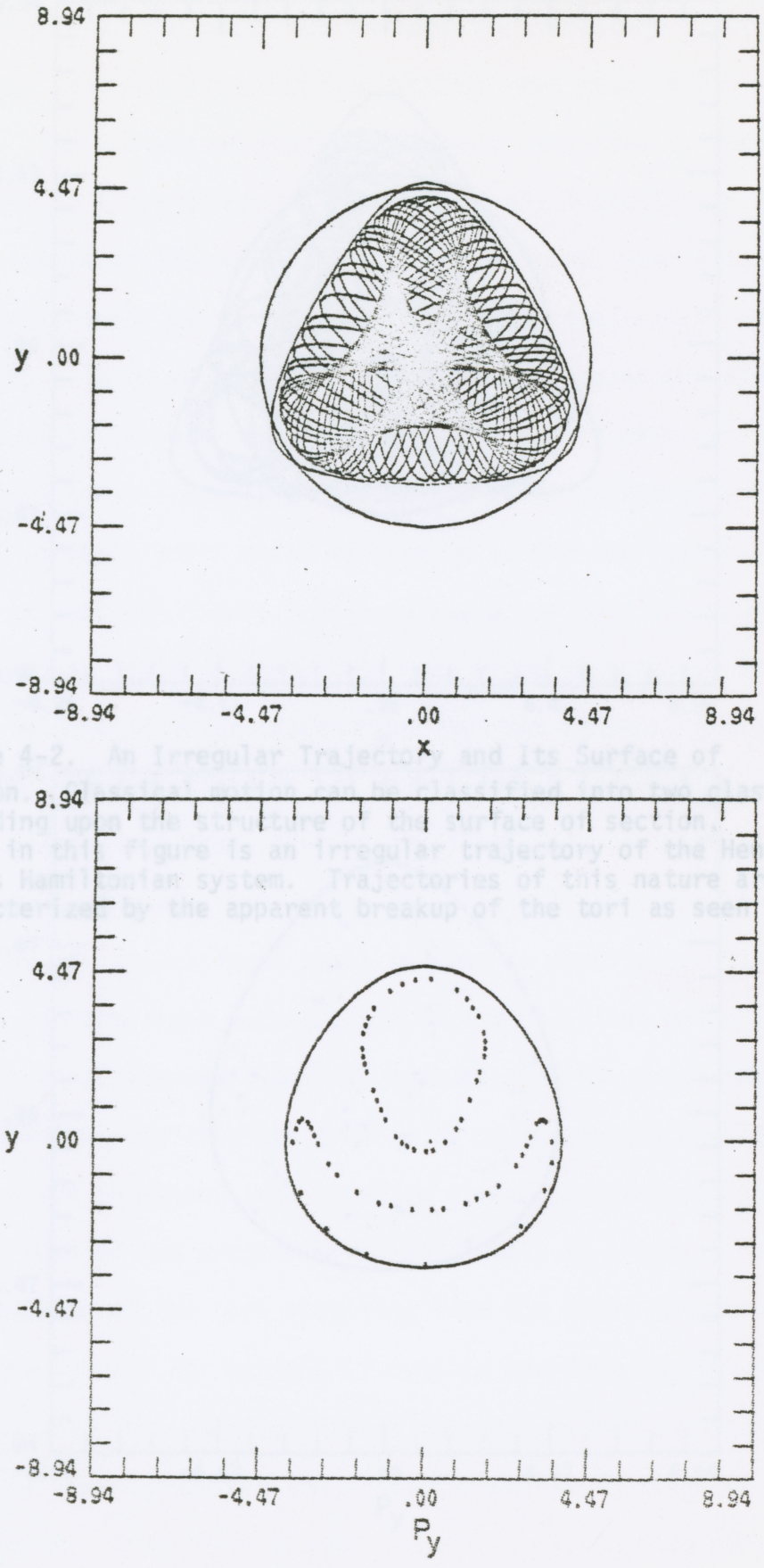

8.94
4.47
y .00
-4.47
-8.94
4.47
y .00
-4.47
-8.94
-8.94
-4.47
.00
4.47
8.94
P_y

Figure 4-1. A Regular Trajectory and its Surface of Section. Classical motion can be classified into two classes depending upon the structure of the surface of section. Shown in this figure is a regular trajectory of the Henon-Heiles Hamiltonian system. Surface of sections of trajectories of this nature are characterized by smooth curves as shown in b). The second class of trajectories are shown in Figure 4-2.


8.94
4.47
y .00
-4.47
-8.94
-8.94
-4.47
.00
4.47
8.94
x
8.94
4.47
y .00
-4.47
-8.94
-8.94
-4.47
.00
4.47
8.94
P_y

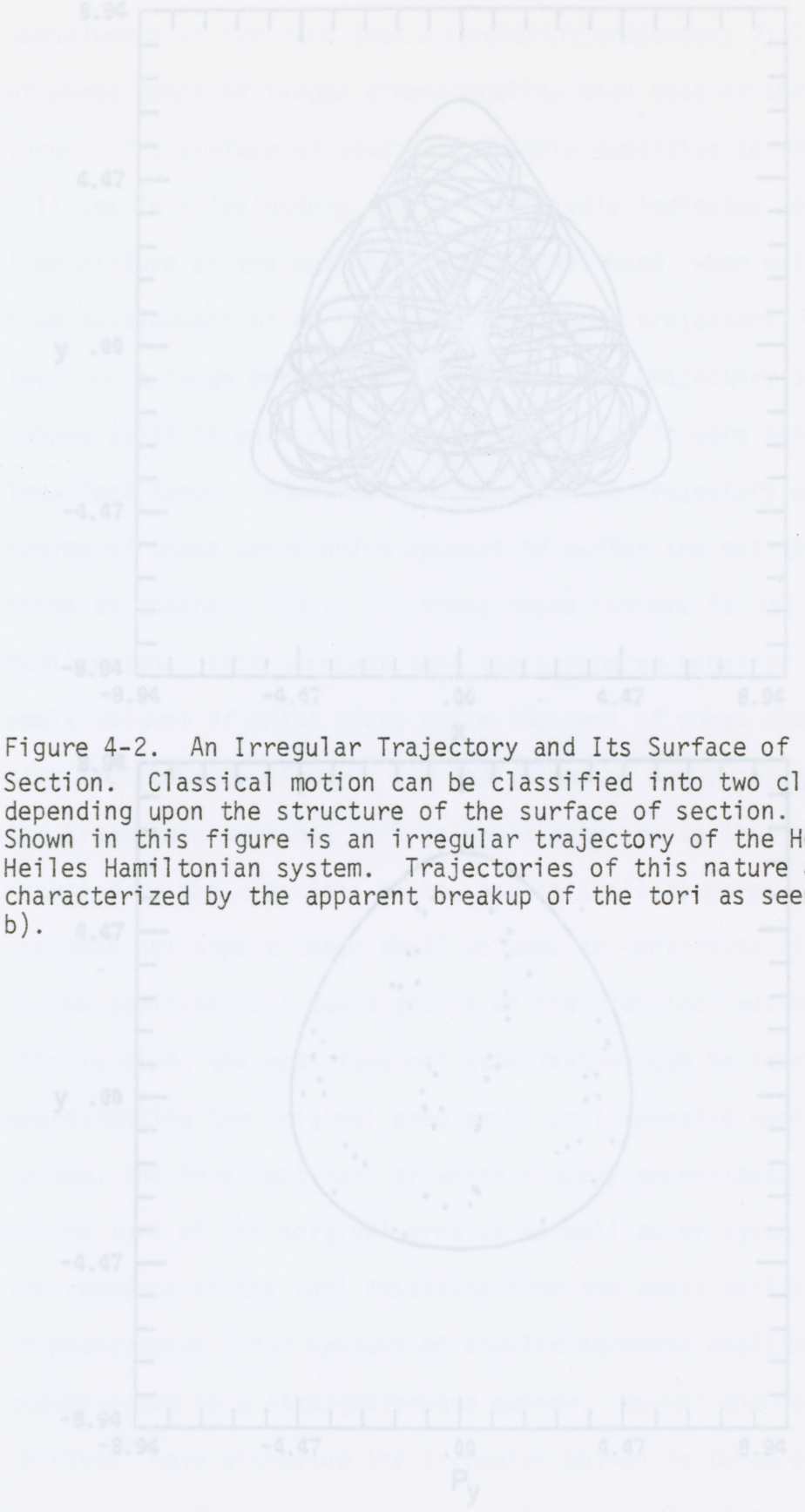
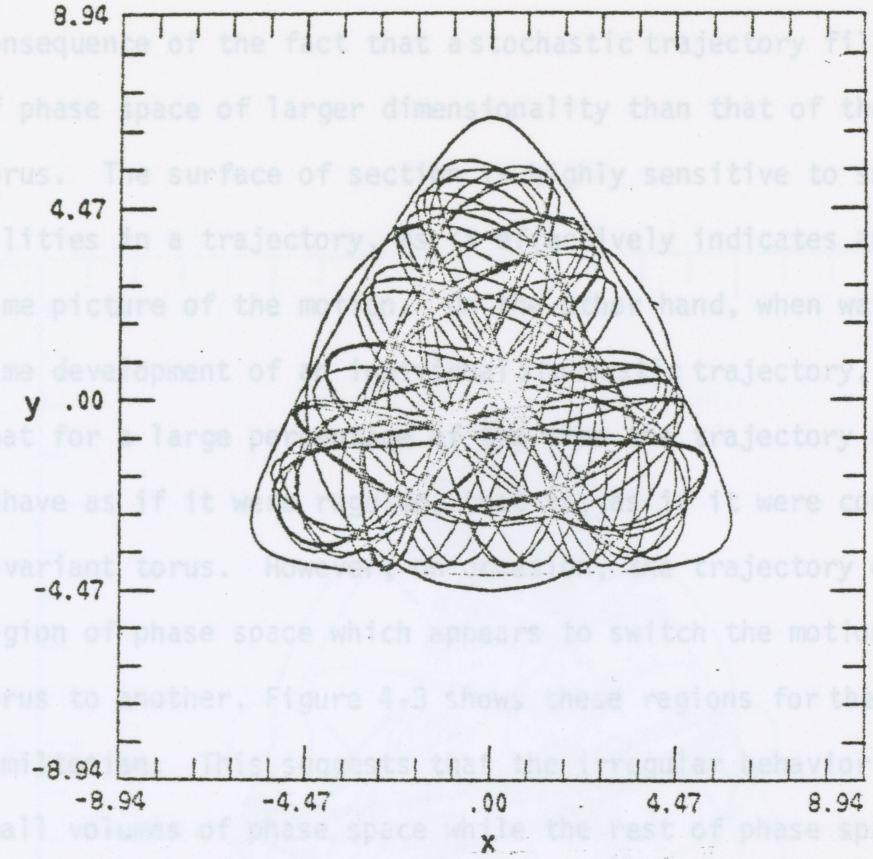
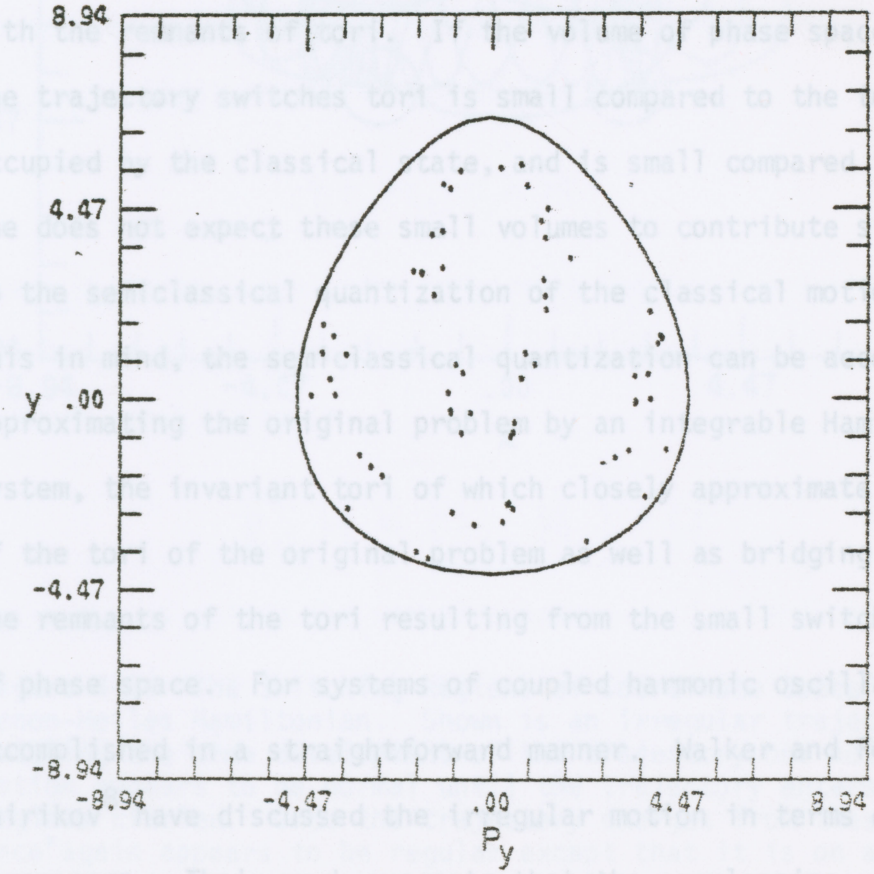


Figure 4-2. An Irregular Trajectory and Its Surface of Section. Classical motion can be classified into two classes depending upon the structure of the surface of section. Shown in this figure is an irregular trajectory of the Henon-Heiles Hamiltonian system. Trajectories of this nature are characterized by the apparent breakup of the tori as seen in b).


8.94
4.47
y .00
-4.47
-8.94
-8.94
-4.47
.00
4.47
8.94
x


8.94
4.47
y .00
-4.47
-8.94
-8.94
-4.47
.00
4.47
8.94
P_y

consequence of the fact that a stochastic trajectory fills a region of phase space of larger dimensionality than that of the invariant torus. The surface of section is highly sensitive to small instabilities in a trajectory, as it effectively indicates an infinite time picture of the motion. On the other hand, when watching the time development of an individual stochastic trajectory, one notices that for a large percentage of the time the trajectory appears to behave as if it were regular, that is, as if it were confined to an invariant torus. However, on occasion, the trajectory enters a region of phase space which appears to switch the motion from one torus to another. Figure 4-3 shows these regions for the Henon-Heiles Hamiltonian. This suggests that the irregular behavior arises in small volumes of phase space while the rest of phase space is filled with the remnants of tori. If the volume of phase space in which the trajectory switches tori is small compared to the total volume occupied by the classical state, and is small compared to $\hbar$, then one does not expect these small volumes to contribute significantly to the semiclassical quantization of the classical motion. With this in mind, the semiclassical quantization can be accomplished by approximating the original problem by an integrable Hamiltonian system, the invariant tori of which closely approximate the remnants of the tori of the original problem as well as bridging the gaps in the remnants of the tori resulting from the small switching volumes of phase space. For systems of coupled harmonic oscillators this is accomplished in a straightforward manner. Walker and Ford[7] and Chirikov[8] have discussed the irregular motion in terms of overlapping resonances. Their work suggests that the overlapping resonances be

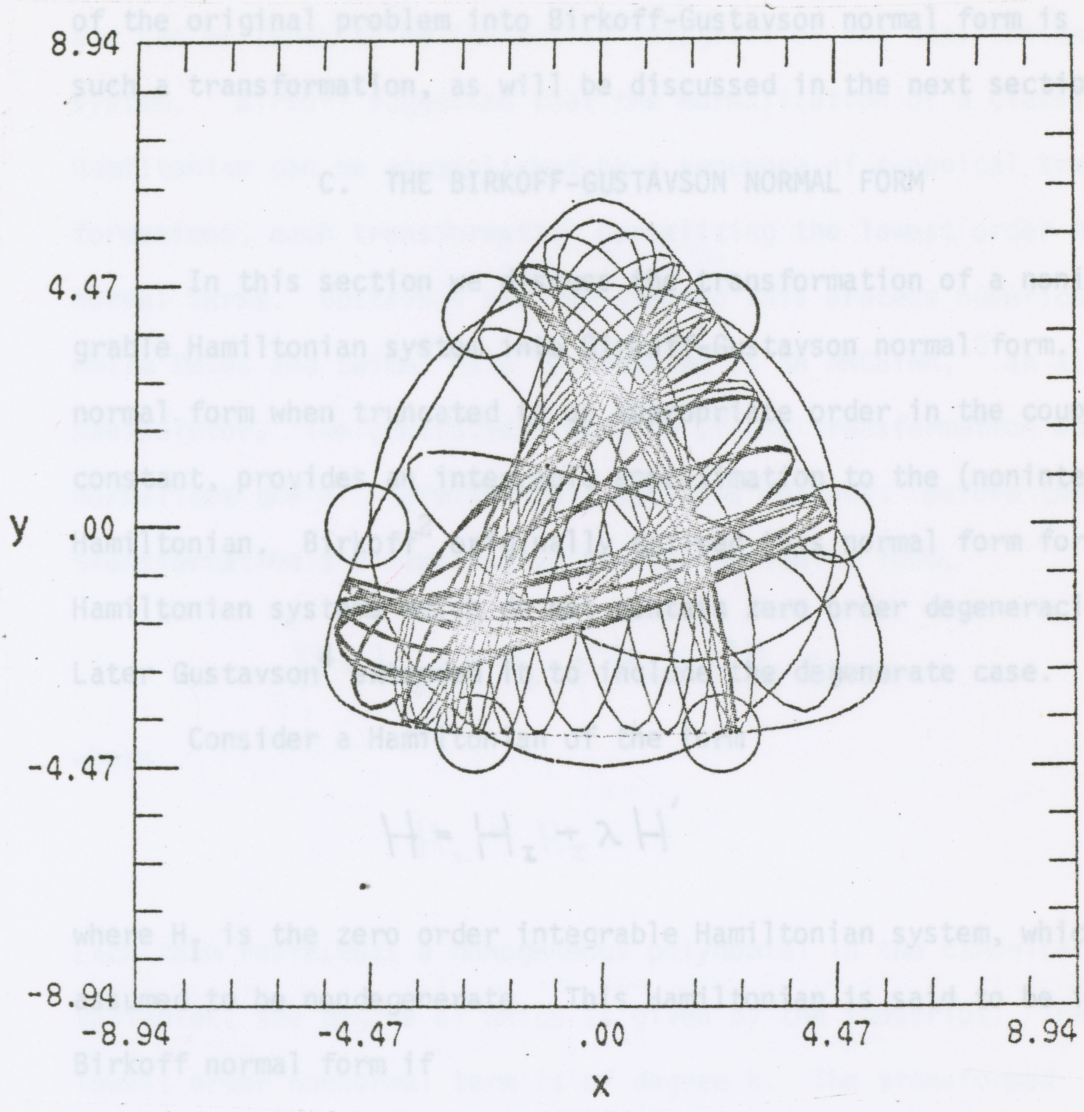


Figure 4-3. The Switching Regions of Coordinate Space for the Henon-Heiles Hamiltonian. Shown is an irregular trajectory. When watching the time development of the trajectory one notices that the motion appears to be normal until the trajectory enters any of the regions circled. Once the trajectory emerges from these regions it once again appears to be regular except that it is on a different torus. This suggests that the irregular regions of phase space contain the remnants of tori.

transformed to high order in the coupling constant, then by truncating the high order terms one can find an integrable approximation of the nonintegrable, classical Hamiltonian. The transformation of the original problem into Birkoff-Gustavson normal form is just such a transformation, as will be discussed in the next section.

C. THE BIRKOFF-GUSTAVSON NORMAL FORM

In this section we discuss the transformation of a nonintegrable Hamiltonian system into Birkoff-Gustavson normal form. This normal form when truncated to an appropriate order in the coupling constant, provides an integrable approximation to the (nonintegrable) Hamiltonian. Birkoff[2] originally defined this normal form for Hamiltonian systems which do not contain zero order degeneracies. Later Gustavson[4] extended it to include the degenerate case.

Consider a Hamiltonian of the form

$$H = H_I + \lambda H' \tag{1}$$

where H_I is the zero order integrable Hamiltonian system, which is assumed to be nondegenerate. This Hamiltonian is said to be in Birkoff normal form if

$$\mathbb{D}_{H_I} H = \{H, H_I\} = 0 \tag{2}$$

where $\mathbb{D}_{H_I}$ is called the normal operator. If a Hamiltonian is in this normal form then it is possible to express it as a rational function of a set of commuting functions, π_i. This set of commuting functions spans the null space of the normal operator,

$$\mathbb{D}_{H_I} \pi_i = 0, \tag{3}$$

and can be taken to be the action integrals of the Hamiltonian system. Birkoff suggested that the normalization of a classical Hamiltonian can be accomplished by a sequence of canonical transformations, each transformation normalizing the lowest order nonnormal terms. Gustavson has implemented this process numerically, while Delos and Swimm[9] have implemented it on MACSYMA,[10] an algebraic manipulator. The generating function of the transformation which normalizes the k^{th} term is constructed as follows. Before the transformation the Hamiltonian has the following form,

$$H = H_2 + \epsilon H_3 + \epsilon^2 H_4 + \epsilon^3 H_5 + \cdots \tag{4}$$

where

$$H_2 = H_I$$

Each term represents a homogeneous polynomial in the canonical variables, the degree of which is given by the subscript. The lowest order nonnormal term is of degree k. The transformed Hamiltonian is of the same form with the exception that the lowest order nonnormal term is of degree k+1. The generating function is assumed to have the form

$$S = \underset{\sim}{q} \cdot \underset{\sim}{P} + \epsilon^{k-2} W_k(\underset{\sim}{q}, \underset{\sim}{P}) \tag{5}$$

where W_k is a homogeneous polynomial of degree k in the old coordinates and the new momenta. Differentiating the generating function

one obtains the transformation equations for the new coordinates and the old momenta,

$$\underset{\sim}{Q} = \underset{\sim}{q} + \epsilon^{k-2} \frac{\partial W_k}{\partial \underset{\sim}{P}} \tag{6a}$$

$$\underset{\sim}{p} = \underset{\sim}{P} + \epsilon^{k-2} \frac{\partial W_k}{\partial \underset{\sim}{q}} \tag{6b}$$

Substituting these equations into the old and the new Hamiltonian, Taylor expanding about the old coordinates and the new momenta, and setting terms of order ϵ^{k-2} equal one finds,

$$\left\{ W_k, H_2 \right\} \Big|_{\substack{\underset{\sim}{p}=\underset{\sim}{P} \\ \underset{\sim}{Q}=\underset{\sim}{q}}} = D_{H_2} W_k \Big|_{\substack{\underset{\sim}{p}=\underset{\sim}{P} \\ \underset{\sim}{Q}=\underset{\sim}{q}}} = \Gamma_k - H_k \Big|_{\substack{\underset{\sim}{p}=\underset{\sim}{P} \\ \underset{\sim}{Q}=\underset{\sim}{q}}} \tag{7}$$

where Γ_k is the k^{th} term of the new Hamiltonian and H_k is the k^{th} term of the old Hamiltonian. In general, the normal operator is singular. As a result, this equation will have a solution if and only if the right hand side is orthogonal to the null space of the transposed problem*.[11] This is equivalent to requiring that the

---

*This is a standard result from linear algebra.[11] Consider the matrix equation, $Mx = y$, where the matrix is singular, $|M| = 0$. This equation has a solution if and only if y is orthogonal to all solutions of the homogeneous transposed problem; $(a_i, y) = 0$, where the set of a_i are all of the functions which satisfy $M^{+}a_i = 0$.

right hand side contain no normal components. This, coupled with the requirement that the k^{th} term of the new Hamiltonian is normal, dictates that this term be chosen to be the normal component of the equivalent term of the old Hamiltonian. Once this choice has been made, Eq. 7 can be solved for the generating function. In order to make this solution unique, it is required that the generating function contain no normal components. Once the generating function has been found, it is a simple matter to transform the Hamiltonian to the new variables.

Gustavson[4] generalizes this transformation to include the case of zero order degeneracies. He notes that the dimension of the null space of the normal operator increases when the zero order problem becomes degenerate. Consequently, the set of functions which span the null space of the normal operator must be enlarged. This can be accomplished if the condition that these functions commute is dropped. A Hamiltonian which can be expressed as a rational function of this enlarged set of functions is said to be in Birkoff-Gustavson normal form.

The sequence of transformations discussed above gives the normal form as a power series in the coupling constant. A small modification of this transformation will accelerate the convergence of the normalization. The transformation just discussed normalizes the lowest order nonnormal terms of the old Hamiltonian, the new transformation normalizes all the nonnormal terms at once. A sequence of these modified transformations converge as ε^{2^n}. This modification is the topic of the next section.

D. THE BIRKOFF-VAN VLECK TRANSFORMATION

This section presents a small modification of the Birkoff-Gustavson transformation which has the effect of accelerating the convergence of the normalization of a classical Hamiltonian. In this modification the entire coupling potential is normalized at each iteration, as opposed to just the lowest order nonnormal term. The new Hamiltonian, at each iteration, is given by the normal part of the old Hamiltonian plus new higher order nonnormal terms.

Consider a Hamiltonian of the form

$$H = H_2 + \lambda H_3 \tag{8}$$

where H_2 represents an integrable problem, and H_3 couples the modes of this problem. The integrable problem is assumed to be a quadratic function of the canonical variables, and the coupling potential is a polynomial in these variables. The subscripts give the degree of the lowest order term. Following the Birkoff-Gustavson transformation the Hamiltonian has the form

$$H = K_2 + \lambda K_3 + \frac{\lambda^2}{2} K_4 + \frac{\lambda^3}{6} K_5 + \cdots \tag{9}$$

where K_3 is in normal form. The generating function is assumed to have the form

$$S = q \cdot \underline{P} + \lambda W_k(q, \underline{P}) \tag{10}$$

where W_k is a polynomial of the old coordinates and the new momenta. The degree of the lowest order term in this function is equal to the degree of the lowest order nonnormal term in the old Hamiltonian. Differentiating the generating function one obtains the

transformation equations for the new coordinates and the old momenta. Substituting these results into the new and old Hamiltonians, Taylor expanding about the new momenta and the old coordinates, and setting terms of order λ equal to each other one obtains

$$\mathbb{D}_{H_2} W_k \Big|_{\substack{\underset{\sim}{P}=\underset{\sim}{P} \\ \underset{\sim}{Q}=\underset{\sim}{q}}} = K_k - H_k \Big|_{\substack{\underset{\sim}{P}=\underset{\sim}{P} \\ \underset{\sim}{Q}=\underset{\sim}{q}}} \quad . \tag{11}$$

The form of this equation is equivalent to that of Eq. 7 in the previous section. As a result, this equation can be solved in the same manner with the exception that in this case the normal operator acts on a large space of functions. Following each transformation the new Hamiltonian can again be written in the form of Eq. 8. Examination of the transformed Hamiltonian reveals that if the lowest order nonnormal term before the transformation is of degree k, after the transformation the lowest order nonnormal term will be of degree 2k. Clearly, this modification accelerates the convergence.

E. THE UNIFORM QUANTIZATION OF THE HENON-HEILES HAMILTONIAN

This section presents the Henon-Heiles Hamiltonian[12] system as an example of the uniform semiclassical quantization of a nonintegrable system. We first briefly outline the procedure. The initial step is to find an integrable approximation to the

nonintegrable problem. This is done by transforming the nonintegrable Hamiltonian into Birkoff-Gustavson normal form to order ε^8, and then truncating the higher order terms. The integrable approximation is then transformed into angle-action like variables. In the new variables the integrable Hamiltonian can be partitioned into two one-dimensional problems. Then the uniform quantization proceeds as in any one-dimensional problem.

1. Normalization of the Henon-Heiles Hamiltonian

The classical Hamiltonian is given by

$$H = \tfrac{1}{2}(p_x^2+x^2) + \tfrac{1}{2}(p_y^2+y^2) + \epsilon y(x^2 - \tfrac{1}{3}y^2) \tag{12}$$

This Hamiltonian is transformed into Birkoff-Gustavson normal form to order ε^8 by three Birkoff-Van Vleck transformations. Recall that in this form the Hamiltonian can be expressed as a rational function of a set of functions which commute with the zero order Hamiltonian. Such a set of functions is

$$\pi_0 = \tfrac{1}{2}(p_x^2+x^2) + \tfrac{1}{2}(p_y^2+y^2) \tag{13a}$$

$$\pi_1 = \tfrac{1}{2}(p_x^2+x^2) - \tfrac{1}{2}(p_y^2+y^2) \tag{13b}$$

$$\pi_2 = p_x y - x p_y \tag{13c}$$

$$\pi_3 = p_x p_y + x y \tag{13d}$$

Expressed in this set of functions the normalized Hamiltonian to order ε^8 is

$$H = \pi_0 + \frac{\epsilon^2}{12}\left\{7\pi_2^2 - 5\pi_0^2\right\}$$

$$+ \frac{\epsilon^4}{9}\left\{\frac{7}{2}\pi_1\left[\pi_1^2 - 3\pi_3^2\right] - \frac{2}{9}\pi_0\left[\pi_0^2 + 5\pi_1^2\right]\right\}$$

$$+ \frac{\epsilon^6}{729}\left\{\frac{1}{16}\left[18887\pi_2^4 - 30246\pi_2^2\pi_0^2 + 11671\pi_0^4\right]\right.$$

$$\left. - 134\pi_0\pi_1\left[\pi_1^2 - 3\pi_3^2\right]\right\} \qquad (14)$$

At this point it is convenient to transform to angle-action like variables. We choose the action like variables to be the total action and the angular momentum. This choice is based on the following observations. 1) The total action is a constant of the motion, that is, the transformed Hamiltonian is not a function of the angle variable corresponding to the total action; and 2) the angular momentum is action like to order ε^4. All other possible choices will be action like to order ε^2. The functions, π_i, in these variables are

$$\pi_0 = J_1 \tag{15a}$$

$$\pi_1 = (J_1^2 - J_2^2)^{1/2} \cos 2\varphi_2 \tag{15b}$$

$$\pi_2 = J_2 \tag{15c}$$

$$\pi_3 = (J_1^2 - J_2^2)^{1/2} \sin 2\varphi_2 \tag{15d}$$

and the Hamiltonian can be written as

$$H = H_1(J_1) + H_2(J_1, J_2, \varphi_2) \tag{16}$$

where

$$H_1(J_1) = J_1 - \frac{5\epsilon^2}{12} J_1^2 - \frac{67\epsilon^4}{432} J_1^3 - \frac{42229\epsilon^6}{155520} J_1^4 \tag{17a}$$

and

$$H_2(J_1, J_2, \varphi_2) = \frac{7\epsilon^2}{12} J_2^2 - \frac{7\epsilon^4}{144} J_1^2 J_2^2 + \frac{7\epsilon^4}{18} (J_1^2 - J_2^2)^{3/2} \cos 6\varphi_2$$

$$- \frac{\epsilon^6 J_2^2}{155520} \left[458682 J_1^2 - 575855 J_2^2 \right]$$

$$- \frac{35\epsilon^6}{648} J_1 J_2^2 (J_1^2 - J_2^2)^{1/2} \cos 2\varphi_2 \tag{17b}$$

$$- \frac{35\epsilon^6}{1458} J_2^2 (J_1^2 - J_2^2) \cos 4\varphi_2$$

$$- \frac{2093\epsilon^6}{2160} J_1 (J_1^2 - J_2^2)^{3/2} \cos 6\varphi_2$$

The period of ψ_1 is 2π and the period of ψ_2 is π. Clearly, each of these terms is a constant of the motion, and consequently, the Hamiltonian can be decoupled and each of the degrees of freedom treated separately.

2. Quantization

We first consider the total action. The Hamiltonian is not a function of the angle variable conjugate to the total action. That is, the total action is a constant of the motion and can be taken to be a good action variable of the approximate problem. Consequently, it can immediately be quantized

$$\overline{J_1} = \frac{1}{2\pi}\int_0^{2\pi} J_1 \, d\varphi_1 = \hbar(n+1) \tag{18}$$

where the path of integration is $\psi_1: 0 \to 2\pi$, $\psi_2 = 0$. Once the total action has been quantized, the problem reduces to a set of one dimensional problems, one for each quantized value of the total action. The decoupled Hamiltonian can be inverted to obtain a polynomial, quartic in the square of the angular momentum,

$$a_8 J_2^8 + a_6 J_2^6 + a_4 J_2^4 + a_2 J_2^2 + a_0 = 0 \tag{19}$$

The coefficients are functions of the total energy, the quantized total action, and the angle like variable conjugate to the angular momentum, (for $\varepsilon^2 = 1/80$)

(20a)

$$a_0 = E^2 - 2EJ_1 + \frac{1}{96}[96+E]J_1^2$$

$$+ \frac{10^{-2}}{13824}[-14400+67E]J_1^3$$

$$+ \frac{10^{-4}}{3981312}[-849600+42229E]J_1^4$$

$$- \frac{32179\times10^{-4}}{3981312}J_1^5 + \frac{16303\times10^{-4}}{38220595 2}J_1^6$$

$$- \frac{98291 21\times10^{-6}}{1100753 14176}J_1^7 - \frac{95713537 67\times10^{-8}}{6340338096 5376}J_1^8$$

$$- \frac{49\times10^{-8}(9600+299J_1)^2}{24461180928}\cos 12\varphi_2$$

(20b)

$$a_2 = -\frac{7}{480}E + \frac{7\times10^{-2}}{4608}(960+E)J_1$$

$$+\frac{7\times10^{-4}}{663552}\left[-86400+10921E\right]J_1^2$$

$$-\frac{26089\times10^{-4}}{221184}J_1^3+\frac{2223557\times10^{-5}}{382205952}J_1^4$$

$$+\frac{1546531\times10^{-5}}{24461180928}J_1^5+\frac{12133881183\times10^{-7}}{10567230160896}J_1^6$$

$$+7\times10^{-6}\left[-995328000(E-J_1)-51840000J_1^2\right.$$

$$\left.+439200J_1^3+15913J_1^4\right]J_1^2\cos4\varphi_2\Big/743008370688$$

$$+\frac{49\times10^{-6}J_1^5}{73383542784}(9600+299J_1)\cos8\varphi_2$$

$$+\frac{49\times10^{-8}J_1^4}{8153726976}(9600+299J_1)^2\cos12\varphi_2$$

(20c)

$$q_4 = \frac{49\times10^{-2}}{9216} - \frac{115171\times10^{-3}}{7962624}E + \frac{114289\times10^{-3}}{7962624}J_1$$

$$- \frac{1574881\times10^{-5}}{95551488}J_1^2 - \frac{13385071\times10^{-5}J_1^3}{2201506283 52}$$

$$+ \frac{114895240019\times10^{-7}J_1^4}{5706304286888384}$$

$$-7\left[-19906560000(E-J_1) - 248832000J_1^2\right.$$

$$\left. + 2390400J_1^3 + 19006 1J_1^4\right]\cos 4\varphi_2 / 14860167413 76$$

$$- \frac{49\times10^{-6}J_1(2332800+72457J_1)}{8916100482 56}\cos 8\varphi_2$$

$$- \frac{49\times10^{-8}J_1^2(9600+299J_1)^2}{8153726976}\cos 12\varphi_2$$

(20d)

$$a_6 = \frac{820309\times10^{-4}}{764411904} + \frac{188503\times10^{-6}\,J_1}{366917771392}$$

$$- \frac{1163008489027\,J_1^2}{142657607172096}$$

$$+ \frac{49\times10^{-5}(-16588800+172800J_1+34537J_1^2)}{118881339310 08}\cos 4\varphi_2$$

$$+ \frac{49\times10^{-6}(2332800+71857J_1)}{1783220089 6512}\cos 8\varphi_2$$

$$+ \frac{49\times10^{-8}(9600+299J_1)^2}{244611809 28}\cos 12\varphi_2$$

$$a_8 = \frac{11938174196 9\times10^{-6}}{228252171475 3536} \qquad \text{(20e)}$$

$$- \frac{806197\times10^{-5}}{118881339310 08}\cos 4\varphi_2$$

$$+ \frac{49\times10^{-4}}{44580502241 28}\cos 8\varphi_2$$

The four roots of this equation occur in pairs which are out of phase with each other. One need only consider one root of each pair. Of these two remaining roots, one has a large negative value and corresponds to motion outside of the potential well. The last root is the physically interesting one. The angular momentum, that is, the square root of this root, is plotted in Figure 4-4 for several different energies, for one value of the total action. From this figure it is clear that the one dimensional problem can be viewed as a threefold hindered rotation. The regions labelled by A, B, and C correspond to the box tori, and the regions labelled D and E correspond to the precessing tori. Since there are disjoint classical regions, one expects quantum tunneling, which joins these regions, to be important. Consequently, one should use a uniform semiclassical quantization condition for this degree of freedom. Miller[13] has derived a uniform semiclassical quantization condition for the threefold hindered rotor. These conditions are

$$\cos\left\{\frac{l\pi}{3}\right\} = \left\{1+e^{2\Theta}\right\}^{1/2}\cos\phi \quad \text{for } l = 0,1,2,\ldots \tag{21}$$

where

$$\phi = \int_{C_1} J_2(J_1, E, \varphi_2)\, d\varphi_2$$

$$\Theta = \int_{C_2} \left| J_2(J_1, E, \varphi_2) \right| d\varphi_2$$

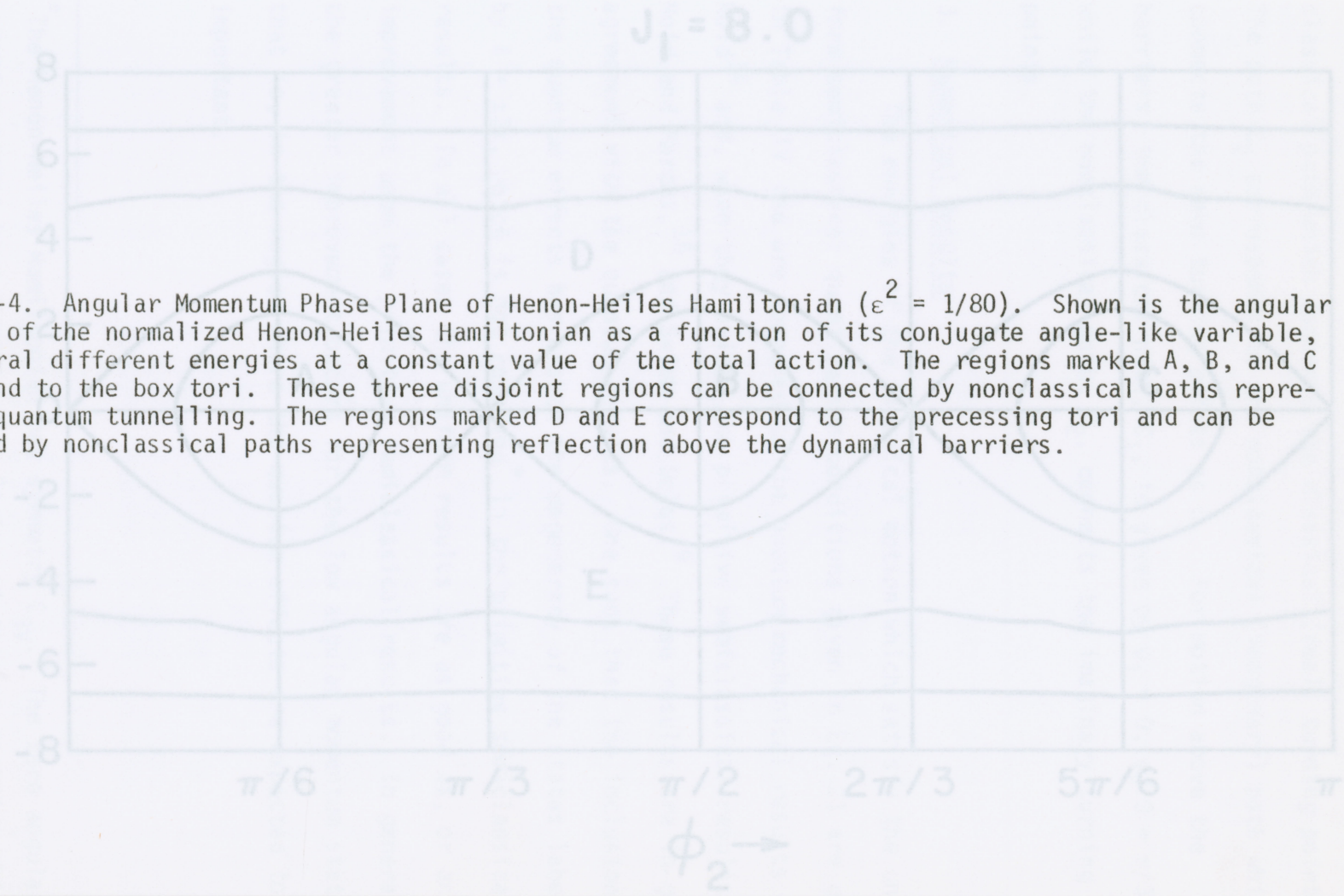
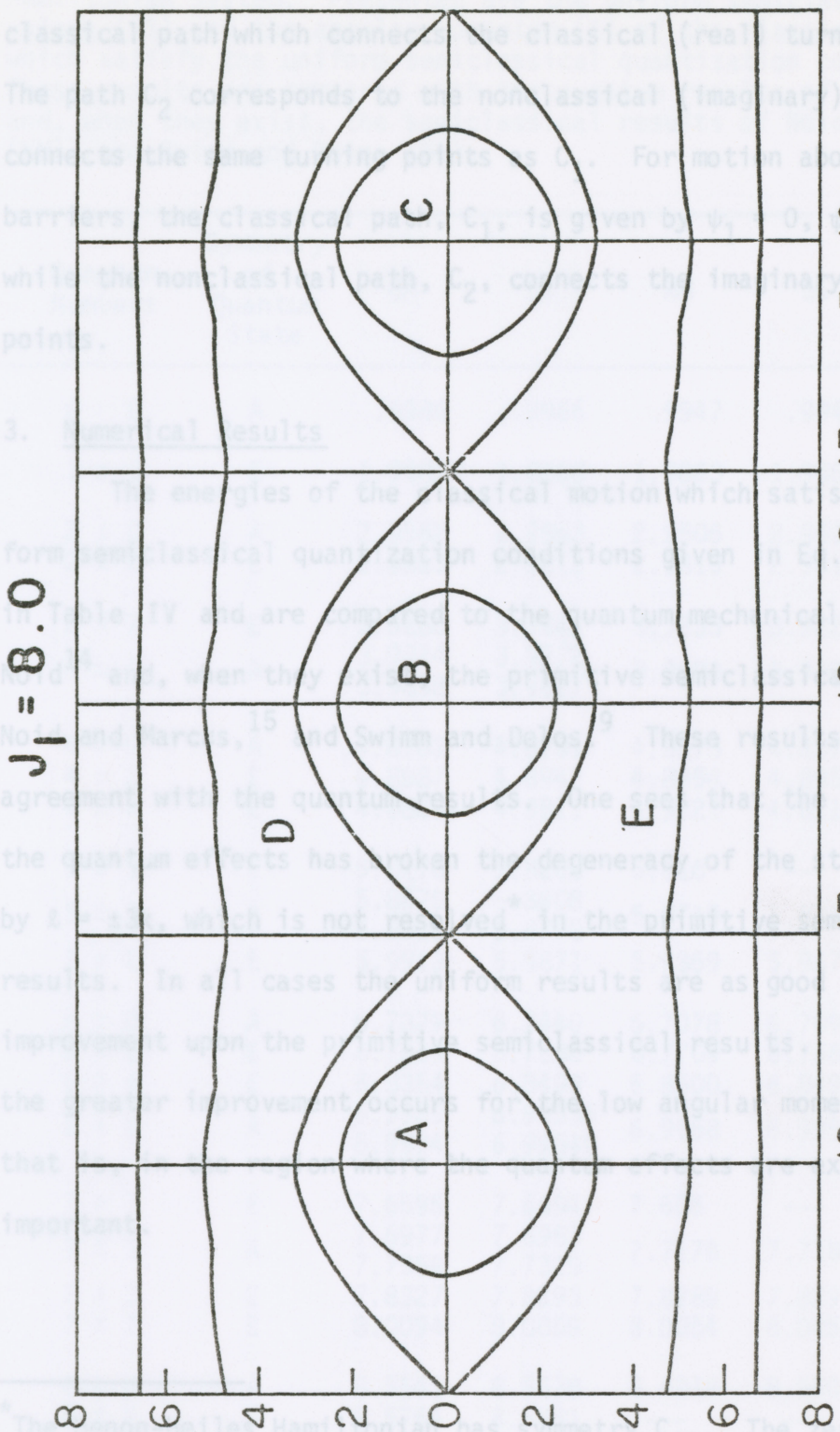


Figure 4-4. Angular Momentum Phase Plane of Henon-Heiles Hamiltonian ($\varepsilon^2 = 1/80$). Shown is the angular momentum of the normalized Henon-Heiles Hamiltonian as a function of its conjugate angle-like variable, for several different energies at a constant value of the total action. The regions marked A, B, and C correspond to the box tori. These three disjoint regions can be connected by nonclassical paths representing quantum tunnelling. The regions marked D and E correspond to the precessing tori and can be connected by nonclassical paths representing reflection above the dynamical barriers.


$J_1 = 8.0$
A
B
C
D
E
J_2
8
6
4
2
0
-2
-4
-6
-8
$\pi/6$
$\pi/3$
$\pi/2$
$2\pi/3$
$5\pi/6$
π
ϕ_2

for motion below the barrier. The path C_1 corresponds to the classical path which connects the classical (real) turning points. The path C_2 corresponds to the nonclassical (imaginary) path which connects the same turning points as C_1. For motion above the barriers, the classical path, C_1, is given by $\psi_1 = 0$, $\psi_2: 0 \rightarrow \pi/3$, while the nonclassical path, C_2, connects the imaginary turning points.

3. Numerical Results

The energies of the classical motion which satisfy the uniform semiclassical quantization conditions given in Eq. 21 are given in Table IV and are compared to the quantum mechanical results of Noid[14] and, when they exist, the primitive semiclassical results of Noid and Marcus,[15] and Swimm and Delos.[9] These results are in good agreement with the quantum results. One sees that the inclusion of the quantum effects has broken the degeneracy of the states labelled by $\ell = \pm 3k$, which is not resolved* in the primitive semiclassical results. In all cases the uniform results are as good as, or an improvement upon the primitive semiclassical results. In general, the greater improvement occurs for the low angular momentum states, that is, in the region where the quantum effects are expected to be important.

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*The Henon-Heiles Hamiltonian has symmetry C_{3V}. The zero angular momentum states have symmetry A_1. States of angular momentum which are not divisible by three have symmetry E and are doubly degenerate. States of angular momentum which are divisible by three mix to form two states of Symmetry A_1 and A_2.

Table IV. The Uniform Semiclassical Eigenvalues of the Henon-Heiles Hamiltonian System. Presented are the uniform semiclassical eigenvalues (US) and the angular momentum (ℓ) of the classical motions which satisfy the uniform semiclassical quantization conditions. These results are compared with the quantum results of Noid (QM) and, when they exist, the semiclassical results of Noid and Marcus (NM), and Swimm and Delos (DS).

Quantum Numbers	Symmetry of Quantum State	QM	US	NM	DS	ℓ
0 0	A	.9986	.9966	.9947	.9947	.501
1 ± 1	E	1.9901	1.9868	1.9863	1.9862	1.038
2 ± 0	A	2.9562	2.9558	2.9506	2.9506	.673
2 ± 2	E	2.9853	2.9812	2.9815	2.9814	2.983
3 ± 1	E	3.9260	3.9241	3.9233	3.9226	1.105
3 ± 3	A	3.9824	3.9772	3.9803	3.9801	2.932
		3.9858	3.9827			3.058
4 ± 0	A	4.8702	4.8731	4.8573	4.8577	.802
4 ± 2	E	4.8987	4.8942	4.8954	4.8954	1.967
4 ± 4	E	4.9863	4.9821	4.9821	4.821	4.000
5 ± 1	E	5.8170	5.8202	5.816	---	1.174
5 ± 3	A	5.8670	5.8608	5.8713	5.8711	2.746
		5.8815	5.8778			3.153
5 ± 5	E	5.9913	5.9871	5.9869	5.9871	5.000
6 ± 0	A	6.7379	6.7440	6.7078	6.7098	.983
6 ± 2	E	6.7649	6.7636	6.7709	6.7663	1.861
6 ± 4	E	6.8354	6.8493	6.8500	6.8492	4.003
6 ± 6	A	6.9989	6.99535	6.9958	6.9951	6.0026
		6.9994	6.99540			6.0033
7 ± 1	E	7.6595	7.6694	7.655	---	1.267
7 ± 3	A	7.6977	7.6953	7.7178	7.7184	2.300
		7.7369	7.7329			3.345
7 ± 5	E	7.8327	7.8293	7.8289	7.8293	4.999
7 ± 7	E	8.0094	8.0059	8.0054	8.0058	7.000
8 ± 0	A	8.5541	8.5638	8.4919	8.5003	1.188
8 ± 2	E	8.5764	8.5881	---	---	1.743
8 ± 4	E	8.6779	8.6730	---	8.6717	4.025
8 ± 6	A	8.8113	8.8088	8.8084	8.8112	5.973
		8.8152	8.8132			6.024
8 ± 8	E	9.0217	9.0193	9.0151	9.0192	8.000

Table IV. (continued)

Quantum Numbers	Symmetry of Quantum State	QM	US	NM	DS	ℓ
9 ± 1	E	9.444	9.4574	---	---	1.379
9 ± 3	A	9.467	9.4850	---	---	1.900
		9.552	9.5486			3.592
9 ± 5	E	9.629	9.6254	---	9.626	4.990
9 ± 7	E	9.794	9.7943	---	9.794	7.000
9 ± 9	A	10.035	10.0350	---	10.035	8.998
		10.036	10.0351			8.999
10 ± 0	A	10.305	10.3238	---	10.221	1.359
10 ± 2	E	10.318	10.3393	---	---	1.592
10 ± 4	E	10.463	10.4591	---	10.455	4.102
10 ± 6	A	10.573	10.5703	---	10.581	5.866
		10.590	10.5893			6.103
10 ± 8	E	10.774	10.7785	---	10.779	8.000
10 ± 10	E	11.050	11.0536	---	11.053	10.000
11 ± 1	E	11.152	11.180	---	---	1.457
11 ± 3	A	11.160	11.192	---	---	1.603
		11.325	11.331			3.817
11 ± 5	E	11.383	11.378	---	11.383	4.922
11 ± 7	E	11.534	11.536	---	11.534	7.002
11 ± 9	A	11.950	11.7637	---	11.750	9.001
		11.752	11.7639			9.003
11 ± 11	E	11.968	12.074	---	12.074	11.000
12 ± 0	A	11.966	12.011	---	11.864	1.459
12 ± 2	E	12.065	12.017	---	---	1.523
12 ± 4	E	12.206	12.217	---	---	4.208
12 ± 6	A	12.277	12.274	---	12.310	5.456
		12.334	12.332			6.295
12 ± 8	E	12.480	12.490	---	12.491	7.999
12 ± 10	E	12.712	12.749	---	12.750	10.000
12 ± 12	A	13.077	13.0975	---	13.097	11.999
		13.087	13.0976			12.000
13 ± 1	E	12.762	12.824	---	---	1.491
13 ± 3	A	12.748	12.827	---	---	1.519
		13.032	13.060			4.114
13 ± 5	E	13.081	13.104	---	---	4.784
13 ± 7	E	13.233	13.238	---	---	7.023
13 ± 9	A	---	13.4397	---	---	8.968
		---	13.4474			9.030
13 ± 11	E	---	13.7351	---	---	11.000

Swimm and Delos[9] obtain their results in a manner very similar to the one reported here. They transform the Hamiltonian into Birkoff-Gustavson normal form by a sequence of Birkoff-Gustavson transformations, and then truncate the high order nonnormal terms. Their next step is to decouple the Hamiltonian by transformation to a set of angle-action like variables. Their choice of these variables, while the obvious one, is unfortunate because the transformed Hamiltonian does not clearly exhibit the symmetry of the problem. They then find the classical motions which satisfy the primitive semiclassical quantization conditions proposed by Noid and Marcus.[15] They are not able to find all of the semiclassical eigenvalues. At this time, the reason for this is not clear.

F. DISCUSSION

This chapter has presented the Henon-Heiles Hamiltonian system as an example of the quantization of a nonintegrable, classical Hamiltonian. The semiclassical quantum results for the motion in the stochastic regions of phase space are excellent. This is attributed to the fact that the volumes of phase space which give rise to the stochastic behavior (rather than those where it appears to occur) are small compared to $\hbar$. The question arises as to how small is small enough. This is an important question which has not been explored. It can be investigated by a series of calculations as presented here with different values of the coupling constant. Quantum mechanically this corresponds to varying the value of $\hbar$. Another question which has not been addressed is how to measure the volumes of the switching regions of phase space.

The normal expansion of a Hamiltonian does not, in general, converge and must be treated as an asymptotic expansion. The truncation of this expansion has serious consequences for the nodal pattern semiclassical wave function.[17] When this formal expansion does converge then there exist angle-action variables.

The methods used in this thesis to carry out the canonical transformations are quite clumsy since the generating function, and hence, the transformation equations, are functions of both the old and the new canonical variables. Lie[17] has developed a transformation theory which avoids this drawback. All of the transformations discussed in this thesis can be reformulated in terms of Lie transforms with the resultant simplification of the numerical methods (see Appendix C).

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SUMMARY

The work reported in this thesis treats the semiclassical quantization of both integrable and nonintegrable Hamiltonian systems. For integrable systems I have developed a sequence of canonical transformations for the transformation of the original Hamiltonian into angle-action variables and have discussed the correct choice of zero order variables. This method is shown to converge rapidly in regions where other iterative processes appear to be in trouble. The semiclassical eigenvalues are then found by evaluating the transformed Hamiltonian at the quantized values of the actions. For nonintegrable systems I have developed a sequence of transformations which transform the Hamiltonian into Birkoff-Gustavson normal form. This sequence of transformations also exhibits accelerated convergence. Once the Hamiltonian has been transformed into this form I show that the system can be decoupled into a set of one dimensional problems, and that each degree of freedom can be quantized individually. In essence this allows the uniform semiclassical quantization of nonseparable Hamiltonian systems.

In conclusion I wish to emphasize that while classical mechanics is very sensitive to instabilities in phase space, the results presented in this thesis indicate that quantum mechanics smooths over these classical instabilities. Consequently, in the semiclassical limit, one need only consider integrable approximations of the classical Hamiltonian. This results in many significant

simplifications of the semiclassical theory of nonseparable Hamiltonian systems.

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APPENDIX A

THE CLASSICAL AND QUANTUM MECHANICAL VAN VLECK TRANSFORMATION

In order to see that the method for constructing tori reported here is indeed the classical limit of Van Vleck's transformation[8] we proceed in the following manner.

In both cases we consider a Hamiltonian of the following form

$$H = H_0 + \epsilon H_1 \tag{A1}$$

In the quantum case (A1) is an operator, and in the classical case (A1) is a function of $(\underset{\sim}{q},\underset{\sim}{p})$. Quantum mechanically, Van Vleck's transformation eliminates terms of order ϵ from H, which connect a state of interest with all other nondegenerate states. Classically, the Van Vleck transformation does much the same, that is, the transformation will eliminate all terms of H that are dependent on the angle "like" variables, i.e., the terms which couple different modes. Quantum mechanically we wish to transform the Hamiltonian in the following manner

$$T^{-1} H T = \mathcal{H}_0 + \epsilon \mathcal{H}_1 + \sum_{l=2}^{\infty} \epsilon^l \mathcal{H}_l \tag{A2}$$

where

$$T = \exp \frac{i}{\hbar} \epsilon W \tag{A3}$$

and $\mathcal{H}_1$ does not couple the state of interest with the rest of the states, that is, the coupling has been transformed to the higher order terms. Expanding Eq. (A3), substituting this result and Eq. (A1) into (A2) and collecting terms of order ε we obtain

$$\mathcal{H}_1 = H_1 - \frac{i}{\hbar}\left[W, H_0\right] \tag{A4}$$

where [,] denotes the usual quantum mechanical commutator. Equation (A4) can now be solved for W which in turn provides the transformation.

Classically the procedure is much the same; however, rather than finding a unitary transformation operator, we seek the generating function of the appropriate canonical transformation,

$$S = q \cdot \underset{\sim}{P} + \epsilon W(q, \underset{\sim}{P}) \tag{A5}$$

In this case we wish to transform the classical Hamiltonian into new variables such that the term of order ε does not depend upon the new angle "like" variables,

$$H = H_0(P) + \epsilon H_1(P, q) = \mathcal{H}_0(\underset{\sim}{P}) + \epsilon \mathcal{H}_1(\underset{\sim}{P}) + \sum_{l=2}^{\infty} \epsilon^l \mathcal{H}_l(\underset{\sim}{P}, \underset{\sim}{Q}) \tag{A6}$$

In order to accomplish this we differentiate Eq. (A5) with respect to q and P. This gives

$$\underset{\sim}{Q} = q + \epsilon \frac{\partial W}{\partial \underset{\sim}{P}} \tag{A7}$$

$$\underset{\sim}{p} = \underset{\sim}{P} + \epsilon \frac{\partial W}{\partial \underset{\sim}{q}} \tag{A8}$$

Substituting Eqs. (A2) and (A8) into Eq. (A6), Taylor expanding and collecting terms of order ε, we find

$$\mathcal{H}_1 = H_1 - \{W, H_0\} \tag{A9}$$

where $\{\ ,\ \}$ is the classical Poisson bracket. It is clear that Eq. (A9) is, of course, the classical equivalent of Eq. (A4) and hence we see that each transformation in our method of constructing the invariant tori is equivalent to a Van Vleck transformation.

APPENDIX B

INVERSION OF EQ. (H) OF SECTION D, CHAPTER II

The problem of inverting Eq. (H) in Section D is a common problem in classical transformation theory. We proceeded in the following manner.

Consider the function

$$\phi(\Theta) = \Theta + \epsilon f(\Theta) \tag{B1}$$

We wish to invert this function to obtain

$$\Theta(\phi) = \phi - \epsilon g(\phi) \tag{B2}$$

Combining Eqs. (B1) and (B2) we find that

$$f(\Theta) = g(\phi) \tag{B3}$$

Fourier analyzing Eq. (B3) with respect to ϕ we obtain,

$$g_\ell = \oint' d\phi \; g(\phi) e^{-i\ell\phi} \tag{B4}$$

Equation (B5) gives the Fourier coefficient of $g(\phi)$. For the numerical calculation the exponential term was expanded in a power series to give

$$g_\ell = \sum_{n=0} \frac{(-i\ell\epsilon)^n}{n!} \oint' d\Theta \left\{ 1 + \epsilon \frac{\partial f}{\partial \Theta} \right\} f(\Theta)^{n+1} e^{-i\ell\Theta} \tag{B6}$$

In practice, good results were obtained from truncation of Eq. (B6) after the seventh term.

APPENDIX C

TRANSFORMATION TO NORMAL FORM VIA AN INFINITE SEQUENCE OF VAN VLECK-LIE TRANSFORMATIONS

In this appendix we consider the formal transformation of a conservative N-dimensional Hamiltonian into normal form. In many simple systems this is equivalent to a canonical transformation to angle-action variables. A similar scheme of Jacobi transformations has been used to decouple the Henon-Heiles Hamiltonian to 8^{th} order.

Initially we consider a Hamiltonian of the form

$$H = H_0(\underline{p},\underline{q}) + \lambda H_1(\underline{p},\underline{q}) \tag{C1}$$

where the zero order term represents an integrable problem and λ is a formal parameter. The equations of motion for this system are

$$\dot{\underline{p}} = -\frac{\partial H}{\partial \underline{q}} = -\frac{\partial H_0}{\partial \underline{q}} - \lambda \frac{\partial H_1}{\partial \underline{q}} = \dot{\underline{p}}_0 - \lambda \frac{\partial H_1}{\partial \underline{q}} \tag{C2a}$$

$$\dot{\underline{q}} = \frac{\partial H}{\partial \underline{p}} = \frac{\partial H_0}{\partial \underline{p}} + \lambda \frac{\partial H_1}{\partial \underline{p}} = \dot{\underline{q}}_0 + \lambda \frac{\partial H_1}{\partial \underline{p}} \tag{C2b}$$

where

$$\dot{\underline{p}}_0 = -\left.\frac{\partial H_0}{\partial \underline{q}_0}\right|_{(\underline{q}_0,\underline{p}_0)\to(\underline{q},\underline{p})} \tag{C3a}$$

$$\dot{\underline{q}}_0 = \left.\frac{\partial H_0}{\partial \underline{p}_0}\right|_{(\underline{q}_0,\underline{p}_0)\to(\underline{q},\underline{p})} \tag{C3b}$$

Integrating these equations one obtains

$$p = p_0 - \lambda \int \frac{\partial H_1}{\partial q} dt \tag{C4a}$$

$$q = q_0 + \lambda \int \frac{\partial H_1}{\partial p} dt \tag{C4b}$$

This suggests a transformation of the form

$$p(q_0, p_0) = p_0 - \lambda \underset{\sim}{f}(q_0, p_0) \tag{C5a}$$

$$q(q_0, p_0) = q_0 + \lambda \underset{\sim}{g}(q_0, p_0) \tag{C5b}$$

The transformation to normal form is such a transformation. The process of normalizing the Hamiltonian can be viewed as a transformation to a new set of variables such that the transformed Hamiltonian can be represented as a rational function of functions which commute with the zero order problem,

$$H(p, q) \longrightarrow H(\pi_i(p, q)) \tag{C6}$$

where

$$\{\pi_i, H_0\} = 0 \tag{C7}$$

It is easy to show that

$$\{H, H_0\} = 0 \tag{C8}$$

This is taken to be the operational definition of the normal form.

In order to construct a transformation such that Eq. 8 is satisfied, we make use of a theorem due to Lie: If the transformation given by

$$H(\underset{\sim}{P}, \underset{\sim}{Q}) = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \mathbb{D}_S^n H(\underset{\sim}{p}, \underset{\sim}{q}) \tag{C9}$$

where $\mathbb{D}_S^0 = 1$, $\mathbb{D}_S^1 = \{\ ,S\}$, and $\mathbb{D}_S^n = \mathbb{D}_S^{n-1}\mathbb{D}_S^1$ for $n \geq 2$, and where S is the determining function, converges then the transformation is canonical. The transformed variables are given by

$$\underset{\sim}{P} = \underset{\sim}{p} + \sum_{n=1}^{\infty} \frac{\lambda^n}{n!} \mathbb{D}_S^n \underset{\sim}{p} \tag{C 10a}$$

$$\underset{\sim}{Q} = \underset{\sim}{q} + \sum_{n=1}^{\infty} \frac{\lambda^n}{n!} \mathbb{D}_S^n \underset{\sim}{q} \tag{C 10b}$$

The determining function in the Lie transformation is analogous to the generating function in Jacobi transformation theory. Hence, the determining function depends only upon the old canonical variables, as opposed to the generating function which depends upon both the old and the new variable. The variable dependence of the determining function results from the relationship of Lie transform to infinitesimal transformations. The group properties of Lie transforms are easily demonstrated. The inverse of Eq. 9 is

$$H(\underset{\sim}{P},\underset{\sim}{q}) = \sum_{m=0}^{\infty} \frac{(-\lambda)^m}{m!} \mathbb{D}_S^m H(\underset{\sim}{P},\underset{\sim}{Q}) \tag{C11}$$

Setting S equal to zero gives the identity transformation. The product of two transformations is itself a transformation; if Eq. 9 is substituted into

$$H(\underset{\sim}{x},\underset{\sim}{y}) = \sum_{m=0}^{\infty} \frac{\lambda^m}{m!} \mathbb{D}_{S'}^m H(\underset{\sim}{P},\underset{\sim}{Q}) \tag{C12}$$

one obtains

$$H(\underset{\sim}{x},\underset{\sim}{y}) = \sum_{m=0}^{\infty} \frac{\lambda^m}{m!} \mathbb{D}_{S'+S}^m H(\underset{\sim}{P},\underset{\sim}{q}) \tag{C13}$$

where

$$\mathbb{D}_{S'+S}^m = \sum_{\ell=0}^{m} \binom{m}{\ell} \mathbb{D}_{S'}^{\ell} \mathbb{D}_S^{m-\ell} \tag{C14}$$

One of the standard approaches to constructing such a transformation is to expand the determining function as a power series in the coupling constant, λ. While expansions of this type are, in general, not convergent, they do provide useful numerical results in regions of phase space which are not characterized by small divisors. If one wishes to treat such regions one must accelerate the convergence of the normalization procedure. This can be accomplished,

recalling that all canonical transformation form a group, by expanding the transformation as a sequence of transformations. Each transformation in this sequence normalizes the nonnormal terms of the Hamiltonian and creates new high order nonnormal terms.

To make this process explicit consider the Hamiltonian given in Eq. 1. We wish to transform this Hamiltonian to the form

$$K(\underset{\sim}{P},\underset{\sim}{Q}) = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} K_n(\underset{\sim}{P},\underset{\sim}{Q}) \tag{C15}$$

Substituting Eq. 1 into Eq. 9 and collecting terms of equal order of λ one obtains

$$K_0 = H_0 \tag{C16a}$$

$$K_1 = H_1 + \mathbb{D}_S H_0 \tag{C16b}$$

$$K_n = \mathbb{D}_S^{n-1}\left\{K_1 + (n-1)H_1\right\} \quad \text{for } n \geq 2 \tag{C16c}$$

Eq. 16b is analogous to Eq. 7 in Chapter IV and can be solved in the same manner. Then the remaining terms of the new Hamiltonian can be constructed by use of Eq. 16c. Clearly by redefining the formal parameter one can rewrite Eq. 15 in the form of Eq. 1 and repeat this process as often as desired.

The process just discussed is the Lie transform equivalent of the Jacobi transformation upon which the numerical work of Chapter IV is based. This method of normalizing the Hamiltonian is not totally satisfactory. Ideally, to discuss the stability of a

Hamiltonian system (and other properties) one wishes to study the flow of the Hamiltonian system associated with the coupling constant (this can be taken as the original parameter). This is not possible in the case just discussed since the parameter is redefined at each step of the process. This shortcoming can be overcome. In the remaining portion of this appendix we outline such a procedure.

We need not reconsider the first transformation. However, for the second transformation rather than rewrite the Hamiltonian, Eq. 15, in the form of Eq. 1, we will substitute Eq. 15 directly into Eq. 9. Then assuming that $S^{(2)} = S_0^{(2)} + \lambda S_1^{(2)}$, we collect terms of equal order in λ to obtain

$$L_0 = K_0$$
$$L_1 = K_1 \qquad \text{(C17a)}$$

$$L_2 = K_2 + \mathbb{D}_{S_0^{(2)}} K_0$$

$$L_3 = K_3 + \mathbb{D}_{S_0^{(2)}} K_1 + \mathbb{D}_{S_1^{(2)}} K_0 \qquad \text{(C17b)}$$

$$\frac{\lambda^4}{4!}\mathbb{R} = K(P(p,q), Q(p,q)) - \left\{L_0 + \lambda L_1 + \frac{\lambda^2}{2} L_2 + \frac{\lambda^3}{6} L_3\right\} \qquad \text{(C17c)}$$

Eq. 17b is solved in a manner analogous to the solution of Eq. 7

in Chapter IV. Generalizing this to the $(n+1)^{th}$ transformation one finds that Eq. 17 becomes

$$H_0^{(\ell+1)} = H_0^{(\ell)}$$

$$- - - -$$

$$H^{(\ell+1)} = H_{2^\ell-1}^{(\ell)} \tag{C18a}$$

$$H_{2^\ell}^{(\ell+1)} = H_{2^\ell}^{(\ell)} + \mathbb{D}_{S_0^{(\ell+1)}} H_0^{(\ell)}$$

$$- - - -$$

(C18b)

$$H_{2^{\ell+1}-1}^{(\ell+1)} = H_{2^{\ell+1}-1}^{(\ell)} + \mathbb{D}_{S_0^{(\ell+1)}} H_{2^\ell-1}^{(\ell)} + \cdots + \mathbb{D}_{S_{2^\ell-1}^{(\ell+1)}} H_0^{(\ell)}$$

$$\frac{\lambda^{2^{\ell+1}}}{(2^{\ell+1})!} \mathbb{R} = H^{(\ell)}\left(\mathcal{P}^{(\ell)}\left(\mathcal{P}^{(\ell+1)}, \mathcal{Q}^{(\ell+1)}\right), \mathcal{Q}^{(\ell)}\left(\mathcal{P}^{(\ell+1)}, \mathcal{Q}^{(\ell+1)}\right)\right)$$

$$- \sum_{k=0}^{2^{\ell+1}-1} H_k^{(\ell+1)}\left(\mathcal{P}^{(\ell+1)}, \mathcal{Q}^{(\ell+1)}\right) \tag{C18c}$$

where we have assumed that the determining function of this transformation has the form

$$S^{(\ell+1)} = \sum_{k=0}^{2^{\ell}-1} \lambda^k S_k^{(\ell+1)} \tag{C19}$$

That this series of transformations can be written as a one-parameter Lie transformation can be demonstrated by showing that the product of the first two transformations is in fact a one-parameter Lie transformation, that is

$$L = \sum_{m=0}^{\infty} \frac{\lambda^m}{m!} \mathbb{D}^m_{S^{(2)}+S^{(1)}} H \tag{C20}$$

where

$$\mathbb{D}^m_{S^{(2)}+S^{(1)}} = \sum_{\ell=0}^{m/2} \binom{m}{\ell} \mathbb{D}^{\ell}_{S^2} \mathbb{D}^{m-2\ell}_{S^1} \tag{C21}$$

Clearly, the product of this transformation and the third transformation of the series can also be written as a one-parameter Lie transform. This process can be continued until the desired degree of approximation is reached.

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