

Chapter 16

Hamiltonian Mechanics

16.1 The Hamiltonian

Recall that $L = L(q, \dot{q}, t)$, and

$$p_\sigma = \frac{\partial L}{\partial \dot{q}_\sigma} . \quad (16.1)$$

The Hamiltonian, $H(q, p)$ is obtained by a Legendre transformation,

$$H(q, p) = \sum_{\sigma=1}^n p_\sigma \dot{q}_\sigma - L . \quad (16.2)$$

Note that

$$\begin{aligned} dH &= \sum_{\sigma=1}^n \left(p_\sigma d\dot{q}_\sigma + \dot{q}_\sigma dp_\sigma - \frac{\partial L}{\partial q_\sigma} dq_\sigma - \frac{\partial L}{\partial \dot{q}_\sigma} d\dot{q}_\sigma \right) - \frac{\partial L}{\partial t} dt \\ &= \sum_{\sigma=1}^n \left(\dot{q}_\sigma dp_\sigma - \frac{\partial L}{\partial q_\sigma} dq_\sigma \right) - \frac{\partial L}{\partial t} dt . \end{aligned} \quad (16.3)$$

Thus, we obtain Hamilton's equations of motion,

$$\frac{\partial H}{\partial p_\sigma} = \dot{q}_\sigma \quad , \quad \frac{\partial H}{\partial q_\sigma} = -\frac{\partial L}{\partial q_\sigma} = -\dot{p}_\sigma \quad (16.4)$$

and

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t} . \quad (16.5)$$

Some remarks:

- As an example, consider a particle moving in three dimensions, described by spherical polar coordinates (r, θ, ϕ) . Then

$$L = \frac{1}{2}m (\dot{r}^2 + r^2 \dot{\theta}^2 + r^2 \sin^2 \theta \dot{\phi}^2) - U(r, \theta, \phi) . \quad (16.6)$$

We have

$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r} \quad , \quad p_\theta = \frac{\partial L}{\partial \dot{\theta}} = mr^2 \dot{\theta} \quad , \quad p_\phi = \frac{\partial L}{\partial \dot{\phi}} = mr^2 \sin^2 \theta \dot{\phi} \quad , \quad (16.7)$$

and thus

$$\begin{aligned} H &= p_r \dot{r} + p_\theta \dot{\theta} + p_\phi \dot{\phi} - L \\ &= \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{p_\phi^2}{2mr^2 \sin^2 \theta} + U(r, \theta, \phi) . \end{aligned} \quad (16.8)$$

Note that H is time-independent, hence $\frac{\partial H}{\partial t} = \frac{dH}{dt} = 0$, and therefore H is a constant of the motion.

- In order to obtain $H(q, p)$ we must invert the relation $p_\sigma = \frac{\partial L}{\partial \dot{q}_\sigma} = p_\sigma(q, \dot{q})$ to obtain $\dot{q}_\sigma(q, p)$. This is possible if the Hessian,

$$\frac{\partial p_\alpha}{\partial \dot{q}_\beta} = \frac{\partial^2 L}{\partial \dot{q}_\alpha \partial \dot{q}_\beta} \quad (16.9)$$

is nonsingular. This is the content of the ‘inverse function theorem’ of multivariable calculus.

- Define the rank $2n$ vector, ξ , by its components,

$$\xi_i = \begin{cases} q_i & \text{if } 1 \leq i \leq n \\ p_{i-n} & \text{if } n < i \leq 2n . \end{cases} \quad (16.10)$$

Then we may write Hamilton’s equations compactly as

$$\dot{\xi}_i = J_{ij} \frac{\partial H}{\partial \xi_j} \quad , \quad (16.11)$$

where

$$J = \begin{pmatrix} \mathbb{O}_{n \times n} & \mathbb{I}_{n \times n} \\ -\mathbb{I}_{n \times n} & \mathbb{O}_{n \times n} \end{pmatrix} \quad (16.12)$$

is a rank $2n$ matrix. Note that $J^t = -J$, *i.e.* J is antisymmetric, and that $J^2 = -\mathbb{I}_{2n \times 2n}$. We shall utilize this ‘symplectic structure’ to Hamilton’s equations shortly.

16.2 Modified Hamilton's Principle

We have that

$$\begin{aligned}
 0 &= \delta \int_{t_a}^{t_b} dt L = \delta \int_{t_a}^{t_b} dt (p_\sigma \dot{q}_\sigma - H) \\
 &= \int_{t_a}^{t_b} dt \left\{ p_\sigma \delta \dot{q}_\sigma + \dot{q}_\sigma \delta p_\sigma - \frac{\partial H}{\partial q_\sigma} \delta q_\sigma - \frac{\partial H}{\partial p_\sigma} \delta p_\sigma \right\} \\
 &= \int_{t_a}^{t_b} dt \left\{ - \left(\dot{p}_\sigma + \frac{\partial H}{\partial q_\sigma} \right) \delta q_\sigma + \left(\dot{q}_\sigma - \frac{\partial H}{\partial p_\sigma} \right) \delta p_\sigma \right\} + (p_\sigma \delta q_\sigma) \Big|_{t_a}^{t_b},
 \end{aligned} \tag{16.13}$$

assuming $\delta q_\sigma(t_a) = \delta q_\sigma(t_b) = 0$. Setting the coefficients of δq_σ and δp_σ to zero, we recover Hamilton's equations.

16.3 Phase Flow is Incompressible

A flow for which $\nabla \cdot \mathbf{v} = 0$ is *incompressible* – we shall see why in a moment. Let's check that the divergence of the phase space velocity does indeed vanish:

$$\begin{aligned}
 \nabla \cdot \dot{\boldsymbol{\xi}} &= \sum_{\sigma=1}^n \left\{ \frac{\partial \dot{q}_\sigma}{\partial q_\sigma} + \frac{\partial \dot{p}_\sigma}{\partial p_\sigma} \right\} \\
 &= \sum_{i=1}^{2n} \frac{\partial \dot{\xi}_i}{\partial \xi_i} = \sum_{i,j} J_{ij} \frac{\partial^2 H}{\partial \xi_i \partial \xi_j} = 0.
 \end{aligned} \tag{16.14}$$

Now let $\rho(\boldsymbol{\xi}, t)$ be a distribution on phase space. Continuity implies

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \dot{\boldsymbol{\xi}}) = 0. \tag{16.15}$$

Invoking $\nabla \cdot \dot{\boldsymbol{\xi}} = 0$, we have that

$$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + \dot{\boldsymbol{\xi}} \cdot \nabla \rho = 0, \tag{16.16}$$

where $D\rho/Dt$ is sometimes called the *convective derivative* – it is the total derivative of the function $\rho(\boldsymbol{\xi}(t), t)$, evaluated at a point $\boldsymbol{\xi}(t)$ in phase space which moves according to the dynamics. This says that the density in the “comoving frame” is locally constant.

16.4 Poincaré Recurrence Theorem

Let g_τ be the ‘ τ -advance mapping’ which evolves points in phase space according to Hamilton’s equations

$$\dot{q}_i = + \frac{\partial H}{\partial p_i} \quad , \quad \dot{p}_i = - \frac{\partial H}{\partial q_i} \quad (16.17)$$

for a time interval $\Delta t = \tau$. Consider a region Ω in phase space. Define $g_\tau^n \Omega$ to be the n^{th} image of Ω under the mapping g_τ . Clearly g_τ is invertible; the inverse is obtained by integrating the equations of motion backward in time. We denote the inverse of g_τ by g_τ^{-1} . By Liouville’s theorem, g_τ is volume preserving when acting on regions in phase space, since the evolution of any given point is Hamiltonian. This follows from the continuity equation for the phase space density,

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\mathbf{u} \varrho) = 0 \quad (16.18)$$

where $\mathbf{u} = \{\dot{\mathbf{q}}, \dot{\mathbf{p}}\}$ is the velocity vector in phase space, and Hamilton’s equations, which say that the phase flow is incompressible, *i.e.* $\nabla \cdot \mathbf{u} = 0$:

$$\begin{aligned} \nabla \cdot \mathbf{u} &= \sum_{i=1}^n \left\{ \frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} \right\} \\ &= \sum_{i=1}^n \left\{ \frac{\partial}{\partial q_i} \left(\frac{\partial H}{\partial p_i} \right) + \frac{\partial}{\partial p_i} \left(- \frac{\partial H}{\partial q_i} \right) \right\} = 0 . \end{aligned} \quad (16.19)$$

Thus, we have that the convective derivative vanishes, *viz.*

$$\frac{D\varrho}{Dt} \equiv \frac{\partial \varrho}{\partial t} + \mathbf{u} \cdot \nabla \varrho = 0 , \quad (16.20)$$

which guarantees that the density remains constant in a frame moving with the flow.

The proof of the recurrence theorem is simple. Assume that g_τ is invertible and volume-preserving, as is the case for Hamiltonian flow. Further assume that phase space volume is finite. Since the energy is preserved in the case of time-independent Hamiltonians, we simply ask that the volume of phase space *at fixed total energy* E be finite, *i.e.*

$$\int d\mu \delta(E - H(\mathbf{q}, \mathbf{p})) < \infty , \quad (16.21)$$

where $d\mu = d\mathbf{q} d\mathbf{p}$ is the phase space uniform integration measure.

Theorem: In any finite neighborhood Ω of phase space there exists a point φ_0 which will return to Ω after n applications of g_τ , where n is finite.

Proof: Assume the theorem fails; we will show this assumption results in a contradiction. Consider the set Υ formed from the union of all sets $g_\tau^m \Omega$ for all m :

$$\Upsilon = \bigcup_{m=0}^{\infty} g_\tau^m \Omega \quad (16.22)$$

We assume that the set $\{g_\tau^m \Omega \mid m \in \mathbb{Z}, m \geq 0\}$ is disjoint. The volume of a union of disjoint sets is the sum of the individual volumes. Thus,

$$\begin{aligned} \text{vol}(\Upsilon) &= \sum_{m=0}^{\infty} \text{vol}(g_\tau^m \Omega) \\ &= \text{vol}(\Omega) \cdot \sum_{m=1}^{\infty} 1 = \infty, \end{aligned} \tag{16.23}$$

since $\text{vol}(g_\tau^m \Omega) = \text{vol}(\Omega)$ from volume preservation. But clearly Υ is a subset of the entire phase space, hence we have a contradiction, because by assumption phase space is of finite volume.

Thus, the assumption that the set $\{g_\tau^m \Omega \mid m \in \mathbb{Z}, m \geq 0\}$ is disjoint fails. This means that there exists some pair of integers k and l , with $k \neq l$, such that $g_\tau^k \Omega \cap g_\tau^l \Omega \neq \emptyset$. Without loss of generality we may assume $k > l$. Apply the inverse g_τ^{-1} to this relation l times to get $g_\tau^{k-l} \Omega \cap \Omega \neq \emptyset$. Now choose any point $\varphi \in g_\tau^n \Omega \cap \Omega$, where $n = k - l$, and define $\varphi_0 = g_\tau^{-n} \varphi$. Then by construction both φ_0 and $g_\tau^n \varphi_0$ lie within Ω and the theorem is proven.

Each of the two central assumptions – invertibility and volume preservation – is crucial. Without either of them, the proof fails. Consider, for example, a volume-preserving map which is not invertible. An example might be a mapping $f: \mathbb{R} \rightarrow \mathbb{R}$ which takes any real number to its fractional part. Thus, $f(\pi) = 0.14159265\dots$. Let us restrict our attention to intervals of width less than unity. Clearly f is then volume preserving. The action of f on the interval $[2, 3)$ is to map it to the interval $[0, 1)$. But $[0, 1)$ remains fixed under the action of f , so no point within the interval $[2, 3)$ will ever return under repeated iterations of f . Thus, f does not exhibit Poincaré recurrence.

Consider next the case of the damped harmonic oscillator. In this case, phase space volumes contract. For a one-dimensional oscillator obeying $\ddot{x} + 2\beta\dot{x} + \Omega_0^2 x = 0$ one has $\nabla \cdot \mathbf{u} = -2\beta < 0$ ($\beta > 0$ for damping). Thus the convective derivative obeys $D_t \varrho = -(\nabla \cdot \mathbf{u})\varrho = +2\beta\varrho$ which says that the density increases exponentially in the comoving frame, as $\varrho(t) = e^{2\beta t} \varrho(0)$. Thus, phase space volumes collapse, and are not preserved by the dynamics. In this case, it is possible for the set Υ to be of finite volume, even if it is the union of an infinite number of sets $g_\tau^n \Omega$, because the volumes of these component sets themselves decrease exponentially, as $\text{vol}(g_\tau^n \Omega) = e^{-2n\beta\tau} \text{vol}(\Omega)$. A damped pendulum, released from rest at some small angle θ_0 , will not return arbitrarily close to these initial conditions.

16.5 Poisson Brackets

The time evolution of any function $F(q, p)$ over phase space is given by

$$\begin{aligned} \frac{d}{dt} F(q(t), p(t), t) &= \frac{\partial F}{\partial t} + \sum_{\sigma=1}^n \left\{ \frac{\partial F}{\partial q_\sigma} \dot{q}_\sigma + \frac{\partial F}{\partial p_\sigma} \dot{p}_\sigma \right\} \\ &\equiv \frac{\partial F}{\partial t} + \{F, H\}, \end{aligned} \tag{16.24}$$

where the *Poisson bracket* $\{\cdot, \cdot\}$ is given by

$$\{A, B\} \equiv \sum_{\sigma=1}^n \left(\frac{\partial A}{\partial q_{\sigma}} \frac{\partial B}{\partial p_{\sigma}} - \frac{\partial A}{\partial p_{\sigma}} \frac{\partial B}{\partial q_{\sigma}} \right) \quad (16.25)$$

$$= \sum_{i,j=1}^{2n} J_{ij} \frac{\partial A}{\partial \xi_i} \frac{\partial B}{\partial \xi_j} . \quad (16.26)$$

Properties of the Poisson bracket:

- Antisymmetry:

$$\{f, g\} = -\{g, f\} . \quad (16.27)$$

- Bilinearity: if λ is a constant, and f , g , and h are functions on phase space, then

$$\{f + \lambda g, h\} = \{f, h\} + \lambda \{g, h\} . \quad (16.28)$$

Linearity in the second argument follows from this and the antisymmetry condition.

- Associativity:

$$\{fg, h\} = f\{g, h\} + g\{f, h\} . \quad (16.29)$$

- Jacobi identity:

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0 . \quad (16.30)$$

Some other useful properties:

- If $\{A, H\} = 0$ and $\frac{\partial A}{\partial t} = 0$, then $\frac{dA}{dt} = 0$, *i.e.* $A(q, p)$ is a constant of the motion.
- If $\{A, H\} = 0$ and $\{B, H\} = 0$, then $\{\{A, B\}, H\} = 0$. If in addition A and B have no explicit time dependence, we conclude that $\{A, B\}$ is a constant of the motion.
- It is easily established that

$$\{q_{\alpha}, q_{\beta}\} = 0 \quad , \quad \{p_{\alpha}, p_{\beta}\} = 0 \quad , \quad \{q_{\alpha}, p_{\beta}\} = \delta_{\alpha\beta} . \quad (16.31)$$

16.6 Canonical Transformations

16.6.1 Point transformations in Lagrangian mechanics

In Lagrangian mechanics, we are free to redefine our generalized coordinates, *viz.*

$$Q_{\sigma} = Q_{\sigma}(q_1, \dots, q_n, t) . \quad (16.32)$$

This is called a “point transformation.” The transformation is invertible if

$$\det\left(\frac{\partial Q_\alpha}{\partial q_\beta}\right) \neq 0 . \quad (16.33)$$

The transformed Lagrangian, \tilde{L} , written as a function of the new coordinates Q and velocities \dot{Q} , is

$$\tilde{L}(Q, \dot{Q}, t) = L(q(Q, t), \dot{q}(Q, \dot{Q}, t)) . \quad (16.34)$$

Finally, Hamilton’s principle,

$$\delta \int_{t_1}^{t_b} dt \tilde{L}(Q, \dot{Q}, t) = 0 \quad (16.35)$$

with $\delta Q_\sigma(t_a) = \delta Q_\sigma(t_b) = 0$, still holds, and the form of the Euler-Lagrange equations remains unchanged:

$$\frac{\partial \tilde{L}}{\partial Q_\sigma} - \frac{d}{dt} \left(\frac{\partial \tilde{L}}{\partial \dot{Q}_\sigma} \right) = 0 . \quad (16.36)$$

The invariance of the equations of motion under a point transformation may be verified explicitly. We first evaluate

$$\frac{d}{dt} \left(\frac{\partial \tilde{L}}{\partial \dot{Q}_\sigma} \right) = \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_\alpha} \frac{\partial \dot{q}_\alpha}{\partial \dot{Q}_\sigma} \right) = \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_\alpha} \frac{\partial q_\alpha}{\partial Q_\sigma} \right) , \quad (16.37)$$

where the relation

$$\frac{\partial \dot{q}_\alpha}{\partial \dot{Q}_\sigma} = \frac{\partial q_\alpha}{\partial Q_\sigma} \quad (16.38)$$

follows from

$$\dot{q}_\alpha = \frac{\partial q_\alpha}{\partial Q_\sigma} \dot{Q}_\sigma + \frac{\partial q_\alpha}{\partial t} . \quad (16.39)$$

Now we compute

$$\begin{aligned} \frac{\partial \tilde{L}}{\partial Q_\sigma} &= \frac{\partial L}{\partial q_\alpha} \frac{\partial q_\alpha}{\partial Q_\sigma} + \frac{\partial L}{\partial \dot{q}_\alpha} \frac{\partial \dot{q}_\alpha}{\partial Q_\sigma} \\ &= \frac{\partial L}{\partial q_\alpha} \frac{\partial q_\alpha}{\partial Q_\sigma} + \frac{\partial L}{\partial \dot{q}_\alpha} \left(\frac{\partial^2 q_\alpha}{\partial Q_\sigma \partial Q_{\sigma'}} \dot{Q}_{\sigma'} + \frac{\partial^2 q_\alpha}{\partial Q_\sigma \partial t} \right) \\ &= \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_\sigma} \right) \frac{\partial q_\alpha}{\partial Q_\sigma} + \frac{\partial L}{\partial \dot{q}_\alpha} \frac{d}{dt} \left(\frac{\partial q_\alpha}{\partial Q_\sigma} \right) \\ &= \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_\sigma} \frac{\partial q_\alpha}{\partial Q_\sigma} \right) = \frac{d}{dt} \left(\frac{\partial \tilde{L}}{\partial \dot{Q}_\sigma} \right) , \end{aligned} \quad (16.40)$$

where the last equality is what we obtained earlier in eqn. 16.37.

16.6.2 Canonical transformations in Hamiltonian mechanics

In Hamiltonian mechanics, we will deal with a much broader class of transformations – ones which mix all the q 's and p 's. The general form for a canonical transformation (CT) is

$$q_\sigma = q_\sigma(Q_1, \dots, Q_n; P_1, \dots, P_n; t) \quad (16.41)$$

$$p_\sigma = p_\sigma(Q_1, \dots, Q_n; P_1, \dots, P_n; t) , \quad (16.42)$$

with $\sigma \in \{1, \dots, n\}$. We may also write

$$\xi_i = \xi_i(\Xi_1, \dots, \Xi_{2n}; t) , \quad (16.43)$$

with $i \in \{1, \dots, 2n\}$. The transformed Hamiltonian is $\tilde{H}(Q, P, t)$.

What sorts of transformations are allowed? Well, if Hamilton's equations are to remain invariant, then

$$\dot{Q}_\sigma = \frac{\partial \tilde{H}}{\partial P_\sigma} , \quad \dot{P}_\sigma = -\frac{\partial \tilde{H}}{\partial Q_\sigma} , \quad (16.44)$$

which gives

$$\frac{\partial \dot{Q}_\sigma}{\partial Q_\sigma} + \frac{\partial \dot{P}_\sigma}{\partial P_\sigma} = 0 = \frac{\partial \dot{\xi}_i}{\partial \Xi_i} . \quad (16.45)$$

I.e. the flow remains incompressible in the new (Q, P) variables. We will also require that phase space volumes are preserved by the transformation, *i.e.*

$$\det \left(\frac{\partial \Xi_i}{\partial \xi_j} \right) = \left\| \frac{\partial(Q, P)}{\partial(q, p)} \right\| = 1 . \quad (16.46)$$

Additional conditions will be discussed below.

16.6.3 Hamiltonian evolution

Hamiltonian evolution itself defines a canonical transformation. Let $\xi_i = \xi_i(t)$ and $\xi'_i = \xi_i(t + dt)$. Then from the dynamics $\dot{\xi}_i = J_{ij} \frac{\partial H}{\partial \xi_j}$, we have

$$\xi_i(t + dt) = \xi_i(t) + J_{ij} \frac{\partial H}{\partial \xi_j} dt + \mathcal{O}(dt^2) . \quad (16.47)$$

Thus,

$$\begin{aligned} \frac{\partial \xi'_i}{\partial \xi_j} &= \frac{\partial}{\partial \xi_j} \left(\xi_i + J_{ik} \frac{\partial H}{\partial \xi_k} dt + \mathcal{O}(dt^2) \right) \\ &= \delta_{ij} + J_{ik} \frac{\partial^2 H}{\partial \xi_j \partial \xi_k} dt + \mathcal{O}(dt^2) . \end{aligned} \quad (16.48)$$

Now, using the result

$$\det(1 + \epsilon M) = 1 + \epsilon \text{Tr } M + \mathcal{O}(\epsilon^2) , \quad (16.49)$$

we have

$$\left\| \frac{\partial \xi'_i}{\partial \xi_j} \right\| = 1 + J_{jk} \frac{\partial^2 H}{\partial \xi_j \partial \xi_k} dt + \mathcal{O}(dt^2) \quad (16.50)$$

$$= 1 + \mathcal{O}(dt^2) . \quad (16.51)$$

16.6.4 Symplectic structure

We have that

$$\dot{\xi}_i = J_{ij} \frac{\partial H}{\partial \xi_j} . \quad (16.52)$$

Suppose we make a time-independent canonical transformation to new phase space coordinates, $\Xi_a = \Xi_a(\xi)$. We then have

$$\dot{\Xi}_a = \frac{\partial \Xi_a}{\partial \xi_j} \dot{\xi}_j = \frac{\partial \Xi_a}{\partial \xi_j} J_{jk} \frac{\partial H}{\partial \xi_k} . \quad (16.53)$$

But if the transformation is canonical, then the equations of motion are preserved, and we also have

$$\dot{\Xi}_a = J_{ab} \frac{\partial \tilde{H}}{\partial \Xi_b} = J_{ab} \frac{\partial \xi_k}{\partial \Xi_b} \frac{\partial H}{\partial \xi_k} . \quad (16.54)$$

Equating these two expressions, we have

$$M_{aj} J_{jk} \frac{\partial H}{\partial \xi_k} = J_{ab} M_{kb}^{-1} \frac{\partial H}{\partial \xi_k} , \quad (16.55)$$

where

$$M_{aj} \equiv \frac{\partial \Xi_a}{\partial \xi_j} \quad (16.56)$$

is the Jacobian of the transformation. Since the equality must hold for all ξ , we conclude

$$MJ = J(M^t)^{-1} \implies MJM^t = J . \quad (16.57)$$

A matrix M satisfying $MM^t = \mathbb{I}$ is of course an *orthogonal* matrix. A matrix M satisfying $MJM^t = J$ is called *symplectic*. We write $M \in \text{Sp}(2n)$, *i.e.* M is an element of the group of *symplectic matrices*¹ of rank $2n$.

The symplectic property of M guarantees that the Poisson brackets are preserved under a

¹Note that the rank of a symplectic matrix is always even. Note also $MJM^t = J$ implies $M^tJM = J$.

canonical transformation:

$$\begin{aligned}
\{A, B\}_\xi &= J_{ij} \frac{\partial A}{\partial \xi_i} \frac{\partial B}{\partial \xi_j} \\
&= J_{ij} \frac{\partial A}{\partial \Xi_a} \frac{\partial \Xi_a}{\partial \xi_i} \frac{\partial B}{\partial \Xi_b} \frac{\partial \Xi_b}{\partial \xi_j} \\
&= (M_{ai} J_{ij} M_{jb}^t) \frac{\partial A}{\partial \Xi_a} \frac{\partial B}{\partial \Xi_b} \\
&= J_{ab} \frac{\partial A}{\partial \Xi_a} \frac{\partial B}{\partial \Xi_b} \\
&= \{A, B\}_\Xi .
\end{aligned} \tag{16.58}$$

16.6.5 Generating functions for canonical transformations

For a transformation to be canonical, we require

$$\delta \int_{t_a}^{t_b} dt \left\{ p_\sigma \dot{q}_\sigma - H(q, p, t) \right\} = 0 = \delta \int_{t_a}^{t_b} dt \left\{ P_\sigma \dot{Q}_\sigma - \tilde{H}(Q, P, t) \right\} . \tag{16.59}$$

This is satisfied provided

$$\left\{ p_\sigma \dot{q}_\sigma - H(q, p, t) \right\} = \lambda \left\{ P_\sigma \dot{Q}_\sigma - \tilde{H}(Q, P, t) + \frac{dF}{dt} \right\} , \tag{16.60}$$

where λ is a constant. For canonical transformations, $\lambda = 1$.² Thus,

$$\begin{aligned}
\tilde{H}(Q, P, t) &= H(q, p, t) + P_\sigma \dot{Q}_\sigma - p_\sigma \dot{q}_\sigma + \frac{\partial F}{\partial q_\sigma} \dot{q}_\sigma + \frac{\partial F}{\partial Q_\sigma} \dot{Q}_\sigma \\
&\quad + \frac{\partial F}{\partial p_\sigma} \dot{p}_\sigma + \frac{\partial F}{\partial P_\sigma} \dot{P}_\sigma + \frac{\partial F}{\partial t} .
\end{aligned} \tag{16.61}$$

Thus, we require

$$\frac{\partial F}{\partial q_\sigma} = p_\sigma \quad , \quad \frac{\partial F}{\partial Q_\sigma} = -P_\sigma \quad , \quad \frac{\partial F}{\partial p_\sigma} = 0 \quad , \quad \frac{\partial F}{\partial P_\sigma} = 0 . \tag{16.62}$$

The transformed Hamiltonian is

$$\tilde{H}(Q, P, t) = H(q, p, t) + \frac{\partial F}{\partial t} . \tag{16.63}$$

²Solutions of eqn. 16.60 with $\lambda \neq 1$ are known as *extended* canonical transformations. We can always rescale coordinates and/or momenta to achieve $\lambda = 1$.

There are four possibilities, corresponding to the freedom to make Legendre transformations with respect to each of the arguments of $F(q, Q)$:

$$F(q, Q, t) = \begin{cases} F_1(q, Q, t) & ; \quad p_\sigma = +\frac{\partial F_1}{\partial q_\sigma} \quad , \quad P_\sigma = -\frac{\partial F_1}{\partial Q_\sigma} \quad (\text{type I}) \\ F_2(q, P, t) - P_\sigma Q_\sigma & ; \quad p_\sigma = +\frac{\partial F_2}{\partial q_\sigma} \quad , \quad Q_\sigma = +\frac{\partial F_2}{\partial P_\sigma} \quad (\text{type II}) \\ F_3(p, Q, t) + p_\sigma q_\sigma & ; \quad q_\sigma = -\frac{\partial F_3}{\partial p_\sigma} \quad , \quad P_\sigma = -\frac{\partial F_3}{\partial Q_\sigma} \quad (\text{type III}) \\ F_4(p, P, t) + p_\sigma q_\sigma - P_\sigma Q_\sigma & ; \quad q_\sigma = -\frac{\partial F_4}{\partial p_\sigma} \quad , \quad Q_\sigma = +\frac{\partial F_4}{\partial P_\sigma} \quad (\text{type IV}) \end{cases}$$

In each case ($\gamma = 1, 2, 3, 4$), we have

$$\tilde{H}(Q, P, t) = H(q, p, t) + \frac{\partial F_\gamma}{\partial t} . \quad (16.64)$$

Let's work out some examples:

- Consider the type-II transformation generated by

$$F_2(q, P) = A_\sigma(q) P_\sigma , \quad (16.65)$$

where $A_\sigma(q)$ is an arbitrary function of the $\{q_\sigma\}$. We then have

$$Q_\sigma = \frac{\partial F_2}{\partial P_\sigma} = A_\sigma(q) \quad , \quad p_\sigma = \frac{\partial F_2}{\partial q_\sigma} = \frac{\partial A_\alpha}{\partial q_\sigma} P_\alpha . \quad (16.66)$$

Thus,

$$Q_\sigma = A_\sigma(q) \quad , \quad P_\sigma = \frac{\partial q_\alpha}{\partial Q_\sigma} p_\alpha . \quad (16.67)$$

This is a general point transformation of the kind discussed in eqn. 16.32. For a general linear point transformation, $Q_\alpha = M_{\alpha\beta} q_\beta$, we have $P_\alpha = p_\beta M_{\beta\alpha}^{-1}$, *i.e.* $Q = Mq$, $P = p M^{-1}$. If $M_{\alpha\beta} = \delta_{\alpha\beta}$, this is the identity transformation. $F_2 = q_1 P_3 + q_3 P_1$ interchanges labels 1 and 3, *etc.*

- Consider the type-I transformation generated by

$$F_1(q, Q) = A_\sigma(q) Q_\sigma . \quad (16.68)$$

We then have

$$p_\sigma = \frac{\partial F_1}{\partial q_\sigma} = \frac{\partial A_\alpha}{\partial q_\sigma} Q_\alpha \quad (16.69)$$

$$P_\sigma = -\frac{\partial F_1}{\partial Q_\sigma} = -A_\sigma(q) . \quad (16.70)$$

Note that $A_\sigma(q) = q_\sigma$ generates the transformation

$$\begin{pmatrix} q \\ p \end{pmatrix} \longrightarrow \begin{pmatrix} -P \\ +Q \end{pmatrix} . \quad (16.71)$$

- A mixed transformation is also permitted. For example,

$$F(q, Q) = q_1 Q_1 + (q_3 - Q_2) P_2 + (q_2 - Q_3) P_3 \quad (16.72)$$

is of type-I with respect to index $\sigma = 1$ and type-II with respect to indices $\sigma = 2, 3$. The transformation effected is

$$Q_1 = p_1 \quad Q_2 = q_3 \quad Q_3 = q_2 \quad (16.73)$$

$$P_1 = -q_1 \quad P_2 = p_3 \quad P_3 = p_2 . \quad (16.74)$$

- Consider the harmonic oscillator,

$$H(q, p) = \frac{p^2}{2m} + \frac{1}{2}kq^2 . \quad (16.75)$$

If we could find a time-independent canonical transformation such that

$$p = \sqrt{2mf(P)} \cos Q \quad , \quad q = \sqrt{\frac{2f(P)}{k}} \sin Q , \quad (16.76)$$

where $f(P)$ is some function of P , then we'd have $\tilde{H}(Q, P) = f(P)$, which is cyclic in Q . To find this transformation, we take the ratio of p and q to obtain

$$p = \sqrt{mk} q \operatorname{ctn} Q , \quad (16.77)$$

which suggests the type-I transformation

$$F_1(q, Q) = \frac{1}{2}\sqrt{mk} q^2 \operatorname{ctn} Q . \quad (16.78)$$

This leads to

$$p = \frac{\partial F_1}{\partial q} = \sqrt{mk} q \operatorname{ctn} Q \quad , \quad P = -\frac{\partial F_1}{\partial Q} = \frac{\sqrt{mk} q^2}{2 \sin^2 Q} . \quad (16.79)$$

Thus,

$$q = \frac{\sqrt{2P}}{\sqrt[4]{mk}} \sin Q \quad \implies \quad f(P) = \sqrt{\frac{k}{m}} P = \omega P , \quad (16.80)$$

where $\omega = \sqrt{k/m}$ is the oscillation frequency. We therefore have

$$\tilde{H}(Q, P) = \omega P , \quad (16.81)$$

whence $P = E/\omega$. The equations of motion are

$$\dot{P} = -\frac{\partial \tilde{H}}{\partial Q} = 0 \quad , \quad \dot{Q} = \frac{\partial \tilde{H}}{\partial P} = \omega , \quad (16.82)$$

which yields

$$Q(t) = \omega t + \varphi_0 \quad , \quad q(t) = \sqrt{\frac{2E}{m\omega^2}} \sin(\omega t + \varphi_0) . \quad (16.83)$$

16.7 Hamilton-Jacobi Theory

We've stressed the great freedom involved in making canonical transformations. Coordinates and momenta, for example, may be interchanged – the distinction between them is purely a matter of convention! We now ask: is there any specially preferred canonical transformation? In this regard, one obvious goal is to make the Hamiltonian $\tilde{H}(Q, P, t)$ and the corresponding equations of motion as simple as possible.

Recall the general form of the canonical transformation:

$$\tilde{H}(Q, P) = H(q, p) + \frac{\partial F}{\partial t} , \quad (16.84)$$

with

$$\frac{\partial F}{\partial q_\sigma} = p_\sigma \quad \frac{\partial F}{\partial p_\sigma} = 0 \quad (16.85)$$

$$\frac{\partial F}{\partial Q_\sigma} = -P_\sigma \quad \frac{\partial F}{\partial P_\sigma} = 0 . \quad (16.86)$$

We now demand that this transformation result in the simplest Hamiltonian possible, that is, $\tilde{H}(Q, P, t) = 0$. This requires we find a function F such that

$$\frac{\partial F}{\partial t} = -H \quad , \quad \frac{\partial F}{\partial q_\sigma} = p_\sigma . \quad (16.87)$$

The remaining functional dependence may be taken to be either on Q (type I) or on P (type II). As it turns out, the generating function F we seek is in fact the action, S , which is the integral of L with respect to time, expressed as a function of its endpoint values.

16.7.1 The action as a function of coordinates and time

We have seen how the action $S[\eta(\tau)]$ is a *functional* of the path $\eta(\tau)$ and a *function* of the endpoint values $\{q_a, t_a\}$ and $\{q_b, t_b\}$. Let us define the action *function* $S(q, t)$ as

$$S(q, t) = \int_{t_a}^t d\tau L(\eta, \dot{\eta}, \tau) , \quad (16.88)$$

where $\eta(\tau)$ starts at (q_a, t_a) and ends at (q, t) . We also require that $\eta(\tau)$ satisfy the Euler-Lagrange equations,

$$\frac{\partial L}{\partial \eta_\sigma} - \frac{d}{d\tau} \left(\frac{\partial L}{\partial \dot{\eta}_\sigma} \right) = 0 \quad (16.89)$$

Let us now consider a new path, $\tilde{\eta}(\tau)$, also starting at (q_a, t_a) , but ending at $(q + dq, t + dt)$,

and also satisfying the equations of motion. The differential of S is

$$\begin{aligned} dS &= S[\tilde{\eta}(\tau)] - S[\eta(\tau)] \\ &= \int_{t_a}^{t+dt} d\tau L(\tilde{\eta}, \dot{\tilde{\eta}}, \tau) - \int_{t_a}^t d\tau L(\eta, \dot{\eta}, \tau) \end{aligned} \quad (16.90)$$

$$\begin{aligned} &= \int_{t_a}^t d\tau \left\{ \frac{\partial L}{\partial \eta_\sigma} [\tilde{\eta}_\sigma(\tau) - \eta_\sigma(\tau)] + \frac{\partial L}{\partial \dot{\eta}_\sigma} [\dot{\tilde{\eta}}_\sigma(\tau) - \dot{\eta}_\sigma(\tau)] \right\} + L(\tilde{\eta}(t), \dot{\tilde{\eta}}(t), t) dt \\ &= \int_{t_a}^t d\tau \left\{ \frac{\partial L}{\partial \eta_\sigma} - \frac{d}{d\tau} \left(\frac{\partial L}{\partial \dot{\eta}_\sigma} \right) \right\} [\tilde{\eta}_\sigma(\tau) - \eta_\sigma(\tau)] \\ &\quad + \left. \frac{\partial L}{\partial \dot{\eta}_\sigma} \right|_t [\tilde{\eta}_\sigma(t) - \eta_\sigma(t)] + L(\tilde{\eta}(t), \dot{\tilde{\eta}}(t), t) dt \\ &= 0 + \pi_\sigma(t) \delta\eta_\sigma(t) + L(\eta(t), \dot{\eta}(t), t) dt + \mathcal{O}(\delta q \cdot dt) , \end{aligned} \quad (16.91)$$

where we have defined

$$\pi_\sigma = \frac{\partial L}{\partial \dot{\eta}_\sigma} , \quad (16.92)$$

and

$$\delta\eta_\sigma(\tau) \equiv \tilde{\eta}_\sigma(\tau) - \eta_\sigma(\tau) . \quad (16.93)$$

Note that the differential dq_σ is given by

$$dq_\sigma = \tilde{\eta}_\sigma(t + dt) - \eta_\sigma(t) \quad (16.94)$$

$$\begin{aligned} &= \tilde{\eta}_\sigma(t + dt) - \tilde{\eta}_\sigma(t) + \tilde{\eta}_\sigma(t) - \eta_\sigma(t) \\ &= \dot{\tilde{\eta}}_\sigma(t) dt + \delta\eta_\sigma(t) \\ &= \dot{q}_\sigma(t) dt + \delta\eta_\sigma(t) + \mathcal{O}(\delta q \cdot dt) . \end{aligned} \quad (16.95)$$

Thus, with $\pi_\sigma(t) \equiv p_\sigma$, we have

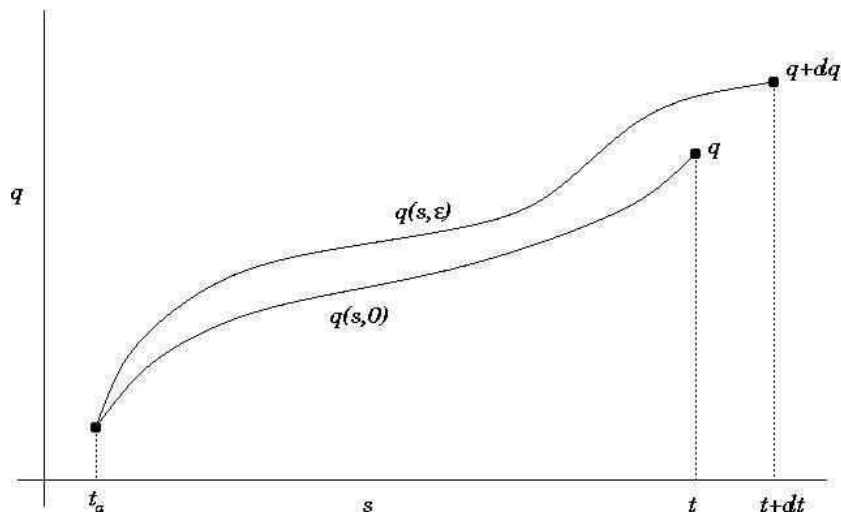
$$\begin{aligned} dS &= p_\sigma dq_\sigma + (L - p_\sigma \dot{q}_\sigma) dt \\ &= p_\sigma dq_\sigma - H dt . \end{aligned} \quad (16.96)$$

We therefore obtain

$$\frac{\partial S}{\partial q_\sigma} = p_\sigma \quad , \quad \frac{\partial S}{\partial t} = -H \quad , \quad \frac{dS}{dt} = L . \quad (16.97)$$

What about the lower limit at t_a ? Clearly there are $n + 1$ constants associated with this limit: $\{q_1(t_a), \dots, q_n(t_a); t_a\}$. Thus, we may write

$$S = S(q_1, \dots, q_n; \Lambda_1, \dots, \Lambda_n, t) + \Lambda_{n+1} , \quad (16.98)$$

Figure 16.1: A one-parameter family of paths $q(s; \epsilon)$.

where our $n + 1$ constants are $\{\Lambda_1, \dots, \Lambda_{n+1}\}$. If we regard S as a mixed generator, which is type-I in some variables and type-II in others, then each Λ_σ for $1 \leq \sigma \leq n$ may be chosen to be either Q_σ or P_σ . We will define

$$\Gamma_\sigma = \frac{\partial S}{\partial \Lambda_\sigma} = \begin{cases} +Q_\sigma & \text{if } \Lambda_\sigma = P_\sigma \\ -P_\sigma & \text{if } \Lambda_\sigma = Q_\sigma \end{cases} \quad (16.99)$$

For each σ , the two possibilities $\Lambda_\sigma = Q_\sigma$ or $\Lambda_\sigma = P_\sigma$ are of course rendered equivalent by a canonical transformation $(Q_\sigma, P_\sigma) \rightarrow (P_\sigma, -Q_\sigma)$.

16.7.2 The Hamilton-Jacobi equation

Since the action $S(q, \Lambda, t)$ has been shown to generate a canonical transformation for which $\tilde{H}(Q, P) = 0$. This requirement may be written as

$$H\left(q_1, \dots, q_n, \frac{\partial S}{\partial q_1}, \dots, \frac{\partial S}{\partial q_n}, t\right) + \frac{\partial S}{\partial t} = 0. \quad (16.100)$$

This is the *Hamilton-Jacobi equation* (HJE). It is a first order partial differential equation in $n + 1$ variables, and in general is nonlinear (since kinetic energy is generally a quadratic function of momenta). Since $\tilde{H}(Q, P, t) = 0$, the equations of motion are trivial, and

$$Q_\sigma(t) = \text{const.} \quad , \quad P_\sigma(t) = \text{const.} \quad (16.101)$$

Once the HJE is solved, one must invert the relations $\Gamma_\sigma = \partial S(q, \Lambda, t)/\partial \Lambda_\sigma$ to obtain $q(Q, P, t)$. This is possible only if

$$\det\left(\frac{\partial^2 S}{\partial q_\alpha \partial \Lambda_\beta}\right) \neq 0, \quad (16.102)$$

which is known as the *Hessian condition*.

It is worth noting that the HJE may have several solutions. For example, consider the case of the free particle, with $H(q, p) = p^2/2m$. The HJE is

$$\frac{1}{2m} \left(\frac{\partial S}{\partial q} \right)^2 + \frac{\partial S}{\partial t} = 0. \quad (16.103)$$

One solution of the HJE is

$$S(q, \Lambda, t) = \frac{m(q - \Lambda)^2}{2t}. \quad (16.104)$$

For this we find

$$\Gamma = \frac{\partial S}{\partial \Lambda} = -\frac{m}{t}(q - \Lambda) \quad \Rightarrow \quad q(t) = \Lambda - \frac{\Gamma}{m} t. \quad (16.105)$$

Here $\Lambda = q(0)$ is the initial value of q , and $\Gamma = -p$ is minus the momentum.

Another equally valid solution to the HJE is

$$S(q, \Lambda, t) = q\sqrt{2m\Lambda} - \Lambda t. \quad (16.106)$$

This yields

$$\Gamma = \frac{\partial S}{\partial \Lambda} = q\sqrt{\frac{2m}{\Lambda}} - t \quad \Rightarrow \quad q(t) = \sqrt{\frac{\Lambda}{2m}}(t + \Gamma). \quad (16.107)$$

For this solution, Λ is the energy and Γ may be related to the initial value of $q(t) = \Gamma\sqrt{\Lambda/2m}$.

16.7.3 Time-independent Hamiltonians

When H has no explicit time dependence, we may reduce the order of the HJE by one, writing

$$S(q, \Lambda, t) = W(q, \Lambda) + T(\Lambda, t). \quad (16.108)$$

The HJE becomes

$$H\left(q, \frac{\partial W}{\partial q}\right) = -\frac{\partial T}{\partial t}. \quad (16.109)$$

Note that the LHS of the above equation is independent of t , and the RHS is independent of q . Therefore, each side must only depend on the constants Λ , which is to say that each side must be a constant, which, without loss of generality, we take to be Λ_1 . Therefore

$$S(q, \Lambda, t) = W(q, \Lambda) - \Lambda_1 t. \quad (16.110)$$

The function $W(q, \Lambda)$ is called *Hamilton's characteristic function*. The HJE now takes the form

$$H\left(q_1, \dots, q_n, \frac{\partial W}{\partial q_1}, \dots, \frac{\partial W}{\partial q_n}\right) = \Lambda_1. \quad (16.111)$$

Note that adding an arbitrary constant C to S generates the same equation, and simply shifts the last constant $\Lambda_{n+1} \rightarrow \Lambda_{n+1} + C$. This is equivalent to replacing t by $t - t_0$ with $t_0 = C/\Lambda_1$, *i.e.* it just redefines the zero of the time variable.

16.7.4 Example: one-dimensional motion

As an example of the method, consider the one-dimensional system,

$$H(q, p) = \frac{p^2}{2m} + U(q) . \quad (16.112)$$

The HJE is

$$\frac{1}{2m} \left(\frac{\partial S}{\partial q} \right)^2 + U(q) = \Lambda . \quad (16.113)$$

which may be recast as

$$\frac{\partial S}{\partial q} = \sqrt{2m[\Lambda - U(q)]} , \quad (16.114)$$

with solution

$$S(q, \Lambda, t) = \sqrt{2m} \int^q dq' \sqrt{\Lambda - U(q')} - \Lambda t . \quad (16.115)$$

We now have

$$p = \frac{\partial S}{\partial q} = \sqrt{2m[\Lambda - U(q)]} , \quad (16.116)$$

as well as

$$\Gamma = \frac{\partial S}{\partial \Lambda} = \sqrt{\frac{m}{2}} \int^{q(t)} \frac{dq'}{\sqrt{\Lambda - U(q')}} - t . \quad (16.117)$$

Thus, the motion $q(t)$ is given by quadrature:

$$\Gamma + t = \sqrt{\frac{m}{2}} \int^{\sqrt{\Lambda - U(q(t))}} \frac{dq'}{\sqrt{\Lambda - U(q')}} , \quad (16.118)$$

where Λ and Γ are constants. The lower limit on the integral is arbitrary and merely shifts t by another constant. Note that Λ is the total energy.

16.7.5 Separation of variables

It is convenient to first work an example before discussing the general theory. Consider the following Hamiltonian, written in spherical polar coordinates:

$$H = \frac{1}{2m} \left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2 \theta} \right) + \overbrace{A(r) + \frac{B(\theta)}{r^2} + \frac{C(\phi)}{r^2 \sin^2 \theta}}^{\text{potential } U(r, \theta, \phi)} . \quad (16.119)$$

We seek a solution with the characteristic function

$$W(r, \theta, \phi) = W_r(r) + W_\theta(\theta) + W_\phi(\phi) . \quad (16.120)$$

The HJE is then

$$\begin{aligned} \frac{1}{2m} \left(\frac{\partial W_r}{\partial r} \right)^2 + \frac{1}{2mr^2} \left(\frac{\partial W_\theta}{\partial \theta} \right)^2 + \frac{1}{2mr^2 \sin^2 \theta} \left(\frac{\partial W_\phi}{\partial \phi} \right)^2 \\ + A(r) + \frac{B(\theta)}{r^2} + \frac{C(\phi)}{r^2 \sin^2 \theta} = \Lambda_1 = E . \end{aligned} \quad (16.121)$$

Multiply through by $r^2 \sin^2 \theta$ to obtain

$$\begin{aligned} \frac{1}{2m} \left(\frac{\partial W_\phi}{\partial \phi} \right)^2 + C(\phi) = -\sin^2 \theta \left\{ \frac{1}{2m} \left(\frac{\partial W_\theta}{\partial \theta} \right)^2 + B(\theta) \right\} \\ - r^2 \sin^2 \theta \left\{ \frac{1}{2m} \left(\frac{\partial W_r}{\partial r} \right)^2 + A(r) - \Lambda_1 \right\} . \end{aligned} \quad (16.122)$$

The LHS is independent of (r, θ) , and the RHS is independent of ϕ . Therefore, we may set

$$\frac{1}{2m} \left(\frac{\partial W_\phi}{\partial \phi} \right)^2 + C(\phi) = \Lambda_2 . \quad (16.123)$$

Proceeding, we replace the LHS in eqn. 16.122 with Λ_2 , arriving at

$$\frac{1}{2m} \left(\frac{\partial W_\theta}{\partial \theta} \right)^2 + B(\theta) + \frac{\Lambda_2}{\sin^2 \theta} = -r^2 \left\{ \frac{1}{2m} \left(\frac{\partial W_r}{\partial r} \right)^2 + A(r) - \Lambda_1 \right\} . \quad (16.124)$$

The LHS of this equation is independent of r , and the RHS is independent of θ . Therefore,

$$\frac{1}{2m} \left(\frac{\partial W_\theta}{\partial \theta} \right)^2 + B(\theta) + \frac{\Lambda_2}{\sin^2 \theta} = \Lambda_3 . \quad (16.125)$$

We're left with

$$\frac{1}{2m} \left(\frac{\partial W_r}{\partial r} \right)^2 + A(r) + \frac{\Lambda_3}{r^2} = \Lambda_1 . \quad (16.126)$$

The full solution is therefore

$$S(q, \Lambda, t) = \sqrt{2m} \int^r dr' \sqrt{\Lambda_1 - A(r') - \frac{\Lambda_3}{r'^2}} \quad (16.127)$$

$$\begin{aligned} + \sqrt{2m} \int^\theta d\theta' \sqrt{\Lambda_3 - B(\theta') - \frac{\Lambda_2}{\sin^2 \theta'}} \\ + \sqrt{2m} \int^\phi d\phi' \sqrt{\Lambda_2 - C(\phi')} - \Lambda_1 t . \end{aligned} \quad (16.128)$$

We then have

$$\Gamma_1 = \frac{\partial S}{\partial \Lambda_1} = \int \frac{\sqrt{\frac{m}{2}} dr'}{\sqrt{\Lambda_1 - A(r') - \Lambda_3 r'^{-2}}} - t \quad (16.129)$$

$$\Gamma_2 = \frac{\partial S}{\partial \Lambda_2} = - \int \frac{\sqrt{\frac{m}{2}} d\theta'}{\sin^2 \theta' \sqrt{\Lambda_3 - B(\theta') - \Lambda_2 \csc^2 \theta'}} + \int \frac{\sqrt{\frac{m}{2}} d\phi'}{\sqrt{\Lambda_2 - C(\phi')}} \quad (16.130)$$

$$\Gamma_3 = \frac{\partial S}{\partial \Lambda_3} = - \int \frac{\sqrt{\frac{m}{2}} dr'}{r'^2 \sqrt{\Lambda_1 - A(r') - \Lambda_3 r'^{-2}}} + \int \frac{\sqrt{\frac{m}{2}} d\theta'}{\sqrt{\Lambda_3 - B(\theta') - \Lambda_2 \csc^2 \theta'}} . \quad (16.131)$$

The game plan here is as follows. The first of the above trio of equations is inverted to yield $r(t)$ in terms of t and constants. This solution is then invoked in the last equation (the upper limit on the first integral on the RHS) in order to obtain an implicit equation for $\theta(t)$, which is invoked in the second equation to yield an implicit equation for $\phi(t)$. The net result is the motion of the system in terms of time t and the six constants $(\Lambda_1, \Lambda_2, \Lambda_3, \Gamma_1, \Gamma_2, \Gamma_3)$. A seventh constant, associated with an overall shift of the zero of t , arises due to the arbitrary lower limits of the integrals.

In general, the separation of variables method begins with³

$$W(q, \Lambda) = \sum_{\sigma=1}^n W_{\sigma}(q_{\sigma}, \Lambda) . \quad (16.132)$$

Each $W_{\sigma}(q_{\sigma}, \Lambda)$ may be regarded as a function of the single variable q_{σ} , and is obtained by satisfying an ODE of the form⁴

$$H_{\sigma} \left(q_{\sigma}, \frac{dW_{\sigma}}{dq_{\sigma}} \right) = \Lambda_{\sigma} . \quad (16.133)$$

We then have

$$p_{\sigma} = \frac{\partial W_{\sigma}}{\partial q_{\sigma}} \quad , \quad \Gamma_{\sigma} = \frac{\partial W}{\partial \Lambda_{\sigma}} + \delta_{\sigma,1} t . \quad (16.134)$$

Note that while each W_{σ} depends on only a single q_{σ} , it may depend on several of the Λ_{σ} .

16.7.6 Example #2 : point charge plus electric field

Consider a potential of the form

$$U(r) = \frac{k}{r} - Fz , \quad (16.135)$$

which corresponds to a charge in the presence of an external point charge plus an external electric field. This problem is amenable to separation in parabolic coordinates, (ξ, η, φ) :

$$x = \sqrt{\xi\eta} \cos \varphi \quad , \quad y = \sqrt{\xi\eta} \sin \varphi \quad , \quad z = \frac{1}{2}(\xi - \eta) . \quad (16.136)$$

³Here we assume *complete separability*. A given system may only be *partially* separable.

⁴ $H_{\sigma}(q_{\sigma}, p_{\sigma})$ may also depend on several of the Λ_{α} . See *e.g.* eqn. 16.126, which is of the form $H_r(r, \partial_r W_r, \Lambda_3) = \Lambda_1$.

Note that

$$\rho \equiv \sqrt{x^2 + y^2} = \sqrt{\xi\eta} \quad (16.137)$$

$$r = \sqrt{\rho^2 + z^2} = \frac{1}{2}(\xi + \eta) . \quad (16.138)$$

The kinetic energy is

$$\begin{aligned} T &= \frac{1}{2}m(\dot{\rho}^2 + \rho^2 \dot{\varphi}^2 + \dot{z}^2) \\ &= \frac{1}{8}m(\xi + \eta) \left(\frac{\dot{\xi}^2}{\xi} + \frac{\dot{\eta}^2}{\eta} \right) + \frac{1}{2}m\xi\eta\dot{\varphi}^2 , \end{aligned} \quad (16.139)$$

and hence the Lagrangian is

$$L = \frac{1}{8}m(\xi + \eta) \left(\frac{\dot{\xi}^2}{\xi} + \frac{\dot{\eta}^2}{\eta} \right) + \frac{1}{2}m\xi\eta\dot{\varphi}^2 - \frac{2k}{\xi + \eta} + \frac{1}{2}F(\xi - \eta) . \quad (16.140)$$

Thus, the conjugate momenta are

$$p_\xi = \frac{\partial L}{\partial \dot{\xi}} = \frac{1}{4}m(\xi + \eta) \frac{\dot{\xi}}{\xi} \quad (16.141)$$

$$p_\eta = \frac{\partial L}{\partial \dot{\eta}} = \frac{1}{4}m(\xi + \eta) \frac{\dot{\eta}}{\eta} \quad (16.142)$$

$$p_\varphi = \frac{\partial L}{\partial \dot{\varphi}} = m\xi\eta\dot{\varphi} , \quad (16.143)$$

and the Hamiltonian is

$$H = p_\xi \dot{\xi} + p_\eta \dot{\eta} + p_\varphi \dot{\varphi} \quad (16.144)$$

$$= \frac{2}{m} \left(\frac{\xi p_\xi^2 + \eta p_\eta^2}{\xi + \eta} \right) + \frac{p_\varphi^2}{2m\xi\eta} + \frac{2k}{\xi + \eta} - \frac{1}{2}F(\xi - \eta) . \quad (16.145)$$

Notice that $\partial H/\partial t = 0$, which means $dH/dt = 0$, *i.e.* $H = E \equiv \Lambda_1$ is a constant of the motion. Also, φ is cyclic in H , so its conjugate momentum p_φ is a constant of the motion.

We write

$$S(q, \Lambda) = W(q, \Lambda) - Et \quad (16.146)$$

$$= W_\xi(\xi, \Lambda) + W_\eta(\eta, \Lambda) + W_\varphi(\varphi, \Lambda) - Et . \quad (16.147)$$

with $E = \Lambda_1$. Clearly we may take

$$W_\varphi(\varphi, \Lambda) = P_\varphi \varphi , \quad (16.148)$$

where $P_\varphi = A_2$. Multiplying the Hamilton-Jacobi equation by $\frac{1}{2}m(\xi + \eta)$ then gives

$$\begin{aligned} \xi \left(\frac{dW_\xi}{d\xi} \right)^2 + \frac{P_\varphi^2}{4\xi} + mk - \frac{1}{4}F\xi^2 - \frac{1}{2}mE\xi \\ = -\eta \left(\frac{dW_\eta}{d\eta} \right)^2 - \frac{P_\varphi^2}{4\eta} - \frac{1}{4}F\eta^2 + \frac{1}{2}mE\eta \equiv \mathcal{Y} , \end{aligned} \quad (16.149)$$

where $\mathcal{Y} = A_3$ is the third constant: $\Lambda = (E, P_\varphi, \mathcal{Y})$. Thus,

$$\begin{aligned} S(\underbrace{\xi, \eta, \varphi}_q; \underbrace{E, P_\varphi, \mathcal{Y}}_\Lambda) &= \int^\xi d\xi' \sqrt{\frac{1}{2}mE + \frac{\mathcal{Y} - mk}{\xi'} + \frac{1}{4}mF\xi' - \frac{P_\varphi^2}{4\xi'^2}} \\ &\quad + \int^\eta d\eta' \sqrt{\frac{1}{2}mE - \frac{\mathcal{Y}}{\eta'} - \frac{1}{4}mF\eta' - \frac{P_\varphi^2}{4\eta'^2}} \\ &\quad + P_\varphi \varphi - Et . \end{aligned} \quad (16.150)$$

16.7.7 Example #3 : Charged Particle in a Magnetic Field

The Hamiltonian is

$$H = \frac{1}{2m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 . \quad (16.151)$$

We choose the gauge $\mathbf{A} = Bx\hat{y}$, and we write

$$S(x, y, P_1, P_2) = W_x(x, P_1, P_2) + W_y(y, P_1, P_2) - P_1 t . \quad (16.152)$$

Note that here we will consider S to be a function of $\{q_\sigma\}$ and $\{P_\sigma\}$.

The Hamilton-Jacobi equation is then

$$\left(\frac{\partial W_x}{\partial x} \right)^2 + \left(\frac{\partial W_y}{\partial y} - \frac{eBx}{c} \right)^2 = 2mP_1 . \quad (16.153)$$

We solve by writing

$$W_y = P_2 y \quad \Rightarrow \quad \left(\frac{dW_x}{dx} \right)^2 + \left(P_2 - \frac{eBx}{c} \right)^2 = 2mP_1 . \quad (16.154)$$

This equation suggests the substitution

$$x = \frac{cP_2}{eB} + \frac{c}{eB} \sqrt{2mP_1} \sin \theta . \quad (16.155)$$

in which case

$$\frac{\partial x}{\partial \theta} = \frac{c}{eB} \sqrt{2mP_1} \cos \theta \quad (16.156)$$

and

$$\frac{\partial W_x}{\partial x} = \frac{\partial W_x}{\partial \theta} \cdot \frac{\partial \theta}{\partial x} = \frac{eB}{c\sqrt{2mP_1}} \frac{1}{\cos \theta} \frac{\partial W_x}{\partial \theta} . \quad (16.157)$$

Substitution this into eqn. 16.154, we have

$$\frac{\partial W_x}{\partial \theta} = \frac{2mcP_1}{eB} \cos^2 \theta , \quad (16.158)$$

with solution

$$W_x = \frac{mcP_1}{eB} \theta + \frac{mcP_1}{2eB} \sin(2\theta) . \quad (16.159)$$

We then have

$$p_x = \frac{\partial W_x}{\partial x} = \frac{\partial W_x}{\partial \theta} \frac{\partial \theta}{\partial x} = \sqrt{2mP_1} \cos \theta \quad (16.160)$$

and

$$p_y = \frac{\partial W_y}{\partial y} = P_2 . \quad (16.161)$$

The type-II generator we seek is then

$$S(q, P, t) = \frac{mcP_1}{eB} \theta + \frac{mcP_1}{2eB} \sin(2\theta) + P_2 y - P_1 t , \quad (16.162)$$

where

$$\theta = \frac{eB}{c\sqrt{2mP_1}} \sin^{-1} \left(x - \frac{cP_2}{eB} \right) . \quad (16.163)$$

Note that, from eqn. 16.155, we may write

$$dx = \frac{c}{eB} dP_2 + \frac{mc}{eB} \frac{1}{\sqrt{2mP_1}} \sin \theta dP_1 + \frac{c}{eB} \sqrt{2mP_1} \cos \theta d\theta , \quad (16.164)$$

from which we derive

$$\frac{\partial \theta}{\partial P_1} = -\frac{\tan \theta}{2P_1} , \quad \frac{\partial \theta}{\partial P_2} = -\frac{1}{\sqrt{2mP_1} \cos \theta} . \quad (16.165)$$

These results are useful in the calculation of Q_1 and Q_2 :

$$\begin{aligned} Q_1 &= \frac{\partial S}{\partial P_1} \\ &= \frac{mc}{eB} \theta + \frac{mcP_1}{eB} \frac{\partial \theta}{\partial P_1} + \frac{mc}{2eB} \sin(2\theta) + \frac{mcP_1}{eB} \cos(2\theta) \frac{\partial \theta}{\partial P_1} - t \\ &= \frac{mc}{eB} \theta - t \end{aligned} \quad (16.166)$$

and

$$\begin{aligned} Q_2 &= \frac{\partial S}{\partial P_2} \\ &= y + \frac{mcP_1}{eB} [1 + \cos(2\theta)] \frac{\partial \theta}{\partial P_2} \\ &= y - \frac{c}{eB} \sqrt{2mP_1} \cos \theta . \end{aligned} \quad (16.167)$$

Now since $\tilde{H}(P, Q) = 0$, we have that $\dot{Q}_\sigma = 0$, which means that each Q_σ is a constant. We therefore have the following solution:

$$x(t) = x_0 + A \sin(\omega_c t + \delta) \quad (16.168)$$

$$y(t) = y_0 + A \cos(\omega_c t + \delta) , \quad (16.169)$$

where $\omega_c = eB/mc$ is the ‘cyclotron frequency’, and

$$x_0 = \frac{cP_2}{eB} , \quad y_0 = Q_2 , \quad \delta \equiv \omega_c Q_1 , \quad A = \frac{c}{eB} \sqrt{2mP_1} . \quad (16.170)$$

16.8 Action-Angle Variables

16.8.1 Circular Phase Orbits: Librations and Rotations

In a completely integrable system, the Hamilton-Jacobi equation may be solved by separation of variables. Each momentum p_σ is a function of only its corresponding coordinate q_σ plus constants – no other coordinates enter:

$$p_\sigma = \frac{\partial W_\sigma}{\partial q_\sigma} = p_\sigma(q_\sigma, \Lambda) . \quad (16.171)$$

The motion satisfies

$$H_\sigma(q_\sigma, p_\sigma) = \Lambda_\sigma . \quad (16.172)$$

The level sets of H_σ are curves \mathcal{C}_σ . In general, these curves each depend on all of the constants Λ , so we write $\mathcal{C}_\sigma = \mathcal{C}_\sigma(\Lambda)$. The curves \mathcal{C}_σ are the *projections* of the full motion onto the (q_σ, p_σ) plane. In general we will assume the motion, and hence the curves \mathcal{C}_σ , is *bounded*. In this case, two types of projected motion are possible: librations and rotations. Librations are periodic oscillations about an equilibrium position. Rotations involve the advancement of an angular variable by 2π during a cycle. This is most conveniently illustrated in the case of the simple pendulum, for which

$$H(p_\phi, \phi) = \frac{p_\phi^2}{2I} + \frac{1}{2}I\omega^2 (1 - \cos \phi) . \quad (16.173)$$

- When $E < I\omega^2$, the momentum p_ϕ vanishes at $\phi = \pm \cos^{-1}(2E/I\omega^2)$. The system executes librations between these extreme values of the angle ϕ .
- When $E > I\omega^2$, the kinetic energy is always positive, and the angle advances monotonically, executing rotations.

In a completely integrable system, each \mathcal{C}_σ is either a libration or a rotation⁵. Both librations and rotations are closed curves. Thus, each \mathcal{C}_σ is in general homotopic to (= “can be

⁵ \mathcal{C}_σ may correspond to a separatrix, but this is a nongeneric state of affairs.

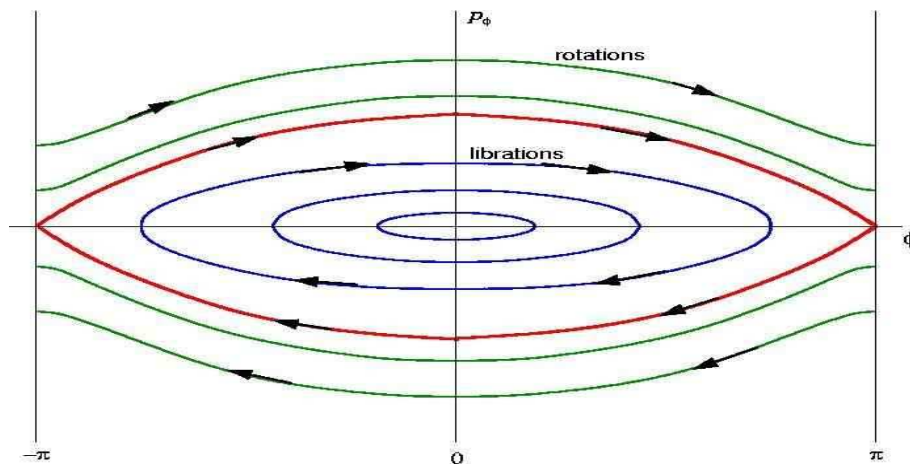


Figure 16.2: Phase curves for the simple pendulum, showing librations (in blue), rotations (in green), and the separatrix (in red). This phase flow is most correctly viewed as taking place on a cylinder, obtained from the above sketch by identifying the lines $\phi = \pi$ and $\phi = -\pi$.

continuously distorted to yield") a circle, \mathbb{S}^1 . For n freedoms, the motion is therefore confined to an n -torus, \mathbb{T}^n :

$$\mathbb{T}^n = \overbrace{\mathbb{S}^1 \times \mathbb{S}^1 \times \cdots \times \mathbb{S}^1}^{n \text{ times}} . \quad (16.174)$$

These are called *invariant tori* (or *invariant manifolds*). There are many such tori, as there are many \mathcal{C}_σ curves in each of the n two-dimensional submanifolds.

Invariant tori never intersect! This is ruled out by the uniqueness of the solution to the dynamical system, expressed as a set of coupled ordinary differential equations.

Note also that phase space is of dimension $2n$, while the invariant tori are of dimension n . Phase space is 'covered' by the invariant tori, but it is in general difficult to conceive of how this happens. Perhaps the most accessible analogy is the $n = 1$ case, where the '1-tori' are just circles. Two-dimensional phase space is covered noninteracting circular orbits. (The orbits are *topologically* equivalent to circles, although *geometrically* they may be distorted.) It is challenging to think about the $n = 2$ case, where a four-dimensional phase space is filled by nonintersecting 2-tori.

16.8.2 Action-Angle Variables

For a completely integrable system, one can transform canonically from (q, p) to new coordinates (ϕ, J) which specify a particular n -torus \mathbb{T}^n as well as the location on the torus, which is specified by n angle variables. The $\{J_\sigma\}$ are 'momentum' variables which specify the torus itself; they are constants of the motion since the tori are invariant. They are

called *action variables*. Since $\dot{J}_\sigma = 0$, we must have

$$\dot{J}_\sigma = -\frac{\partial H}{\partial \phi_\sigma} = 0 \implies H = H(J) . \quad (16.175)$$

The $\{\phi_\sigma\}$ are the *angle variables*.

The coordinate ϕ_σ describes the projected motion along \mathcal{C}_σ , and is normalized by

$$\oint_{\mathcal{C}_\sigma} d\phi_\sigma = 2\pi \quad (\text{once around } \mathcal{C}_\sigma) . \quad (16.176)$$

The dynamics of the angle variables are given by

$$\dot{\phi}_\sigma = \frac{\partial H}{\partial J_\sigma} \equiv \nu_\sigma(J) . \quad (16.177)$$

Thus,

$$\phi_\sigma(t) = \phi_\sigma(0) + \nu_\sigma(J)t . \quad (16.178)$$

The $\{\nu_\sigma(J)\}$ are *frequencies* describing the rate at which the \mathcal{C}_σ are traversed; $T_\sigma(J) = 2\pi/\nu_\sigma(J)$ is the period.

16.8.3 Canonical Transformation to Action-Angle Variables

The $\{J_\sigma\}$ determine the $\{\mathcal{C}_\sigma\}$; each q_σ determines a point on \mathcal{C}_σ . This suggests a type-II transformation, with generator $F_2(q, J)$:

$$p_\sigma = \frac{\partial F_2}{\partial q_\sigma} \quad , \quad \phi_\sigma = \frac{\partial F_2}{\partial J_\sigma} . \quad (16.179)$$

Note that⁶

$$2\pi = \oint_{\mathcal{C}_\sigma} d\phi_\sigma = \oint_{\mathcal{C}_\sigma} d\left(\frac{\partial F_2}{\partial J_\sigma}\right) = \oint_{\mathcal{C}_\sigma} \frac{\partial^2 F_2}{\partial J_\sigma \partial q_\sigma} dq_\sigma = \frac{\partial}{\partial J_\sigma} \oint_{\mathcal{C}_\sigma} p_\sigma dq_\sigma , \quad (16.180)$$

which suggests the definition

$$J_\sigma = \frac{1}{2\pi} \oint_{\mathcal{C}_\sigma} p_\sigma dq_\sigma . \quad (16.181)$$

I.e. J_σ is $(2\pi)^{-1}$ times the area enclosed by \mathcal{C}_σ .

If, separating variables,

$$W(q, A) = \sum_\sigma W_\sigma(q_\sigma, A) \quad (16.182)$$

⁶In general, we should write $d(\frac{\partial F_2}{\partial J_\sigma}) = \frac{\partial^2 F_2}{\partial J_\sigma \partial q_\alpha} dq_\alpha$ with a sum over α . However, in eqn. 16.180 all coordinates and momenta other than q_σ and p_σ are held fixed. Thus, $\alpha = \sigma$ is the only term in the sum which contributes.

is Hamilton's characteristic function for the transformation $(q, p) \rightarrow (Q, P)$, then

$$J_\sigma = \frac{1}{2\pi} \oint_{\mathcal{C}_\sigma} \frac{\partial W_\sigma}{\partial q_\sigma} dq_\sigma = J_\sigma(\Lambda) \quad (16.183)$$

is a function only of the $\{\Lambda_\alpha\}$ and not the $\{\Gamma_\alpha\}$. We then invert this relation to obtain $\Lambda(J)$, to finally obtain

$$F_2(q, J) = W(q, \Lambda(J)) = \sum_\sigma W_\sigma(q_\sigma, \Lambda(J)) . \quad (16.184)$$

Thus, the recipe for canonically transforming to action-angle variable is as follows:

- (1) Separate and solve the Hamilton-Jacobi equation for $W(q, \Lambda) = \sum_\sigma W_\sigma(q_\sigma, \Lambda)$.
- (2) Find the orbits \mathcal{C}_σ – the level sets of satisfying $H_\sigma(q_\sigma, p_\sigma) = \Lambda_\sigma$.
- (3) Invert the relation $J_\sigma(\Lambda) = \frac{1}{2\pi} \oint_{\mathcal{C}_\sigma} \frac{\partial W_\sigma}{\partial q_\sigma} dq_\sigma$ to obtain $\Lambda(J)$.
- (4) $F_2(q, J) = \sum_\sigma W_\sigma(q_\sigma, \Lambda(J))$ is the desired type-II generator⁷.

16.8.4 Example : Harmonic Oscillator

The Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 q^2 , \quad (16.185)$$

hence the Hamilton-Jacobi equation is

$$\left(\frac{dW}{dq}\right)^2 + m^2\omega_0^2 q^2 = 2m\Lambda . \quad (16.186)$$

Thus,

$$p = \frac{dW}{dq} = \pm \sqrt{2m\Lambda - m^2\omega_0^2 q^2} . \quad (16.187)$$

We now define

$$q \equiv \left(\frac{2\Lambda}{m\omega_0^2}\right)^{1/2} \sin \theta \quad \Rightarrow \quad p = \sqrt{2m\Lambda} \cos \theta , \quad (16.188)$$

in which case

$$J = \frac{1}{2\pi} \oint p dq = \frac{1}{2\pi} \cdot \frac{2\Lambda}{\omega_0} \cdot \int_0^{2\pi} d\theta \cos^2 \theta = \frac{\Lambda}{\omega_0} . \quad (16.189)$$

⁷Note that $F_2(q, J)$ is time-independent. *I.e.* we are not transforming to $\tilde{H} = 0$, but rather to $\tilde{H} = \tilde{H}(J)$.

Solving the HJE, we write

$$\frac{dW}{d\theta} = \frac{\partial q}{\partial \theta} \cdot \frac{dW}{dq} = 2J \cos^2 \theta . \quad (16.190)$$

Integrating,

$$W = J\theta + \frac{1}{2}J \sin 2\theta , \quad (16.191)$$

up to an irrelevant constant. We then have

$$\phi = \left. \frac{\partial W}{\partial J} \right|_q = \theta + \frac{1}{2} \sin 2\theta + J(1 + \cos 2\theta) \left. \frac{\partial \theta}{\partial J} \right|_q . \quad (16.192)$$

To find $(\partial \theta / \partial J)_q$, we differentiate $q = \sqrt{2J/m\omega_0} \sin \theta$:

$$dq = \frac{\sin \theta}{\sqrt{2m\omega_0 J}} dJ + \sqrt{\frac{2J}{m\omega_0}} \cos \theta d\theta \Rightarrow \left. \frac{\partial \theta}{\partial J} \right|_q = -\frac{1}{2J} \tan \theta . \quad (16.193)$$

Plugging this result into eqn. 16.192, we obtain $\phi = \theta$. Thus, the full transformation is

$$q = \left(\frac{2J}{m\omega_0} \right)^{1/2} \sin \phi , \quad p = \sqrt{2m\omega_0 J} \cos \phi . \quad (16.194)$$

The Hamiltonian is

$$H = \omega_0 J , \quad (16.195)$$

hence $\dot{\phi} = \frac{\partial H}{\partial J} = \omega_0$ and $\dot{J} = -\frac{\partial H}{\partial \phi} = 0$, with solution $\phi(t) = \phi(0) + \omega_0 t$ and $J(t) = J(0)$.

16.8.5 Example : Particle in a Box

Consider a particle in an open box of dimensions $L_x \times L_y$ moving under the influence of gravity. The bottom of the box lies at $z = 0$. The Hamiltonian is

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + mgz . \quad (16.196)$$

Step one is to solve the Hamilton-Jacobi equation via separation of variables. The Hamilton-Jacobi equation is written

$$\frac{1}{2m} \left(\frac{\partial W_x}{\partial x} \right)^2 + \frac{1}{2m} \left(\frac{\partial W_y}{\partial y} \right)^2 + \frac{1}{2m} \left(\frac{\partial W_z}{\partial z} \right)^2 + mgz = E \equiv \Lambda_z . \quad (16.197)$$

We can solve for $W_{x,y}$ by inspection:

$$W_x(x) = \sqrt{2m\Lambda_x} x , \quad W_y(y) = \sqrt{2m\Lambda_y} y . \quad (16.198)$$

We then have⁸

$$W'_z(z) = -\sqrt{2m(\Lambda_z - \Lambda_x - \Lambda_y - mgz)} \quad (16.199)$$

$$W_z(z) = \frac{2\sqrt{2}}{3\sqrt{mg}} (\Lambda_z - \Lambda_x - \Lambda_y - mgz)^{3/2} . \quad (16.200)$$

⁸Our choice of signs in taking the square roots for W'_x , W'_y , and W'_z is discussed below.

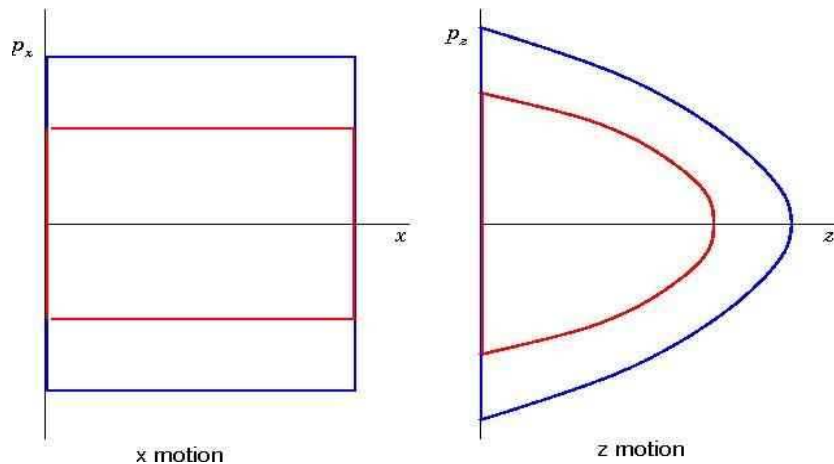


Figure 16.3: The librations \mathcal{C}_z and \mathcal{C}_x . Not shown is \mathcal{C}_y , which is of the same shape as \mathcal{C}_x .

Step two is to find the \mathcal{C}_σ . Clearly $p_{x,y} = \sqrt{2m\Lambda_{x,y}}$. For fixed p_x , the x motion proceeds from $x = 0$ to $x = L_x$ and back, with corresponding motion for y . For x , we have

$$p_z(z) = W'_z(z) = \sqrt{2m(\Lambda_z - \Lambda_x - \Lambda_y - mgz)} , \quad (16.201)$$

and thus \mathcal{C}_z is a truncated parabola, with $z_{\max} = (\Lambda_z - \Lambda_x - \Lambda_y)/mg$.

Step three is to compute $J(\Lambda)$ and invert to obtain $\Lambda(J)$. We have

$$J_x = \frac{1}{2\pi} \oint_{\mathcal{C}_x} p_x dx = \frac{1}{\pi} \int_0^{L_x} dx \sqrt{2m\Lambda_x} = \frac{L_x}{\pi} \sqrt{2m\Lambda_x} \quad (16.202)$$

$$J_y = \frac{1}{2\pi} \oint_{\mathcal{C}_y} p_y dy = \frac{1}{\pi} \int_0^{L_y} dy \sqrt{2m\Lambda_y} = \frac{L_y}{\pi} \sqrt{2m\Lambda_y} \quad (16.203)$$

and

$$\begin{aligned} J_z &= \frac{1}{2\pi} \oint_{\mathcal{C}_z} p_z dz = \frac{1}{\pi} \int_0^{z_{\max}} dz \sqrt{2m(\Lambda_z - \Lambda_x - \Lambda_y - mgz)} \\ &= \frac{2\sqrt{2}}{3\pi\sqrt{m}g} (\Lambda_z - \Lambda_x - \Lambda_y)^{3/2} . \end{aligned} \quad (16.204)$$

We now invert to obtain

$$\Lambda_x = \frac{\pi^2}{2mL_x^2} J_x^2 \quad , \quad \Lambda_y = \frac{\pi^2}{2mL_y^2} J_y^2 \quad (16.205)$$

$$\Lambda_z = \left(\frac{3\pi\sqrt{m}g}{2\sqrt{2}} \right)^{2/3} J_z^{2/3} + \frac{\pi^2}{2mL_x^2} J_x^2 + \frac{\pi^2}{2mL_y^2} J_y^2 . \quad (16.206)$$

$$F_2(x, y, z, J_x, J_y, J_z) = \frac{\pi x}{L_x} J_x + \frac{\pi y}{L_y} J_y + \pi \left(J_z^{2/3} - \frac{2m^{2/3} g^{1/3} z}{(3\pi)^{2/3}} \right)^{3/2}. \quad (16.207)$$

We now find

$$\phi_x = \frac{\partial F_2}{\partial J_x} = \frac{\pi x}{L_x}, \quad \phi_y = \frac{\partial F_2}{\partial J_y} = \frac{\pi y}{L_y} \quad (16.208)$$

and

$$\phi_z = \frac{\partial F_2}{\partial J_z} = \pi \sqrt{1 - \frac{2m^{2/3} g^{1/3} z}{(3\pi J_z)^{2/3}}} = \pi \sqrt{1 - \frac{z}{z_{\max}}}, \quad (16.209)$$

where

$$z_{\max}(J_z) = \frac{(3\pi J_z)^{2/3}}{2m^{2/3} g^{1/3}}. \quad (16.210)$$

The momenta are

$$p_x = \frac{\partial F_2}{\partial x} = \frac{\pi J_x}{L_x}, \quad p_y = \frac{\partial F_2}{\partial y} = \frac{\pi J_y}{L_y} \quad (16.211)$$

and

$$p_z = \frac{\partial F_2}{\partial z} = -\sqrt{2m} \left(\left(\frac{3\pi\sqrt{m}g}{2\sqrt{2}} \right)^{2/3} J_z^{2/3} - mgz \right)^{1/2}. \quad (16.212)$$

We note that the angle variables $\phi_{x,y,z}$ seem to be restricted to the range $[0, \pi]$, which seems to be at odds with eqn. 16.180. Similarly, the momenta $p_{x,y,z}$ all seem to be positive, whereas we know the momenta reverse sign when the particle bounces off a wall. The origin of the apparent discrepancy is that when we solved for the functions $W_{x,y,z}$, we had to take a square root in each case, and we chose a particular branch of the square root. So rather than $W_x(x) = \sqrt{2m\Lambda_x} x$, we should have taken

$$W_x(x) = \begin{cases} \sqrt{2m\Lambda_x} x & \text{if } p_x > 0 \\ \sqrt{2m\Lambda_x} (2L_x - x) & \text{if } p_x < 0. \end{cases} \quad (16.213)$$

The relation $J_x = (L_x/\pi)\sqrt{2m\Lambda_x}$ is unchanged, hence

$$W_x(x) = \begin{cases} (\pi x/L_x) J_x & \text{if } p_x > 0 \\ 2\pi J_x - (\pi x/L_x) J_x & \text{if } p_x < 0. \end{cases} \quad (16.214)$$

and

$$\phi_x = \begin{cases} \pi x/L_x & \text{if } p_x > 0 \\ \pi(2L_x - x)/L_x & \text{if } p_x < 0. \end{cases} \quad (16.215)$$

Now the angle variable ϕ_x advances by 2π during the cycle \mathcal{C}_x . Similar considerations apply to the y and z sectors.

16.8.6 Kepler Problem in Action-Angle Variables

This is discussed in detail in standard texts, such as Goldstein. The potential is $V(r) = -k/r$, and the problem is separable. We write⁹

$$W(r, \theta, \varphi) = W_r(r) + W_\theta(\theta) + W_\varphi(\varphi) , \quad (16.216)$$

hence

$$\frac{1}{2m} \left(\frac{\partial W_r}{\partial r} \right)^2 + \frac{1}{2mr^2} \left(\frac{\partial W_\theta}{\partial \theta} \right)^2 + \frac{1}{2mr^2 \sin^2 \theta} \left(\frac{\partial W_\varphi}{\partial \varphi} \right)^2 + V(r) = E \equiv \Lambda_r . \quad (16.217)$$

Separating, we have

$$\frac{1}{2m} \left(\frac{dW_\varphi}{d\varphi} \right)^2 = \Lambda_\varphi \quad \Rightarrow \quad J_\varphi = \oint_{\mathcal{C}_\varphi} d\varphi \frac{dW_\varphi}{d\varphi} = 2\pi \sqrt{2m\Lambda_\varphi} . \quad (16.218)$$

Next we deal with the θ coordinate:

$$\begin{aligned} \frac{1}{2m} \left(\frac{dW_\theta}{d\theta} \right)^2 &= \Lambda_\theta - \frac{\Lambda_\varphi}{\sin^2 \theta} \quad \Rightarrow \\ J_\theta &= 4\sqrt{2m\Lambda_\theta} \int_0^{\theta_0} d\theta \sqrt{1 - (\Lambda_\varphi/\Lambda_\theta) \csc^2 \theta} \\ &= 2\pi\sqrt{2m} \left(\sqrt{\Lambda_\theta} - \sqrt{\Lambda_\varphi} \right) , \end{aligned} \quad (16.219)$$

where $\theta_0 = \sin^{-1}(\Lambda_\varphi/\Lambda_\theta)$. Finally, we have¹⁰

$$\begin{aligned} \frac{1}{2m} \left(\frac{dW_r}{dr} \right)^2 &= E + \frac{k}{r} - \frac{\Lambda_\theta}{r^2} \quad \Rightarrow \\ J_r &= \oint_{\mathcal{C}_r} dr \sqrt{2m \left(E + \frac{k}{r} - \frac{\Lambda_\theta}{r^2} \right)} \\ &= -(J_\theta + J_\varphi) + \pi k \sqrt{\frac{2m}{|E|}} , \end{aligned} \quad (16.220)$$

where we've assumed $E < 0$, *i.e.* bound motion.

Thus, we find

$$H = E = -\frac{2\pi^2 mk^2}{(J_r + J_\theta + J_\varphi)^2} . \quad (16.221)$$

Note that the frequencies are completely degenerate:

$$\nu \equiv \nu_{r,\theta,\varphi} = \frac{\partial H}{\partial J_{r,\theta,\varphi}} = \frac{4\pi^2 mk^2}{(J_r + J_\theta + J_\varphi)^3} = \left(\frac{\pi^2 mk^2}{2|E|^3} \right)^{1/2} . \quad (16.222)$$

⁹We denote the azimuthal angle by φ to distinguish it from the AA variable ϕ .

¹⁰The details of performing the integral around \mathcal{C}_r are discussed in *e.g.* Goldstein.

This threefold degeneracy may be removed by a transformation to new AA variables,

$$\left\{ (\phi_r, J_r), (\phi_\theta, J_\theta), (\phi_\varphi, J_\varphi) \right\} \longrightarrow \left\{ (\phi_1, J_1), (\phi_2, J_2), (\phi_3, J_3) \right\}, \quad (16.223)$$

using the type-II generator

$$F_2(\phi_r, \phi_\theta, \phi_\varphi; J_1, J_2, J_3) = (\phi_\varphi - \phi_\theta) J_1 + (\phi_\theta - \phi_r) J_2 + \phi_r J_3, \quad (16.224)$$

which results in

$$\phi_1 = \frac{\partial F_2}{\partial J_1} = \phi_\varphi - \phi_\theta \qquad J_r = \frac{\partial F_2}{\partial \phi_r} = J_3 - J_2 \quad (16.225)$$

$$\phi_2 = \frac{\partial F_2}{\partial J_2} = \phi_\theta - \phi_r \qquad J_\theta = \frac{\partial F_2}{\partial \phi_\theta} = J_2 - J_1 \quad (16.226)$$

$$\phi_3 = \frac{\partial F_2}{\partial J_3} = \phi_r \qquad J_\varphi = \frac{\partial F_2}{\partial \phi_\varphi} = J_1. \quad (16.227)$$

The new Hamiltonian is

$$H(J_1, J_2, J_3) = -\frac{2\pi^2 m k^2}{J_3^2}, \quad (16.228)$$

whence $\nu_1 = \nu_2 = 0$ and $\nu_3 = \nu$.

16.8.7 Charged Particle in a Magnetic Field

For the case of the charged particle in a magnetic field, studied above in section 16.7.7, we found

$$x = \frac{cP_2}{eB} + \frac{c}{eB} \sqrt{2mP_1} \sin \theta \quad (16.229)$$

and

$$p_x = \sqrt{2mP_1} \cos \theta \qquad , \qquad p_y = P_2. \quad (16.230)$$

The action variable J is then

$$J = \oint p_x dx = \frac{2mcP_1}{eB} \int_0^{2\pi} d\theta \cos^2 \theta = \frac{mcP_1}{eB}. \quad (16.231)$$

We then have

$$W = J\theta + \frac{1}{2}J \sin(2\theta) + Py, \quad (16.232)$$

where $P \equiv P_2$. Thus,

$$\begin{aligned} \phi &= \frac{\partial W}{\partial J} \\ &= \theta + \frac{1}{2} \sin(2\theta) + J [1 + \cos(2\theta)] \frac{\partial \theta}{\partial J} \\ &= \theta + \frac{1}{2} \sin(2\theta) + 2J \cos^2 \theta \cdot \left(-\frac{\tan \theta}{2J} \right) \\ &= \theta. \end{aligned} \quad (16.233)$$

The other canonical pair is (Q, P) , where

$$Q = \frac{\partial W}{\partial P} = y - \sqrt{\frac{2cJ}{eB}} \cos \phi . \quad (16.234)$$

Therefore, we have

$$x = \frac{cP}{eB} + \sqrt{\frac{2cJ}{eB}} \sin \phi \quad , \quad y = Q + \sqrt{\frac{2cJ}{eB}} \cos \phi \quad (16.235)$$

and

$$p_x = \sqrt{\frac{2eBJ}{c}} \cos \phi \quad , \quad p_y = P . \quad (16.236)$$

The Hamiltonian is

$$\begin{aligned} H &= \frac{p_x^2}{2m} + \frac{1}{2m} \left(p_y - \frac{eBx}{c} \right)^2 \\ &= \frac{eBJ}{mc} \cos^2 \phi + \frac{eBJ}{mc} \sin^2 \phi \\ &= \omega_c J , \end{aligned} \quad (16.237)$$

where $\omega_c = eB/mc$. The equations of motion are

$$\dot{\phi} = \frac{\partial H}{\partial J} = \omega_c \quad , \quad \dot{J} = -\frac{\partial H}{\partial \phi} = 0 \quad (16.238)$$

and

$$\dot{Q} = \frac{\partial H}{\partial P} = 0 \quad , \quad \dot{P} = -\frac{\partial H}{\partial Q} = 0 . \quad (16.239)$$

Thus, Q , P , and J are constants, and $\phi(t) = \phi_0 + \omega_c t$.

16.8.8 Motion on Invariant Tori

The angle variables evolve as

$$\phi_\sigma(t) = \nu_\sigma(J) t + \phi_\sigma(0) . \quad (16.240)$$

Thus, they wind around the invariant torus, specified by $\{J_\sigma\}$ at constant rates. In general, while each ϕ_σ executed periodic motion around a circle, the motion of the system as a whole is not periodic, since the frequencies $\nu_\sigma(J)$ are not, in general, commensurate. In order for the motion to be periodic, there must exist a set of integers, $\{l_\sigma\}$, such that

$$\sum_{\sigma=1}^n l_\sigma \nu_\sigma(J) = 0 . \quad (16.241)$$

This means that the ratio of any two frequencies ν_σ/ν_α must be a rational number. On a given torus, there are several possible orbits, depending on initial conditions $\phi(0)$. However, since the frequencies are determined by the action variables, which specify the tori, on a given torus either all orbits are periodic, or none are.

In terms of the original coordinates q , there are two possibilities:

$$\begin{aligned} q_\sigma(t) &= \sum_{\ell_1=-\infty}^{\infty} \cdots \sum_{\ell_n=-\infty}^{\infty} A_{\ell_1 \ell_2 \dots \ell_n}^{(\sigma)} e^{i\ell_1 \phi_1(t)} \dots e^{i\ell_n \phi_n(t)} \\ &\equiv \sum_{\ell} A_{\ell}^{\sigma} e^{i\ell \cdot \phi(t)} \quad (\text{libration}) \end{aligned} \quad (16.242)$$

or

$$q_\sigma(t) = q_\sigma^\circ \phi_\sigma(t) + \sum_{\ell} B_{\ell}^{\sigma} e^{i\ell \cdot \phi(t)} \quad (\text{rotation}) . \quad (16.243)$$

For rotations, the variable $q_\sigma(t)$ increased by $\Delta q_\sigma = 2\pi q_\sigma^\circ \cdot R$

16.9 Canonical Perturbation Theory

16.9.1 Canonical Transformations and Perturbation Theory

Suppose we have a Hamiltonian

$$H(\xi, t) = H_0(\xi, t) + \epsilon H_1(\xi, t) , \quad (16.244)$$

where ϵ is a small dimensionless parameter. Let's implement a type-II transformation, generated by $S(q, P, t)$:¹¹

$$\tilde{H}(Q, P, t) = H(q, p, t) + \frac{\partial}{\partial t} S(q, P, t) . \quad (16.245)$$

Let's expand everything in powers of ϵ :

$$q_\sigma = Q_\sigma + \epsilon q_{1,\sigma} + \epsilon^2 q_{2,\sigma} + \dots \quad (16.246)$$

$$p_\sigma = P_\sigma + \epsilon p_{1,\sigma} + \epsilon^2 p_{2,\sigma} + \dots \quad (16.247)$$

$$\tilde{H} = \tilde{H}_0 + \epsilon \tilde{H}_1 + \epsilon^2 \tilde{H}_2 + \dots \quad (16.248)$$

$$S = \underbrace{q_\sigma P_\sigma}_{\substack{\text{identity} \\ \text{transformation}}} + \epsilon S_1 + \epsilon^2 S_2 + \dots . \quad (16.249)$$

Then

$$\begin{aligned} Q_\sigma &= \frac{\partial S}{\partial P_\sigma} = q_\sigma + \epsilon \frac{\partial S_1}{\partial P_\sigma} + \epsilon^2 \frac{\partial S_2}{\partial P_\sigma} + \dots \\ &= Q_\sigma + \left(q_{1,\sigma} + \frac{\partial S_1}{\partial P_\sigma} \right) \epsilon + \left(q_{2,\sigma} + \frac{\partial S_2}{\partial P_\sigma} \right) \epsilon^2 + \dots \end{aligned} \quad (16.250)$$

¹¹Here, $S(q, P, t)$ is not meant to signify Hamilton's principal function.

and

$$p_\sigma = \frac{\partial S}{\partial q_\sigma} = P_\sigma + \epsilon \frac{\partial S_1}{\partial q_\sigma} + \epsilon^2 \frac{\partial S_2}{\partial q_\sigma} + \dots \quad (16.251)$$

$$= P_\sigma + \epsilon p_{1,\sigma} + \epsilon^2 p_{2,\sigma} + \dots \quad (16.252)$$

We therefore conclude, order by order in ϵ ,

$$q_{k,\sigma} = -\frac{\partial S_k}{\partial P_\sigma} \quad , \quad p_{k,\sigma} = +\frac{\partial S_k}{\partial q_\sigma} \quad (16.253)$$

Now let's expand the Hamiltonian:

$$\tilde{H}(Q, P, t) = H_0(q, p, t) + \epsilon H_1(q, p, t) + \frac{\partial S}{\partial t} \quad (16.254)$$

$$\begin{aligned} &= H_0(Q, P, t) + \frac{\partial H_0}{\partial Q_\sigma} (q_\sigma - Q_\sigma) + \frac{\partial H_0}{\partial P_\sigma} (p_\sigma - P_\sigma) \\ &\quad + \epsilon H_1(Q, P, t) + \epsilon \frac{\partial}{\partial t} S_1(Q, P, t) + \mathcal{O}(\epsilon^2) \\ &= H_0(Q, P, t) + \left(-\frac{\partial H_0}{\partial Q_\sigma} \frac{\partial S_1}{\partial P_\sigma} + \frac{\partial H_0}{\partial P_\sigma} \frac{\partial S_1}{\partial Q_\sigma} + \frac{\partial S_1}{\partial t} + H_1 \right) \epsilon + \mathcal{O}(\epsilon^2) \\ &= H_0(Q, P, t) + \left(H_1 + \{S_1, H_0\} + \frac{\partial S_1}{\partial t} \right) \epsilon + \mathcal{O}(\epsilon^2) . \end{aligned} \quad (16.255)$$

In the above expression, we evaluate $H_k(q, p, t)$ and $S_k(q, P, t)$ at $q = Q$ and $p = P$ and expand in the differences $q - Q$ and $p - P$. Thus, we have derived the relation

$$\tilde{H}(Q, P, t) = \tilde{H}_0(Q, P, t) + \epsilon \tilde{H}_1(Q, P, t) + \dots \quad (16.256)$$

with

$$\tilde{H}_0(Q, P, t) = H_0(Q, P, t) \quad (16.257)$$

$$\tilde{H}_1(Q, P, t) = H_1 + \{S_1, H_0\} + \frac{\partial S_1}{\partial t} \quad (16.258)$$

The problem, though, is this: we have one equation, eqn, 16.258, for the two unknowns \tilde{H}_1 and S_1 . Thus, the problem is underdetermined. Of course, we could choose $\tilde{H}_1 = 0$, which basically recapitulates standard Hamilton-Jacobi theory. But we might just as well demand that \tilde{H}_1 satisfy some other requirement, such as that $\tilde{H}_0 + \epsilon \tilde{H}_1$ being integrable.

Incidentally, this treatment is paralleled by one in quantum mechanics, where a unitary transformation may be implemented to eliminate a perturbation to lowest order in a small parameter. Consider the Schrödinger equation,

$$i\hbar \frac{\partial \psi}{\partial t} = (\mathcal{H}_0 + \epsilon \mathcal{H}_1) \psi \quad , \quad (16.259)$$

and define χ by

$$\psi \equiv e^{iS/\hbar} \chi , \quad (16.260)$$

with

$$S = \epsilon S_1 + \epsilon^2 S_2 + \dots . \quad (16.261)$$

As before, the transformation $U \equiv \exp(iS/\hbar)$ collapses to the identity in the $\epsilon \rightarrow 0$ limit. Now let's write the Schrödinger equation for χ . Expanding in powers of ϵ , one finds

$$i\hbar \frac{\partial \chi}{\partial t} = \mathcal{H}_0 \chi + \epsilon \left(\mathcal{H}_1 + \frac{1}{i\hbar} [S_1, \mathcal{H}_0] + \frac{\partial S_1}{\partial t} \right) \chi + \dots \equiv \tilde{\mathcal{H}} \chi , \quad (16.262)$$

where $[A, B] = AB - BA$ is the commutator. Note the classical-quantum correspondence,

$$\{A, B\} \longleftrightarrow \frac{1}{i\hbar} [A, B] . \quad (16.263)$$

Again, what should we choose for S_1 ? Usually the choice is made to make the $\mathcal{O}(\epsilon)$ term in $\tilde{\mathcal{H}}$ vanish. But this is not the only possible simplifying choice.

16.9.2 Canonical Perturbation Theory for $n = 1$ Systems

Henceforth we shall assume $H(\xi, t) = H(\xi)$ is time-independent, and we write the perturbed Hamiltonian as

$$H(\xi) = H_0(\xi) + \epsilon H_1(\xi) . \quad (16.264)$$

Let (ϕ_0, J_0) be the action-angle variables for H_0 . Then

$$\tilde{H}_0(\phi_0, J_0) = H_0(q(\phi_0, J_0), p(\phi_0, J_0)) = \tilde{H}_0(J_0) . \quad (16.265)$$

We define

$$\tilde{H}_1(\phi_0, J_0) = H_1(q(\phi_0, J_0), p(\phi_0, J_0)) . \quad (16.266)$$

We assume that $\tilde{H} = \tilde{H}_0 + \epsilon \tilde{H}_1$ is integrable¹², so it, too, possesses action-angle variables, which we denote by (ϕ, J) ¹³. Thus, there must be a canonical transformation taking $(\phi_0, J_0) \rightarrow (\phi, J)$, with

$$\tilde{H}(\phi_0(\phi, J), J_0(\phi, J)) \equiv K(J) = E(J) . \quad (16.267)$$

We solve via a type-II canonical transformation:

$$S(\phi_0, J) = \phi_0 J + \epsilon S_1(\phi_0, J) + \epsilon^2 S_2(\phi_0, J) + \dots , \quad (16.268)$$

where $\phi_0 J$ is the identity transformation. Then

$$J_0 = \frac{\partial S}{\partial \phi_0} = J + \epsilon \frac{\partial S_1}{\partial \phi_0} + \epsilon^2 \frac{\partial S_2}{\partial \phi_0} + \dots \quad (16.269)$$

$$\phi = \frac{\partial S}{\partial J} = \phi_0 + \epsilon \frac{\partial S_1}{\partial J} + \epsilon^2 \frac{\partial S_2}{\partial J} + \dots , \quad (16.270)$$

¹²This is always true, in fact, for $n = 1$.

¹³We assume the motion is bounded, so action-angle variables may be used.

and

$$E(J) = E_0(J) + \epsilon E_1(J) + \epsilon^2 E_2(J) + \dots \quad (16.271)$$

$$= \tilde{H}_0(\phi_0, J_0) + \tilde{H}_1(\phi_0, J_0) . \quad (16.272)$$

We now expand $\tilde{H}(\phi_0, J_0)$ in powers of $J_0 - J$:

$$\tilde{H}(\phi_0, J_0) = \tilde{H}_0(\phi_0, J_0) + \epsilon \tilde{H}_1(\phi_0, J_0) \quad (16.273)$$

$$\begin{aligned} &= \tilde{H}_0(J) + \frac{\partial \tilde{H}_0}{\partial J} (J_0 - J) + \frac{1}{2} \frac{\partial^2 \tilde{H}_0}{\partial J^2} (J_0 - J)^2 + \dots \\ &\quad + \epsilon \tilde{H}_1(\phi_0, J_0) + \epsilon \frac{\partial \tilde{H}_1}{\partial J} (J_0 - J) + \dots \\ &= \tilde{H}_0(J) + \left(\tilde{H}_1(\phi_0, J_0) + \frac{\partial \tilde{H}_0}{\partial J} \frac{\partial S_1}{\partial \phi_0} \right) \epsilon \\ &\quad + \left(\frac{\partial \tilde{H}_0}{\partial J} \frac{\partial S_2}{\partial \phi_0} + \frac{1}{2} \frac{\partial^2 \tilde{H}_0}{\partial J^2} \left(\frac{\partial S_1}{\partial \phi_0} \right)^2 + \frac{\partial \tilde{H}_1}{\partial J} \frac{\partial S_1}{\partial \phi_0} \right) \epsilon^2 + \dots . \end{aligned} \quad (16.274)$$

Equating terms, then,

$$E_0(J) = \tilde{H}_0(J) \quad (16.275)$$

$$E_1(J) = \tilde{H}_1(\phi_0, J) + \frac{\partial \tilde{H}_0}{\partial J} \frac{\partial S_1}{\partial \phi_0} \quad (16.276)$$

$$E_2(J) = \frac{\partial \tilde{H}_0}{\partial J} \frac{\partial S_2}{\partial \phi_0} + \frac{1}{2} \frac{\partial^2 \tilde{H}_0}{\partial J^2} \left(\frac{\partial S_1}{\partial \phi_0} \right)^2 + \frac{\partial \tilde{H}_1}{\partial J} \frac{\partial S_1}{\partial \phi_0} . \quad (16.277)$$

How, one might ask, can we be sure that the LHS of each equation in the above hierarchy depends only on J when each RHS seems to depend on ϕ_0 as well? The answer is that we use the freedom to choose each S_k to make this so. We demand each RHS be independent of ϕ_0 , which means it must be equal to its average, $\langle \text{RHS}(\phi_0) \rangle$, where

$$\langle f(\phi_0) \rangle = \int_0^{2\pi} \frac{d\phi_0}{2\pi} f(\phi_0) . \quad (16.278)$$

The average is performed *at fixed J and not at fixed J_0* . In this regard, we note that holding J constant and increasing ϕ_0 by 2π also returns us to the same starting point. Therefore, J is a periodic function of ϕ_0 . We must then be able to write

$$S_k(\phi_0, J) = \sum_{m=-\infty}^{\infty} S_k(J; m) e^{im\phi_0} \quad (16.279)$$

for each $k > 0$, in which case

$$\left\langle \frac{\partial S_k}{\partial \phi_0} \right\rangle = \frac{1}{2\pi} [S_k(2\pi) - S_k(0)] = 0 . \quad (16.280)$$

Let's see how this averaging works to the first two orders of the hierarchy. Since $\tilde{H}_0(J)$ is independent of ϕ_0 and since $\partial S_1/\partial\phi_0$ is periodic, we have

$$E_1(J) = \langle \tilde{H}_1(\phi_0, J) \rangle + \frac{\partial \tilde{H}_0}{\partial J} \overbrace{\left\langle \frac{\partial S_1}{\partial \phi_0} \right\rangle}^{\text{this vanishes!}} \quad (16.281)$$

and hence S_1 must satisfy

$$\frac{\partial S_1}{\partial \phi_0} = \frac{\langle \tilde{H}_1 \rangle - \tilde{H}_1}{\nu_0(J)}, \quad (16.282)$$

where $\nu_0(J) = \partial \tilde{H}_0/\partial J$. Clearly the RHS of eqn. 16.282 has zero average, and must be a periodic function of ϕ_0 . The solution is $S_1 = S_1(\phi_0, J) + g(J)$, where $g(J)$ is an arbitrary function of J . However, $g(J)$ affects only the difference $\phi - \phi_0$, changing it by a constant value $g'(J)$. So there is no harm in taking $g(J) = 0$.

Next, let's go to second order in ϵ . We have

$$E_2(J) = \left\langle \frac{\partial \tilde{H}_1}{\partial J} \frac{\partial S_1}{\partial \phi_0} \right\rangle + \frac{1}{2} \frac{\partial \nu_0}{\partial J} \left\langle \left(\frac{\partial S_1}{\partial \phi_1} \right)^2 \right\rangle + \nu_0(J) \overbrace{\left\langle \frac{\partial S_2}{\partial \phi_0} \right\rangle}^{\text{this vanishes!}}. \quad (16.283)$$

The equation for S_2 is then

$$\begin{aligned} \frac{\partial S_2}{\partial \phi_0} = \frac{1}{\nu_0^2(J)} \left\{ \left\langle \frac{\partial \tilde{H}_1}{\partial J} \right\rangle \langle \tilde{H}_0 \rangle - \left\langle \frac{\partial \tilde{H}_1}{\partial J} \tilde{H}_0 \right\rangle - \frac{\partial \tilde{H}_1}{\partial J} \langle \tilde{H}_1 \rangle + \frac{\partial \tilde{H}_1}{\partial J} \tilde{H}_1 \right. \\ \left. + \frac{1}{2} \frac{\partial \ln \nu_0}{\partial J} \left(\langle \tilde{H}_1^2 \rangle - 2\langle \tilde{H}_1 \rangle^2 + 2\langle \tilde{H}_1 \rangle - \tilde{H}_1^2 \right) \right\}. \end{aligned} \quad (16.284)$$

The expansion for the energy $E(J)$ is then

$$\begin{aligned} E(J) = \tilde{H}_0(J) + \epsilon \langle \tilde{H}_1 \rangle + \frac{\epsilon^2}{\nu_0(J)} \left\{ \left\langle \frac{\partial \tilde{H}_1}{\partial J} \right\rangle \langle \tilde{H}_1 \rangle - \left\langle \frac{\partial \tilde{H}_1}{\partial J} \tilde{H}_1 \right\rangle \right. \\ \left. + \frac{1}{2} \frac{\partial \ln \nu_0}{\partial J} \left(\langle \tilde{H}_1^2 \rangle - \langle \tilde{H}_1 \rangle^2 \right) \right\} + \mathcal{O}(\epsilon^3). \end{aligned} \quad (16.285)$$

Note that we don't need S to find $E(J)$! The perturbed frequencies are

$$\nu(J) = \frac{\partial E}{\partial J}. \quad (16.286)$$

Sometimes the frequencies are all that is desired. However, we can of course obtain the full motion of the system via the succession of canonical transformations,

$$(\phi, J) \longrightarrow (\phi_0, J_0) \longrightarrow (q, p). \quad (16.287)$$

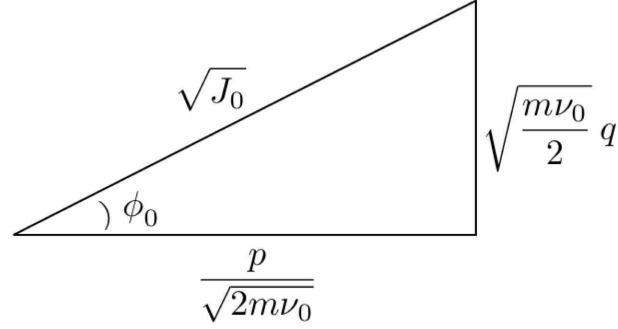


Figure 16.4: Action-angle variables for the harmonic oscillator.

16.9.3 Example : Nonlinear Oscillator

Consider the nonlinear oscillator with Hamiltonian

$$H(q, p) = \overbrace{\frac{p^2}{2m} + \frac{1}{2}m\nu_0^2 q^2}^{H_0} + \frac{1}{4}\epsilon\alpha q^4. \quad (16.288)$$

The action-angle variables for the harmonic oscillator Hamiltonian H_0 are

$$\phi_0 = \tan^{-1}(mvq/p) \quad , \quad J_0 = \frac{p^2}{2m\nu_0} + \frac{1}{2}m\nu_0 q^2, \quad (16.289)$$

and the relation between (ϕ_0, J_0) and (q, p) is further depicted in fig. 16.4. Note $H_0 = \nu_0 J_0$. For the full Hamiltonian, we have

$$\begin{aligned} \tilde{H}(\phi_0, J_0) &= \nu_0 J_0 + \frac{1}{4}\epsilon\alpha \left(\sqrt{\frac{2J_0}{m\nu_0}} \sin \phi_0 \right)^4 \\ &= \nu_0 J_0 + \frac{\epsilon\alpha}{m^2\nu_0^2} J_0^2 \sin^4 \phi_0. \end{aligned} \quad (16.290)$$

We may now evaluate

$$E_1(J) = \langle \tilde{H}_1 \rangle = \frac{\alpha J^2}{m^2\nu_0^2} \int_0^{2\pi} \frac{d\phi_0}{2\pi} \sin^4 \phi_0 = \frac{3\alpha J^2}{8m^2\nu_0^2}. \quad (16.291)$$

The frequency, to order ϵ , is

$$\nu(J) = \nu_0 + \frac{3\epsilon\alpha J}{4m^2\nu_0^2}. \quad (16.292)$$

Now to lowest order in ϵ , we may replace J by $J_0 = \frac{1}{2}m\nu_0 A^2$, where A is the amplitude of the q motion. Thus,

$$\nu(A) = \nu_0 + \frac{3\epsilon\alpha}{8m\nu_0}. \quad (16.293)$$

This result agrees with that obtained via heavier lifting, using the Poincaré-Lindstedt method.

Next, let's evaluate the canonical transformation $(\phi_0, J_0) \rightarrow (\phi, J)$. We have

$$\begin{aligned} \nu_0 \frac{\partial S_1}{\partial \phi_0} &= \frac{\alpha J^2}{m^2 \nu_0^2} \left(\frac{3}{8} - \sin^4 \phi_0 \right) \quad \Rightarrow \\ S(\phi_0, J) &= \phi_0 J + \frac{\epsilon \alpha J^2}{8 m^2 \nu_0^3} (3 + 2 \sin^2 \phi_0) \sin \phi_0 \cos \phi_0 + \mathcal{O}(\epsilon^2). \end{aligned} \quad (16.294)$$

Thus,

$$\phi = \frac{\partial S}{\partial J} = \phi_0 + \frac{\epsilon \alpha J}{4 m^2 \nu_0^3} (3 + 2 \sin^2 \phi_0) \sin \phi_0 \cos \phi_0 + \mathcal{O}(\epsilon^2) \quad (16.295)$$

$$J_0 = \frac{\partial S}{\partial \phi_0} = J + \frac{\epsilon \alpha J^2}{8 m^2 \nu_0^3} (4 \cos 2\phi_0 - \cos 4\phi_0) + \mathcal{O}(\epsilon^2). \quad (16.296)$$

Again, to lowest order, we may replace J by J_0 in the above, whence

$$J = J_0 - \frac{\epsilon \alpha J_0^2}{8 m^2 \nu_0^3} (4 \cos 2\phi_0 - \cos 4\phi_0) + \mathcal{O}(\epsilon^2) \quad (16.297)$$

$$\phi = \phi_0 + \frac{\epsilon \alpha J_0}{8 m^2 \nu_0^3} (3 + 2 \sin^2 \phi_0) \sin 2\phi_0 + \mathcal{O}(\epsilon^2). \quad (16.298)$$

To obtain (q, p) in terms of (ϕ, J) is not analytically tractable – the relations cannot be analytically inverted.

16.9.4 $n > 1$ Systems : Degeneracies and Resonances

Generalizing the procedure we derived for $n = 1$, we obtain

$$J_0^\alpha = \frac{\partial S}{\partial \phi_0^\alpha} = J^\alpha + \epsilon \frac{\partial S_1}{\partial \phi_0^\alpha} + \epsilon^2 \frac{\partial S_2}{\partial \phi_0^\alpha} + \dots \quad (16.299)$$

$$\phi^\alpha = \frac{\partial S}{\partial J^\alpha} = \phi_0^\alpha + \epsilon \frac{\partial S_1}{\partial J^\alpha} + \epsilon^2 \frac{\partial S_2}{\partial J^\alpha} + \dots \quad (16.300)$$

and

$$E_0(\mathbf{J}) = \tilde{H}_0(\mathbf{J}) \quad (16.301)$$

$$E_1(\mathbf{J}) = \tilde{H}_0(\phi_0, \mathbf{J}) + \nu_0^\alpha(\mathbf{J}) \frac{\partial S_1}{\partial \phi_0^\alpha} \quad (16.302)$$

$$E_2(\mathbf{J}) = \frac{\partial \tilde{H}_0}{\partial J^\alpha} \frac{\partial S_2}{\partial \phi_0^\alpha} + \frac{1}{2} \frac{\partial \nu_0^\alpha}{\partial J^\beta} \frac{\partial S_1}{\partial \phi_0^\alpha} \frac{\partial S_1}{\partial \phi_0^\beta} + \nu_0^\alpha \frac{\partial S_1}{\partial \phi_0^\alpha}. \quad (16.303)$$

We now implement the averaging procedure, with

$$\langle f(J^1, \dots, J^n) \rangle = \int_0^{2\pi} \frac{d\phi_0^1}{2\pi} \dots \int_0^{2\pi} \frac{d\phi_0^n}{2\pi} f(\phi_0^1, \dots, \phi_0^n, J^1, \dots, J^n). \quad (16.304)$$

The equation for S_1 is

$$\nu_0^\alpha \frac{\partial S_1}{\partial \phi_0^\alpha} = \langle \tilde{H}_1 \rangle - \tilde{H}_1 \equiv -\sum'_{\boldsymbol{\ell}} V_{\boldsymbol{\ell}} e^{i\boldsymbol{\ell} \cdot \boldsymbol{\phi}} , \quad (16.305)$$

where $\boldsymbol{\ell} = \{\ell^1, \ell^2, \dots, \ell^n\}$, with each ℓ^σ an integer, and with $\boldsymbol{\ell} \neq 0$. The solution is

$$S_1(\boldsymbol{\phi}_0, \mathbf{J}) = i \sum'_l \frac{V_{\boldsymbol{\ell}}}{\boldsymbol{\ell} \cdot \boldsymbol{\nu}_0} e^{i\boldsymbol{\ell} \cdot \boldsymbol{\phi}} . \quad (16.306)$$

where $\boldsymbol{\ell} \cdot \boldsymbol{\nu}_0 = l^\alpha \nu_0^\alpha$. When two or more of the frequencies $\nu_\alpha(J)$ are *commensurate*, there exists a set of integers l such that the denominator of $D(l)$ vanishes. But even when the frequencies are not rationally related, one can approximate the ratios $\nu_0^\alpha / \nu_0^{\alpha'}$ by rational numbers, and for large enough l the denominator can become arbitrarily small.

Periodic time-dependent perturbations present a similar problem. Consider the system

$$H(\boldsymbol{\phi}, \mathbf{J}, t) = H_0(\mathbf{J}) + \epsilon V(\boldsymbol{\phi}, \mathbf{J}, t) , \quad (16.307)$$

where $V(t+T) = V(t)$. This means we may write

$$V(\boldsymbol{\phi}, \mathbf{J}, t) = \sum_k V_k(\boldsymbol{\phi}, \mathbf{J}) e^{-ik\Omega t} \quad (16.308)$$

$$= \sum_k \sum_{\boldsymbol{\ell}} \hat{V}_{k,\boldsymbol{\ell}}(\mathbf{J}) e^{i\boldsymbol{\ell} \cdot \boldsymbol{\phi}} e^{-ik\Omega t} . \quad (16.309)$$

by Fourier transforming from both time and angle variables; here $\Omega = 2\pi/T$. Note that $V(\boldsymbol{\phi}, \mathbf{J}, t)$ is real if $V_{k,\boldsymbol{\ell}}^* = V_{-k,-\boldsymbol{\ell}}$. The equations of motion are

$$\dot{J}^\alpha = -\frac{\partial H}{\partial \phi^\alpha} = -i\epsilon \sum_{k,\boldsymbol{\ell}} l^\alpha \hat{V}_{k,\boldsymbol{\ell}}(\mathbf{J}) e^{i\boldsymbol{\ell} \cdot \boldsymbol{\phi}} e^{-ik\Omega t} \quad (16.310)$$

$$\dot{\phi}^\alpha = +\frac{\partial H}{\partial J^\alpha} = \nu_0^\alpha(\mathbf{J}) + \epsilon \sum_{k,\boldsymbol{\ell}} \frac{\partial \hat{V}_{k,\boldsymbol{\ell}}(\mathbf{J})}{\partial J^\alpha} e^{i\boldsymbol{\ell} \cdot \boldsymbol{\phi}} e^{-ik\Omega t} . \quad (16.311)$$

We now expand in ϵ :

$$\phi^\alpha = \phi_0^\alpha + \epsilon \phi_1^\alpha + \epsilon^2 \phi_2^\alpha + \dots \quad (16.312)$$

$$J^\alpha = J_0^\alpha + \epsilon J_1^\alpha + \epsilon^2 J_2^\alpha + \dots . \quad (16.313)$$

To order ϵ^0 , $J^\alpha = J_0^\alpha$ and $\phi_0^\alpha = \nu_0^\alpha t + \beta_0^\alpha$. To order ϵ^1 ,

$$\dot{J}_1^\alpha = -i \sum_{k,\boldsymbol{\ell}} l^\alpha \hat{V}_{k,\boldsymbol{\ell}}(\mathbf{J}_0) e^{i(\boldsymbol{\ell} \cdot \boldsymbol{\nu}_0 - k\Omega)t} e^{i\boldsymbol{\ell} \cdot \boldsymbol{\beta}_0} \quad (16.314)$$

and

$$\dot{\phi}_1^\alpha = \frac{\partial \nu_0^\alpha}{\partial J^\beta} J_1^\beta + \sum_{k,\boldsymbol{\ell}} \frac{\partial \hat{V}_{k,\boldsymbol{\ell}}(\mathbf{J})}{\partial J^\alpha} e^{i(\boldsymbol{\ell} \cdot \boldsymbol{\nu}_0 - k\Omega)t} e^{i\boldsymbol{\ell} \cdot \boldsymbol{\beta}_0} , \quad (16.315)$$

where derivatives are evaluated at $\mathbf{J} = \mathbf{J}_0$. The solution is:

$$J_1^\alpha = \sum_{k,\ell} \frac{l^\alpha \hat{V}_{k,\ell}(J_0)}{k\Omega - \ell \cdot \boldsymbol{\nu}_0} e^{i(\ell \cdot \boldsymbol{\nu}_0 - k\Omega)t} e^{i\ell \cdot \boldsymbol{\beta}_0} \quad (16.316)$$

$$\phi_1^\alpha = \left\{ \frac{\partial \nu_0^\alpha}{\partial J^\beta} \frac{l^\beta \hat{V}_{k,\ell}(J_0)}{(k\Omega - \ell \cdot \boldsymbol{\nu}_0)^2} + \frac{\partial \hat{V}_{k,\ell}(J)}{\partial J^\alpha} \frac{1}{k\Omega - \ell \cdot \boldsymbol{\nu}_0} \right\} e^{i(\ell \cdot \boldsymbol{\nu}_0 - k\Omega)t} e^{i\ell \cdot \boldsymbol{\beta}_0} . \quad (16.317)$$

When the resonance condition,

$$k\Omega = \ell \cdot \boldsymbol{\nu}_0(\mathbf{J}_0) , \quad (16.318)$$

holds, the denominators vanish, and the perturbation theory breaks down.

16.9.5 Particle-Wave Interaction

Consider a particle of charge e moving in the presence of a constant magnetic field $\mathbf{B} = B\hat{z}$ and a space- and time-varying electric field $\mathbf{E}(\mathbf{x}, t)$, described by the Hamiltonian

$$H = \frac{1}{2m} (\mathbf{p} - \frac{e}{c}\mathbf{A})^2 + \epsilon eV_0 \cos(k_\perp x + k_z z - \omega t) , \quad (16.319)$$

where ϵ is a dimensionless expansion parameter. Working in the gauge $\mathbf{A} = Bx\hat{y}$, from our earlier discussions in section 16.7.7, we may write

$$H = \omega_c J + \frac{p_z^2}{2m} + \epsilon eV_0 \cos \left(k_z z + \frac{k_\perp P}{m\omega_c} + k_\perp \sqrt{\frac{2J}{m\omega_c}} \sin \phi - \omega t \right) . \quad (16.320)$$

Here,

$$x = \frac{P}{m\omega_c} + \sqrt{\frac{2J}{m\omega_c}} \sin \phi \quad , \quad y = Q + \sqrt{\frac{2J}{m\omega_c}} \cos \phi , \quad (16.321)$$

with $\omega_c = eB/mc$, the cyclotron frequency. We now make a mixed canonical transformation, generated by

$$F = \phi J' + \left(k_z z + \frac{k_\perp P}{m\omega_c} - \omega t \right) K' - PQ' , \quad (16.322)$$

where the new sets of conjugate variables are $\{(\phi', J'), (Q', P'), (\psi', K')\}$. We then have

$$\phi' = \frac{\partial F}{\partial J'} = \phi \quad \quad \quad J = \frac{\partial F}{\partial \phi} = J' \quad (16.323)$$

$$Q = -\frac{\partial F}{\partial P} = -\frac{k_\perp K'}{m\omega_c} + Q' \quad \quad \quad P' = -\frac{\partial F}{\partial Q'} = P \quad (16.324)$$

$$\psi' = \frac{\partial F}{\partial K'} = k_z z + \frac{k_\perp P}{m\omega_c} - \omega t \quad \quad \quad p_z = \frac{\partial F}{\partial z} = k_z K' . \quad (16.325)$$

The transformed Hamiltonian is

$$\begin{aligned} H' &= H + \frac{\partial F}{\partial t} \\ &= \omega_c J' + \frac{k_z^2}{2m} K'^2 - \omega K' + \epsilon eV_0 \cos \left(\psi' + k_\perp \sqrt{\frac{2J'}{m\omega_c}} \sin \phi' \right) . \end{aligned} \quad (16.326)$$

We will now drop primes and simply write $H = H_0 + \epsilon H_1$, with

$$H_0 = \omega_c J + \frac{k_z^2}{2m} K^2 - \omega K \quad (16.327)$$

$$H_1 = eV_0 \cos \left(\psi + k_\perp \sqrt{\frac{2J}{m\omega_c}} \sin \phi \right). \quad (16.328)$$

When $\epsilon = 0$, the frequencies associated with the ϕ and ψ motion are

$$\omega_\phi^0 = \frac{\partial H_0}{\partial \phi} = \omega_c \quad , \quad \omega_\psi^0 = \frac{\partial H_0}{\partial \psi} = \frac{k_z^2 K}{m} - \omega = k_z v_z - \omega \quad , \quad (16.329)$$

where $v_z = p_z/m$ is the z -component of the particle's velocity. Now let us solve eqn. 16.305:

$$\omega_\phi^0 \frac{\partial S_1}{\partial \phi} + \omega_\psi^0 \frac{\partial S_1}{\partial \psi} = \langle H_1 \rangle - H_1. \quad (16.330)$$

This yields

$$\begin{aligned} \omega_c \frac{\partial S_1}{\partial \phi} + \left(\frac{k_z^2 K}{m} - \omega \right) \frac{\partial S_1}{\partial \psi} &= -eA_0 \cos \left(\psi + k_\perp \sqrt{\frac{2J}{m\omega_c}} \sin \phi \right) \\ &= -eA_0 \sum_{n=-\infty}^{\infty} J_n \left(k_\perp \sqrt{\frac{2J}{m\omega_c}} \right) \cos(\psi + n\phi) \quad , \end{aligned} \quad (16.331)$$

where we have used the result

$$e^{iz \sin \theta} = \sum_{n=-\infty}^{\infty} J_n(z) e^{in\theta}. \quad (16.332)$$

The solution for S_1 is

$$S_1 = \sum_n \frac{eV_0}{\omega - n\omega_c - k_z^2 \bar{K}/m} J_n \left(k_\perp \sqrt{\frac{2\bar{J}}{m\omega_c}} \right) \sin(\psi + n\phi). \quad (16.333)$$

We then have new action variables \bar{J} and \bar{K} , where

$$J = \bar{J} + \epsilon \frac{\partial S_1}{\partial \phi} + \mathcal{O}(\epsilon^2) \quad (16.334)$$

$$K = \bar{K} + \epsilon \frac{\partial S_1}{\partial \psi} + \mathcal{O}(\epsilon^2). \quad (16.335)$$

Defining the dimensionless variable

$$\lambda \equiv k_\perp \sqrt{\frac{2\bar{J}}{m\omega_c}} \quad , \quad (16.336)$$

we obtain the result

$$\left(\frac{m\omega_c^2}{2eV_0 k_\perp^2} \right) \bar{\lambda}^2 = \left(\frac{m\omega_c^2}{2eV_0 k_\perp^2} \right) \lambda^2 - \epsilon \sum_n \frac{n J_n(\lambda) \cos(\psi + n\phi)}{\frac{\omega}{\omega_c} - n - \frac{k_z^2 \bar{K}}{m\omega_c}} + \mathcal{O}(\epsilon^2) \quad , \quad (16.337)$$

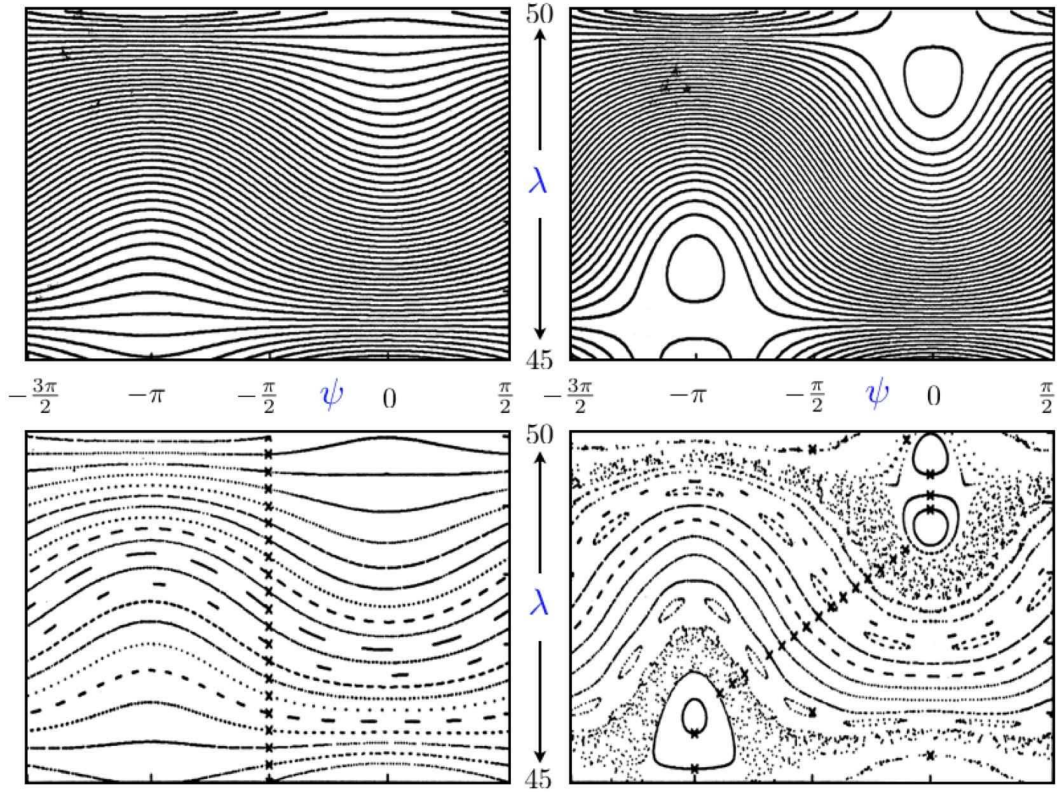


Figure 16.5: Plot of λ versus ψ for $\phi = 0$ (Poincaré section) for $\omega = 30.11 \omega_c$. Top panels are nonresonant invariant curves calculated to first order. Bottom panels are exact numerical dynamics, with x symbols marking the initial conditions. Left panels: weak amplitude (no trapping). Right panels: stronger amplitude (shows trapping). From Lichtenberg and Lieberman (1983).

where $\bar{\lambda} = k_{\perp} \sqrt{2J/m\omega_c}$.¹⁴

We see that resonances occur whenever

$$\frac{\omega}{\omega_c} - \frac{k_z^2 K}{m\omega_c} = n, \quad (16.338)$$

for any integer n . Let us consider the case $k_z = 0$, in which the resonance condition is $\omega = n\omega_c$. We then have

$$\frac{\bar{\lambda}^2}{2\alpha} = \frac{\lambda^2}{2\alpha} - \sum_n \frac{n J_n(\lambda) \cos(\psi + n\phi)}{\frac{\omega}{\omega_c} - n}, \quad (16.339)$$

where

$$\alpha = \frac{E_0}{B} \cdot \frac{ck_{\perp}}{\omega_c} \quad (16.340)$$

¹⁴Note that the argument of J_n in eqn. 16.337 is λ and not $\bar{\lambda}$. This arises because we are computing the new action \bar{J} in terms of the old variables (ϕ, J) and (ψ, K) .

is a dimensionless measure of the strength of the perturbation, with $E_0 \equiv k_{\perp} V_0$. In Fig. 16.5 we plot the level sets for the RHS of the above equation $\lambda(\psi)$ for $\phi = 0$, for two different values of the dimensionless amplitude α , for $\omega/\omega_c = 30.11$ (*i.e.* off resonance). Thus, when the amplitude is small, the level sets are far from a primary resonance, and the analytical and numerical results are very similar (left panels). When the amplitude is larger, resonances may occur which are not found in the lowest order perturbation treatment. However, as is apparent from the plots, the gross features of the phase diagram are reproduced by perturbation theory. What is missing is the existence of ‘chaotic islands’ which initially emerge in the vicinity of the trapping regions.

16.10 Adiabatic Invariants

Adiabatic perturbations are slow, smooth, time-dependent perturbations to a dynamical system. A classic example: a pendulum with a slowly varying length $l(t)$. Suppose $\lambda(t)$ is the adiabatic parameter. We write $H = H(q, p; \lambda(t))$. All explicit time-dependence to H comes through $\lambda(t)$. Typically, a dimensionless parameter ϵ may be associated with the perturbation:

$$\epsilon = \frac{1}{\omega_0} \left| \frac{d \ln \lambda}{dt} \right|, \quad (16.341)$$

where ω_0 is the natural frequency of the system when λ is constant. We require $\epsilon \ll 1$ for adiabaticity. In adiabatic processes, the action variables are conserved to a high degree of accuracy. These are the *adiabatic invariants*. For example, for the harmonic oscillator, the action is $J = E/\nu$. While E and ν may vary considerably during the adiabatic process, their ratio is very nearly fixed. As a consequence, assuming small oscillations,

$$E = \nu J = \frac{1}{2} m g l \theta_0^2 \quad \Rightarrow \quad \theta_0(l) \approx \frac{2J}{m\sqrt{g} l^{3/2}}, \quad (16.342)$$

so $\theta_0(l) \propto l^{-3/4}$.

Suppose that for fixed λ the Hamiltonian is transformed to action-angle variables via the generator $S(q, J; \lambda)$. The transformed Hamiltonian is

$$\tilde{H}(\phi, J, t) = H(\phi, J; \lambda) + \frac{\partial S}{\partial \lambda} \frac{d\lambda}{dt}, \quad (16.343)$$

where

$$H(\phi, J; \lambda) = H(q(\phi, J; \lambda), p(\phi, J; \lambda); \lambda). \quad (16.344)$$

We assume $n = 1$ here. Hamilton’s equations are now

$$\dot{\phi} = + \frac{\partial \tilde{H}}{\partial J} = \nu(J; \lambda) + \frac{\partial^2 S}{\partial \lambda \partial J} \frac{d\lambda}{dt} \quad (16.345)$$

$$\dot{J} = - \frac{\partial \tilde{H}}{\partial \phi} = - \frac{\partial^2 S}{\partial \lambda \partial \phi} \frac{d\lambda}{dt}. \quad (16.346)$$

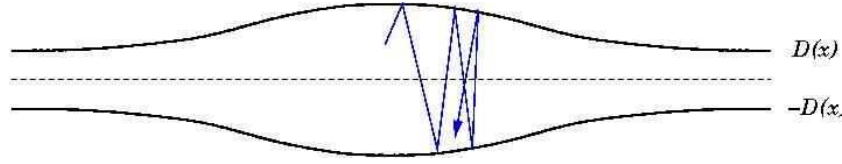


Figure 16.6: A mechanical mirror.

The second of these may be Fourier decomposed as

$$\dot{J} = -i\dot{\lambda} \sum_m m \frac{\partial S_m(J; \lambda)}{\partial \lambda} e^{im\phi}, \quad (16.347)$$

hence

$$\Delta J = J(t = +\infty) - J(t = -\infty) = -i \sum_m m \int_{-\infty}^{\infty} dt \frac{\partial S_m(J; \lambda)}{\partial \lambda} \frac{d\lambda}{dt} e^{im\phi}. \quad (16.348)$$

Since $\dot{\lambda}$ is small, we have $\phi(t) = \nu t + \beta$, to lowest order. We must therefore evaluate integrals such as

$$\mathcal{I}_m = \int_{-\infty}^{\infty} dt \frac{\partial S_m(J; \lambda)}{\partial \lambda} \frac{d\lambda}{dt} e^{im\nu t}. \quad (16.349)$$

The term in curly brackets is a smooth, slowly varying function of t . Call it $f(t)$. We presume $f(t)$ can be analytically continued off the real t axis, and that its closest singularity in the complex t plane lies at $t = \pm i\tau$, in which case \mathcal{I} behaves as $\exp(-|m|\nu\tau)$. Consider, for example, the Lorentzian,

$$f(t) = \frac{\mathcal{C}}{1 + (t/\tau)^2} \Rightarrow \int_{-\infty}^{\infty} dt f(t) e^{im\nu t} = \pi\tau e^{-|m|\nu\tau}, \quad (16.350)$$

which is exponentially small in the time scale τ . Because of this, only $m = \pm 1$ need be considered. What this tells us is that the change ΔJ may be made arbitrarily small by a sufficiently slowly varying $\lambda(t)$.

16.10.1 Example: mechanical mirror

Consider a two-dimensional version of a mechanical mirror, depicted in fig. 16.6. A particle bounces between two curves, $y = \pm D(x)$, where $|D'(x)| \ll 1$. The bounce time is $\tau_{b\perp} = 2D/v_y$. We assume $\tau \ll L/v_x$, where $v_{x,y}$ are the components of the particle's velocity, and L is the total length of the system. There are, therefore, many bounces, which means the particle gets to sample the curvature in $D(x)$.

The adiabatic invariant is the action,

$$J = \frac{1}{2\pi} \int_{-D}^D dy m v_y + \frac{1}{2\pi} \int_D^{-D} dy m (-v_y) = \frac{2}{\pi} m v_y D(x) . \quad (16.351)$$

Thus,

$$E = \frac{1}{2} m (v_x^2 + v_y^2) = \frac{1}{2} m v_x^2 + \frac{\pi^2 J^2}{8mD^2(x)} , \quad (16.352)$$

or

$$v_x^2 = \frac{2E}{m} - \left(\frac{\pi J}{2mD(x)} \right)^2 . \quad (16.353)$$

The particle is reflected in the throat of the device at horizontal coordinate x^* , where

$$D(x^*) = \frac{\pi J}{\sqrt{8mE}} . \quad (16.354)$$

16.10.2 Example: magnetic mirror

Consider a particle of charge e moving in the presence of a uniform magnetic field $\mathbf{B} = B\hat{z}$. Recall the basic physics: velocity in the parallel direction v_z is conserved, while in the plane perpendicular to \mathbf{B} the particle executes circular ‘cyclotron orbits’, satisfying

$$\frac{mv_{\perp}^2}{\rho} = \frac{e}{c} v_{\perp} B \quad \Rightarrow \quad \rho = \frac{mc v_{\perp}}{eB} , \quad (16.355)$$

where ρ is the radial coordinate in the plane perpendicular to \mathbf{B} . The period of the orbits is $T = 2\pi\rho \cdot v_{\perp} = 2\pi mc/eB$, hence their frequency is the cyclotron frequency $\omega_c = eB/mc$.

Now assume that the magnetic field is spatially dependent. Note that a spatially varying \mathbf{B} -field cannot be unidirectional:

$$\nabla \cdot \mathbf{B} = \nabla_{\perp} \cdot \mathbf{B}_{\perp} + \frac{\partial B_z}{\partial z} = 0 . \quad (16.356)$$

The non-collinear nature of \mathbf{B} results in the *drift* of the cyclotron orbits. Nevertheless, if the field \mathbf{B} felt by the particle varies slowly on the time scale $T = 2\pi/\omega_c$, then the system possesses an adiabatic invariant:

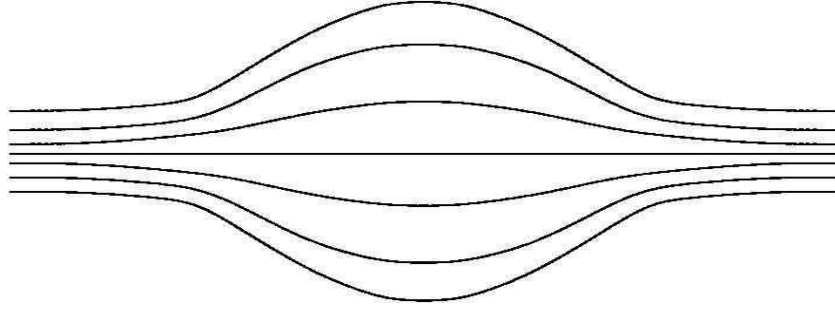
$$J = \frac{1}{2\pi} \oint_C \mathbf{p} \cdot d\boldsymbol{\ell} = \frac{1}{2\pi} \oint_C (m\mathbf{v} + \frac{e}{c} \mathbf{A}) \cdot d\boldsymbol{\ell} \quad (16.357)$$

$$= \frac{m}{2\pi} \oint_C \mathbf{v} \cdot d\boldsymbol{\ell} + \frac{e}{2\pi c} \oint_{\text{int}(C)} \mathbf{B} \cdot \hat{\mathbf{n}} d\Sigma . \quad (16.358)$$

The last two terms are of opposite sign, and one has

$$J = -\frac{m}{2\pi} \cdot \frac{\rho e B_z}{mc} \cdot 2\pi\rho + \frac{e}{2\pi c} \cdot B_z \cdot \pi\rho^2 \quad (16.359)$$

$$= -\frac{eB_z\rho^2}{2c} = -\frac{e}{2\pi c} \cdot \Phi_B(C) = -\frac{m^2 v_{\perp}^2 c}{2eB_z} , \quad (16.360)$$

Figure 16.7: \mathbf{B} field lines in a magnetic bottle.

where $\Phi_B(\mathcal{C})$ is the magnetic flux enclosed by \mathcal{C} .

The energy is

$$E = \frac{1}{2}mv_{\perp}^2 + \frac{1}{2}mv_z^2, \quad (16.361)$$

hence we have

$$v_z = \sqrt{\frac{2}{m}(E - MB)}. \quad (16.362)$$

where

$$M \equiv -\frac{e}{mc} J = \frac{e^2}{2\pi mc^2} \Phi_B(\mathcal{C}) \quad (16.363)$$

is the *magnetic moment*. Note that v_z vanishes when $B = B_{\max} = E/M$. When this limit is reached, the particle turns around. This is a *magnetic mirror*. A pair of magnetic mirrors may be used to confine charged particles in a *magnetic bottle*, depicted in fig. 16.7.

Let $v_{\parallel,0}$, $v_{\perp,0}$, and $B_{\parallel,0}$ be the longitudinal particle velocity, transverse particle velocity, and longitudinal component of the magnetic field, respectively, at the point of injection. Our two conservation laws (J and E) guarantee

$$v_{\parallel}^2(z) + v_{\perp}^2(z) = v_{\parallel,0}^2 + v_{\perp,0}^2 \quad (16.364)$$

$$\frac{v_{\perp}(z)^2}{B_{\parallel}(z)} = \frac{v_{\perp,0}^2}{B_{\parallel,0}}. \quad (16.365)$$

This leads to reflection at a longitudinal coordinate z^* , where

$$B_{\parallel}(z^*) = B_{\parallel,0} \sqrt{1 + \frac{v_{\parallel,0}^2}{v_{\perp,0}^2}}. \quad (16.366)$$

The physics is quite similar to that of the mechanical mirror.

16.10.3 Resonances

When $n > 1$, we have

$$j^\alpha = -i\lambda \sum_m m^\alpha \frac{\partial S_m(J; \lambda)}{\partial \lambda} e^{im \cdot \phi} \quad (16.367)$$

$$\Delta J = -i \sum_m m^\alpha \int_{-\infty}^{\infty} dt \frac{\partial S_m(J; \lambda)}{\partial \lambda} \frac{d\lambda}{dt} e^{im \cdot \nu t} e^{im \cdot \beta} . \quad (16.368)$$

Therefore, when $\mathbf{m} \cdot \boldsymbol{\nu}(J) = 0$ we have a resonance, and the integral grows linearly with time – a violation of the adiabatic invariance of J^α .

16.11 Appendix : Canonical Perturbation Theory

Consider the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 q^2 + \frac{1}{3}\epsilon m\omega_0^2 \frac{q^3}{a} ,$$

where ϵ is a small dimensionless parameter.

(a) Show that the oscillation frequency satisfies $\nu(J) = \omega_0 + \mathcal{O}(\epsilon^2)$. That is, show that the first order (in ϵ) frequency shift vanishes.

Solution: It is good to recall the basic formulae

$$q = \sqrt{\frac{2J_0}{m\omega_0}} \sin \phi_0 \quad , \quad p = \sqrt{2m\omega_0 J_0} \cos \phi_0 \quad (16.369)$$

as well as the results

$$J_0 = \frac{\partial S}{\partial \phi_0} = J + \epsilon \frac{\partial S_1}{\partial \phi_0} + \epsilon^2 \frac{\partial S_2}{\partial \phi_0} + \dots \quad (16.370)$$

$$\phi = \frac{\partial S}{\partial J} = \phi_0 + \epsilon \frac{\partial S_1}{\partial J} + \epsilon^2 \frac{\partial S_2}{\partial J} + \dots , \quad (16.371)$$

and

$$E_0(J) = \tilde{H}_0(J) \quad (16.372)$$

$$E_1(J) = \tilde{H}_1(\phi_0, J) + \frac{\partial \tilde{H}_0}{\partial J} \frac{\partial S_1}{\partial \phi_0} \quad (16.373)$$

$$E_2(J) = \frac{\partial \tilde{H}_0}{\partial J} \frac{\partial S_2}{\partial \phi_0} + \frac{1}{2} \frac{\partial^2 \tilde{H}_0}{\partial J^2} \left(\frac{\partial S_1}{\partial \phi_0} \right)^2 + \frac{\partial \tilde{H}_1}{\partial J} \frac{\partial S_1}{\partial \phi_0} . \quad (16.374)$$

Expressed in action-angle variables,

$$\tilde{H}_0(\phi_0, J) = \omega_0 J \quad (16.375)$$

$$\tilde{H}_1(\phi_0, J) = \frac{2}{3} \sqrt{\frac{2\omega_0}{ma^2}} J^{3/2} \sin^3 \phi_0 . \quad (16.376)$$

Thus, $\nu_0 = \frac{\partial \tilde{H}_0}{\partial J} = \omega_0$.

Averaging the equation for $E_1(J)$ yields

$$E_1(J) = \langle \tilde{H}_1(\phi_0, J) \rangle = \frac{2}{3} \sqrt{\frac{2\omega_0}{ma^2}} J^{3/2} \langle \sin^3 \phi_0 \rangle = 0 . \quad (16.377)$$

(b) Compute the frequency shift $\nu(J)$ to second order in ϵ .

Solution : From the equation for E_1 , we also obtain

$$\frac{\partial S_1}{\partial \phi_0} = \frac{1}{\nu_0} \left(\langle \tilde{H}_1 \rangle - \tilde{H}_1 \right) . \quad (16.378)$$

Inserting this into the equation for $E_2(J)$ and averaging then yields

$$E_2(J) = \frac{1}{\nu_0} \left\langle \frac{\partial \tilde{H}_1}{\partial J} \left(\langle \tilde{H}_1 \rangle - \tilde{H}_1 \right) \right\rangle = -\frac{1}{\nu_0} \left\langle \tilde{H}_1 \frac{\partial \tilde{H}_1}{\partial J} \right\rangle \quad (16.379)$$

$$= -\frac{4\nu_0 J^2}{3ma^2} \langle \sin^6 \phi_0 \rangle \quad (16.380)$$

In computing the average of $\sin^6 \phi_0$, it is good to recall the binomial theorem, or the Fibonacci tree. The sixth order coefficients are easily found to be $\{1, 6, 15, 20, 15, 6, 1\}$, whence

$$\sin^6 \phi_0 = \frac{1}{(2i)^6} (e^{i\phi_0} - e^{-i\phi_0})^6 \quad (16.381)$$

$$= \frac{1}{64} (-2 \sin 6\phi_0 + 12 \sin 4\phi_0 - 30 \sin 2\phi_0 + 20) . \quad (16.382)$$

Thus,

$$\langle \sin^6 \phi_0 \rangle = \frac{5}{16} , \quad (16.383)$$

whence

$$E(J) = \omega_0 J - \frac{5}{12} \epsilon^2 \frac{J^2}{ma^2} \quad (16.384)$$

and

$$\nu(J) = \frac{\partial E}{\partial J} = \omega_0 - \frac{5}{6} \epsilon^2 \frac{J}{ma^2} . \quad (16.385)$$

(c) Find $q(t)$ to order ϵ . Your result should be finite for all times.

Solution : From the equation for $E_1(J)$, we have

$$\frac{\partial S_1}{\partial \phi_0} = -\frac{2}{3} \sqrt{\frac{2J^3}{m\omega_0 a^2}} \sin^3 \phi_0 . \quad (16.386)$$

Integrating, we obtain

$$S_1(\phi_0, J) = \frac{2}{3} \sqrt{\frac{2J^3}{m\omega_0 a^2}} \left(\cos \phi_0 - \frac{1}{3} \cos^3 \phi_0 \right) \quad (16.387)$$

$$= \frac{J^{3/2}}{\sqrt{2m\omega_0 a^2}} \left(\cos \phi_0 - \frac{1}{9} \cos 3\phi_0 \right) . \quad (16.388)$$

Thus, with

$$S(\phi_0, J) = \phi_0 J + \epsilon S_1(\phi_0, J) + \dots , \quad (16.389)$$

we have

$$\phi = \frac{\partial S}{\partial J} = \phi_0 + \frac{3}{2} \frac{\epsilon J^{1/2}}{\sqrt{2m\omega_0 a^2}} \left(\cos \phi_0 - \frac{1}{9} \cos 3\phi_0 \right) \quad (16.390)$$

$$J_0 = \frac{\partial S}{\partial \phi_0} = J - \frac{\epsilon J^{3/2}}{\sqrt{2m\omega_0 a^2}} \left(\sin \phi_0 - \frac{1}{3} \sin 3\phi_0 \right) . \quad (16.391)$$

Inverting, we may write ϕ_0 and J_0 in terms of ϕ and J :

$$\phi_0 = \phi + \frac{3}{2} \frac{\epsilon J^{1/2}}{\sqrt{2m\omega_0 a^2}} \left(\frac{1}{9} \cos 3\phi - \cos \phi \right) \quad (16.392)$$

$$J_0 = J + \frac{\epsilon J^{3/2}}{\sqrt{2m\omega_0 a^2}} \left(\frac{1}{3} \sin 3\phi - \sin \phi \right) . \quad (16.393)$$

Thus,

$$q(t) = \sqrt{\frac{2J_0}{m\omega_0}} \sin \phi_0 \quad (16.394)$$

$$= \sqrt{\frac{2J}{m\omega_0}} \sin \phi \cdot \left(1 + \frac{\delta J}{2J} + \dots \right) \left(\sin \phi + \delta \phi \cos \phi + \dots \right) \quad (16.395)$$

$$= \sqrt{\frac{2J}{m\omega_0}} \sin \phi - \frac{\epsilon J}{m\omega_0 a} \left(1 + \frac{1}{3} \cos 2\phi \right) + \mathcal{O}(\epsilon^2) , \quad (16.396)$$

with

$$\phi(t) = \phi(0) + \nu(J) t . \quad (16.397)$$