Chapter 9

Hamilton-Jacobi equations. Poisson brackets. Canonical Transformations

9.1 Hamilton-Jacobi equations

We have stated from the beginning that the general action priniciple is

$$\delta W = G_1 - G_2, \quad G = \sum_a p_a \delta q_a - H\delta t, \tag{9.1}$$

where the generators arise from the endpoint variations. Suppose we now regard the end time $t_1 = t$ to be a variable, and that the action is a function of that time and of the dynamical variables at that time, $q_a(t) = q_a$, $p_a(t) = p_a$,

$$W = W(q_a, p_a, t). \tag{9.2}$$

From the above generator statement,

$$\frac{\partial W}{\partial t} = -H(q_a, p_q, t), \quad \frac{\partial W}{\partial q_a} = p_a, \tag{9.3}$$

so if these equations are combined, we obtain

$$\frac{\partial W}{\partial t} + H\left(q_a, \frac{\partial W}{\partial q_a}, t\right) = 0. \tag{9.4}$$

This is the Hamilton-Jacobi equation. (W is conventionally called S.)

For a system with s degrees of freedom, there are $s+1$ arbitrary constants of integration. (A "complete integral" contains as many arbitrary constants as there are variables.) Because the Hamilton-Jacobi equation involves only derivatives of the action, one of them must be an additive constant, so we may write

$$W = f(q_1, q_2, \ldots, q_s; \alpha_1, \alpha_2, \ldots, \alpha_s; t) + A, \tag{9.5}$$

where the αs are the remaining constants of integration. Then, we define new constants β_a by

$$\frac{\partial W}{\partial \alpha_a} = \beta_a. \tag{9.6}$$

This equation, together with

$$\frac{\partial W}{\partial q_a} = p_a, \tag{9.7}$$

allows us to completely solve the problem.

Let us illustrate this in the simple case of a one-dimensional harmonic oscillator, described by the Lagrangian

$$L = \frac{m}{2}\dot{q}^2 - \frac{k}{2}q^2, \tag{9.8}$$

and the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}kq^2. \tag{9.9}$$

The Hamilton-Jacobi equation now reads

$$\frac{\partial W}{\partial t} + \frac{1}{2m}\left(\frac{\partial W}{\partial q}\right)^2 + \frac{k}{2}q^2 = 0. \tag{9.10}$$

Since the Hamiltonian in this case possesses no explicit time dependence, $\partial W/\partial t$ must be a constant,

$$\frac{d}{dt}\left(\frac{\partial W}{\partial t}\right) = -\frac{dH}{dt} = -\frac{\partial H}{\partial t} = 0, \tag{9.11}$$

which constant, naturally, we will $-E$. Then the Hamilton-Jacobi equation implies

$$\frac{\partial W}{\partial q} = \sqrt{2m\left(E - \frac{k}{2}q^2\right)}. \tag{9.12}$$

This can be explicitly integrated,

$$W = -Et + \frac{q}{2}\sqrt{1 - \frac{k}{2E}q^2} + \frac{1}{2}\sqrt{\frac{2E}{k}}\arcsin\left(\sqrt{\frac{k}{2E}}q\right), \tag{9.13}$$

but this is not necessary because only derivatives of the action are required. In fact we now use Eq. (9.6) to write

$$\beta = \frac{\partial W}{\partial E} = -t + m\int dq \frac{1}{\sqrt{2m\left(E - \frac{k}{2}q^2\right)}} = -t + \sqrt{\frac{m}{k}}\arcsin\sqrt{\frac{k}{2E}}q, \tag{9.14}$$

which is instantly inverted to

$$q = \sqrt{\frac{2E}{k}} \sin \sqrt{\frac{k}{m}}(\beta + t), \tag{9.15}$$

so we see β defines the amplitude at $t = 0$ (specifies the phase of the sinusoidal motion), and then from the remaining equation (9.7) we get

$$p = \frac{\partial W}{\partial q} = \sqrt{2m\left(E - \frac{k}{2}q^2\right)} = \sqrt{2mE}\cos\sqrt{\frac{k}{m}}(\beta + t), \tag{9.16}$$

as expected. Evidently E is indeed the conserved energy

$$E = \frac{1}{2m}p^2 + \frac{k}{2}q^2. \tag{9.17}$$

9.2 Poisson brackets

For any two functions of dynamical variables, $f(\{q_a\}, \{p_a\}, t)$, $g(\{q_a\}, \{p_a\}, t)$, the Poisson bracket is defined by (there are variations in notation and sign)

$$\{f, g\} = \sum_a \left(\frac{\partial f}{\partial p_a}\frac{\partial g}{\partial q_a} - \frac{\partial f}{\partial q_a}\frac{\partial g}{\partial p_a} \right). \tag{9.18}$$

We see immediately that

$$\{q_a, q_b\} = \{p_a, p_b\} = 0, \quad \{p_a, q_b\} = \delta_{ab}. \tag{9.19}$$

Moreover,

$$\{q_a, f\} = -\frac{\partial f}{\partial p_a}, \quad \{p_a, f\} = \frac{\partial f}{\partial q_a}, \tag{9.20}$$

and so, from Hamilton's equations,

$$\{H, q_a\} = \dot{q}_a, \quad \{H, p_a\} = \dot{p}_a. \tag{9.21}$$

It follows that

$$\{H, f\} = \sum_a \left(\frac{\partial f}{\partial p_a}\dot{p}_a + \frac{\partial f}{\partial q_a}\dot{q}_a \right) = \frac{df}{dt} - \frac{\partial f}{\partial t}, \tag{9.22}$$

or

$$\frac{d}{dt}f = \frac{\partial}{\partial t}f + \{H, f\}. \tag{9.23}$$

The properties of the Poisson bracket are mostly quite obvious: It is antisymmetric,

$$\{f, g\} = -\{g, f\}, \tag{9.24a}$$

the Poisson bracket with a constant vanishes,

$$\{f, c\} = 0, \tag{9.24b}$$

it is linear in the first and second argument,

$$\{f+\lambda g, h\} = \{f, h\} + \lambda\{g, h\}, \tag{9.24c}$$

it satisfies Leibnitz' product rule in the sense

$$\{fg, h\} = f\{g, h\} + \{f, h\}g, \tag{9.24d}$$

and it satisfies Jacobi's identity,

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0. \tag{9.24e}$$

A proof of the latter is given in Landau and Lifshitz.

The total derivative of a Poisson bracket is also distributive:

$$\begin{aligned}
\frac{d}{dt}\{f, g\} &= \frac{\partial}{\partial t}\{f, g\} + \{H, \{f, g\}\} \\
&= \left\{\frac{\partial f}{\partial t}, g\right\} + \left\{f, \frac{\partial g}{\partial t}\right\} - \{f, \{g, H\}\} - \{g, \{H, f\}\} \\
&= \left\{\frac{\partial f}{\partial t} + \{H, f\}, g\right\} + \left\{f, \left\{\frac{\partial g}{\partial t} + \{H, g\}\right\}\right\} \\
&= \left\{\frac{df}{dt}, g\right\} + \left\{f, \frac{dg}{dt}\right\}.
\end{aligned} \tag{9.25}$$

The latter means if f and g are both constants of the motion, so is their Poisson bracket. This can be a useful way to construct constants of the motion.

Perhaps the most important aspect of the Poisson bracket is that it makes an easy transition to quantum mechanics, where it becomes the commutator:

$$\{\ ,\ \} \to \frac{i}{\hbar}[\ ,\ ], \tag{9.26}$$

where for operators corresponding to physical observables,

$$[A, B] = AB - BA. \tag{9.27}$$

Thus we recognize

$$\{q_a, p_b\} = -\delta_{ab} \Rightarrow [q_a, p_b] = i\hbar\delta_{ab}, \tag{9.28}$$

and all the above properties for the Poisson brackets pass over to corresponding properties of the commutators, including the Jacobi identity.

9.3 Canonical Transformations

A *point transformation* is just a change in coordinates,

$$\{q_a\}_{a=1}^s \to \{Q_a(\{q_b\}, t)\}_{a=1}^s. \tag{9.29}$$

This does not alter the form of either Lagrange's or Hamilton's equations.

We want to consider a more general transformation,

$$Q_a = Q_a(\{q\},\{p\},t), \quad P_a = P_a(\{q\},\{p\},t), \tag{9.30}$$

which we will call *canonical* if Hamilton's equations still hold, that it, there is a transformed Hamiltonian H', a function of the new coordinates and momenta, $H'(\{Q\},\{P\},t)$, such that

$$\dot{Q}_a = \frac{\partial H'}{\partial P_a}, \quad \dot{P}_a = -\frac{\partial H'}{\partial Q_a}. \tag{9.31}$$

What's required for this to be true is seen from the action principle, which in terms of the old and new coordinates reads

$$\delta \int \left(\sum_a p_a dq_a\right) - H dt = G_1 - G_2, \quad \delta \int \left(\sum_a P_a dQ_a\right) - H' dt = G_1' - G_2', \tag{9.32}$$

and the requirement that these be equivalent entails

$$\sum_a (p_a dq_a - P_a dQ_a) - (H - H')dt = dF. \tag{9.33}$$

Here $F(\{q\},\{p\},t)$ is the *generating function* of the canonical transformation, which shifts the generators,

$$G' = G + \delta F = \sum_a P_a \delta Q_a - H'\delta t, \tag{9.34}$$

and we have

$$p_a = \frac{\partial F}{\partial q_a}, \quad P_a = -\frac{\partial F}{\partial Q_a}, \quad H' = H + \frac{\partial F}{\partial t}. \tag{9.35}$$

If we want $\Phi(\{q\},\{P\},t)$ as the generating function, do a Legendre transformation,

$$d(F + \sum_a P_a Q_a) = d\Phi(\{q\},\{P\},t) = \sum_a (p_a dq_a + Q_a dP_a) + (H' - H)dt, \tag{9.36}$$

so

$$p_a = \frac{\partial \Phi}{\partial q_a}, \quad Q_a = \frac{\partial \Phi}{\partial P_a}, \quad H' = H + \frac{\partial \Phi}{\partial t}. \tag{9.37}$$

Note that if the generating function is independent of time, the Hamiltonian is unchanged, it just needs to be expressed in terms of the new coordinates and momenta, Q_a and P_a.

A simple example of a canonical transformation is

$$Q_a = p_a, \quad P_a = -q_a, \tag{9.38}$$

which is generated by

$$F = \sum_a q_a Q_a. \tag{9.39}$$

This shows there is no real distinction between what we call coordinates and momenta, they are just conjugate dynamical variables.

An important property of a canonical transformation is that it preserves the Poisson bracket,

$$\{f, g\}_{p,q} = \{f, g\}_{P,Q}. \tag{9.40}$$

The proof is straightforward. Consider the time independent case, since the effect of time in the transformation is just parametric. Then by use of the chain rule

$$\begin{aligned}
\{f, g\}_{p,q} &= \sum_a \left(\frac{\partial f}{\partial p_a}\frac{\partial g}{\partial q_a} - \frac{\partial f}{\partial q_a}\frac{\partial g}{\partial p_a}\right) \\
&= \sum_{abc} \Bigg[\left(\frac{\partial f}{\partial P_b}\frac{\partial P_b}{\partial p_a} + \frac{\partial f}{\partial Q_b}\frac{\partial Q_b}{\partial p_a}\right)\left(\frac{\partial g}{\partial P_c}\frac{\partial P_c}{\partial q_a} + \frac{\partial g}{\partial Q_c}\frac{\partial Q_c}{\partial q_a}\right) \\
&\qquad - \left(\frac{\partial f}{\partial P_b}\frac{\partial P_b}{\partial q_a} + \frac{\partial f}{\partial Q_b}\frac{\partial Q_b}{\partial q_a}\right)\left(\frac{\partial g}{\partial P_c}\frac{\partial P_c}{\partial p_a} + \frac{\partial g}{\partial Q_c}\frac{\partial Q_c}{\partial p_a}\right)\Bigg] \\
&= \frac{\partial f}{\partial P_b}\frac{\partial g}{\partial Q_c}\{P_b, Q_c\}_{p,q} + \frac{\partial f}{\partial Q_b}\frac{\partial g}{\partial P_c}\{Q_b, P_c\}_{p,q} \\
&\qquad + \frac{\partial f}{\partial P_b}\frac{\partial g}{\partial P_c}\{P_b, P_c\}_{p,q} + \frac{\partial f}{\partial Q_b}\frac{\partial g}{\partial Q_c}\{Q_b, Q_c\}_{p,q}.
\end{aligned} \tag{9.41}$$

Now if the canonical relations for the new coordinates and momenta hold,

$$\{Q_b, Q_c\}_{p,q} = \{P_b, P_c\}_{p,q} = 0, \quad \{P_b, Q_c\}_{p,q} = \delta_{b,c}, \tag{9.42}$$

which must be true, since the new coordinates and momenta are just as good as the old ones, then it follows that Eq. (9.40) is proved. In other words, the p, q subscripts on the Poisson bracket are unnecessary. The Poisson bracket is an invariant object, defined independently from the coordinate system. The form is invariant. That this is true is fundamentally because the form of the generators is unchanged by a canonical transformation. This is probably most easily seen through the quantum-mechanical correspondence (9.28). The associated commutator is independent of the basis, and the structure of the canonical commutation relations are determined by the generators.[1]

Finally, we note that time evolution is itself a canonical transformation. The dynamical variables at one time q_t, p_t are mapped to the dynamical variables at a later time, $q_{t+\tau}, p_{t+\tau}$. From the action principle, the difference between the generators at the two times is

$$\delta W = G_1 - G_2 = \sum_a ((p_a)_{t+\tau}\delta(q_a)_{t+\tau} - (p_a)_t\delta(q_a)_t) - (H_{t+\tau} - H_t)\delta t. \tag{9.43}$$

[1] For further details, see my book, *Schwinger's Quantum Action Principle* (Springer, 2015).

This is the structure of a canonical transformation, as seen in Eq. (9.33), from which we see that the generating function of this transformtion is the negative of the action, $-W$.

9.4 Axial vector revisited

Let us return to the Coulomb problem, defined by the Hamiltonian

$$H = \frac{p^2}{2m} - \frac{\alpha}{r}, \tag{9.44}$$

Recall that not only is the angular momentum conserved,

$$\dot{\mathbf{L}} = \{H, \mathbf{L}\} = 0, \quad \mathbf{L} = \mathbf{r} \times \mathbf{p}, \tag{9.45}$$

which also says that H is a scalar under rotations, as well as the Hamiltonian,

$$\frac{dH}{dt} = \{H, H\} = 0, \tag{9.46}$$

but there is an additional, independent, conserved quantity which we called the axial vector,

$$\mathbf{A} = \mathbf{v} \times \mathbf{L} - \alpha\hat{\mathbf{r}}. \tag{9.47}$$

Now in homework you proved that

$$\{L_i, r_j\} = -\epsilon_{ijk} r_k, \quad \{L_i, p_j\} = -\epsilon_{ijk} p_k, \tag{9.48}$$

so that for any vector constructed from $\mathbf{r}$ and $\mathbf{p}$ the same form must hold, so, in particular we obtain the Poisson bracket relation for angular momentum

$$\{L_i, L_j\} = -\epsilon_{ijk} L_k. \tag{9.49}$$

The same form must hold true for the axial vector,

$$\{L_i, A_j\} = -\epsilon_{ijk} A_k. \tag{9.50}$$

To complete the story we need to evaluate the Poisson bracket $\{A_i, A_j\}$. To this end, we first note that

$$\begin{aligned} A^2 &= (\mathbf{v} \times \mathbf{L}) \cdot (\mathbf{v} \times \mathbf{L}) - 2\alpha \mathbf{L} \cdot \hat{\mathbf{r}} \times \mathbf{v} + \alpha^2 = v^2 L^2 - \frac{2\alpha}{mr} L^2 + \alpha^2 \\ &= \frac{2}{m} H L^2 + \alpha^2. \end{aligned} \tag{9.51}$$

(Incidentally, if we consider a circular orbit so that $\mathbf{A} = 0$ (why?), this implies

$$H = -\frac{m\alpha^2}{2L^2}, \tag{9.52}$$

which if we import from quantum mechanics the notion that angular momentum is quantized, $L = n\hbar$, $\hbar$ being Planck's constant, we get Bohr's formula for the energy levels of the hydrogenic atom,

$$E_n = -\frac{mZ^2e^4}{2n^2\hbar^2}.) \tag{9.53}$$

Now in spite of its name, $\mathbf{A}$ is a polar vector, while $\mathbf{L}$ is an axial vector, meaning that under a spatial reflection, $\mathbf{r} \to -\mathbf{r}$, $\mathbf{p} \to -\mathbf{p}$,

$$\mathbf{A} \to -\mathbf{A}, \quad \mathbf{L} \to \mathbf{L}, \tag{9.54}$$

and therefore the form of the desired Poisson bracket is

$$\{A_i, A_j\} = C\epsilon_{ijk}L_k. \tag{9.55}$$

So all we must do is determine the constant C. We can compute $\{\mathbf{A}, A^2\}$ in two ways. On the one hand,

$$\begin{aligned}\{A_x, A^2\} &= \{A_x, A_y^2 + A_z^2\} = 2\{A_x, A_y\}A_y + 2\{A_x, A_z\}A_z \\ &= 2C(L_zA_y - L_yA_z).\end{aligned} \tag{9.56}$$

But using Eq. (9.51) we can also write

$$\begin{aligned}\{A_x, A^2\} &= \frac{2}{m}H\{A_x, L^2\} = \frac{2H}{m}\left(2\{A_x, L_x\}L_x + 2\{A_x, L_y\}L_y + 2\{A_x, L_z\}L_z\right) \\ &= -\frac{4H}{m}(A_zL_y - A_yL_z),\end{aligned} \tag{9.57}$$

so by comparing with Eq. (9.56) we have

$$C = \frac{2H}{m}, \tag{9.58}$$

which is negative for a bound state ($H < 0$). Therefore we conclude that

$$\{A_x, A_y\} = \frac{2H}{m}L_z, \tag{9.59}$$

or, generally,

$$\{A_i, A_j\} = \frac{2H}{m}\epsilon_{ijk}L_k. \tag{9.60}$$

Now we can present this result in another way, if we define

$$\mathbf{J}^{(\pm)} = \frac{1}{2}\left(\mathbf{L} \pm \sqrt{\frac{m}{-2H}}\mathbf{A}\right). \tag{9.61}$$

We see immediately that

$$\{J_x^{(\pm)}, J_y^{(\pm)}\} = -\frac{1}{2}\left(L_z \pm \sqrt{\frac{m}{-2H}}A_z\right) = -J_z^{(\pm)}, \tag{9.62}$$

while

$$\{J_x^{(\pm)}, J_y^{(\mp)}\} = 0. \tag{9.63}$$

So $\mathbf{J}^{(\pm)}$ constitute two independent angular momenta. Thus the symmetry group of the hydrogen atom is not the two-dimensionic rotation group, $O_3 \cong SU_2$ but $O_3 \times O_3 \cong SU_2 \times SU_2 \cong O_4$.

9.5 Problems for Chapter 9

1. Important in classical statistical mechanics is the concept of phase space. If we have a system of s degrees of freedom, described by $\{q_a\}_{a=1}^s$, $\{p_a\}_{a=1}^s$, the element of phase space is defined by

$$d\Gamma = dp_1 \dots dp_s dq_1 \dots dq_s. \tag{9.64}$$

The total phase space of the system is just the integral of this:

$$\Gamma = \int d\Gamma. \tag{9.65}$$

Show that this integral is invariant under a canonical transformation. You may follow the argument given in Landau and Lifshitz, Sec. 46, but then you must supply the details. Then, in view of the above remarks, show that as the system evolves in time, the total phase-space volume is preserved.