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5.6 Liouville's theorem

The formalism and results we've developed allow us to now prove easily the following result. Consider a region $V \subseteq \mathcal{P}$ in phase space. Its volume is

$$\text{vol}(V) = \int_V dq_1 \cdots dq_n dp_1 \cdots dp_n . \quad (5.102)$$

Now consider a map from phase space to itself which in coordinates is described by $\mathbf{q} \rightarrow \mathbf{Q} = \mathbf{Q}(\mathbf{q}, \mathbf{p}, t)$, $\mathbf{p} \rightarrow \mathbf{P} = \mathbf{P}(\mathbf{q}, \mathbf{p}, t)$. Under this map the region V transforms to another region \tilde{V} with volume

$$\text{vol}(\tilde{V}) = \int_{\tilde{V}} dQ_1 \cdots dQ_n dP_1 \cdots dP_n . \quad (5.103)$$

If the map is a *canonical transformation* then the volume is *preserved*, i.e. $\text{vol}(V) = \text{vol}(\tilde{V})$. This is straightforward to see using the symplectic property of canonical transformations. Writing $(y_1, \dots, y_{2n}) = (q_1, \dots, q_n, p_1, \dots, p_n)$, $(Y_1, \dots, Y_{2n}) = (Q_1, \dots, Q_n, P_1, \dots, P_n)$, the transformed volume integral may be written as

$$\text{vol}(\tilde{V}) = \int_{\tilde{V}} dY_1 \cdots dY_{2n} = \int_V |\det \mathcal{J}| dy_1 \cdots dy_{2n} , \quad (5.104)$$

where $\mathcal{J}_{\alpha\beta} = \partial Y_\alpha / \partial y_\beta$ is the Jacobian matrix. But the symplectic condition (5.54) immediately implies that $(\det \mathcal{J})^2 = 1$, and thus $|\det \mathcal{J}| = 1$. We thus conclude that $\text{vol}(\tilde{V}) = \text{vol}(V)$.

Recall that we may regard Hamiltonian flow as a one-parameter family of maps from phase space to itself, parametrized by time t . Thus $(\mathbf{q}, \mathbf{p}) = (\mathbf{q}(0), \mathbf{p}(0)) \rightarrow (\mathbf{Q}, \mathbf{P}) = (\mathbf{q}(t), \mathbf{p}(t))$. If one chooses a region $V = V(0) \subseteq \mathcal{P}$ at time $t = 0$ then under Hamiltonian flow this region will change shape to $V(t) \subseteq \mathcal{P}$. Since we showed in the last subsection that Hamiltonian flow is a canonical transformation for all t , we have thus proven

Liouville's Theorem: The volume of any region in phase space is invariant under Hamiltonian evolution.

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In other words, $\frac{d}{dt}V = 0$.

The physical applications of this result take us in the direction of statistical physics. So far we've been describing the classical mechanics of a single particle, or more precisely the single "quasi-particle" described at the end of section 2.1. This traces out a single curve in phase space under Hamiltonian evolution. But we might instead want to think about a system with many such particles, each of which is described by the same Hamiltonian – for example, a gas. One is then not interested in keeping track of the individual behaviours of the particles, but rather wants to understand the average behaviour. In this situation we may introduce a *density function* $\rho(\mathbf{q}, \mathbf{p}, t)$ on $\mathcal{P} \times \mathbb{R}$, where the number of particles in a small region of phase space δV centred at $(\mathbf{q}, \mathbf{p}) \in \mathcal{P}$ at time t is $\delta N = \rho(\mathbf{q}, \mathbf{p}, t) \delta V$. The total number of particles is

$$N = \int_{\mathcal{P}} \rho(\mathbf{q}, \mathbf{p}, t) dq_1 \cdots dq_n dp_1 \cdots dp_n, \quad (5.105)$$

which is fixed, *i.e.* we assume that particles are not created or destroyed. In fact the latter is a *local* property. In particular if we follow the Hamiltonian evolution of a small number of particles δN centred at $(\mathbf{q}, \mathbf{p}) = (\mathbf{q}(0), \mathbf{p}(0))$ at time $t = 0$, then this will evolve to $\delta N = \rho(\mathbf{q}(t), \mathbf{p}(t), t) \delta V(t)$ at a later time t . Since particles are not created or destroyed, δN must be independent of time t . But we've also shown that $\delta V(t) = \delta V(0)$ is also independent of time. We thus conclude that

$$\frac{d\rho}{dt} = 0, \quad (5.106)$$

holds under Hamiltonian evolution. Using (5.28) we may rewrite this as

$$\{\rho, H\} + \frac{\partial \rho}{\partial t} = 0, \quad (5.107)$$

which is often referred to as *Liouville's equation*. Equation (5.106) says that the density of states is constant along every trajectory in phase space.

5.7 The Hamilton-Jacobi equation

The Hamilton-Jacobi equation provides yet another approach to classical mechanics. Again, it has its own particular advantages – for example, this equation can be useful for finding conserved

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quantities. On a more conceptual level, the Hamilton-Jacobi equation provides a particularly direct link with quantum mechanics and the Schrödinger equation.

We begin by reconsidering the action S , which we discussed briefly in the Hamiltonian formalism in section 5.5, equation (5.92). Recall that the action is extremized over all paths $\mathbf{q}(t)$ with fixed boundary conditions to find the equations of motion. More precisely, let's take the fixed boundary conditions for the paths to be $\mathbf{q}(t_0) = \mathbf{q}^{(0)}$ at time $t = t_0$, and $\mathbf{q}(t_f) = \mathbf{q}^f$ at time $t = t_f$. The action for any path $\mathbf{q}(t)$ satisfying these boundary conditions is

$$S[\mathbf{q}(t)] = \int_{t_0}^{t_f} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) dt, \quad (5.108)$$

and the classical path taken by the system extremizes this, resulting in a (we assume unique) solution $\mathbf{q}(t) = \mathbf{q}^{\text{classical}}(t)$. We now take this classical solution and substitute it back into the action (5.108). Of course doing this we get a number, but that number depends on the fixed final time t_f and fixed final point \mathbf{q}^f . We may then consider varying these final boundary conditions, which defines a function

$$\mathcal{S}(\mathbf{q}^f, t_f) = S[\mathbf{q}^{\text{classical}}(t)]. \quad (5.109)$$

Of course this also depends on the initial time t_0 and initial point $\mathbf{q}^{(0)}$, but we keep these absolutely fixed. Physicists usually refer to the action evaluated on the classical solution as the *on-shell action* (with the words “on-shell” really referring to a notion in special relativity, so this is another physics misnomer).

Now under *any* variation $\delta\mathbf{q}(t)$ of a path we have

$$\delta S = \sum_{a=1}^n \left\{ \int_{t_0}^{t_f} \left[\frac{\partial L}{\partial q_a} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_a} \right) \right] \delta q_a(t) dt + \left[\frac{\partial L}{\partial \dot{q}_a} \delta q_a(t) \right]_{t_0}^{t_f} \right\}. \quad (5.110)$$

If we vary the path so that the initial conditions are fixed, meaning $\delta\mathbf{q}(t_0) = \mathbf{0}$, but at the final point $\delta\mathbf{q}(t_f) = \delta\mathbf{q}^f$, then when (5.110) is evaluated on the classical path solving the Lagrange equations of motion with these boundary conditions we have simply

$$\delta S = \sum_{a=1}^n \left. \frac{\partial L}{\partial \dot{q}_a} \right|_{t=t_f} \delta q_a^f. \quad (5.111)$$

In terms of (5.109) this means that

$$\frac{\partial \mathcal{S}}{\partial \mathbf{q}^f} = \mathbf{p}^f, \quad (5.112)$$

where $\mathbf{p}^f = \partial L / \partial \dot{\mathbf{q}}|_{t=t_f}$ is the final momentum of the classical path. We may similarly consider varying the final time t_f . From the fundamental theorem of calculus

$$\frac{d\mathcal{S}}{dt_f} = L = L(\mathbf{q}^{\text{classical}}(t_f), \dot{\mathbf{q}}^{\text{classical}}(t_f), t_f) = L(\mathbf{q}^f, \dot{\mathbf{q}}^f, t_f), \quad (5.113)$$

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where $\dot{\mathbf{q}}^f$ is the final velocity. On the other hand via the chain rule

$$\frac{d\mathcal{S}}{dt_f} = \frac{\partial \mathcal{S}}{\partial t_f} + \sum_{a=1}^n \frac{\partial \mathcal{S}}{\partial q_a^f} \dot{q}_a^f = \frac{\partial \mathcal{S}}{\partial t} + \sum_{a=1}^n p_a^f \dot{q}_a^f. \quad (5.114)$$

Combining these last two equations we find

$$\frac{\partial \mathcal{S}}{\partial t_f} = L(\mathbf{q}^f, \dot{\mathbf{q}}^f, t_f) - \sum_{a=1}^n p_a^f \dot{q}_a^f = -H(\mathbf{q}^f, \mathbf{p}^f, t_f), \quad (5.115)$$

where $H(\mathbf{q}^f, \mathbf{p}^f, t_f)$ is the Hamiltonian evaluated on the final data.

Now that we have finished varying paths, we relabel the final data as $\mathbf{q}^f \rightarrow \mathbf{q}$, $t_f \rightarrow t$, so that (5.109) defines a function $\mathcal{S}(\mathbf{q}, t)$ on $\mathcal{Q} \times \mathbb{R}$. It is called *Hamilton's principal function*, and we've just shown that it satisfies

$$\frac{\partial \mathcal{S}}{\partial t} + H(\mathbf{q}, \mathbf{p}, t) = 0, \quad \text{where} \quad \mathbf{p} = \frac{\partial \mathcal{S}}{\partial \mathbf{q}}. \quad (5.116)$$

In other words $\mathcal{S}(\mathbf{q}, t)$ satisfies the first order partial differential equation

$$\frac{\partial \mathcal{S}}{\partial t} + H\left(q_1, \dots, q_n, \frac{\partial \mathcal{S}}{\partial q_1}, \dots, \frac{\partial \mathcal{S}}{\partial q_n}, t\right) = 0. \quad (5.117)$$

This is the *Hamilton-Jacobi equation*.

Since we have a single first order PDE in $n + 1$ independent variables, general PDE theory says we should have $n + 1$ constants of integration in the general solution (called a *complete integral*). Notice that one of these constants of integration is easy to identify: \mathcal{S} enters (5.117) only through its partial derivatives, so if $\mathcal{S}(\mathbf{q}, t)$ is a solution then so is $\mathcal{S}(\mathbf{q}, t) + c$ for any constant c . We then write the general solution to (5.117) as

$$\mathcal{S} = \mathcal{S}_0(q_1, \dots, q_n, t; \alpha_1, \dots, \alpha_n) + A, \quad (5.118)$$

where $\alpha_1, \dots, \alpha_n$ and A are the $n + 1$ integration constants.

The equations (5.116) may look familiar from our discussion of generating functions in section 5.5. Indeed, consider a generating function of the second kind $F_2 = F_2(\mathbf{q}, \mathbf{P}, t)$, where (\mathbf{q}, \mathbf{p}) and (\mathbf{Q}, \mathbf{P}) are the old and new coordinates, respectively. As discussed around equation (5.98), this generates the canonical transformation

$$\mathbf{p} = \frac{\partial F_2}{\partial \mathbf{q}}, \quad \mathbf{Q} = \frac{\partial F_2}{\partial \mathbf{P}}, \quad K = H + \frac{\partial F_2}{\partial t}. \quad (5.119)$$

In particular, if we choose our generating function F_2 so that the new Hamiltonian $K = 0$ is identically zero, then in the new coordinates the dynamics is trivial: $\dot{\mathbf{P}} = \mathbf{0} = \dot{\mathbf{Q}}$. The transformed position and momenta are then conserved quantities, and we may write $\mathbf{Q} = \boldsymbol{\beta}$, and $\mathbf{P} = \boldsymbol{\alpha}$, where $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n)$, $\boldsymbol{\beta} = (\beta_1, \dots, \beta_n)$ are altogether $2n$ constants. In particular notice that $F_2 = F_2(\mathbf{q}, \boldsymbol{\alpha}, t)$. Denoting this generating function by $F_2 = \mathcal{S}$, we see that (5.119) are simply the equations (5.116), while the generating function F_2 itself is simply Hamilton's principal function,

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with the conserved momenta $\mathbf{P} = \boldsymbol{\alpha}$ in the new coordinates being interpreted as the integration constants in the general solution (5.118). Moreover, the second equation in (5.119) tells us that

$$\mathbf{Q} = \boldsymbol{\beta} = \frac{\partial \mathcal{S}}{\partial \boldsymbol{\alpha}} \tag{5.120}$$

are also conserved quantities.

What we've done might seem miraculous, so it's perhaps worth taking stock. Given a Hamiltonian function we construct the Hamilton-Jacobi equation (5.117), which is a first order PDE for $\mathcal{S}(\mathbf{q}, t)$ with general solution (5.118) depending on the $n + 1$ integration constants $\alpha_1, \dots, \alpha_n$ and A . We then impose the n algebraic equations (5.120), where $\boldsymbol{\beta}$ are constant. Having done this we may interpret the general solution (5.118) to the Hamilton-Jacobi equation as a generating function of the second kind. This generates a canonical transformation which trivialises the Hamiltonian $K = 0$ in the new coordinates, and where $\boldsymbol{\alpha} = \mathbf{P}$ are interpreted as the conserved momenta in the new coordinates. The constants $\boldsymbol{\beta} = \mathbf{Q}$ are correspondingly the conserved positions in the new coordinates. Since we've solved Hamilton's equations in the new coordinates, via the canonical transformation generated by \mathcal{S} we have also solved Hamilton's equations in the original coordinates. Notice we have $2n$ integration constants in total, as expected.

We can also think of this slightly differently. If one manages to solve the Hamilton-Jacobi equation to find the complete integral (5.118), essentially one has solved half of the dynamical problem. Specifically, this determines the momenta

$$\mathbf{p} = \frac{\partial \mathcal{S}}{\partial \mathbf{q}} \tag{5.121}$$

as a function of \mathbf{q}, t and the integration constants $\boldsymbol{\alpha}$. One can then substitute this into the remaining n Hamilton equations

$$\dot{\mathbf{q}} = \left. \frac{\partial H}{\partial \mathbf{p}} \right|_{\mathbf{p}=\partial \mathcal{S}/\partial \mathbf{q}} . \tag{5.122}$$

These are now n *first order* differential equations for $\mathbf{q}(t)$, giving rise to another n integration constants (again, $2n$ in total). In this approach it's less clear that we have in fact solved Hamilton's equations. But this is easily checked from (5.121):

$$\dot{p}_a = \frac{d}{dt} \left(\frac{\partial \mathcal{S}}{\partial q_a} \right) = \frac{\partial^2 \mathcal{S}}{\partial t \partial q_a} + \sum_{b=1}^n \frac{\partial^2 \mathcal{S}}{\partial q_a \partial q_b} \dot{q}_b . \tag{5.123}$$

On the other hand taking the partial derivative of the Hamilton-Jacobi equation (5.116) with respect to q_a gives

$$\frac{\partial^2 \mathcal{S}}{\partial t \partial q_a} = -\frac{\partial H}{\partial q_a} - \sum_{b=1}^n \frac{\partial H}{\partial p_b} \frac{\partial^2 \mathcal{S}}{\partial q_a \partial q_b} = -\frac{\partial H}{\partial q_a} - \sum_{b=1}^n \frac{\partial^2 \mathcal{S}}{\partial q_a \partial q_b} \dot{q}_b , \tag{5.124}$$

where in the first equality we used (5.121), and in the second equality we used (5.122). Substituting this into (5.123) we thus find

$$\dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}} . \tag{5.125}$$

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When the Hamiltonian is independent of time, so $\partial H/\partial t = 0$, one can solve the time-dependence of the Hamilton-Jacobi equation via

$$\mathcal{S}(\mathbf{q}, t) = W(\mathbf{q}) - Et, \quad (5.126)$$

where E is constant and the time-independent function W on configuration space \mathcal{Q} is sometimes called *Hamilton's characteristic function*. This leads to a reduced Hamilton-Jacobi equation

$$H\left(q_1, \dots, q_n, \frac{\partial W}{\partial q_1}, \dots, \frac{\partial W}{\partial q_n}\right) = E, \quad (5.127)$$

where E is then interpreted as the energy.

Separation of variables

Of course for this approach to be of any practical use, one needs to be able to solve the Hamilton-Jacobi equation (5.117), or in the time-independent setting the slightly easier (5.127). Either way, one has to solve a first order PDE. In general one could proceed via the method of characteristics, but this precisely converts the PDE back into ODEs, *i.e.* effectively Hamilton's equations! However, in certain cases we may solve the PDE via separation of variables. Of course whether or not there are separable solutions will depend both on the Hamiltonian and on the particular coordinates being used: a Hamiltonian may separate in one coordinate system, but not in another. There's a whole theory here, but we'll content ourselves with looking at some examples.

Suppose that the coordinate q_1 and derivative term $\partial_{q_1} \mathcal{S}$ appear in the Hamilton-Jacobi equation only through the combination $f(q_1, \partial_{q_1} \mathcal{S})$, for some function f . That is, the equation can be written in the form

$$\Phi[f(q_1, \partial_{q_1} \mathcal{S}), q_2, \dots, q_n, \partial_{q_2} \mathcal{S}, \dots, \partial_{q_n} \mathcal{S}, t] = 0. \quad (5.128)$$

When then seek a separable solution

$$\mathcal{S}(q_1, \dots, q_n, t) = \tilde{\mathcal{S}}(q_2, \dots, q_n, t) + \mathcal{S}_1(q_1). \quad (5.129)$$

With this ansatz the Hamilton-Jacobi equation (5.128) becomes

$$\Phi\left[f\left(q_1, \frac{d\mathcal{S}_1}{dq_1}\right), q_2, \dots, q_n, \partial_{q_2} \tilde{\mathcal{S}}, \dots, \partial_{q_n} \tilde{\mathcal{S}}, t\right] = 0. \quad (5.130)$$

Since the dependence on q_1 is entirely in the first entry of the function Φ , a solution must satisfy

$$f\left(q_1, \frac{d\mathcal{S}_1}{dq_1}\right) = \alpha_1, \quad (5.131)$$

where α_1 is constant. This is a first order ODE for $\mathcal{S}_1(q_1)$, which may be solved, and substituting $f = \alpha_1$ back into (5.117) the remaining Hamilton-Jacobi equation has one fewer independent variables.

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In some cases one can successively solve for and eliminate all the variables in this way. In particular in the time-independent case (5.127) this means one can solve the Hamilton-Jacobi equation with the ansatz

$$\mathcal{S}(q_1, \dots, q_n, t) = \sum_{a=1}^n \mathcal{S}_a(q_a) - Et, \quad (5.132)$$

where each $\mathcal{S}_a = \mathcal{S}_a(q_a)$ is a function of one variable only, leading to n first order ODEs in one variable. The Hamilton-Jacobi equation is then said to be *completely separable*. This results in n integration constants $\alpha_1, \dots, \alpha_n$, as in (5.118). Notice that $E = E(\alpha_1, \dots, \alpha_n)$ is not an independent integration constant, but rather is determined by substituting the solution $W = \sum_{a=1}^n \mathcal{S}_a(q_a)$ into (5.127).

A special case of the above discussion is an ignorable coordinate, *i.e.* q_1 doesn't appear in the Hamiltonian, $\partial H / \partial q_1 = 0$, and thus doesn't appear in the Hamilton-Jacobi equation either. This means that $f = f(\partial \mathcal{S} / \partial q_1)$ above, and (5.131) integrates to $\mathcal{S}_1(q_1) = \alpha_1 q_1$, giving

$$\mathcal{S}(q_1, \dots, q_n, t) = \tilde{\mathcal{S}}(q_2, \dots, q_n, t) + \alpha_1 q_1. \quad (5.133)$$

Notice then that $p_1 = \partial \mathcal{S} / \partial q_1 = \alpha_1$ is simply the corresponding conserved momenta. Similarly, the $-Et$ term in (5.132) for a time-independent system corresponds to separation of the "ignorable coordinate" t .

Example: We consider the reduced two-body problem Lagrangian

$$L_{\text{reduced}} = \frac{1}{2} \mu (\dot{\varrho}^2 + \varrho^2 \dot{\phi}^2) - V(\varrho), \quad (5.134)$$

describing motion in the plane with polar coordinates (ϱ, ϕ) . The Hamiltonian is

$$H = H(q_1, q_2, p_1, p_2) = \frac{1}{2\mu} \left(p_1^2 + \frac{p_2^2}{q_1^2} \right) + V(q_1), \quad (5.135)$$

where $q_1 = \varrho$, $q_2 = \phi$. The Hamilton-Jacobi equation (5.117) hence reads

$$\frac{\partial \mathcal{S}}{\partial t} + \frac{1}{2\mu} \left(\frac{\partial \mathcal{S}}{\partial q_1} \right)^2 + \frac{1}{2\mu q_1^2} \left(\frac{\partial \mathcal{S}}{\partial q_2} \right)^2 + V(q_1) = 0. \quad (5.136)$$

Since $\partial H / \partial t = 0$ and $\partial H / \partial q_2 = 0$ our general discussion above implies we can separate variables, seeking a solution

$$\mathcal{S}(q_1, q_2, t) = \mathcal{S}_1(q_1) + \mathcal{S}_2(q_2) - Et. \quad (5.137)$$

Substituting this into (5.136) and rearranging slightly gives

$$\left(\frac{d\mathcal{S}_2}{dq_2} \right)^2 = 2\mu q_1^2 \left[E - V(q_1) - \frac{1}{2\mu} \left(\frac{d\mathcal{S}_1}{dq_1} \right)^2 \right]. \quad (5.138)$$

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Since the left hand side depends only on q_2 , while the right hand side depends only on q_1 , both sides must be constant and in particular we may integrate

$$\mathcal{S}_2(q_2) = \alpha_2 q_2, \quad (5.139)$$

with α_2 constant (which is the conserved angular momentum), and (5.138) becomes the first order ODE

$$\frac{d\mathcal{S}_1}{dq_1} = \left(2\mu E - 2\mu V(q_1) - \frac{\alpha_2^2}{q_1^2} \right)^{1/2} \equiv F(q_1; E, \alpha_2). \quad (5.140)$$

We have thus reduced the problem to quadratures, with the final solution to the Hamilton-Jacobi equation being

$$\mathcal{S}(q_1, q_2, t) = -Et + \alpha_2 q_2 + \int^{q_1} F(x; E, \alpha_2) dx. \quad (5.141)$$

There is a trivial additive integration constant from integrating the final ODE. The two non-trivial integration constants are $\alpha_1 = E$ and α_2 .

Recall that to solve Hamilton's equations we must now impose (5.120). This leads to the equations

$$\beta_1 = \frac{\partial \mathcal{S}}{\partial E} = -t + \int^{q_1} \frac{\mu}{F(x; E, \alpha_2)} dx, \quad (5.142)$$

$$\beta_2 = \frac{\partial \mathcal{S}}{\partial \alpha_2} = q_2 - \int^{q_1} \frac{\alpha_2}{x^2 F(x; E, \alpha_2)} dx. \quad (5.143)$$

It may not look like it, but we have in fact solved the equations of motion. To see this in a more familiar guise, recall that in the original variables the energy E is (see equation (2.100))

$$E = \frac{1}{2}\mu\dot{\varrho}^2 + \frac{p_\phi^2}{2\mu\varrho^2} + V(\varrho), \quad (5.144)$$

where $\alpha_2 = p_\phi = \mu\varrho^2\dot{\phi}$. The equations of motion may then be written

$$\dot{\varrho} = \frac{1}{\mu}F(\varrho), \quad \frac{d\phi}{dr} = \frac{\alpha_2}{\varrho^2 F(\varrho)}, \quad (5.145)$$

which integrate to (5.142) and (5.143).

5.8 * Quantum mechanics

We end these lectures with a few further remarks about the relationship between classical mechanics and quantum mechanics. We already briefly described how the principle of least action enters the Feynman formulation of quantum mechanics via the path integral (an integral over all paths) in section 2.6.

Those who have studied quantum mechanics will certainly have recognized the Poisson bracket structure we encountered in section 5.3. This similarity was first noticed by Dirac, who postulated

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that a classical system may be “quantized” by taking the classical Poisson brackets and mapping them to commutator brackets of operators

$$\{f, g\} \longrightarrow -\frac{i}{\hbar}[\hat{f}, \hat{g}] . \quad (5.146)$$

The time evolution then maps as

$$\frac{df}{dt} = \{f, H\} \longrightarrow i\hbar \frac{d\hat{f}}{dt} = [\hat{f}, \hat{H}] , \quad (5.147)$$

which is the equation for the time evolution of an operator in the Heisenberg picture. Of course for all this to make sense to each function f on classical phase space we must associate an operator \hat{f} acting on an appropriate Hilbert space \mathcal{H} of wave functions, so that (5.146) holds. There is a beautiful way to do this, under appropriate conditions, called *geometric quantization*. This mathematically constructs the Hilbert space directly from the phase space, and provides an explicit formula for mapping an appropriate class of classical observables f on phase space to operators \hat{f} acting on \mathcal{H} . The geometric quantization procedure is engineered so that (5.146) and (5.147) then hold for the operators \hat{f} . This is all wonderful – when the method can be applied. But there is no general mathematical procedure called “quantization” that works in all circumstances. On the other hand, from a physics point of view it’s not clear why one would expect there to be.

While the Poisson bracket representation of Hamiltonian mechanics relates to the Heisenberg picture of quantum mechanics, the Hamilton-Jacobi equation relates to the Schrödinger equation. In fact this was one of Schrödinger’s motivations in finding his equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi , \quad (5.148)$$

describing a quantum particle of mass m moving under the influence of a potential V . In the WKB approximation one substitutes the ansatz

$$\psi(\mathbf{q}, t) = A(\mathbf{q}, t, \hbar) \exp \left[\frac{i}{\hbar} \mathcal{S}(\mathbf{q}, t) \right] , \quad (5.149)$$

where A is the real amplitude, and expands in an asymptotic series in \hbar , as we take $\hbar \rightarrow 0$. Substituting this into (5.148) the leading term gives

$$\frac{\partial \mathcal{S}}{\partial t} + H \left(\mathbf{q}, \mathbf{p} = \frac{\partial \mathcal{S}}{\partial \mathbf{q}}, t \right) = 0 , \quad (5.150)$$

where

$$H(\mathbf{q}, \mathbf{p}, t) = \frac{|\mathbf{p}|^2}{2m} + V(\mathbf{q}) , \quad (5.151)$$

is precisely the classical Hamiltonian. Thus the leading behaviour of the Schrödinger equation as $\hbar \rightarrow 0$ is governed by the Hamilton-Jacobi equation, with Hamilton’s principal function $\mathcal{S}(\mathbf{q}, t)$ (which is also the classical action) determining the phase of the wave function.