

1 The Hamilton-Jacobi equation

When we change from old phase space variables to new ones, one equation that we have is

$$K = H + \frac{\partial F}{\partial t} \quad (1)$$

where K is the new Hamiltonian. What would happen if we arrange things so that $K = 0$? Then since the equations of motion for the new phase space variables are given by K

$$\dot{Q} = \frac{\partial K}{\partial P}, \quad \dot{P} = -\frac{\partial K}{\partial Q} \quad (2)$$

we would find that

$$\dot{Q} = 0, \quad \dot{P} = 0 \quad (3)$$

and it would seem that at least in these new coordinates there is no dynamics, nothing seems to move. How can such a thing be possible?

Note that when we change variables, we can make the changes explicitly time dependent. The following are time *independent* canonical transformations

$$Q = p, \quad P = -q, \quad Q = 2q + p^2, \quad P = \frac{p}{2} \quad (4)$$

while the following are time *dependent* ones

$$Q = q + t^2, \quad P = p, \quad Q = \frac{q}{t}, \quad P = p t \quad (5)$$

Note that in taking Poisson brackets, you can treat t as a constant, since Poisson brackets are taken at any given point of time. But the change from old to new coordinates can be made time dependent, as the above examples show.

Now consider the harmonic oscillator. Its solution is

$$q = A \sin(\omega t + \phi) \quad (6)$$

where A, ϕ are constants depending on initial conditions. What happens if we make a new coordinate as

$$Q = q - A_0 \sin(\omega t + \phi_0) \quad (7)$$

where A_0, ϕ_0 are some constants that we choose. Then if we happened to have the motion where the amplitude A equalled A_0 , and the phase ϕ equalled ϕ_0 , then we would find

$$Q = 0 \quad (8)$$

for all time t . So we *can* make coordinate changes where the coordinate does not change with t , even though the system is dynamical: the oscillator is still oscillating, but the way we made the new coordinate Q was such that value q and the *definition* of Q both changed with time in such a way that there was no net change in Q .

But the above example is not yet of the kind that we are after. If we had taken an amplitude $A \neq A_0$ or a phase $\phi \neq \phi_0$ then we would get

$$Q = q - A_0 \sin(\omega t + \phi_0) = A \sin(\omega t + \phi) - A_0 \sin(\omega t + \phi_0) \neq 0 \quad (9)$$

Note that we cannot change our definition of Q away from (7); once we define $Q = Q(q, t)$ we have to stick with that definition. So we see that for general trajectories of the oscillator we have still not managed to make Q constant in time.

Now let us use the other part of phase space, the momentum p . If q is given by (6), then

$$p = m\omega A \cos(\omega t + \phi) \quad (10)$$

We want to get rid of t in our new coordinate, no matter what trajectory the system might take; i.e., no matter what the A, ϕ for the solution be. Note that

$$q^2 + \left(\frac{1}{m\omega}\right)^2 p^2 = A^2 \quad (11)$$

So let us try

$$Q = q^2 + \left(\frac{1}{m\omega}\right)^2 p^2 \quad (12)$$

This is a good definition of a new variable. It turned out to not involve t explicitly; we just had $Q = Q(q, p)$, but that is fine, we got lucky that it worked without t . We see that in any motion, Q will stay a constant. The value of this constant will be different for different motions, since A (the amplitude) will in general be different for different motions. But this is a good thing, since we want to have Q as a phase space variable; different values of Q *should* try to describe different motions.

We are not done though, since we also have to make our new P . We already have different values of A covered by different choices of Q . We may therefore expect that P should say something about ϕ ; in that case the combination Q, P would be able to tell us both A, ϕ , and that would be enough to specify the dynamics. We note that

$$\frac{q}{p} = \frac{1}{m\omega} \tan(\omega t + \phi) \quad (13)$$

Thus

$$\phi = \tan^{-1}\left[m\omega \frac{q}{p}\right] - \omega t \quad (14)$$

So we can try to write

$$P = \tan^{-1}\left[m\omega \frac{q}{p}\right] - \omega t \quad (15)$$

This time we have $P = P(q, p, t)$, so we see an explicit time dependence. But this new P will be just like the new Q : it will not change with time along the motion, since ϕ is fixed for a given oscillation. P *will* be different for motions with different ϕ , but that is a good thing, since we want P to be a coordinate on phase space and so it should be different for different motions in general.

So we now have new variables Q, P , but we have not checked if they are canonical. We have

$$\{Q, P\} = \frac{\partial Q}{\partial q} \frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p} \frac{\partial P}{\partial q} = -\frac{2}{m\omega} \quad (16)$$

So the transformation is not quite canonical, but since $\{Q, P\}$ came out to be a constant we can easily fix this. We can take

$$Q = q^2 + \left(\frac{1}{m\omega}\right)^2 p^2, \quad P = -\frac{m\omega}{2} \tan^{-1}\left[m\omega \frac{q}{p}\right] + \frac{m\omega^2}{2} t \quad (17)$$

and then we will have

$$\{Q, P\} = 1 \quad (18)$$

So at the end we have canonical variables, $Q(q, p, t), P(q, p, t)$; since they are canonical, their evolution is given by Hamilton's equations with some Hamiltonian K , and we have $K = 0$. This means that Q, P will remain constant during the evolution, and we have explicitly seen that this will be so.

2 The geometric picture

But why have we taken the trouble to do all this, and what is the geometric picture of the new Q, P ?

Imagine that we plot the trajectories of the system in q, p, t space. This implies that someone has solved the dynamics completely, and then given us $q(t), p(t)$ for all possible initial conditions. Now we look at this whole set up and ask if we want some new coordinates to describe the evolution.

Take any given time $t = t_0$. Each dynamical trajectory passes through some point q, p in the $t = t_0$ plane. At this plane, let us take each trajectory and give it a 'tag'; i.e., we label it with a pair of numbers which we call Q, P . The trajectory will carry this tag with it through its entire evolution. Thus at a later time t the trajectory will be at a different q, p but it will still carry the same tag Q, P . It can be seen that $Q = Q(q, p, t), P = P(q, p, t)$, with the t dependence being such that it 'cancels' the changes of q, p with time; thus the Q, P are able to stay the same at all times.

Thus Q, P are interesting coordinates of the kind that we made in the above section. Thus we can interpret the coordinates we made in the last section as a set of tags attached to dynamical trajectories. The coordinates Q, P do not change with time because they are tags for the entire trajectory, and so they will stay the same wherever the trajectory goes.

But we can attach the tags to trajectories in many different ways. Are all these choices of Q, P equally good? In the present geometric discussion we have obtained Q, P that are time independent but we have not yet tried to make sure that they are canonical. Only some choices of tags will be canonical coordinates Q, P ; other will not be. How do we find canonical choices?

3 The Hamilton-Jacobi equation

To find canonical coordinates Q, P it may be helpful to use the idea of generating functions. Let us use $F(q, Q, t)$. Then we will have

$$p = \frac{\partial F}{\partial q}, \quad P = -\frac{\partial F}{\partial Q}, \quad 0 = H + \frac{\partial F}{\partial t} \quad (19)$$

If we know F , we can find the canonical transformation, since the first two equations are two relations for two unknowns Q, P , which can, with some algebra, be expressed in terms of q, p, t . To find F , we can use the last equation. Working with the harmonic oscillator, we have

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 \quad (20)$$

Since we are trying to find $F(q, Q)$, we want to keep our ‘favorite’ variables q, Q in all equations, and remove p, P where ever we see them. We see p in H , and so we remove it by writing $p = \frac{\partial F(q, Q, t)}{\partial q}$. Then we will have the equation

$$\frac{\partial F(q, Q, t)}{\partial t} + \frac{1}{2m} \left(\frac{\partial F(q, Q, t)}{\partial q} \right)^2 + \frac{1}{2}m\omega^2 q^2 = 0 \quad (21)$$

Now it is indeed true that we can find $F(q, Q, t)$, and thus find our required canonical transformation; all we have to do is solve the above equation. But it is a partial differential equation, and so it has a very large number of solutions! In fact, we can choose any form of the function F at $t = 0$

$$F(q, Q, 0) = f(q, Q) \quad (22)$$

and then (21) will find F all other t , thus providing a solution to the problem. When we find Q, P from F , we will pick up this time dependence; we had already seen in the last section that we expect the definitions of these variables to be time dependent.

Let us try to solve (21). The equation involves derivatives in t and q ; the variable Q is more of a spectator. First we see that we can separate the variables q, t by writing

$$F(q, Q, T) = W(q, Q) - V(Q)t \quad (23)$$

We let the t part be simple, since we can see that a first derivative in t will remove t , and there is no t elsewhere in the equation. The variable q is more complicated, since it appears in the potential term as well, so we have left an undetermined function $W(q, Q)$ in F .

Now we get

$$\frac{1}{2m} \left(\frac{\partial W(q, Q)}{\partial q} \right)^2 + \frac{1}{2}m\omega^2 q^2 = V(Q) \quad (24)$$

Note that Q will be one of our canonical coordinates at the end. We are not very particular at this point about exactly which coordinate Q will be, so we might as well choose $\tilde{Q} = V(Q)$ to be our new coordinate. This will simplify the equation

$$\frac{1}{2m} \left(\frac{\partial \tilde{W}(q, \tilde{Q})}{\partial q} \right)^2 + \frac{1}{2}m\omega^2 q^2 = \tilde{Q} \quad (25)$$

where $\tilde{W}(q, \tilde{Q}) = W(q, Q)$. We do not want to carry the symbol tilde along, so for convenience we rewrite variables in (25) to get

$$\frac{1}{2m} \left(\frac{\partial W(q, Q)}{\partial q} \right)^2 + \frac{1}{2} m \omega^2 q^2 = Q \quad (26)$$

We have now used up all our choices of simplifications, and have to work to solve this equation for W . We have

$$\frac{\partial W(q, Q)}{\partial q} = \sqrt{2mQ - m^2 \omega^2 q^2} \quad (27)$$

so that

$$W(q, Q) = \int dq \sqrt{2mQ - m^2 \omega^2 q^2} + g(Q) \quad (28)$$

Since all we want is to get one solution to the equation, we might as well set $g(Q) = 0$ so that

$$W(q, Q) = \int dq \sqrt{2mQ - m^2 \omega^2 q^2} \quad (29)$$

and

$$F(q, Q, t) = \int dq \sqrt{2mQ - m^2 \omega^2 q^2} - Qt \quad (30)$$

Now we can return to our other equations

$$p = \frac{\partial F(q, Q, t)}{\partial q} \quad (31)$$

This is easily solved, since differentiating in q just cancels the integration

$$p = \sqrt{2mQ - m^2 \omega^2 q^2} \quad (32)$$

The other equation is

$$P = -\frac{\partial F(q, Q, t)}{\partial Q} = -m \int \frac{dq}{\sqrt{2mQ - m^2 \omega^2 q^2}} + t \quad (33)$$

Eq. (32) gives

$$Q = \frac{1}{2m} [p^2 + m^2 \omega^2 q^2] \quad (34)$$

This is not so different from (17); it only differs from the Q there by an overall multiplicative constant, which we could have chosen according to our wish anyway. Note however that this time we did not have to get Q by ‘guesswork’; it came from our canonical transformation equation.

Eq. (33) gives

$$P = -\frac{1}{\omega} \sin^{-1} \sqrt{\frac{m \omega^2 q^2}{2Q}} + t \quad (35)$$

Substituting the value of Q found in (34) we get

$$P = -\frac{1}{\omega} \sin^{-1} \frac{m \omega q}{\sqrt{p^2 + m^2 \omega^2 q^2}} + t \quad (36)$$

We can also rewrite this as

$$P = -\frac{1}{\omega} \tan^{-1} \frac{m\omega q}{p} + t \quad (37)$$

This is just like the variable P in (17), after we take into account the different scalings of the Q variable in the two cases.

Thus we see that by using the method of generating functions, we could arrive at the canonical transformation that we needed without guesswork at any stage.

But one may still ask: what was the point of obtaining the new variables Q, P . The answer is, that in doing all this we have solved the dynamical equation of the harmonic oscillator, though we have not yet explicitly realized this. Since the new Hamiltonian $K = 0$, we know that Q, P will be constant in time. From (35) we see that we have an equation that gives q in terms of t , in terms of two constants Q, P . All we have to do is the algebra needed to invert (35). Doing this algebra, we get

$$q = -\sqrt{\frac{2Q}{m\omega^2}} \sin[\omega(P - t)] \quad (38)$$

The two constants Q, P thus give, with some scalings, the amplitude and the phase of the oscillator. Thus we have found the sinusoidal vibrations of the oscillator, complete with its two arbitrary constants of motion, without having explicitly written an equation of the form $\ddot{q} + \omega^2 q = 0$. Of course this was a simple problem, and we already knew the solution. But in a more complicated case, it may well be that the solution obtained by this Hamilton-Jacobi way might be easier than the solution obtained by directly solving the equation of motion.

4 The interpretation of F as the action

We have used the action S to get the dynamics from a variational principle. We asked that S be extremized with q, t held fixed at the endpoints. Once we extremized S , we got the dynamical path, but the *value* of S at this extremum was not of interest to us. Now we will see that this value has an important role. We will also see what happens if we change the endpoints q, t .

Let the dynamical path go from t_0, q_0 to q, t . The action is

$$S = \int_{t_0, q_0}^{t, q} L(q, \dot{q}, t) dt \quad (39)$$

Suppose we change the endpoint from t, q to $t, q + dq$. We had

$$\delta S = \int dt \left[\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right] = \int dt \left[\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \frac{d}{dt} (\delta q) \right] \quad (40)$$

Integration by parts gave

$$\delta S = \int dt \left[\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right] \delta q - \left[\frac{\partial L}{\partial \dot{q}} \delta q \right]_{t_0, q_0} + \left[\frac{\partial L}{\partial \dot{q}} \delta q \right]_{t, q} \quad (41)$$

If our path satisfies the equations of motion then the first term vanishes. We plan to hold fixed the endpoint t_0, q_0 , so the next term vanishes as well. We are holding fixed t , but changing q . So we will write our change as

$$\frac{\partial S}{\partial q} = \frac{\partial L}{\partial \dot{q}}(t) = p(t) \quad (42)$$

Thus we see that if we compute S along the extremized path, then move the endpoint slightly, and again compute S along the new extremized path, then the difference will be given by the momentum at the endpoint which is moved!

This is a remarkable relation, but we have one more such relation to find: we will now move t while keeping q fixed. From the figure drawn in class, we can see that the extra time interval dt contributes an amount $L(t)dt$ to the change δS , but we also find that we must change q at the endpoint by an amount $-\dot{q}dt$. This change will make the action change by

$$\delta S = p\delta q = -p\dot{q}dt \quad (43)$$

Thus the overall change of S is

$$\delta S = -(p\dot{q} - L)dt \quad (44)$$

and we can write

$$\frac{\partial S}{\partial t} = -(p\dot{q} - L) = -H \quad (45)$$

or

$$H + \frac{\partial S}{\partial t} = 0 \quad (46)$$

We now notice something remarkable: the equations (42),(46) are just like the first and third equations in (19), which defined the canonical transformation needed to map the dynamical variables to variables that were time independent (i.e., they labeled dynamical trajectories). In fact these are the two equations that we used to find F and solve for the motion; the last middle equation in (19) just helped us find the variable P that formed a canonical pair with Q . We thus see that S is the generating function that maps the dynamical variables q, p to variables Q, P that remain constant with time; in other words, it finds the ‘tags’ that labels whole dynamical trajectories, and thus solves the dynamical problem.

5 The Schrodinger equation

This equation is

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \quad (47)$$

If we have $H = \frac{p^2}{2m} + V(q)$, then we get

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial q^2} + V(q)\psi \quad (48)$$

Write

$$\psi = e^{i\frac{S}{\hbar}} \quad (49)$$

Such an expansion is used in the WKB approximation where S is real to leading order; at this point we have not said anything about the reality of S , so the above equation is just a mathematical identity. Then we have

$$-\frac{\partial S}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 S}{\partial q^2} + \left(\frac{\partial S}{\partial q}\right)^2 + V(q) \quad (50)$$

If we assume that $\hbar \rightarrow 0$, which is the ‘classical limit’ in quantum mechanics, then we see that

$$-\frac{\partial S}{\partial t} = \left(\frac{\partial S}{\partial q}\right)^2 + V(q) \quad (51)$$

More generally,

$$\frac{\partial S}{\partial t} + H\left(q, \frac{\partial S}{\partial q}\right) = 0 \quad (52)$$

which is just the Hamilton-Jacobi equation. Thus we see that in the classical limit $\hbar \rightarrow 0$ the Schrodinger equation is just the Hamilton-Jacobi equation. The H-J equation was a partial differential equation that could be solved with any choice of function at $t = 0$. This function acts like the wavefunction that we encounter in quantum mechanics. For the H-J equation we will take a real solution S , and thus we will indeed be dropping the \hbar order term from the Schrodinger equation. We will thus have

$$|\psi| = |e^{i\frac{S}{\hbar}}| = 1 \quad (53)$$

so the waveform extends over all space q , not falling off at large q . It looks like a plane fronted wave, and we can ask what the wavelength is. The phase will return to its value after

$$\delta S = 2\pi\hbar \quad (54)$$

This implies

$$\delta q = \left(\frac{\partial S}{\partial q}\right)^{-1} \delta S = \frac{2\pi\hbar}{p} \quad (55)$$

This gives

$$\lambda = \frac{h}{p} \quad (56)$$

which is a familiar equation in quantum mechanics.

6 An example of a H-J problem

Problem Consider a particle of mass m in one dimension with a linear potential $V = kx$. The Lagrangian is therefore

$$L = \frac{1}{2}m\dot{x}^2 - kx$$

The goal of this problem is to solve for the motion of this particle by the Hamilton-Jacobi method. Recall that this method uses a generating function $F_2(q, p', t) \equiv S$ to map the variables q, p to a set of variables q', p' that are constant. The function of type F_2 gives the following canonical transformation relations

$$p = \frac{\partial F_2}{\partial q}, \quad q' = \frac{\partial F_2}{\partial p'}, \quad H' = H + \frac{\partial F_2}{\partial t}$$

(a) Write the Hamilton-Jacobi equation for S .

(b) Write a separation of variables ansatz for S and use this ansatz to find an expression for S (you may not want to solve all the integrals occurring in S).

(c) Use the result of (b) to find the variables q, p explicitly as functions of time, with two free constants appearing in your solution.

Solution :

(a)

$$\frac{1}{2m} \left(\frac{\partial S}{\partial x} \right)^2 + kx + \frac{\partial S}{\partial t} = 0$$

(b)

$$\begin{aligned} S &= -\alpha t + W(x) \\ \frac{1}{2m} \left(\frac{dW}{dx} \right)^2 + kx &= \alpha \\ S &= \int dx \sqrt{2m(\alpha - kx)} - \alpha t \end{aligned}$$

(c)

$$\begin{aligned} \beta &= \int dx m \frac{1}{\sqrt{2m(\alpha - kx)}} - t = -\frac{1}{k} \sqrt{2m(\alpha - kx)} - t \\ x &= -\frac{1}{k} \frac{1}{2m} [k(\beta + t)]^2 + \frac{\alpha}{k} \\ p &= \frac{\partial S}{\partial x} = \sqrt{2m(\alpha - kx)} = -k(\beta + t) \end{aligned}$$

(Sign needs to be checked explicitly.)