PY 421/621 - Advanced Computing in Physics

Lecture notes.

1 Classical limit of the Schrödinger equation.

The path integral formulation of quantum mechanics shows that in the classical limit $\hbar \to 0$ the evolution of the wave function is dominated by trajectories which cluster around a trajectory that makes the action stationary. This is the classical trajectory, which satisfies the Euler-Lagrange equations of motion. We expect therefore that, in the classical limit, the wave function will have a phase of the form

$$e^{\frac{\imath S(x,t)}{\hbar}} \tag{1}$$

where $S(x,t)$ is the classical action. This motivates us to express in general the complex wave function in terms of its amplitude and phase, including an explicit factor of $1/\hbar$ in the phase

$$\psi(x,t) = A(x,t)\, e^{\frac{\imath S(x,t)}{\hbar}} \tag{2}$$

and to reformulate the Schrödinger equation

$$\imath\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \tag{3}$$

as a pair of coupled equations for A and S. Substituting Eq. 2 into Eq. 3 we get

$$\imath\hbar \left[\frac{\partial A(x,t)}{\partial t} + A(x,t) \frac{\imath}{\hbar} \frac{\partial S(x,t)}{\partial t} \right] e^{-\frac{\imath S(x,t)}{\hbar}} =$$
$$-\frac{\hbar^2}{2m} \left[\frac{\partial^2 A(x,t)}{\partial x^2} + 2 \frac{\partial A(x,t)}{\partial x} \frac{\imath}{\hbar} \frac{\partial S(x,t)}{\partial x} + A(x,t) \frac{\imath}{\hbar} \frac{\partial^2 S(x,t)}{\partial x^2} \right.$$
$$\left. + A(x,t) \left(\frac{\imath}{\hbar} \frac{\partial S(x,t)}{\partial x} \right)^2 \right] e^{\frac{\imath S(x,t)}{\hbar}} + V(x) A(x,t)\, e^{\frac{\imath S(x,t)}{\hbar}} \tag{4}$$

Multiplying by $\exp(-\imath S(x,t)/\hbar)$ and comparing real and imaginary parts we get

$$
\begin{aligned}
-A(x,t)\frac{\partial S(x,t)}{\partial t} &= -\frac{\hbar^2}{2m}\frac{\partial^2 A(x,t)}{\partial x^2} + \frac{1}{2m}A(x,t)\left(\frac{\partial S(x,t)}{\partial x}\right)^2 \\
&+ V(x)A(x,t) \qquad (5) \\
\frac{\partial A(x,t)}{\partial t} &= -\frac{1}{m}\frac{\partial A(x,t)}{\partial x}\frac{\partial S(x,t)}{\partial x} - \frac{1}{2m}A(x,t)\frac{\partial^2 A(x,t)}{\partial x^2} \qquad (6)
\end{aligned}
$$

We go to the classical limit by letting $\hbar \to 0$ in these two equations. Equation 5 reduces to an equation for $S(x,t)$ only, namely

$$
-\frac{\partial S(x,t)}{\partial t} = \frac{1}{2m}\left(\frac{\partial S(x,t)}{\partial x}\right)^2 + V(x) \qquad (7)
$$

while the other equation, which does not contain any explicit dependence on $\hbar$, can be taken as an equation for $A(x,t)$ once Eq. 7 has been solved for S.

Equation 7 is the equation of Hamilton-Jacobi of classical mechanics. It is an equation for the stationary action which is obtained by substituting $\partial S(x,t)/\partial x$ for the momentum p in the Hamiltonian $H(x,p) = p^2/(2m) + V(x)$ and equating $-\partial S/\partial t$ to $H(x, \partial S(x,t)/\partial x)$. The replacement $p \to \partial S(x,t)/\partial x$ can be intuitively understood by recalling that the momentum operator of quantum mechanics is $\hat{p} = -\imath\hbar\partial/\partial x$, so that

$$
\hat{p}\, e^{\frac{\imath S(x,t)}{\hbar}} = \frac{\partial S(x,t)}{\partial x}\, e^{\frac{\imath S(x,t)}{\hbar}} \qquad (8)
$$

The equation of Hamilton-Jacobi is the equation for the “geometrical optics” limit of the Schrödinger equation. It should be observed, though, that it was derived from classical mechanics independently and much earlier than the Schrödinger equation. If anything, the fact that the Schrödinger equation reduces to the equation of Hamilton-Jacobi for $\hbar \to 0$ can be taken as a consistency check of the classical limit, and can also be the starting point for semiclassical approximations to quantum mechanics.

2 Bellman’s principle of optimization.

We will derive the equation of Hamilton-Jacobi from the requirement that the classical trajectory gives origin to a stationary action, but in order to better understand the derivation it will be useful to make a digression into a seemingly unrelated field. We want to solve the following industrial problem. We must install a certain number x of machines over a given number n of quarters, and we must find the acquisition strategy, i.e. x_1 machines installed at the end of quarter 1, and then $x_2, x_3 \dots$ up to the final number $x = x_n$, which minimizes the total cost of the procedure. In the calculation of the cost we must fold the following parameters:

- Each machine has a given unit cost c. This will contribute to the total cost a fixed amount cx_n independent of the acquisition strategy, and so we can neglect it.

- There is a penalty for installing several machines during the same term, for example because of the extra cost induced by the crowding of operations. We parametrize this extra cost by $m(\Delta x)^2/2$, where $\Delta x = x_n - x_{n-1}$ is the number of machines installed during the n^{th} quarter. (The reason for the factor of 1/2 will become apparent in the next section.)

- Once the machines have been installed they can be put into production, giving a return proportional to their number, which reduces the total cost. We parametrize this return by $-g(x_n + x_{n-1})/2$. (We use $(x_n + x_{n-1})/2$ as the average number of machines in production during the n^{th} quarter.)

With this, the cost associated to a certain acquisition strategy will be

$$C(x_1, x_2, \dots x_n) = \sum_{i=1,n} \left[\frac{m}{2}(x_i - x_{i-1})^2 - \frac{g}{2}(x_i + x_{i-1}) \right] \tag{9}$$

Let us denote by $S(x_n, n)$ the optimal, i.e. minimal cost for having x_n machines installed at the end of quarter n. Bellman makes the crucial observation that the optimal strategy will be optimal all the way. If the number of machines installed at the end of quarter $n-1$ is x_{n-1}, the cost incurred to install these machines will be $S(x_{n-1}, n-1)$, i.e. the optimal cost, because otherwise we could have reduced the final cost by following an acquisition strategy which reduces the cost sustained for acquiring those x_{n-1} machines. This leads to the following equation for the optimal cost

$$S(x_n, n) = \min_{x_{n-1}} \left[S(x_{n-1}, n-1) + \frac{m}{2}(x_n - x_{n-1})^2 - \frac{g}{2}(x_n + x_{n-1}) \right] \tag{10}$$

where the last two terms in the r.h.s. of the equation represent the cost of adding the final $x_n - x_{n-1}$ machines during the last quarter.

The Bellman equation can be solved by recursion. Staring from $S(0,0) = 0$ we can solve Eq. 10 progressively for $n = 1, 2, \ldots$ to find the optimal costs along the whole acquisition process, and, as a byproduct, also the corresponding numbers of installed machines, i.e. the optimal acquisition strategy. This solution also shows how it is advantageous to focus on the optimal cost, rather then directly on the optimal number of installed machines. The program bhj.f90 implements the solution of Bellman's equations for this particular example.

3 The equation of Hamilton-Jacobi.

We can make contact with classical mechanics by taking the continuum limit of our acquisition process. We take the number of machines installed to be a real number $x(t)$ which varies continuously in time and characterize the acquisition process by the function, or trajectory $x = x(t)$. For the cost itself, we imagine that the total time interval $0 \to t$ is subdivided into n subintervals of equal duration dt and, in order to get a meaningful continuum limit, rescale the parameters m and g by $m \to m/dt$, $g \to g\,dt$. Then the cost of the acquisition trajectory becomes

$$C(x(t)) = \sum_{i=1,n} \left[\frac{m}{2} \frac{(x_i - x_{i-1})^2}{dt} - \frac{g}{2}(x_i + x_{i-1})\, dt \right] \tag{11}$$

which in the limit $dt \to 0$ becomes

$$C(x(t)) = \int \left[\frac{m}{2} \left(\frac{d(x(t)}{dt} \right)^2 - g x(t) \right] dt \tag{12}$$

We recognize in this equation the action associated with the motion along the x-axis of a particle of mass m and subject to a potential $V(x) = gx$.

Let us denote by $S(x,t)$ the minimal action. As a matter of fact the consideration that follow do not require the action to be minimal, but apply also to a stationary action. We will nevertheless use the term "minimal" for convenience of notation. At $t - dt$ the trajectory will be at $x - dx$, with minimal action $S(x - dx, t - dt)$. Bellman's equation, generalized to this continuum process, states that $S(x,t)$ will satisfy the condition

$$S(x,t) = \min_{dx}\left[S(x-dx,t-dt) + \left(\frac{m}{2}\Big(\frac{d(x(t)}{dt}\Big)^2 - gx(t)\right)\right] dt \qquad (13)$$

where the term in square brackets in the r.h.s. represents the contribution to the action coming from part of the trajectory between $t-dt$ and t. The minimum must be taken over all positions $x-dx$ at $t-dt$. It is convenient to parametrize dx in terms of the final velocity v

$$dx = v\,dt \qquad (14)$$

Equation 13 can be reformulated in terms of v

$$S(x,t) = \min_v\left[S(x-v\,dx,t-dt) + \left(\frac{m}{2}v^2 - gx\right) dt\right] \qquad (15)$$

Expanding to first order in dt this becomes

$$S(x,t) = \min_v\left[S(x,t) - \frac{\partial S}{\partial x}v\,dt - \frac{\partial S}{\partial t}\,dt + \left(\frac{m}{2}v^2 - gx\right) dt\right] \qquad (16)$$

or, eliminating $S(x,t)$ first, and then dt from the two sides of the equation

$$0 = \min_v\left[-\frac{\partial S}{\partial x}v - \frac{\partial S}{\partial t} + \left(\frac{m}{2}v^2 - gx\right)\right] \qquad (17)$$

The minimum of the r.h.s. occurs at the value of v which makes the derivative of the r.h.s. with respect to v vanish, namely for

$$v = \frac{1}{m}\frac{\partial S}{\partial x} \qquad (18)$$

Substituting this value into into Eq. 17 we finally get

$$-\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 - \frac{\partial S}{\partial t} - gx = 0 \qquad (19)$$

i.e. the Hamilton-Jacobi Eq. 7 with $V(x) = gx$.

Note that the contribution from the trajectory segment between $t-dt$ and t in Eq. 15, namely $[(m/2)v^2 - gx]\,dt$, is equal to $L(x,v)\,dt$, where $L(x,v)$

is the Lagrangian of the system. This will be true in general. Thus, in the most general case Eq. 17 will take the form

$$0 = \min_v \left[-\frac{\partial S}{\partial x} v - \frac{\partial S}{\partial t} + L(x, v) \right] \tag{20}$$

The minimum will occur for

$$\frac{\partial S}{\partial x} = \frac{\partial L(x, v)}{\partial v} \tag{21}$$

But the r.h.s. of this equation is the momentum p conjugate to the variable x. Thus at the minimum

$$\frac{\partial S}{\partial x} = p \tag{22}$$

Substituting into Eq. 20 we then find

$$-\frac{\partial S}{\partial t} = pv - L(x, v) = H(x, p) \tag{23}$$

where $H(x, p)$ is the Hamiltonian of the system. According to Eq. 22 p must be replaced by $\partial S/\partial x$ and thus we recover the equation of Hamilton-Jacobi in its general form

$$-\frac{\partial S}{\partial t} = H(x, \partial S/\partial x) \tag{24}$$