Hamiltonian formulation

The Lagrangian formalism describes a system by specifying a set of N generalized coordinates q_i and its corresponding time derivative $\dot{q}_i$:

$$\mathcal{L} = \mathcal{L}(q_1, q_2, \ldots, \dot{q}_1, \dot{q}_2, \ldots) \tag{1}$$

From the Lagrangian we then derive a set of N second order equations (the Euler-Lagrange equations).

There is also another formulation of mechanics due to Hamilton which uses instead the N coordinates q_i and their corresponding generalized momenta

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \tag{2}$$

This formulation has several advantages from a formal point of view and is also more convenient to treat complex problems. But most importantly, the Hamiltonian framework is the one in which we usually <u>quantize</u> a theory; ie, where we transform a classical theory into a quantum theory.

To go to a description in terms of q_i and p_i we use the energy of the system

$$E = \sum_i \dot{q}_i p_i - \mathcal{L} \tag{3}$$

but expressed in terms of q_i and p_i; ie, we must invert Eq (2) to express $\dot{q}_i$ as a function of q_i and p_i.

The energy expressed in terms of q_i and p_i is called the Hamiltonian

$$\boxed{H = \sum_i \dot{q}_i p_i - \mathcal{L}} \tag{4}$$

It is a function of $q_1, q_2, \ldots$ and $p_1, p_2, \ldots$.

The operation done in Eq (4) is called a Legendre transformation. You may have seen it before in thermodynamics, when we want to transform the internal energy into enthalpy or free energy.

Let us check that H is indeed a function of q_i and p_i. For this we compute

$$dH = \sum_i \left[(d\dot{q}_i) p_i + \dot{q}_i \, dp_i \right] - d\mathcal{L} \tag{5}$$

But

$$d\mathcal{L} = \sum_i \left\{ \frac{\partial \mathcal{L}}{\partial q_i} dq_i + \frac{\partial \mathcal{L}}{\partial \dot{q}_i} d\dot{q}_i \right\}$$

$$= \sum_i \left\{ \dot{p}_i \, dq_i + p_i \, d\dot{q}_i \right\} \tag{6}$$

Here I used the definition of the generalized momentum, Eq (2), in the second term. And in the first I used the Euler-Lagrange equations

$$\dot{p}_i = \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i} \right) = \frac{\partial \mathcal{L}}{\partial q_i} \tag{7}$$

Substituting (6) in (5) we find

$$dH = \sum_i \left\{ p_i \, d\dot{q}_i + \dot{q}_i \, dp_i - \dot{p}_i \, dq_i - p_i \, d\dot{q}_i \right\}$$

$$dH = \sum_i \left\{ -\dot{p}_i \, dq_i + \dot{q}_i \, dp_i \right\} \tag{8}$$

The term involving $d\dot{q}_i$ vanishes and we indeed find that H is only a function of q_i and p_i. If you are confused, note that to establish on which variables a function depends we have to look at the differentials, not the multiplying coefficients.

In fact, for a function $H(q_i, p_i)$, we have in general

$$dH = \sum_i \left\{ \frac{\partial H}{\partial q_i} \, dq_i + \frac{\partial H}{\partial p_i} \, dp_i \right\} \tag{9}$$

[cf. Eq (6)]. Thus, by comparing (8) and (9) we conclude that

$$\boxed{\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i} \\ \dot{p}_i &= -\frac{\partial H}{\partial q_i} \end{aligned}} \tag{10}$$

These are called the Hamilton's equations of motion. They are equivalent to the Euler-Lagrange equations, but expressed as $2N$ first order equations (instead of N second order ones). Due to their importance they are also called the canonical equations (the word canonical means "important")

The procedure is therefore the following:

1) Obtain $\mathcal{L}$ in terms of q_i and $\dot{q}_i$

2) Compute $p_i = \partial \mathcal{L} / \partial \dot{q}_i$ and invert to find $\dot{q}_i$ in terms of q's and p's

3) Compute the Hamiltonian as $H = \sum_i \dot{q}_i p_i - \mathcal{L}$ and express it as a function of q's and p's (eliminate any $\dot{q}_i$'s).

4) Obtain the canonical equations as $\dot{q}_i = \partial H / \partial p_i$ and $\dot{p}_i = -\partial H / \partial q_i$

Example: cartesian coordinates

$$\mathcal{L} = \frac{1}{2} m (\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - U(x, y, z)$$

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}_i} = m \dot{x}_i \quad \Rightarrow \quad \dot{x}_i = \frac{p_i}{m}$$

$$H = \sum_i \dot{x}_i p_i - \mathcal{L}$$

$$= \frac{p_x^2 + p_y^2 + p_z^2}{m} + \frac{1}{2} m \left(\frac{p_x^2 + p_y^2 + p_z^2}{m^2} \right) + U$$

$$\therefore \quad H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + U(x, y, z)$$

Or, more succinctly,

$$\boxed{H = \frac{p^2}{2m} + U} \qquad (11)$$

Now we use the canonical equations

$$\dot{x}_i = \frac{\partial H}{\partial p_i} = \frac{p_i}{m} \qquad (12)$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} = -\frac{\partial U}{\partial q_i} = F_i$$

We therefore recover the usual results.

Example: spherical coordinates

$$\mathcal{L} = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\dot{\phi}^2\sin^2\theta) - U(r,\phi,\theta) \tag{13}$$

$$p_r = \frac{\partial \mathcal{L}}{\partial \dot{r}} = m\dot{r} \quad \Rightarrow \quad \dot{r} = \frac{p_r}{m}$$

$$p_\theta = \frac{\partial \mathcal{L}}{\partial \dot{\theta}} = mr^2\dot{\theta} \quad \Rightarrow \quad \dot{\theta} = \frac{p_\theta}{mr^2} \tag{14}$$

$$p_\phi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = mr^2\dot{\phi}\sin^2\theta \quad \Rightarrow \quad \dot{\phi} = \frac{p_\phi}{mr^2\sin^2\theta}$$

If you want, you can first compute the energy in terms of q_i and $\dot{q}_i$ and then change from q_i to p_i. For instance, we already know from Euler's theorem on homogeneous functions that

$$E = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\dot{\phi}^2\sin^2\theta) + U \tag{15}$$

Now we substitute (14). When the energy is written in terms of q_i and p_i we call it H:

$$H = \frac{1}{2m}\left\{ p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2\sin^2\theta} \right\} + U \tag{16}$$

We may then obtain the equations of motion

$$\dot{r} = \frac{\partial H}{\partial p_r} = \frac{p_r}{m} \qquad \dot{\theta} = \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{mr^2} \qquad \dot{\phi} = \frac{\partial H}{\partial p_\phi} = \frac{p_\phi}{mr^2\sin^2\theta}$$

which are just (14) again, as expected

The other equations are

$$\dot{p}_r = -\frac{\partial H}{\partial r} = \frac{p_\theta^2}{mr^3} + \frac{p_\phi^2}{mr^3 \sin^2\theta} - \frac{\partial U}{\partial r}$$

$$\dot{p}_\theta = -\frac{\partial H}{\partial \theta} = \frac{p_\phi^2}{mr^2 \sin^3\theta}\cos\theta - \frac{\partial U}{\partial \theta} \qquad (17)$$

$$\dot{p}_\phi = -\frac{\partial H}{\partial \phi} = -\frac{\partial U}{\partial \phi}$$

The use of <u>cyclic coordinates</u> is also quite evident in the Hamiltonian formulation:

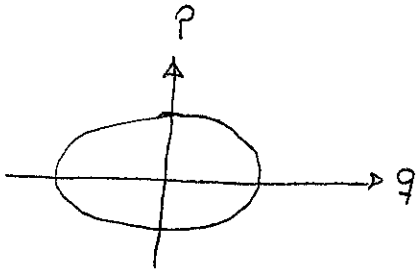
> If q_i does not appear in $H \Rightarrow$ p_i = constant (18)

In the Hamiltonian (16), ϕ is a cyclic coordinate when U does not depend on ϕ. Consequently, p_ϕ is conserved. This can also be seen in (17).

Liouville's theorem and phase space

A system with N degrees of freedom is described by N generalized coordinates $q_1, \ldots, q_N$ and N generalized momenta $p_1, \ldots, p_N$. Thus, one realization of the motion means specifying $2N$ function of time. We can imagine this as a trajectory in a $2N$ dimensional space which we call phase space.

When $N = 1$, the phase space is two dimensional. So, for instance, a trajectory of a harmonic oscilator in phase space looks like this



For $N = 4$ the phase space becomes 4 dimensional and we can no longer visualize it in an easy way. But mathematically the concept is well defined.

A point in phase space is specified by a $2N$ dimensional vector

$$z(t) = (q_1, \ldots, q_N, p_1, \ldots, p_N) \tag{19}$$

In certain situations we call this a <u>microstate</u> because it contains all the microscopic information of all degrees of freedom.

Trajectories in phase space satisfy (at least) two very important properties. The first is that two trajectories in phase space never cross each other. This is easy to understand. Hamilton's equations completely specify, for any point in phase space, where the system will go next. The motion is deterministic. If at time t you are at $\vec{z}(t)$, then at time $t + \Delta t$, you will for sure be at $\vec{z}(t+\Delta t)$.

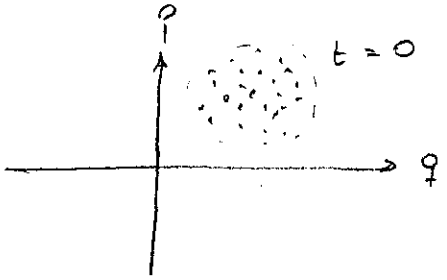
So if two trajectories were to cross, you would have, for a given point in phase space, two possibilities for where to go next. And that cannot happen.

Newton's law or the Euler-Lagrange equations are second order in time, whereas Hamilton's equation are first order. When you have a first order equation, knowing where you are now completely specifies where you will be later.

Note also that what I'm saying is that two trajectories in phase space never cross each other. I'm not talking about trajectories in the real world $\mathbb{R}^3$. I'm talking about trajectories in a mathematical space of dimension $2N$.

The other important property about phase space is called Liouville's theorem. It says that trajectories in phase space move in time like an incompressible fluid.

what this means is the following. Suppose you integrate the equations of motion starting with several random initial conditions



this swarm of points will evolve in time each in its own complicated way. But according to Liouville this will occur in such a way that the total area in phase space is conserved.

In a sense, this is a consequence of the fact that the trajectories never cross each other. If you imagine each individual trajectory as being a tiny piece of fluid flowing in the river, then the statement that the area is preserved is tantamount to saying that the fluid is incompressible.

when we studied the velocity Verlet numerical integration scheme, I said that the method was symplectic. A symplectic method is one which conserves areas in phase space. So even though the velocity Verlet does not conserve the energy, it preserves areas in phase space. That is why it is so useful for long-term stability.

There are many ways to prove Liouville's theorem. The simplest one is to note that if δ is the velocity of a fluid, the statement of incompressibility implies that $\nabla \cdot \delta = 0$.

In our case, we are talking about the $2N$ dimensional phase space $z(t)$ and therefore a velocity $\dot{z}$. The generalization of $\nabla \cdot \delta = 0$ is then

$$\sum_{a=1}^{2N} \frac{\partial}{\partial z_a} \dot{z}_a \stackrel{?}{=} 0$$

Splitting into q's and p's this gives

$$\sum_a \frac{\partial \dot{z}_a}{\partial z_a} = \sum_{i=1}^{N} \left\{ \frac{\partial}{\partial q_i} \dot{q}_i + \frac{\partial}{\partial p_i} \dot{p}_i \right\}$$

Using Hamilton's equations (10) we find

$$\sum_a \frac{\partial \dot{z}_a}{\partial z_a} = \sum_{i=1}^{N} \left\{ \frac{\partial}{\partial q_i} \left(\frac{\partial H}{\partial p_i} \right) + \frac{\partial}{\partial p_i} \left(-\frac{\partial H}{\partial q_i} \right) \right\}$$

$$= \sum_{i=1}^{N} \left\{ \frac{\partial^2 H}{\partial q_i \partial p_i} - \frac{\partial^2 H}{\partial p_i \partial q_i} \right\}$$

$$= 0$$

This proves Liouville's theorem: trajectories in phase space behave like an incompressible fluid.

Poisson brackets

Let $f(q_i, p_i, t)$ be some function of the coordinates, the momenta and time. Its total time derivative is

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_i \left\{ \frac{\partial f}{\partial q_i} \dot{q}_i + \frac{\partial f}{\partial p_i} \dot{p}_i \right\} \tag{20}$$

Substituting Hamilton's equations for $\dot{q}_i$ and $\dot{p}_i$ we get

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_i \left\{ \frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right\} \tag{21}$$

we define a new quantity called the <u>Poisson bracket</u> as

$$\boxed{[f, H] = \sum_i \left\{ \frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right\}} \tag{22}$$

we may then write

$$\boxed{\frac{df}{dt} = \frac{\partial f}{\partial t} + [f, H]} \tag{23}$$

Let us now ask about the conditions for f to be an <u>integral of motion</u>. By definition, this means that $\frac{df}{dt} = 0$ so for f to be a constant of the motion we must have

$$\frac{\partial f}{\partial t} + [f, H] = 0 \tag{24}$$

In particular, if f does not depend explicitly on time, then the condition for f to be a constant of the motion is

$$[f, H] = 0 \tag{25}$$

This gives a systematic test to see if a certain quantity is an integral of the motion.

The Poisson bracket is defined not only for f and H. For any two quantities f and g we define

$$[f, g] = \sum_i \left\{ \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right\} \tag{26}$$

In particular, if $g = q_j$ we get

$$[f, q_j] = \sum_i \left\{ \frac{\partial f}{\partial q_i} \frac{\partial q_j}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial q_j}{\partial q_i} \right\}$$

But $\frac{\partial q_j}{\partial p_i} = 0$ and $\frac{\partial q_j}{\partial q_i} = \delta_{ij}$. Thus

$$[f, q_j] = -\frac{\partial f}{\partial p_j} \tag{27a}$$

Similarly,

$$[f, p_j] = \frac{\partial f}{\partial q_j} \tag{27b}$$

With these formulas we may obtain some beautiful results. First, if we use $f = H$ in (27a) and (27b) we get

$$[H, q_i] = -\frac{\partial H}{\partial p_i} = -\dot{q}_i$$

$$[H, p_i] = \frac{\partial H}{\partial q_i} = -\dot{p}_i$$

Hence, Hamilton's equations may be rewritten compactly as

$$\begin{aligned} \dot{q}_i &= -[H, q_i] \\ \dot{p}_i &= -[H, p_i] \end{aligned} \tag{28}$$

If you wish to get rid of the minus sign, note that, from the definition (26),

$$[f, g] = -[g, f] \tag{29}$$

Thus we get

$$\begin{aligned} \dot{q}_i &= [q_i, H] \\ \dot{p}_i &= [p_i, H] \end{aligned} \tag{30}$$

We may combine both equations using that vector z_a defined in (19). We then get

$$\boxed{\dot{z}_a = [H, z_a]} \tag{31}$$

This gives the equations of motion in a very compact form.

Another nice thing we can do with (27) is to find the Poisson brackets between q's and p's. Using $f = q_u$ in (27a) we get

$$[q_u, q_j] = 0 \tag{32a}$$

using $f = p_u$ in (27b) we get

$$[p_u, p_j] = 0 \tag{32b}$$

and finally, using $f = q_u$ in (27b) gives

$$\boxed{[q_u, p_j] = \delta_{uj}} \tag{32c}$$

You may have seen a very similar relation in quantum mechanics.

The action as a function of the coordinates

The action is

$$S = \int_{t_1}^{t_2} \mathcal{L}\, dt \tag{33}$$

Now let us recall the derivation of the Euler-Lagrange equations from the principle of least action. we had, for one degree of freedom,

$$\delta S = \int_{t_1}^{t_2} \mathcal{L}(q+\delta q,\ \dot{q}+\delta\dot{q}, t)dt - \int_{t_1}^{t_2} \mathcal{L}(q, \dot{q}, t)dt$$

$$\approx \int_{t_1}^{t_2} \left\{ \frac{\partial \mathcal{L}}{\partial q}\delta q + \frac{\partial \mathcal{L}}{\partial \dot{q}}\delta\dot{q} \right\} dt$$

Integrating the second term by parts:

$$\int_{t_1}^{t_2} \frac{\partial \mathcal{L}}{\partial \dot{q}} \frac{d}{dt}(\delta q)\, dt = \left[\frac{\partial \mathcal{L}}{\partial \dot{q}}\delta q \right]_{t_1}^{t_2} - \int_{t_1}^{t_2} \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}}\right)\delta q\, dt$$

Usually we throw away the first term argueing that for the true path $\delta q(t_1) = \delta q(t_2) = 0$.

Now I want to do something different. I want to regard the action as a function of the coordinates at the end of the motion, $\delta q(t_2)$, still assuming $\delta q(t_1) = 0$.

This means that we will not minimize the action (yet). We will leave it as a function of t_2 and $\delta q(t_2)$, knowing that the minimum of the action occurs at $\delta q(t_2) = 0$.

we then get

$$\delta S = \left[\frac{\partial \mathcal{L}}{\partial \dot{q}} \delta q \right]_{t_1}^{t_2} + \int_{t_1}^{t_2} \left\{ \frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}} \right) \right] \delta q \, dt$$

The last term is zero since the system satisfies the Euler-Lagrange equations. Substituting $p = \frac{\partial \mathcal{L}}{\partial \dot{q}}$ and denoting t_2 by t we get

$$\delta S = p \delta q$$

The generalization to many degrees of freedom is straightforward:

$$\delta S = \sum_i p_i \delta q_i \tag{34}$$

Conclusion: if we regard S as a function of q_i and t, then

$$\boxed{\frac{\partial S}{\partial q_i} = p_i} \tag{35}$$

As for the dependence on time, we have

$$\frac{dS}{dt} = \frac{\partial S}{\partial t} + \sum_i \frac{\partial S}{\partial q_i} \dot{q}_i$$

$$= \frac{\partial S}{\partial t} + \sum_i p_i \dot{q}_i$$

On the other hand, from the definition (33) we have

$$\frac{dS}{dt} = L$$

Hence we see that

$$\frac{\partial S}{\partial t} = L - \sum_i p_i \dot{q}_i = -H$$

Thus

$$\boxed{\frac{\partial S}{\partial q_i} = p_i \qquad \frac{\partial S}{\partial t} = -H} \tag{36}$$

where I emphasize, these relations hold if S is interpreted as a function of the coordinates and time

$$S = S(q_1, \ldots, q_N, t) \tag{37}$$

Eq (36) may be written as

$$\frac{\partial S}{\partial t} = -H\left(q_1, \ldots, q_N, p_1, \ldots, p_N\right) \tag{38}$$

But $p_i = \partial S / \partial q_i$ so we may write

$$\boxed{\frac{\partial S}{\partial t} + H\left(q_1, \ldots, q_N, \frac{\partial S}{\partial q_1}, \ldots, \frac{\partial S}{\partial q_N}\right) = 0} \tag{39}$$

This is called the Hamilton-Jacobi equation. It corresponds to yet another way of formulating the dynamics of a mechanical system. This is now a partial differential equation for the variable $S(q_1, \ldots, q_N, t)$.

For instance, if

$$H = \frac{p^2}{2m} + U(x) \tag{40}$$

then the Hamiltan-Jacobi equation reads

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + U(x) = 0 \tag{41}$$

which is a non-linear partial differential equation for $S(q,t)$.

When $H = E$ is a conserved quantity, the time dependence of S becomes simple. From (36) we see that

$$S(q,t) = S_0(q) - E\,t \tag{42}$$

The Hamiltan-Jacobi equation (39) then becomes

$$\boxed{H\left(q_1, \ldots, q_N, \frac{\partial S_0}{\partial q_1}, \ldots \frac{\partial S_0}{\partial q_N}\right) = E} \tag{43}$$

Or, for the Hamiltonian (40),

$$\boxed{\frac{1}{2m}\left(\frac{\partial S_0}{\partial x}\right)^2 + U(x) = E} \tag{44}$$

Quantum mechanics according to Schrödinger

Schrödinger used Eq (44) as a starting point to derive his famous equation. I will now retrace his steps exactly as done in

E. Schrödinger, Annalen der Physik (1926) vol 79

His first step was to change variables from S to a new function ψ, as

$$S = K \log \psi \tag{45}$$

where K is a constant. After he solved the hydrogen atom he realized that for consistency it was necessary to have $K = \hbar$. Thus

$$S = \hbar \log \psi \tag{46}$$

Eq (44) may then be written as

$$\frac{\hbar^2}{2m}\left(\frac{\partial \psi}{\partial x}\right)^2 + [U(x) - E]\psi^2 = 0 \tag{47}$$

This is still the Hamilton-Jacobi equation, so thus far we haven't done anything new.

This equation can be solved for a given value of E. Remember that E is a constant of the motion and varies continuously. But Schrödinger knew that in the quantum world the energy levels were quantized.

So Schrödinger's brilliant insight was not to try to solve Eq (47), which can be done for any E. Instead, he considered what happens when the integral of that equation over all of space is an extremum.

Let

$$J = \int_{-\infty}^{\infty} dx \left\{ \frac{\hbar^2}{2m} \left(\frac{\partial \psi}{\partial x} \right)^2 + [U(x) - E] \psi^2 \right\} \tag{48}$$

This is a functional of ψ. We find the extremum just like we did in the principle of least action. We let

$$\psi(x) \to \psi(x) + \epsilon \phi(x) \tag{49}$$

where $\phi(x)$ is an arbitrary variation and ϵ is a tiny parameter we then have

$$\psi^2 \to (\psi + \epsilon\phi)^2 \simeq \psi^2 + 2\epsilon \psi\phi + \mathcal{O}(\epsilon)^2$$

and

$$(\partial_x \psi)^2 \to (\partial_x \psi + \epsilon \partial_x \phi)^2 \simeq (\partial_x \psi)^2 + 2\epsilon (\partial_x \psi)(\partial_x \phi) + \mathcal{O}(\epsilon)^2$$

Thus

$$\delta J = \int dx \left\{ \frac{\hbar^2}{2m} 2\epsilon (\partial_x \psi)(\partial_x \phi) + [U(x) - E] 2\epsilon \psi\phi \right\}$$

we now integrate by parts the first term so that we can write δJ as a function of ϕ.

we have

$$\int_{-\infty}^{\infty} dx\, (\partial_x \psi)(\partial_x \phi) = (\partial_x \psi)\phi \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} (\partial_x^2 \psi)\, \phi \, dx$$

To get rid of the cross term we need to assume that $\phi(\pm\infty) \to 0$. when we do that we arrive at

$$\delta J = \int_{-\infty}^{\infty} dx\, 2\epsilon\phi \left\{ -\frac{\hbar^2}{2m} \partial_x^2 \psi + [U(x) - E]\psi \right\} \tag{50}$$

If we impose that J must be an extremum then $\delta J = 0$ and we conclude that for this to happen, ψ must satisfy

$$\boxed{-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U(x)\psi = E\psi} \tag{51}$$

which is the famous Schrödinger equation.

Canonical quantization

Starting with any Lagrangian $\mathcal{L}(q_1, \ldots, q_N, \dot{q}_1, \ldots, \dot{q}_N)$, there is a general recipe to obtain the corresponding quantum theory which always works. It is called canonical quantization.

Starting with a Lagrangian, obtain the generalized momenta p_i and the Hamiltonian $H(q_i, p_i)$. To quantize the Hamiltonian we must promote q_i and p_i to new objects called <u>operators</u>. We write them with hats, $\hat{q}_i$ and $\hat{p}_i$. The difference between operators and numbers is that when you multiply two operators, the order is important:

$$\hat{q}_i \hat{p}_i \neq \hat{p}_i \hat{q}_i \tag{52}$$

It is convenient to define the commutator between two operators as

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{53}$$

We use the same notation as Poisson brackets, Eq (26). This is not a coincidence. Much of the quantum theory is carried over from the classical case by replacing Poisson brackets with commutators.

For $\hat{q}_i$ and $\hat{p}_i$ the canonical quantization recipe is to set

$$\boxed{[\hat{q}_j, \hat{p}_k] = i\hbar\,\delta_{jk}} \tag{54}$$

compare with (32c).

So the recipe is this: starting with a Lagrangian, find the p_i and convert to a Hamiltonian formulation. Then transform H into an operator $\hat{H}$ by promoting q_i and p_i to operators satisfying (54).

To see why this works, suppose we have only one degree of freedom, with

$$H = \frac{p^2}{2m} + U(x) \tag{55}$$

Then we promote x and p to operators $\hat{x}$ and $\hat{p}$ satisfying

$$[\hat{x}, \hat{p}] = i\hbar \tag{56}$$

When we do this we may either work with abstract operators or we can choose a specific <u>representation</u>. The most famous one is called the <u>coordinate representation</u>

$$\begin{aligned} \hat{x} &\to x \quad \text{(a number)} \\ \hat{p} &\to -i\hbar \frac{\partial}{\partial x} \end{aligned} \tag{57}$$

This choice satisfies (56). But to see that it is easier to act on both sides with some arbitrary function $f(x)$.

Then

$$\begin{aligned} [\hat{x}, \hat{p}] f(x) &= \left(\hat{x}\hat{p} - \hat{p}\hat{x}\right) f(x) \\ &= -i\hbar x \frac{\partial f}{\partial x} + i\hbar \frac{\partial}{\partial x}(xf) \\ &= -i\hbar x \frac{\partial f}{\partial x} + i\hbar \left\{ f + x \frac{\partial f}{\partial x} \right\} \\ &= i\hbar f \end{aligned}$$

Since this must hold for any $f(x)$, we arrive at (56). Thus we now have promoted the Hamiltonian (55) to the operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x) \tag{58}$$

This operator needs something to act on so we finally introduce a wave function ψ and write

$$\hat{H}\psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right]\psi = E\psi \tag{59}$$

which is Schrödinger's equation.