## Quantizing Classical Mechanics

## Lagrangian and Hamiltonian Classical Mechanics

Before I tell you how to quantize a classical mechanical system, let me remind you how the classical mechanics works in the Lagrangian or the Hamiltonian formulations. For simplicity, I'll focus on systems without any friction or dissipative forces, so the energy flows between the bodies we are interested in but does not get lost to heat or other nonmechanical forms. For such systems, the Lagrangian or the Hamiltonian formulations of mechanics are mathematically equivalent to the original Newtonian formulations, but they are more convenient for describing constrained motion like a pendulum hanging from the bottom of another pendulum, or a body sliding off another moving body. Indeed, the Lagrangian or the Hamiltonian description of such systems allows non-Cartesian coordinates which resolve all the constrains and yields the equations of motion for any such coordinates without bothering to calculate the normal forces between the bodies in contact. OOH , the Newtonian description is designed for the Cartesian coordinates of all the bodies and involve calculating all the forces, including the normal forces.

## Lagrangian formulation

Consider a system described by some $N$ independent dynamical variables $\left(q_{1}, \ldots, q_{N}\right)$, for example 3 coordinates ( $x, y, z$ ) of some moving particle, or $3 n$ coordinates of $n$ interacting particles. The Lagrangian description starts with the Lagrangian function

$$
\begin{equation*}
L\left(q_{1}, \ldots, q_{N} ; \dot{q}_{1}, \ldots, \dot{q}_{N}\right) \tag{1}
\end{equation*}
$$

of all the dynamical variables $q_{i}$ and their time derivatives (velocities) $\dot{q}_{i}=d q_{i} / d t$. Typically

$$
\begin{align*}
L & =E_{\text {kinetic }}-E_{\text {potential }} \\
\text { such as } \quad L & =\sum_{i=1}^{n} \frac{m_{i}}{2} \dot{\mathbf{x}}_{i}^{2}-V\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right) . \tag{2}
\end{align*}
$$

Then for any conceivable path $\left(q_{1}(t), \ldots, q_{N}(t)\right)$ through the coordinate space, we define the
action integral

$$
\begin{equation*}
S\left[\text { all } q_{i}(t) \text { at all } t\right]=\int_{t_{\text {start }}}^{t_{\text {fnish }}} d t L\left(q_{1}(t), \ldots, q_{N}(t) ; \dot{q}_{1}(t), \ldots, \dot{q}_{N}(t)\right) \tag{3}
\end{equation*}
$$

Note: while the Lagrangian is an ordinary function of $2 N$ arguments, the action is a functional of the entire history of motion, i.e. of $N$ whole functions $q_{i}(t)$ rather than of its values at some particular point of time.

The action functional (3) is defined for any path $\left(q_{1}(t), \ldots, q_{N}(t)\right)$, regardless of whether it obeys the Newton laws or does not bother; even a completely random drunkard's walk has a well-defined action. But the least action principle states that the path $\left(q_{1}(t), \ldots, q_{N}(t)\right)$ which obeys the Laws of Motion has the least action among all differentiable paths starting at the same point $\left(q_{1}, \ldots, q_{N}\right)_{1}$ at the initial time $t_{1}$ and finishing at the same point $\left(q_{1}, \ldots, q_{N}\right)_{2}$ at the final time $t_{2}$.

Formally, minimizing the action functional is the matter of variational calculus: We allow for infinitesimal variations $q_{i}(t) \rightarrow q_{i}(t)+\delta q_{i}(t)$ and then demand that the first variation $\delta S$ must vanish for all $\delta q_{i}(t)$, which eventually translates to the differential equations for the $q_{i}(t)$. Let me skip this step and simply present you with the resulting Euler-Lagrange equations

$$
\begin{equation*}
\forall i=1, \ldots, N: \quad \frac{d}{d t}\left(\frac{\partial L}{\partial \dot{q}_{i}} @ t\right)=\frac{\partial L}{\partial q_{i}} @ t . \tag{4}
\end{equation*}
$$

For example, for a single particle with the Lagrangian

$$
\begin{equation*}
L=\frac{m}{2} \dot{\mathbf{x}}^{2}-V(\mathbf{x}) \tag{5}
\end{equation*}
$$

we have

$$
\begin{equation*}
\frac{\partial L}{\partial \dot{x}_{i}}=m \dot{x}_{i}, \quad \frac{\partial L}{\partial x_{i}}=-\frac{\partial V}{\partial x_{i}}, \tag{6}
\end{equation*}
$$

so the Euler-Lagrange equation (4) becomes

$$
\begin{equation*}
\frac{d}{d t}\left(m \dot{x}_{i}\right)=-\frac{\partial V}{\partial x_{i}} \tag{7}
\end{equation*}
$$

or in vector notations

$$
\begin{equation*}
\frac{d}{d t}(m \dot{\mathbf{x}})=-\nabla V(\mathbf{x})=\mathbf{F}(\mathbf{x}) \tag{8}
\end{equation*}
$$

The last formula here is the good old Second Law of Newton for the potential force $\mathbf{F}=-\nabla V$, and that's why we have started with the Lagrangian (5) in the first place.

## Hamiltonian formulation

In the Lagrangian formulation, the Euler-Lagrange equations are second-order differential equations, and there is one such equation for each independent coordinate $q_{i}(t)$. The Hamiltonian formulation doubles the number of variables: besides the $N$ position variables $q_{i}(t)$ there are also $N$ canonical momenta $p_{i}(t)$, and all these $2 N$ variables are subject to $2 N$ first-order differential equations. Here is how this works:

1. Given $N$ position variables $\left(q_{1}, \ldots, q_{N}\right)$ and the Lagrangian $L\left(q_{1}, \ldots, q_{N} ; \dot{q}_{1}, \ldots, \dot{q}_{N}\right)$, we start by defining the canonical momentum $p_{i}$ for each position $q_{i}$ according to

$$
\begin{equation*}
p_{i} \stackrel{\text { def }}{=} \frac{\partial L}{\partial \dot{q}_{i}}\left\langle\left\langle\text { at fixed } q_{j} \text { and } \dot{q}_{j \neq i}\right\rangle\right\rangle . \tag{9}
\end{equation*}
$$

2. Second, we calculate the net energy of the system $H$ as

$$
\begin{equation*}
H=\sum_{i=1}^{N} p_{i} \dot{q}_{i}-L \tag{10}
\end{equation*}
$$

3. Third, we treat eq. (9) as equations for the velocities $\dot{q}_{i}$ in terms of the momenta $p_{i}$ and solve these equations. This gives us the velocities $\dot{q}_{i}$ as functions of the momenta $p_{i}$.
4. Fourth, we plug these functions into eq. (10) and rewrite the energy $H$ as a function $H(q, p)$ of positions and canonical momenta rather than positions and velocities. This function is called the Hamiltonian.
5. Given the Hamiltonian function $H\left(q_{1}, \ldots, q_{N} ; p_{1}, \ldots p_{N}\right)$, the time-dependence of all the positions and all the momenta is governed by the first-order Hamilton equations

$$
\begin{equation*}
\forall i=1, \ldots, N: \quad \frac{d q_{i}}{d t}=+\frac{\partial H(q, p)}{\partial p_{i}}, \quad \frac{d p_{i}}{d t}=-\frac{\partial H(q, p)}{\partial q_{i}} . \tag{11}
\end{equation*}
$$

As a simple example, let's go back to the single 3d particle in the potential $V(\mathbf{x})$,

$$
\begin{equation*}
L=\frac{m}{2} \dot{\mathbf{v}}^{2}-V(\mathbf{x}) \quad \text { for } \mathbf{v} \stackrel{\text { def }}{=} \dot{\mathbf{x}}=\frac{d \mathbf{x}}{d t} . \tag{5}
\end{equation*}
$$

For this system, the canonical momentum $\mathbf{p}$ is the usual momentum $m \mathbf{v}$, indeed

$$
\begin{equation*}
p_{i}=\frac{\partial L}{\partial v_{i}}=m v_{i} \quad \Longrightarrow \quad \mathbf{p}=m \mathbf{v} \tag{12}
\end{equation*}
$$

hence

$$
\begin{equation*}
H=\mathbf{p} \cdot \mathbf{v}-L=m \mathbf{v} \cdot \mathbf{v}-\frac{m \mathbf{v}^{2}}{2}+V(\mathbf{x})=+\frac{m \mathbf{v}^{2}}{2}+V(\mathbf{x}) \tag{13}
\end{equation*}
$$

or in terms of positions and momenta

$$
\begin{equation*}
H(\mathbf{x}, \mathbf{p})=V(\mathbf{x})+\frac{\mathbf{p}^{2}}{2 m} \tag{14}
\end{equation*}
$$

Consequently, the Hamilton equations (11) become

$$
\begin{align*}
& \frac{d \mathbf{x}}{d t}=+\frac{\partial H}{\partial \mathbf{p}}=\frac{\mathbf{p}}{m}  \tag{15}\\
& \frac{d \mathbf{p}}{d t}=-\frac{\partial H}{\partial \mathbf{x}}=-\nabla V(\mathbf{x})=+\mathbf{F}(\mathbf{x})
\end{align*}
$$

which together reproduce the good old Second Law of Newton.

## Charged particle example

As a more interesting example, consider a charged particle in electric and magnetic fields. For simplicity, let's assume a non-relativistic particle of charge $Q$ without any build-in spin or magnetic moment. Then its Lagrangian is

$$
\begin{equation*}
L(\mathbf{x}, \mathbf{v})=\frac{m \mathbf{v}^{2}}{2}-Q \Phi(\mathbf{x})+\frac{Q}{c} \mathbf{v} \cdot \mathbf{A}(\mathbf{x}) \tag{16}
\end{equation*}
$$

where $\Phi(\mathbf{x})$ is the scalar electric potential, $\mathbf{A}(\mathbf{x})$ is the vector magnetic potential (in Gauss units), and both potentials are evaluated at the particle's location $\mathbf{x}$. Note that the third term here - the magnetic term - depends on both the velocity and the position of the particle.

Let me skip the Euler-Lagrange equation for the charged particle and go directly to the Hamiltonian formulation. First of all, the canonical momentum $\mathbf{p}$ of the charged particle is different from its usual kinematic momentum $\vec{\pi}=m \mathbf{v}$ ! Instead,

$$
\begin{equation*}
\mathbf{p} \stackrel{\text { def }}{=} \frac{\partial L}{\partial \mathbf{v}}=m \mathbf{v}+\frac{Q}{c} \mathbf{A}(\mathbf{x}) . \tag{17}
\end{equation*}
$$

Next, the energy of the charged particle is

$$
\begin{align*}
H & =\mathbf{p} \cdot \mathbf{v}-L \\
& =m \mathbf{v} \cdot \mathbf{v}+\frac{Q}{c} \mathbf{A}(\mathbf{x}) \cdot \mathbf{v}-\frac{m \mathbf{v}^{2}}{2}+Q \Phi(\mathbf{x})-\frac{Q}{c} \mathbf{A}(\mathbf{x}) \cdot \mathbf{v}  \tag{18}\\
& =+\frac{m \mathbf{v}^{2}}{2}+Q \Phi(\mathbf{x})
\end{align*}
$$

At first blush this energy seems to be independent of the vector potential $\mathbf{A}$ and hence of the magnetic field. However, when we re-express this energy in terms of the canonical momentum p rather than velocity or the kinematic momentum $\vec{\pi}$, we end up with a Hamiltonian which does depend on A. Specifically,

$$
\begin{equation*}
H=+\frac{\vec{\pi}^{2}}{2 m}+Q \Phi(\mathbf{x})=\frac{1}{2 m}\left(\mathbf{p}-\frac{Q}{c} \mathbf{A}(\mathbf{x})\right)^{2}+Q \Phi(\mathbf{x}) \tag{19}
\end{equation*}
$$

Consequently, the Hamilton equations for the charged particle are

$$
\begin{equation*}
\frac{d \mathbf{x}}{d t}=+\frac{\partial H}{\partial \mathbf{p}}=\frac{1}{m}\left(\mathbf{p}-\frac{Q}{c} \mathbf{A}(\mathbf{x})\right)=\frac{\vec{\pi}}{m} \tag{20}
\end{equation*}
$$

and

$$
\begin{equation*}
\frac{d \mathbf{p}}{d t}=-\frac{\partial H}{\partial \mathbf{x}}=-Q \nabla \Phi(\mathbf{x})+\frac{Q}{m c}\left(p_{j}-\frac{Q}{c} A_{j}(\mathbf{x})\right) \nabla A_{j}(\mathbf{x}) . \tag{21}
\end{equation*}
$$

To make physical sense of of this equation, let's restate it in terms of the kinematic momentum

$$
\begin{equation*}
\vec{\pi}=m \mathbf{v}=\mathbf{p}-\frac{Q}{c} \mathbf{A}(\mathbf{x}) \quad \text { (cf. eq. (20)) } \tag{22}
\end{equation*}
$$

In terms of $\vec{\pi}(t)$, eq. (21) becomes

$$
\begin{equation*}
\frac{d}{d t}\left(\vec{\pi}(t)+\frac{Q}{c} \mathbf{A}(\mathbf{x}(t))\right)=-Q \nabla \Phi(\mathbf{x})+\frac{Q}{m c} \pi_{j} \nabla A_{j}(\mathbf{x}) . \tag{23}
\end{equation*}
$$

On the LHS here, the vector potential $\mathbf{A}(\mathbf{x}(t))$ is evaluated at the position $\mathbf{x}(t)$ of the moving particle, so it depends on dime due to $d \mathbf{x} / d t$ even in a static magnetic field,

$$
\begin{equation*}
\frac{d}{d t} \mathbf{A}(\mathbf{x}(t))=v_{j} \frac{\partial \mathbf{A}}{\partial x_{j}} \tag{24}
\end{equation*}
$$

In a time-dependent magnetic field, we also get a term due to time-dependence of $\mathbf{A}$ at a fixed location, thus

$$
\begin{equation*}
\frac{d}{d t} \mathbf{A}(\mathbf{x}(t), t)=\frac{\partial \mathbf{A}}{\partial t}+v_{j} \frac{\partial \mathbf{A}}{\partial x_{j}} . \tag{25}
\end{equation*}
$$

Plugging this term into eq. (23), we get

$$
\begin{equation*}
\frac{d \vec{\pi}}{d t}+\frac{Q}{c} \frac{\partial \mathbf{A}}{\partial t}+\frac{Q}{c} v_{j} \frac{\partial \mathbf{A}}{\partial x_{j}}=-Q \nabla \Phi+\frac{Q}{c}\left(\frac{\pi_{j}}{m}=v_{j}\right) \nabla A_{j}, \tag{26}
\end{equation*}
$$

and hence

$$
\begin{equation*}
\frac{d \vec{\pi}}{d t}=Q\left(-\nabla \Phi-\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}\right)+\frac{Q}{c}\left(v_{j} \nabla A_{j}-v_{j} \nabla_{j} \mathbf{A}\right) . \tag{27}
\end{equation*}
$$

On the RHS here, the first term is the electric force $Q \mathbf{E}$, indeed

$$
\begin{equation*}
-\nabla \Phi(\mathbf{x}, t)-\frac{1}{c} \frac{\partial \mathbf{A}(\mathbf{x}, t)}{\partial t}=\mathbf{E}(\mathbf{x}, t) \tag{28}
\end{equation*}
$$

is the electric field. As to the second term in eq. (27), the expression inside ( $\cdots$ ) amounts
to $\mathbf{v} \times \mathbf{B}$, indeed

$$
\begin{align*}
\left(v_{j} \nabla A_{j}-v_{j} \nabla_{j} \mathbf{A}\right)_{i} & =v_{j}\left(\nabla_{i} A_{j}-\nabla_{j} A_{i}\right) \\
& =v_{j}\left(\delta_{i \ell} \delta_{j m}-\delta_{i m} \delta_{j \ell}\right) \nabla_{\ell} A_{m}=v_{j} \epsilon_{i j k} \epsilon_{k \ell m} \nabla_{\ell} A_{m} \\
& =v_{j} \epsilon_{i j k}\left(\epsilon_{k \ell m} \nabla_{\ell} A_{m}=(\nabla \times \mathbf{A})_{k}=B_{k}\right)  \tag{29}\\
& =\epsilon_{i j k} v_{j} B_{k}=(\mathbf{v} \times \mathbf{B})_{i},
\end{align*}
$$

so the second term in (27) is the Lorentz force

$$
\begin{equation*}
\mathbf{F}_{L}=\frac{Q}{c} \mathbf{v} \times \mathbf{B}(\mathbf{x}, t) . \tag{30}
\end{equation*}
$$

Altogether, eq. (27) amounts to

$$
\begin{equation*}
\frac{d \vec{\pi}}{d t}=Q \mathbf{E}(\mathbf{x}, t)+\frac{Q}{c} \mathbf{v} \times \mathbf{B}(\mathbf{x}, t) . \tag{31}
\end{equation*}
$$

In other words, the two Hamilton equations (20) and (21) amount to the Newton Law for the charged particle subject to the electric an magnetic forces,

$$
\begin{equation*}
\frac{d}{d t}(m \mathbf{v})=\mathbf{F}_{E M}=Q \mathbf{E}(\mathbf{x}, t)+\frac{Q}{c} \mathbf{v} \times \mathbf{B}(\mathbf{x}, t) \tag{32}
\end{equation*}
$$

Experimentally, we know that the equation of motion (32) is correct. And that's how we know that we have started with the correct Lagrangian (16) and Hamiltonian (19).

## Quantization

There are two ways of turning a classical mechanical system into a quantum system or a classical field theory into a quantum field theory:

1. The canonical quantization. One starts with the Hamiltonian formulation of the classical system in terms 'position' variables $q_{i}(t)$, the canonical momenta $p_{i}(t)$, and the Hamilton function $H(q, p)$. Then one turns the positions and the momenta into linear operators $\hat{q}_{i}$ and $\hat{p}_{i}$ in some Hilbert space and constructs the Hamiltonian operator $\hat{H}=H(\hat{q}, \hat{p})$ which governs the time evolution of the system.
2. The functional quantization also known as the path integral method. In this method one skips over the operators and calculates the quantum evolution amplitudes from the classical action functional by integrating over all differentiable trajectories from the initial point to the final point,

$$
\begin{equation*}
U\left(q_{1} @ t_{1} \rightarrow q_{2} @ t_{2}\right)=\iiint \int_{q\left(t_{1}\right)=q_{1}}^{q\left(t_{2}\right)=q_{2}} \mathcal{D}[q(t)] \exp (i S[q(t)] / \hbar) . \tag{33}
\end{equation*}
$$

In this class we shall focus on the canonical quantization. But I shall spend a lecture or two - or more likely an extra lecture or two - introducing the path integrals.

## Canonical Quantization of Mechanics

In Quantum Mechanics, the classical position and momentum variables $q_{i}(t)$ and $p_{i}(t)$ become linear operators $\hat{q}_{i}$ and $\hat{p}_{i}$ in some Hilbert space. For systems of only a few degrees of freedom this Hilbert space is usually defined in terms of wave functions $\psi\left(q_{1}, \ldots, q_{N}\right)$ obeying suitable integrability conditions, but for our purposes we do not care about the gory details of this Hilbert space. Instead, let's focus on the canonical commutation relations between the position and the momentum operators: however you realize those operators, they must obey

$$
\begin{equation*}
\left[\hat{q}_{i}, \hat{q}_{j}\right]=0, \quad\left[\hat{p}_{i}, \hat{p}_{j}\right]=0, \quad\left[\hat{q}_{i}, \hat{p}_{j}\right]=i \hbar \delta_{i j} \tag{34}
\end{equation*}
$$

Note that the momentum operators in these relations are the canonical momenta whose classical counterparts obtain from eq. (9), and for other kinds of momenta the commutation relations might be different. For example, consider the kinematic momentum $\vec{\pi}=m \mathbf{v}$ of a charged particle; defining its quantum counterpart as

$$
\begin{equation*}
\hat{\vec{\pi}} \stackrel{\text { def }}{=} \hat{\mathbf{p}}-\frac{Q}{c} \mathbf{A}(\hat{\mathbf{x}}), \tag{35}
\end{equation*}
$$

we get

$$
\begin{equation*}
\left[\hat{x}_{i}, \hat{x}_{j}\right]=0 \quad \text { and } \quad\left[\hat{x}_{i}, \hat{\pi}_{j}\right]=i \hbar \delta_{i j} \tag{36}
\end{equation*}
$$

but

$$
\begin{equation*}
\left[\hat{\pi}_{i}, \hat{\pi}_{j}\right]=\frac{i \hbar Q}{c} \epsilon_{i j k} B_{k}(\hat{\mathbf{x}}) \neq 0 \tag{37}
\end{equation*}
$$

Indeed,

$$
\begin{align*}
{\left[\hat{\pi}_{i}, \hat{\pi}_{j}\right] } & =-\frac{Q}{c}\left[A_{i}(\hat{\mathbf{x}}), \hat{\pi}_{j}\right]-\frac{Q}{c}\left[\hat{\pi}_{i}, A_{j}(\hat{\mathbf{x}})\right] \\
& =-\frac{i \hbar Q}{c}\left(\nabla_{j} A_{i}(\hat{\mathbf{x}})\right)+\frac{i \hbar Q}{c}\left(\nabla_{i} A_{j}(\hat{\mathbf{x}})\right) \\
& =\frac{i \hbar Q}{c}\left(\nabla_{i} A_{j}-\nabla_{j} A_{i}\right) \tag{38}
\end{align*}
$$

where

$$
\begin{align*}
\nabla_{i} A_{j}-\nabla_{j} A_{i} & =\epsilon_{i j k} \epsilon_{k \ell m} \nabla_{\ell} A_{m} \\
& =\epsilon_{i j k}(\nabla \times \mathbf{A})_{k}=\epsilon_{i j k} B_{k}(\hat{\mathbf{x}}) . \tag{39}
\end{align*}
$$

In the Hamiltonian formalism, the kinematic momentum $\vec{\pi}$ is an example of a dependent variable, i.e., a function of the positions and the canonical momentum. In general, a classical system may have all kinds of interesting dependent variables

$$
\begin{equation*}
F(t)=\mathcal{F}\left(q_{1}, \ldots, q_{N} ; p_{1}, \ldots, p_{N}\right) @(\text { time }=t), \tag{40}
\end{equation*}
$$

and in the quantum system all such variables become operators in the Hilbert space constructed as

$$
\begin{equation*}
\hat{F}=\mathcal{F}\left(\hat{q}_{1}, \ldots, \hat{q}_{N} ; \hat{p}_{1}, \ldots, \hat{p}_{N}\right) \tag{41}
\end{equation*}
$$

modulo operator ordering. That is, if the same term in $\mathcal{F}$ involves both position and momentum operators, the order of their product is ambiguous; it has to be second-guessed or determined experimentally. More generally,

$$
\begin{equation*}
\hat{F}=\mathcal{F}\left(\hat{q}_{1}, \ldots, \hat{q}_{N} ; \hat{p}_{1}, \ldots, \hat{p}_{N}\right)+O(\hbar) \tag{42}
\end{equation*}
$$

where the order $-\hbar$ correction cannot be determined from the classical theory alone.

The most important dependent variable of any classical system is the Hamiltonian $H(q, p)$; like the other dependent variables, its quantum counterpart is the Hamiltonian operator

$$
\begin{equation*}
\hat{H}=H(\hat{q}, \hat{p})+O(\hbar) \tag{43}
\end{equation*}
$$

where the $O(\hbar)$ correction stems from the ordering ambiguities of a function of both position and momentum operators. For the simple classical Hamiltonians like

$$
\begin{equation*}
H(q, p)=V(q)+K(p), \tag{44}
\end{equation*}
$$

their quantum counterparts are

$$
\begin{equation*}
\hat{H}=\hat{V}+\hat{K}=V(\hat{q})+K(\hat{p}) \tag{45}
\end{equation*}
$$

without any quantum ambiguities (and hence without the $O(\hbar)$ corrections), but in more general cases there are terms involving both positions and momenta so we must resolve the ordering ambiguity. There are no standard recipies this resolution, but there is two simple rule: whatever you do, the Hamiltonian operator $\hat{H}$ you build must be Hermitian.

The Hamiltonian operator determines the time evolution of the quantum system, but the specific nature of this time evolution is different in different pictures of Quantum Mechanics. In the Schrödinger picture the operators are time independent. That is, they act on a wave function in the same way at all times, for example

$$
\begin{equation*}
\hat{\mathbf{x}} \psi(\mathbf{x})=\mathbf{x} \psi(\mathbf{x}) \quad \text { and } \quad \hat{\mathbf{p}} \psi(\mathbf{x})=-i \hbar \bar{\nabla} \psi(\mathbf{x}) . \tag{46}
\end{equation*}
$$

On the other hand, the quantum states evolve with time according to the Schrödinger equation

$$
\begin{equation*}
i \hbar \frac{d}{d t}|\psi\rangle=\hat{H}|\psi\rangle . \tag{47}
\end{equation*}
$$

In the Heisenberg picture it's the states which are time independent, same $|\psi\rangle(t)$ at all $t$; on
the other hand, the operators evolve with time according to the Heisenberg equation

$$
\begin{equation*}
i \hbar \frac{d}{d t} \hat{F}(t)=[\hat{F}, \hat{H}]=\hat{F} \hat{H}-\hat{H} \hat{F} \tag{48}
\end{equation*}
$$

Fortunately, the expectation values of the operators have the same time dependence in all pictures; specifically, they obey the Heisenberg-Dirac equations

$$
\begin{equation*}
i \hbar \frac{d}{d t}\langle\psi| \hat{F}|\psi\rangle=\langle\psi|[\hat{F}, \hat{H}]|\psi\rangle . \tag{49}
\end{equation*}
$$

In the Schrödinger picture the canonical commutation relations (34) between position and momentum operators are time independent, but in the Heisenberg picture those commutation relations work only at equal times:

$$
\begin{align*}
\text { for } t=t^{\prime}: & {\left[\hat{q}_{i}(t), \hat{q}_{j}\left(t^{\prime}\right)\right]=0, \quad\left[\hat{p}_{i}(t), \hat{p}_{j}\left(t^{\prime}\right)\right]=0, \quad\left[\hat{q}_{i}(t), \hat{p}_{j}\left(t^{\prime}\right)\right]=i \hbar \delta_{i j}, }  \tag{50}\\
\text { but for } t \neq t^{\prime} & {\left[\hat{q}_{i}(t), \hat{q}_{j}\left(t^{\prime}\right)\right]=? ?, \quad\left[\hat{p}_{i}(t), \hat{p}_{j}\left(t^{\prime}\right)\right]=? ?, \quad\left[\hat{q}_{i}(t), \hat{p}_{j}\left(t^{\prime}\right)\right]=? ? } \tag{51}
\end{align*}
$$

For example, for a harmonic oscillator solving the Heisenberg equations gives us

$$
\begin{equation*}
\hat{q}(t)=\hat{q}(0) \times \cos (\omega t)+\frac{\hat{p}(0)}{m \omega} \times \sin (\omega t), \quad \hat{p}(t)=\hat{p}(0) \times \cos (\omega t)-m \omega \hat{q}(0) \times \sin (\omega t), \tag{52}
\end{equation*}
$$

and therefore

$$
\begin{align*}
{\left[\hat{q}\left(t_{1}\right), \hat{q}\left(t_{2}\right)\right] } & =\frac{i \hbar}{m \omega} \times \sin (\omega \Delta t), \\
{\left[\hat{p}\left(t_{1}\right), \hat{p}\left(t_{2}\right)\right] } & =i \hbar m \omega \times \sin (\omega \Delta t)  \tag{53}\\
{\left[\hat{q}\left(t_{1}\right), \hat{p}\left(t_{2}\right)\right] } & =i \hbar \times \cos (\omega \Delta t)
\end{align*}
$$

## Poisson Brackets and Commutator Brackets

Both classical mechanics and quantum mechanics use bi-linear brackets of variables with similar algebraic properties. In classical mechanics the variables are functions of the canonical coordinates and momenta, and the Poisson bracket of two such variables $A(q, p)$ and $B(q, p)$ are defined as

$$
\begin{equation*}
[A, B]_{P} \stackrel{\text { def }}{=} \sum_{i}\left(\frac{\partial A}{\partial q_{i}} \frac{\partial B}{\partial p_{i}}-\frac{\partial A}{\partial p_{i}} \frac{\partial B}{\partial q_{i}}\right) \tag{54}
\end{equation*}
$$

In quantum mechanics the variables are linear operators in some Hilbert space, and the commutator bracket of two operators is

$$
\begin{equation*}
[A, B]_{C} \stackrel{\text { def }}{=} A B-B A . \tag{55}
\end{equation*}
$$

Both types of brackets have similar algebraic properties:

1. Linearity: $\left[\alpha_{1} A_{1}+\alpha_{2} A_{2}, B\right]=\alpha_{1}\left[A_{1}, B\right]+\alpha_{2}\left[A_{2}, B\right]$ and $\left[A, \beta_{1} B_{1}+\beta_{2} B_{2}\right]=\beta_{1}\left[A, B_{1}\right]+$ $\beta_{2}\left[A, B_{2}\right]$.
2. Antisymmetry: $[A, B]=-[B, A]$.
3. Leibniz rules: $[A B, C]=A[B, C]+[A, C] B$ and $[A, B C]=B[A, C]+[A, B] C$.
4. Jacobi Identity: $[A,[B, C]]+[B,[C, A]]+[C,[A, B]]=0$.

Also, both types of brackets involving the Hamiltonian can be used to describe the time dependence of the classical/quantum variables. In classical mechanics,

$$
\begin{align*}
\frac{d}{d t} A(q, p)= & \sum_{i}\left(\frac{\partial A}{\partial q_{i}} \frac{d q_{i}}{d t}+\frac{\partial A}{\partial p_{i}} \frac{d p_{i}}{d t}\right) \\
& \langle\langle\text { by the Hamilton equations }\rangle\rangle \\
= & \sum_{i}\left(\frac{\partial A}{\partial q_{i}} \frac{\partial H}{\partial p_{i}}-\frac{\partial A}{\partial p_{i}} \frac{\partial H}{\partial q_{i}}\right)  \tag{56}\\
\equiv & {[A, H]_{P}, }
\end{align*}
$$

while in quantum mechanics we have the Heisenberg-Dirac equation

$$
\begin{equation*}
i \hbar \frac{d}{d t}\langle\psi| \hat{A}|\psi\rangle=\langle\psi|[\hat{A}, \hat{H}]_{C}|\psi\rangle \tag{57}
\end{equation*}
$$

which in the Heisenberg picture of QM becomes simply

$$
\begin{equation*}
i \hbar \frac{d}{d t} \hat{A}=[\hat{A}, \hat{H}]_{C} . \tag{58}
\end{equation*}
$$

The similarity between the classical Poisson brackets and the quantum commutator brackets stems from the following theorem: Once we generalize the Poisson brackets to the non-commuting variables of quantum mechanics, they become proportional to the commutator brackets,

$$
\begin{equation*}
[\hat{A}, \hat{B}]_{P}=\frac{\hat{A} \hat{B}-\hat{B} \hat{A}}{i \hbar} . \tag{59}
\end{equation*}
$$

Mathematically speaking: for any non-commutative but associative variables, any bracket $[A, B]$ with the algebraic properties $1-4$ is proportional to the commutator bracket:

$$
\begin{equation*}
[A, B]=c(A B-B A) \tag{60}
\end{equation*}
$$

for a universal constant $c$ (same $c$ for all variables); in Physics $c=1 / i \hbar$.
Proof: Take any 4 variables $A, B, U, V$ and calculate $[A U, B V]$ using the Leibniz rules, first for the $A U$ and then for the $B V$ :

$$
\begin{align*}
{[A U, B V] } & =A[U, B V]+[A, B V] U  \tag{61}\\
& =A B[U, V]+A[U, B] V+B[A, V] U+[A, B] V U .
\end{align*}
$$

OOH , if we use the two Leibniz rules in the opposite order we get a different expression

$$
\begin{align*}
{[A U, B V] } & =B[A U, V]+[A U, B] V \\
& =B A[U, V]+B[A, V] U+A[U, B] V+[A, B] U V \tag{62}
\end{align*}
$$

To make sure the two expressions are equal to each other we need


On the last line here, the LHS depends only on the $U$ and $V$ while the RHS depends only
on the $A$ and $B$, and the only way a relation like that can work for any unrelated variables is if the ratios on both sides of equations are equal to the same universal constant $c$, thus

$$
\begin{equation*}
[A, B]=c(A B-B A) \quad \text { and } \quad[U, V]=c(U V-V U) \tag{64}
\end{equation*}
$$

Quod erat demonstrandum.
Thanks to this theorem, we may quantize a classical theory described in terms of noncanonical variables $\xi_{1}, \ldots, \xi_{2 N}$ (instead of the canonical $q_{1}, \ldots, q_{N}$ and $p_{1}, \ldots, p_{N}$ ) as long as we have a consistent algebra of Poisson brackets. (Their definition would be different from eqs. (54), but they have to obey the algebraic rules 1-4.) Given the classical Poisson algebra, the quantization maps it to the commutator algebra of operators in some Hilbert space. That is, if classically $[A, B]_{P}=C$, then the corresponding operators in quantum mechanics should obey $[\hat{A}, \hat{B}]=i \hbar \hat{C}$.

In particular, if we do have classical canonical variables $q_{i}$ and $p_{i}$, then

$$
\begin{equation*}
\left[q_{i}, q_{j}\right]_{P}=0, \quad\left[p_{i}, p_{j}\right]_{P}=0, \quad\left[q_{i}, p_{j}\right]_{P}=\delta_{i j} \tag{65}
\end{equation*}
$$

so the corresponding quantum operators should obey the canonical commutation relations

$$
\begin{equation*}
\left[\hat{q}_{i}, \hat{q}_{j}\right]_{C}=0, \quad\left[\hat{p}_{i}, \hat{p}_{j}\right]_{C}=0, \quad\left[\hat{q}_{i}, \hat{p}_{j}\right]_{C}=i \hbar \delta_{i j} \tag{66}
\end{equation*}
$$

