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 non-mechanical 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 $(q_1, \ldots, q_N)$, for example 3 coordinates (x, y, z) of some moving particle, or $3n$ coordinates of n interacting particles. The Lagrangian description starts with the Lagrangian function

$$L(q_1, \ldots, q_N; \dot{q}_1, \ldots, \dot{q}_N) \tag{1}$$

of all the dynamical variables q_i and their time derivatives (velocities) $\dot{q}_i = dq_i/dt$. Typically

$$\begin{aligned} L &= E_{\text{kinetic}} - E_{\text{potential}} \\ \text{such as} \quad L &= \sum_{i=1}^{n} \frac{m_i}{2} \dot{\mathbf{x}}_i^2 - V(\mathbf{x}_1, \ldots, \mathbf{x}_n). \end{aligned} \tag{2}$$

Then for any conceivable path $\big(q_1(t), \ldots, q_N(t)\big)$ through the coordinate space, we define the

action integral

$$S[\text{all } q_i(t) \text{ at all } t] \;=\; \int\limits_{t_{\text{start}}}^{t_{\text{finish}}} dt\, L\big(q_1(t),\ldots,q_N(t);\dot q_1(t),\ldots,\dot q_N(t)\big). \tag{3}$$

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

The action functional (3) is defined for any path $\big(q_1(t),\ldots,q_N(t)\big)$, 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* $\big(q_1(t),\ldots,q_N(t)\big)$ *which obeys the Laws of Motion has the least action* among all differentiable paths starting at the same point $(q_1,\ldots,q_N)_1$ at the initial time t_1 and finishing at the same point $(q_1,\ldots,q_N)_2$ at the final time t_2.

Formally, minimizing the action functional is the matter of variational calculus: We allow for infinitesimal variations $q_i(t) \to q_i(t) + \delta q_i(t)$ and then demand that the first variation δS 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*

$$\forall i = 1,\ldots,N: \quad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot q_i}@t\right) \;=\; \frac{\partial L}{\partial q_i}@t. \tag{4}$$

For example, for a single particle with the Lagrangian

$$L \;=\; \frac{m}{2}\,\dot{\mathbf{x}}^2 \;-\; V(\mathbf{x}) \tag{5}$$

we have

$$\frac{\partial L}{\partial \dot x_i} \;=\; m\dot x_i\,, \quad \frac{\partial L}{\partial x_i} \;=\; -\frac{\partial V}{\partial x_i}\,, \tag{6}$$

so the Euler–Lagrange equation (4) becomes

$$\frac{d}{dt}(m\dot x_i) \;=\; -\frac{\partial V}{\partial x_i}\,, \tag{7}$$

or in vector notations

$$\frac{d}{dt}(m\dot{\mathbf{x}}) \;=\; -\nabla V(\mathbf{x}) \;=\; \mathbf{F}(\mathbf{x}). \tag{8}$$

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 $2N$ variables are subject to $2N$ first-order differential equations. Here is how this works:

1. Given N position variables $(q_1, \ldots, q_N)$ and the Lagrangian $L(q_1, \ldots, q_N; \dot{q}_1, \ldots, \dot{q}_N)$, we start by defining the *canonical momentum* p_i for each position q_i according to

$$p_i \;\stackrel{\text{def}}{=}\; \frac{\partial L}{\partial \dot{q}_i} \quad \langle\!\langle \text{ at fixed } q_j \text{ and } \dot{q}_{j\neq i} \,\rangle\!\rangle. \tag{9}$$

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

$$H \;=\; \sum_{i=1}^{N} p_i \dot{q}_i \;-\; L. \tag{10}$$

3. Third, we change independent variables from the velocities to the momenta. Thus, we treat eq. (9) as equations for the velocities $\dot{q}_i$ in terms of the given momenta p_i, and solve these equations. This gives us the velocities $\dot{q}_i$ as functions of the momenta p_i (and perhaps also of the coordinates q_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 $H(q_1, \ldots, q_N; p_1, \ldots p_N)$, the time-dependence of all the positions and all the momenta is governed by the first-order *Hamilton equations*

$$\forall i = 1, \ldots, N: \qquad \frac{dq_i}{dt} \;=\; +\frac{\partial H(q,p)}{\partial p_i}\,, \qquad \frac{dp_i}{dt} \;=\; -\frac{\partial H(q,p)}{\partial q_i}\,. \tag{11}$$

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

$$L \;=\; \frac{m}{2}\dot{\mathbf{v}}^2 \;-\; V(\mathbf{x}) \qquad \text{for } \mathbf{v} \stackrel{\text{def}}{=} \dot{\mathbf{x}} \;=\; \frac{d\mathbf{x}}{dt}\,. \tag{5}$$

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

$$p_i \;=\; \frac{\partial L}{\partial v_i} \;=\; m v_i \quad\Longrightarrow\quad \mathbf{p} \;=\; m\mathbf{v}, \tag{12}$$

hence

$$H \;=\; \mathbf{p}\cdot\mathbf{v} \;-\; L \;=\; m\mathbf{v}\cdot\mathbf{v} \;-\; \frac{m\mathbf{v}^2}{2} \;+\; V(\mathbf{x}) \;=\; +\frac{m\mathbf{v}^2}{2} \;+\; V(\mathbf{x}), \tag{13}$$

or in terms of positions and momenta

$$H(\mathbf{x},\mathbf{p}) \;=\; V(\mathbf{x}) \;+\; \frac{\mathbf{p}^2}{2m}\,. \tag{14}$$

Consequently, the Hamilton equations (11) become

$$\begin{aligned} \frac{d\mathbf{x}}{dt} \;&=\; +\frac{\partial H}{\partial \mathbf{p}} \;=\; \frac{\mathbf{p}}{m}\,, \\ \frac{d\mathbf{p}}{dt} \;&=\; -\frac{\partial H}{\partial \mathbf{x}} \;=\; -\nabla V(\mathbf{x}) \;=\; +\mathbf{F}(\mathbf{x}), \end{aligned} \tag{15}$$

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

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

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,

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

Next, the energy of the charged particle is

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

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 $\mathbf{p}$ rather than velocity or the kinematic momentum $\vec{\pi}$, we end up with a Hamiltonian which does depend on $\mathbf{A}$. Specifically,

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

Consequently, the Hamilton equations for the charged particle are

$$\frac{d\mathbf{x}}{dt} \;=\; +\frac{\partial H}{\partial \mathbf{p}} \;=\; \frac{1}{m}\left(\mathbf{p} \,-\, \frac{Q}{c}\mathbf{A}(\mathbf{x})\right) \;=\; \frac{\vec{\pi}}{m} \tag{20}$$

and

$$\frac{d\mathbf{p}}{dt} \;=\; -\frac{\partial H}{\partial \mathbf{x}} \;=\; -Q\nabla\Phi(\mathbf{x}) \;+\; \frac{Q}{mc}\left(p_j \,-\, \frac{Q}{c}A_j(\mathbf{x})\right)\nabla A_j(\mathbf{x}). \tag{21}$$

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

$$\vec{\pi} \;=\; m\mathbf{v} \;=\; \mathbf{p} \,-\, \frac{Q}{c}\mathbf{A}(\mathbf{x}) \qquad (\textit{cf.}\text{ eq. (20)}). \tag{22}$$

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

$$\frac{d}{dt}\left(\vec{\pi}(t) \,+\, \frac{Q}{c}\mathbf{A}(\mathbf{x}(t))\right) \;=\; -Q\nabla\Phi(\mathbf{x}) \;+\; \frac{Q}{mc}\,\pi_j\nabla A_j(\mathbf{x}). \tag{23}$$

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 time due to $d\mathbf{x}/dt$ even in a static magnetic field,

$$\frac{d}{dt}\mathbf{A}(\mathbf{x}(t)) \;=\; v_j\frac{\partial \mathbf{A}}{\partial x_j}\,. \tag{24}$$

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

$$\frac{d}{dt}\mathbf{A}(\mathbf{x}(t),t) \;=\; \frac{\partial \mathbf{A}}{\partial t} \;+\; v_j\,\frac{\partial \mathbf{A}}{\partial x_j}\,. \tag{25}$$

Plugging this time derivative into eq. (23), we get

$$\frac{d\vec{\pi}}{dt} \;+\; \frac{Q}{c}\frac{\partial \mathbf{A}}{\partial t} \;+\; \frac{Q}{c}\,v_j\frac{\partial \mathbf{A}}{\partial x_j} \;=\; -Q\nabla\Phi \;+\; \frac{Q}{c}\left(\frac{\pi_j}{m} = v_j\right)\nabla A_j\,, \tag{26}$$

and hence

$$\frac{d\vec{\pi}}{dt} \;=\; Q\left(-\nabla\Phi \,-\, \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}\right) \;+\; \frac{Q}{c}\Big(v_j\nabla A_j \,-\, v_j\nabla_j\mathbf{A}\Big). \tag{27}$$

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

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

is the electric field. As to the second term in eq. (27), the expression inside $(\cdots)$ amounts

to $\mathbf{v}\times\mathbf{B}$, indeed

$$\begin{aligned}\Big(v_j\nabla A_j \,-\, v_j\nabla_j\mathbf{A}\Big)_i \;&=\; v_j\big(\nabla_i A_j \,-\, \nabla_j A_i\big)\\ &=\; v_j\big(\delta_{i\ell}\delta_{jm}-\delta_{im}\delta_{j\ell}\big)\nabla_\ell A_m \;=\; v_j\,\epsilon_{ijk}\epsilon_{k\ell m}\,\nabla_\ell A_m\\ &=\; v_j\,\epsilon_{ijk}\Big(\epsilon_{k\ell m}\nabla_\ell A_m \;=\; \big(\nabla\times\mathbf{A}\big)_k \;=\; B_k\Big)\\ &=\; \epsilon_{ijk}v_jB_k \;=\; (\mathbf{v}\times\mathbf{B})_i\,,\end{aligned} \tag{29}$$

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

$$\mathbf{F}_L \;=\; \frac{Q}{c}\,\mathbf{v}\times\mathbf{B}(\mathbf{x},t). \tag{30}$$

Altogether, eq. (27) amounts to

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

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,

$$\frac{d}{dt}(m\mathbf{v}) \;=\; \mathbf{F}_{EM} \;=\; Q\mathbf{E}(\mathbf{x},t) \;+\; \frac{Q}{c}\,\mathbf{v}\times\mathbf{B}(\mathbf{x},t). \tag{32}$$

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,

$$U(q_1@t_1 \to q_2@t_2) \;=\; \iint\limits_{q(t_1)=q_1}^{q(t_2)=q_2} \mathcal{D}[q(t)]\, \exp(iS[q(t)]/\hbar). \tag{33}$$

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 $\psi(q_1, \ldots, q_N)$ 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

$$[\hat{q}_i, \hat{q}_j] \;=\; 0, \quad [\hat{p}_i, \hat{p}_j] \;=\; 0, \quad [\hat{q}_i, \hat{p}_j] \;=\; i\hbar\delta_{ij}\,. \tag{34}$$

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

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

we get

$$[\hat{x}_i, \hat{x}_j] \;=\; 0 \quad \text{and} \quad [\hat{x}_i, \hat{\pi}_j] \;=\; i\hbar\delta_{ij} \tag{36}$$

but

$$[\hat{\pi}_i, \hat{\pi}_j] \;=\; \frac{i\hbar Q}{c}\,\epsilon_{ijk} B_k(\hat{\mathbf{x}}) \;\neq\; 0. \tag{37}$$

Indeed,

$$\begin{aligned}
[\hat{\pi}_i, \hat{\pi}_j] \;&=\; -\frac{Q}{c}\,[A_i(\hat{\mathbf{x}}), \hat{\pi}_j] \;-\; \frac{Q}{c}\,[\hat{\pi}_i, A_j(\hat{\mathbf{x}})] \\
&=\; -\frac{i\hbar Q}{c}\,(\nabla_j A_i(\hat{\mathbf{x}})) \;+\; \frac{i\hbar Q}{c}(\nabla_i A_j(\hat{\mathbf{x}})) \\
&=\; \frac{i\hbar Q}{c}\big(\nabla_i A_j - \nabla_j A_i\big)
\end{aligned} \tag{38}$$

where

$$\begin{aligned}
\nabla_i A_j \;-\; \nabla_j A_i \;&=\; \epsilon_{ijk}\epsilon_{k\ell m}\nabla_\ell A_m \\
&=\; \epsilon_{ijk}\big(\nabla \times \mathbf{A}\big)_k \;=\; \epsilon_{ijk} B_k(\hat{\mathbf{x}}).
\end{aligned} \tag{39}$$

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

$$F(t) \;=\; \mathcal{F}(q_1, \ldots, q_N; p_1, \ldots, p_N)@(\text{time} = t), \tag{40}$$

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

$$\hat{F} \;=\; \mathcal{F}(\hat{q}_1, \ldots, \hat{q}_N; \hat{p}_1, \ldots, \hat{p}_N) \tag{41}$$

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,

$$\hat{F} \;=\; \mathcal{F}(\hat{q}_1, \ldots, \hat{q}_N; \hat{p}_1, \ldots, \hat{p}_N) \;+\; O(\hbar) \tag{42}$$

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*

$$\hat{H} \;=\; H(\hat{q},\hat{p}) \;+\; O(\hbar) \tag{43}$$

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

$$H(q,p) \;=\; V(q) \;+\; K(p), \tag{44}$$

their quantum counterparts are

$$\hat{H} \;=\; \hat{V} \;+\; \hat{K} \;=\; V(\hat{q}) \;+\; K(\hat{p}) \tag{45}$$

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 recipes this resolution, but there is a general 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

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

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

$$i\hbar\frac{d}{dt}\left|\psi\right\rangle \;=\; \hat{H}\left|\psi\right\rangle. \tag{47}$$

In the *Heisenberg picture*, it's the states which are time independent, same $\left|\psi\right\rangle(t)$ at all t;

on the other hand, the operators evolve with time according to the Heisenberg equation

$$i\hbar\frac{d}{dt}\hat{F}(t) \;=\; [\hat{F},\hat{H}] \;=\; \hat{F}\hat{H} \;-\; \hat{H}\hat{F}. \tag{48}$$

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

$$i\hbar\frac{d}{dt}\left\langle\psi\right|\hat{F}\left|\psi\right\rangle \;=\; \left\langle\psi\right|[\hat{F},\hat{H}]\left|\psi\right\rangle. \tag{49}$$

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:*

$$\text{for } t=t': \quad [\hat{q}_i(t),\hat{q}_j(t')] \;=\; 0, \quad [\hat{p}_i(t),\hat{p}_j(t')] \;=\; 0, \quad [\hat{q}_i(t),\hat{p}_j(t')] \;=\; i\hbar\delta_{ij}\,, \tag{50}$$

$$\text{but for } t\neq t' \quad [\hat{q}_i(t),\hat{q}_j(t')] \;=??, \quad [\hat{p}_i(t),\hat{p}_j(t')] \;=??, \quad [\hat{q}_i(t),\hat{p}_j(t')] \;=??\,. \tag{51}$$

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

$$\hat{q}(t) \;=\; \hat{q}(0)\times\cos(\omega t) + \frac{\hat{p}(0)}{m\omega}\times\sin(\omega t), \qquad \hat{p}(t) \;=\; \hat{p}(0)\times\cos(\omega t) \;-\; m\omega\hat{q}(0)\times\sin(\omega t), \tag{52}$$

and therefore

$$\begin{aligned} [\hat{q}(t_1),\hat{q}(t_2)] \;&=\; \frac{i\hbar}{m\omega}\times\sin(\omega\Delta t), \\ [\hat{p}(t_1),\hat{p}(t_2)] \;&=\; i\hbar m\omega\times\sin(\omega\Delta t), \\ [\hat{q}(t_1),\hat{p}(t_2)] \;&=\; i\hbar\times\cos(\omega\Delta t). \end{aligned} \tag{53}$$

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

$$[A,B]_P \stackrel{\text{def}}{=} \sum_i \left(\frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} \right). \tag{54}$$

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

$$[A,B]_C \stackrel{\text{def}}{=} AB - BA. \tag{55}$$

Both types of brackets have similar algebraic properties:

1. Linearity: $[\alpha_1 A_1 + \alpha_2 A_2, B] = \alpha_1[A_1,B] + \alpha_2[A_2,B]$ and $[A, \beta_1 B_1 + \beta_2 B_2] = \beta_1[A,B_1] + \beta_2[A,B_2]$.
2. Antisymmetry: $[A,B] = -[B,A]$.
3. Leibniz rules: $[AB,C] = A[B,C] + [A,C]B$ and $[A,BC] = B[A,C] + [A,B]C$.
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,

$$\begin{aligned} \frac{d}{dt}A(q,p) &= \sum_i \left(\frac{\partial A}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial A}{\partial p_i}\frac{dp_i}{dt} \right) \\ &\qquad \langle\!\langle \text{ by the Hamilton equations } \rangle\!\rangle \\ &= \sum_i \left(\frac{\partial A}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial H}{\partial q_i} \right) \\ &\equiv [A,H]_P\,, \end{aligned} \tag{56}$$

while in quantum mechanics we have the Heisenberg–Dirac equation

$$i\hbar \frac{d}{dt} \langle\psi|\, \hat{A}\, |\psi\rangle = \langle\psi|\, [\hat{A},\hat{H}]_C\, |\psi\rangle\,, \tag{57}$$

which in the Heisenberg picture of QM becomes simply

$$i\hbar\frac{d}{dt}\hat{A} \;=\; [\hat{A},\hat{H}]_C\,. \tag{58}$$

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,

$$[\hat{A},\hat{B}]_P \;=\; \frac{\hat{A}\hat{B}-\hat{B}\hat{A}}{i\hbar}\,. \tag{59}$$

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:*

$$[A,B] \;=\; c(AB-BA) \tag{60}$$

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 $[AU,BV]$ using the Leibniz rules, first for the AU and then for the BV:

$$\begin{aligned}[AU,BV] \;&=\; A[U,BV] \;+\; [A,BV]U \\ &=\; AB[U,V] \;+\; A[U,B]V \;+\; B[A,V]U \;+\; [A,B]VU.\end{aligned} \tag{61}$$

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

$$\begin{aligned}[AU,BV] \;&=\; B[AU,V] \;+\; [AU,B]V \\ &=\; BA[U,V] \;+\; B[A,V]U \;+\; A[U,B]V \;+\; [A,B]UV.\end{aligned} \tag{62}$$

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

$$\begin{aligned} AB[U,V] \;+\; [A,B]VU &= \; BA[U,V] \;+\; [A,B]UV \\ &\Downarrow \\ (AB-BA)[U,V] &= \; [A,B](UV-VU) \\ &\Downarrow \\ [U,V](UV-VU)^{-1} &= \; (AB-BA)^{-1}[A,B] \end{aligned} \tag{63}$$

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

$$[A,B] \;=\; c(AB-BA) \quad \text{and} \quad [U,V] \;=\; c(UV-VU). \tag{64}$$

Quod erat demonstrandum.

Thanks to this theorem, we may quantize a classical theory described in terms of non-canonical variables $\xi_1,\ldots,\xi_{2N}$ (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

$$[q_i,q_j]_P \;=\; 0, \quad [p_i,p_j]_P \;=\; 0, \quad [q_i,p_j]_P \;=\; \delta_{ij}\,, \tag{65}$$

so the corresponding quantum operators should obey the *canonical commutation relations*

$$[\hat{q}_i,\hat{q}_j]_C \;=\; 0, \quad [\hat{p}_i,\hat{p}_j]_C \;=\; 0, \quad [\hat{q}_i,\hat{p}_j]_C \;=\; i\hbar\delta_{ij}\,. \tag{66}$$