

# 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,

$$U(q_1 @ t_1 \rightarrow q_2 @ t_2) = \iiint_{q(t_1)=q_1}^{q(t_2)=q_2} \mathcal{D}[q(t)] \exp(iS[q(t)]/\hbar). \quad (1)$$

In field theory, the functional quantization makes relativity manifest but obscures unitarity. Also, it makes a bit easier to derive the Feynman rules but makes much harder to see the field–particle correspondence. On the other hand, the canonical quantization is manifestly unitary but obscures relativity. Also, it makes the field-particle relations easy to see — and we shall see how it works in a couple of lectures, — but deriving the Feynman rules takes a few extra steps.

In this class, I shall use the canonical quantization throughout the first semester. The functional quantization will have to wait until the middle of the second semester.

## Hamiltonian Formulation of Classical Mechanics

Let’s start with some classical system with  $N$  dynamical variables  $q_1(t), \dots, q_N(t)$  and the Lagrangian  $L(q_1, \dots, q_n; \dot{q}_1, \dots, \dot{q}_N)$ . Before we quantize, we need to convert the Lagrangian formulation of the classical system to the Hamiltonian formulation. First, we

define  $N$  canonical momenta  $p_1, \dots, p_N$  — one momentum  $p_i$  for each ‘position’ variable  $q_i$  — according to

$$p_i \stackrel{\text{def}}{=} \frac{\partial L}{\partial \dot{q}_i}. \quad (2)$$

Second, we calculate the systems energy  $H$  as

$$H = \sum_{i=1}^N p_i \dot{q}_i - L. \quad (3)$$

Third, given  $N$  positions  $q_1, \dots, q_N$  and  $N$  momenta  $p_1, \dots, p_N$  we solve eqs. (2) for the velocities  $\dot{q}_1, \dots, \dot{q}_N$ , plug the solutions into eq. (3), and rewrite the energy  $H$  as a function  $H(q, p)$  of positions and momenta rather than positions and velocities. Given such function  $H(q, p)$  — called the classical Hamiltonian — we can write the Hamilton equations for the time dependence of all the coordinates and momenta:

$$\forall i = 1, \dots, N : \quad \frac{dq_i}{dt} = +\frac{\partial H}{\partial p_i} \quad \text{and} \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}. \quad (4)$$

Note: The Hamilton equations are first-order in the time derivative, but there are  $2N$  equations, so altogether there are  $N$  degrees of freedom. By comparison, in the Lagrangian formalism the same  $N$  degrees of freedom are described by  $N$  second-order Euler–Lagrange equations.

As an example of a Hamiltonian and Hamilton equations consider a non-relativistic particle subject to the potential  $V(\mathbf{x})$ , thus the Lagrangian

$$L = \frac{m}{2} \mathbf{v}^2 - V(\mathbf{x}) \quad \text{for } \mathbf{v} \stackrel{\text{def}}{=} \dot{\mathbf{x}}. \quad (5)$$

For this Lagrangian, the canonical momenta (2) form a 3-vector

$$\mathbf{p} = \frac{\partial L}{\partial \mathbf{v}} = m\mathbf{v} \quad (6)$$

hence the energy

$$H = \mathbf{p} \cdot \mathbf{v} - L = m\mathbf{v}^2 - \frac{m}{2} \mathbf{v}^2 + V(\mathbf{x}) = \frac{m}{2} \mathbf{v}^2 + V(\mathbf{x}). \quad (7)$$

In terms of the momentum (6) the velocity is  $\mathbf{v} = \mathbf{p}/m$ , so as a function of the position and

the momentum the energy (7) becomes

$$H(\mathbf{x}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}). \quad (8)$$

Given this Hamiltonian function, the Hamilton equations (4) become

$$\frac{d\mathbf{x}}{dt} = +\frac{\partial H}{\partial \mathbf{p}} = \frac{\mathbf{p}}{m} \quad (9)$$

— which recovers  $\mathbf{v} = \mathbf{p}/m$ , — and the Newton's Law

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{x}} = -\nabla V(\mathbf{x}) = +\mathbf{F}(\mathbf{x}). \quad (10)$$

For a more interesting example, consider a charged particle moving in electric and magnetic fields. For simplicity, assume given static EM fields with potentials  $\Phi(\mathbf{x})$  and  $\mathbf{A}(\mathbf{x})$ . This time, the Lagrangian is

$$L = \frac{m}{2} \mathbf{v}^2 - Q\Phi(\mathbf{x}) + \frac{Q}{c} \mathbf{v} \cdot \mathbf{A}(\mathbf{x}). \quad (11)$$

Note that the magnetic term here depends on both the position and the velocity of the charged particle. For the Lagrangian (11), the *canonical momentum* of the charged particle is

$$\mathbf{p} = \frac{\partial L}{\partial \mathbf{v}} = m\mathbf{v} + \frac{Q}{c} \mathbf{A}(\mathbf{x}), \quad (12)$$

which is quite different from the *kinematic momentum*  $\vec{\pi} = m\mathbf{v}$ . As to the energy  $H$ , at first blush we get

$$\begin{aligned} H &= \mathbf{p} \cdot \mathbf{v} - L \\ &= m\mathbf{v}^2 + \frac{Q}{c} \mathbf{A}(\mathbf{x}) \cdot \mathbf{v} - \frac{m}{2} \mathbf{v}^2 + Q\Phi(\mathbf{x}) - \frac{Q}{c} \mathbf{v} \cdot \mathbf{A}(\mathbf{x}) \\ &= \frac{m}{2} \mathbf{v}^2 + Q\Phi(\mathbf{x}), \end{aligned} \quad (13)$$

regardless of the vector potential  $\mathbf{A}$  for the magnetic field. However, when we re-express this energy in terms of the canonical momentum  $\mathbf{p}$  rather than the velocity  $\mathbf{v}$  or the kinematic

momentum  $\vec{\pi} = m\mathbf{v}$ , the dependence on the magnetic potential comes back,

$$H(\mathbf{x}, \mathbf{p}) = \frac{\vec{\pi}^2}{2m} + Q\Phi(\mathbf{x}) = \frac{1}{2m} \left( \mathbf{p} - \frac{Q}{c} \mathbf{A}(\mathbf{x}) \right)^2 + Q\Phi(\mathbf{x}). \quad (14)$$

To save time, let me skip the Hamilton equations for this system. But if you have a little time left over from the regular homework, I suggest you write down these Hamilton equations and then convert them into the Newton Law for a particle subject to electric and Lorentz forces.

## 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  $\psi(q_1, \dots, q_N)$  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

$$[\hat{q}_i, \hat{q}_j] = 0, \quad [\hat{p}_i, \hat{p}_j] = 0, \quad [\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij}. \quad (15)$$

Note that the momentum operators in these relations are the *canonical momenta* whose classical counterparts obtain from eq. (2), 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

$$\hat{\vec{\pi}} \stackrel{\text{def}}{=} \hat{\mathbf{p}} - \frac{Q}{c} \mathbf{A}(\hat{\mathbf{x}}), \quad (16)$$

we get

$$[\hat{x}_i, \hat{x}_j] = 0 \quad \text{and} \quad [\hat{x}_i, \hat{\pi}_j] = i\hbar\delta_{ij} \quad (17)$$

but

$$\begin{aligned}
[\hat{\pi}_i, \hat{\pi}_j] &= -\frac{Q}{c} [A_i(\hat{\mathbf{x}}), \hat{\pi}_j] - \frac{Q}{c} [\hat{\pi}_i, A_j(\hat{\mathbf{x}})] \\
&= -\frac{i\hbar Q}{c} (\nabla_j A_i(\hat{\mathbf{x}})) + \frac{i\hbar Q}{c} (\nabla_i A_j(\hat{\mathbf{x}})) \\
&= \frac{i\hbar Q}{c} \epsilon_{ijk} B_k(\hat{\mathbf{x}}).
\end{aligned} \tag{18}$$

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

$$F(t) = \mathcal{F}(q_1, \dots, q_N; p_1, \dots, p_N) @(\text{time} = t), \tag{19}$$

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

$$\hat{F} = \mathcal{F}(\hat{q}_1, \dots, \hat{q}_N; \hat{p}_1, \dots, \hat{p}_N) \tag{20}$$

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,

$$\hat{F} = \mathcal{F}(\hat{q}_1, \dots, \hat{q}_N; \hat{p}_1, \dots, \hat{p}_N) + O(\hbar) \tag{21}$$

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*

$$\hat{H} = H(\hat{q}, \hat{p}) + O(\hbar) \tag{22}$$

which determines the time evolution of the quantum system. The exact 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

$$\hat{\mathbf{x}}\psi(\mathbf{x}) = \mathbf{x}\psi(\mathbf{x}) \quad \text{and} \quad \hat{\mathbf{p}}\psi(\mathbf{x}) = -i\hbar\bar{\nabla}\psi(\mathbf{x}). \quad (23)$$

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

$$i\hbar\frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle. \quad (24)$$

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

$$i\hbar\frac{d}{dt}\hat{F}(t) = [\hat{F}, \hat{H}] = \hat{F}\hat{H} - \hat{H}\hat{F}. \quad (25)$$

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

$$i\hbar\frac{d}{dt}\langle\psi|\hat{F}|\psi\rangle = \langle\psi|[\hat{F}, \hat{H}]|\psi\rangle. \quad (26)$$

In the Schrödinger picture the canonical commutation relations (15) between position and momentum operators are time independent, but in the Heisenberg picture those commutation relations work *only at equal times*:

$$\text{for } t = t' : [\hat{q}_i(t), \hat{q}_j(t')] = 0, \quad [\hat{p}_i(t), \hat{p}_j(t')] = 0, \quad [\hat{q}_i(t), \hat{p}_j(t')] = i\hbar\delta_{ij}, \quad (27)$$

$$\text{but for } t \neq t' \quad [\hat{q}_i(t), \hat{q}_j(t')] = ??, \quad [\hat{p}_i(t), \hat{p}_j(t')] = ??, \quad [\hat{q}_i(t), \hat{p}_j(t')] = ??. \quad (28)$$

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

$$\hat{q}(t) = \hat{q}(0) \times \cos(\omega t) + \frac{\hat{p}(0)}{m\omega} \times \sin(\omega t), \quad \hat{p}(t) = \hat{p}(0) \times \cos(\omega t) - m\omega\hat{q}(0) \times \sin(\omega t), \quad (29)$$

and therefore

$$\begin{aligned} [\hat{q}(t_1), \hat{q}(t_2)] &= \frac{i\hbar}{m\omega} \times \sin(\omega\Delta t), \\ [\hat{p}(t_1), \hat{p}(t_2)] &= i\hbar m\omega \times \sin(\omega\Delta t), \\ [\hat{q}(t_1), \hat{p}(t_2)] &= i\hbar \times \cos(\omega\Delta t). \end{aligned} \quad (30)$$

## 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

$$[A, B]_P \stackrel{\text{def}}{=} \sum_i \left( \frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right). \quad (31)$$

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

$$[A, B]_C \stackrel{\text{def}}{=} AB - BA. \quad (32)$$

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,

$$\begin{aligned} \frac{d}{dt} A(q, p) &= \sum_i \left( \frac{\partial A}{\partial q_i} \frac{dq_i}{dt} + \frac{\partial A}{\partial p_i} \frac{dp_i}{dt} \right) \\ &\quad \langle\langle \text{by the Hamilton equations} \rangle\rangle \\ &= \sum_i \left( \frac{\partial A}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial H}{\partial q_i} \right) \\ &\equiv [A, H]_P, \end{aligned} \quad (33)$$

while in quantum mechanics we have the Heisenberg–Dirac equation

$$i\hbar \frac{d}{dt} \langle \psi | \hat{A} | \psi \rangle = \langle \psi | [\hat{A}, \hat{H}]_C | \psi \rangle, \quad (34)$$

which in the Heisenberg picture of QM becomes simply

$$i\hbar \frac{d}{dt} \hat{A} = [\hat{A}, \hat{H}]_C. \quad (35)$$

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,

$$[\hat{A}, \hat{B}]_P = \frac{\hat{A}\hat{B} - \hat{B}\hat{A}}{i\hbar}. \quad (36)$$

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:*

$$[A, B] = c(AB - BA) \quad (37)$$

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  $BV$ :

$$\begin{aligned} [AU, BV] &= A[U, BV] + [A, BV]U \\ &= AB[U, V] + A[U, B]V + B[A, V]U + [A, B]VU. \end{aligned} \quad (38)$$

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

$$\begin{aligned} [AU, BV] &= B[AU, V] + [AU, B]V \\ &= BA[U, V] + B[A, V]U + A[U, B]V + [A, B]UV. \end{aligned} \quad (39)$$

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

$$\begin{aligned} AB[U, V] + [A, B]VU &= BA[U, V] + [A, B]UV \\ &\Downarrow \\ (AB - BA)[U, V] &= [A, B](UV - VU) \\ &\Downarrow \\ [U, V](UV - VU)^{-1} &= (AB - BA)^{-1}[A, B] \end{aligned} \quad (40)$$

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

$$[A, B] = c(AB - BA) \quad \text{and} \quad [U, V] = c(UV - VU). \quad (41)$$

*Quod erat demonstrandum.*

Thanks to this theorem, we may quantize a classical theory described in terms of non-canonical variables  $\xi_1, \dots, \xi_{2N}$  (instead of the canonical  $q_1, \dots, q_N$  and  $p_1, \dots, p_N$ ) as long as we have a consistent algebra of Poisson brackets. (Their definition would be different from eqs. (31), 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

$$[q_i, q_j]_P = 0, \quad [p_i, p_j]_P = 0, \quad [q_i, p_j]_P = \delta_{ij}, \quad (42)$$

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

$$[\hat{q}_i, \hat{q}_j]_C = 0, \quad [\hat{p}_i, \hat{p}_j]_C = 0, \quad [\hat{q}_i, \hat{p}_j]_C = i\hbar\delta_{ij}. \quad (43)$$