LECTURE 2 — 09/23/2020
CLASSICAL V.S. QUANTUM

1. Classical Mechanics in $T^*\mathbb{R}^n$

Consider the simplest system in classical physics: a free particle moving in a force field in $\mathbb{R}^n$. Here, "free" means there is no other outer force acting on the particle. Denote by $V(x)$ the potential energy function of the force field, which will be assumed to be time-independent. For simplicity we take the particle mass $m = 1$. Denote by

$$x(t) = (x_1(t), \cdots, x_n(t))$$

the position vector of the particle at time t, so that the movement of the particle is described by a curve

$$t \mapsto x(t) \in \mathbb{R}^n$$

in the *configuration space* $\mathbb{R}^n$. The only force acting on the particle is

$$F = -\nabla V$$

which depends only on the position of the particle. According to the famous Newton's rule, the position vector of the particle satisfies the *Newton's second law*

$$\ddot{x}(t) = F(x(t)) = -(\nabla V)(x(t)), \tag{1}$$

Here and in the future, dot (or dots) means taking derivatives with respect to t. A remarkable fact of the system (which is of course a trivial application of the Newton's rule) is the conservation law, which claims that the *energy function* of the system,

$$E = \frac{1}{2}|\dot{x}(t)|^2 + V(x(t)), \tag{2}$$

is a conserved quantity, i.e. is a constant independent of t.

In many situation, when describing such a system, it is very important to describe not only the position vector of the particle, but also the momentum vector

$$\xi(t) = \dot{x}(t) = (\xi_1(t), \cdots, \xi_n(t))$$

of the particle. By using the vector ξ, one can rewrite the Newton's equation as

$$\begin{cases} \dot{x}(t) = \xi(t), \\ \dot{\xi}(t) = -\nabla V. \end{cases}$$

This is of course trivial in the theory of ordinary differential equations: one can always rewrite a higher order differential equation as a system of several first order differential equations by introducing new variables. However, it opens a new door to

both physicists and mathematicians: inside this door it is Hamiltonian mechanics, or in the language of mathematics, symplectic geometry.

In Hamiltonian mechanics, instead of using the configuration space $\mathbb{R}^n$ as the background space, people use the *phase space*

$$T^*\mathbb{R}^n = \mathbb{R}^n \times \mathbb{R}^n = \{(x,\xi)|x \in \mathbb{R}^n, \xi \in \mathbb{R}^n\}$$

as the background space. The movement of the particle is then described by a curve

$$t \mapsto \gamma(t) = (x(t), \xi(t)) \in \mathbb{R}^n \times \mathbb{R}^n$$

in the phase space. We will call this curve the *classical trajectory* of the system. In this language any point in the phase space (usually called a *classical state*) describes a possible situation of the system. Moreover, the total energy of a given system represented by a state (x,ξ) is the value of the energy function (always called the *energy observable*, or the *Hamiltonian*)

$$H = \frac{1}{2}|\xi|^2 + V(x) \in C^\infty(T^*\mathbb{R}^n) \tag{3}$$

at the point (x,ξ). Using the Hamiltonian H, one can rewrite the system of equations above as

$$\begin{cases} \dot{x}_k(t) = \frac{\partial H}{\partial \xi_k}(x(t),\xi(t)), \\ \dot{\xi}_k(t) = -\frac{\partial H}{\partial x_k}(x(t),\xi(t)). \end{cases} \tag{4}$$

This is usually referred to as the *system of Hamilton's equations*. If we denote Ξ_H be the vector field (called the *Hamiltonian vector field* associated to H)

$$\Xi_H = \sum_k \left(\frac{\partial H}{\partial \xi_k}\frac{\partial}{\partial x_k} - \frac{\partial H}{\partial x_k}\frac{\partial}{\partial \xi_k} \right), \tag{5}$$

then the system of Hamilton's equations can be rewritten as

$$\dot{\gamma}(t) = \Xi_H(\gamma(t)). \tag{6}$$

In other words, the solution curve $\gamma = \gamma(t)$ with initial value $\gamma(0) = \gamma_0 = (x_0, \xi_0)$ is the integral curve of the vector field Ξ_H starting at the point γ_0.

Now given any initial data $\gamma(0) = (x_0, \xi_0)$, one can solve the system (6), at least locally near $t = 0$. For simplicity we will assume that the solution exists for all t, in other words, we assume the vector field Ξ_H to be complete[1]. The advantage of introducing the Hamiltonian vector field is the following: it generates a *flow*[2] (called the *Hamiltonian flow* associated with H),

$$\rho_t = e^{t\Xi_H} : \mathbb{R}^{2n} \to \mathbb{R}^{2n}, \quad \gamma(0) \mapsto \rho_t(\gamma(0)) := \gamma(t), \tag{7}$$

[1]The solution may "blow up at finite time" even if V is smooth. But Ξ_H is complete if we have a nice control of V, e.g. if V has a polynomial growth at infinity.

[2]A flow is a family of maps $\rho_t : X \to X$, depending continuously or smoothly in $t \in \mathbb{R}$, such that $\rho_t \circ \rho_s = \rho_{t+s}$.

which tells us how the system evolutes in time, given *any* initial state. In particular, the *conservation of energy* has the following form in this context:

Proposition 1.1. *The Hamiltonian H is invariant under the Hamiltonian flow ρ_t:*

$$H(\rho_t(\gamma_0)) = H(\gamma_0).$$

Proof. This follows from a simple direct computation:

$$\frac{d}{dt}H(\rho_t(\gamma_0)) = \frac{d}{dt}H(x(t),\xi(t)) = \frac{\partial H}{\partial x}\dot{x} + \frac{\partial H}{\partial \xi}\dot{\xi} = 0.$$

□

Remark. In particular, we see that each *energy surface*

$$H^{-1}(E) = \{(x,\xi) \in \mathbb{R}^{2n} \mid H(x,\xi) = E\}$$

is invariant under the flow $\rho(t)$. In applications we will assume E to be a regular value of H, and assume H is proper, so that $H^{-1}(E)$ is a compact smooth submanifold.

More generally, one calls any real valued smooth function $a = a(x,\xi)$ defined on the phase space a *classical observable*. Any physical experiment concerning the system should lead to quantities which can be described by the values of some classical observables. It is important to study the rate of change of a classical observable $a(x,\xi)$ of a classical system as t changes, which can be viewed as a generalization of "the law of conservation of the energy observable" to any observable:

Proposition 1.2. *If we denote $a(t) = a(x(t),\xi(t))$ for any classical observable a, then*

$$\dot{a}(t) = \sum_k \left(\frac{\partial a}{\partial x_k}\frac{\partial H}{\partial \xi_k} - \frac{\partial a}{\partial \xi_k}\frac{\partial H}{\partial x_k} \right), \tag{8}$$

where H is the Hamiltonian (3) described above.

Proof. The computation is almost the same as above:

$$\dot{a}(t) = \sum_k \frac{\partial a}{\partial x_k}\dot{x}_k + \frac{\partial a}{\partial \xi_k}\dot{\xi}_k = \sum_k \left(\frac{\partial a}{\partial x_k}\frac{\partial H}{\partial \xi_k} - \frac{\partial a}{\partial \xi_k}\frac{\partial H}{\partial x_k} \right).$$

□

It is thus natural to introduce the following notion:

Definition 1.3. The *Poisson bracket* of two smooth functions $f, g \in C^\infty(\mathbb{R}^n \times \mathbb{R}^n)$ is the smooth function

$$\{f,g\} = \sum_{k=1}^n \left(\frac{\partial f}{\partial \xi_k}\frac{\partial g}{\partial x_k} - \frac{\partial f}{\partial x_k}\frac{\partial g}{\partial \xi_k} \right) \in C^\infty(\mathbb{R}^n \times \mathbb{R}^n). \tag{9}$$

So we can rewrite the evolution equation (8) of a classical observable a simply as

$$\dot{a}(t) = \{H, a\}. \tag{10}$$

But, where is symplectic geometry? Well, for a more complicated system, the phase space is a *symplectic manifold*, i.e. a smooth manifold M together with a non-degenerate closed 2-form ω. For example in the case $M = T^*\mathbb{R}^n$ one just take

$$\omega = \sum dx_k \wedge d\xi_k.$$

Note that the Hamiltonian vector field Ξ_H associated to H defined by the formula (5) is related to H by the symplectic form via the following equation (which can be called *Hamilton's equations* because the system of Hamilton's equations alluded to above is just the integral curves of Ξ_H)

$$\iota_{\Xi_H}\omega = dH. \tag{11}$$

Everything above generalize to symplectic manifolds: A smooth function H (called the *Hamiltonian*) will play the role of the energy observable above. The Hamiltonian H is preserved along any *classical trajectory*, which is the trajectory of the *Hamiltonian flow* associated to the *Hamiltonian vector field*. One still has the notion of *Poisson bracket* in this abstract setting, and the equation of motion is again

$$\dot{a} = \{H, a\}.$$

Although it is very interesting to consider quite general symplectic manifolds, in this course we will mainly focus on a special class of symplectic manifolds: the cotangent bundle $M = T^*X$ of a smooth manifold X, which, as we will see in the future, admits a natural symplectic structure.

2. Quantum Mechanics in $L^2(\mathbb{R}^n)$

Quantum mechanics is much more difficult to understand. The mathematical theory to describe a quantum mechanical system is functional analysis. The space of states is usually a complex Hilbert space $(\mathcal{H}, \langle\cdot,\cdot\rangle)$, or more precisely, the projectified Hilbert space $\mathbb{P}\mathcal{H}$ which consists of the unit vectors in $\mathcal{H}$. (But we will always work on $\mathcal{H}$ itself instead of on $\mathbb{P}\mathcal{H}$ because the results for $\mathcal{H}$ implies the results for $\mathbb{P}\mathcal{H}$, while $\mathcal{H}$ is much easier to handle.)

In the case that the phase space of a classical system is the cotangent bundle $T^*\mathbb{R}^n$ as we just described, one usually take

$$\mathcal{H} = L^2(\mathbb{R}^n),$$

with the usual L^2-inner product

$$\langle f, g\rangle = \int_{\mathbb{R}^n} f(x)\overline{g(x)}dx.$$

A (t-independent) *quantum state* (or a *wave function*) is a function $\psi \in L^2(\mathbb{R}^n)$ satisfying

$$\int_{\mathbb{R}^n} |\psi(x)|^2 dx = 1.$$

Note that in quantum mechanics, the position of a particle is no longer a determined quantity: one can only compute the probability of finding a particle in a certain region. In the language of Hilbert space above, the probability of finding a quantum particle with wave function ψ in a measurable region $U \subset \mathbb{R}^n$ is

$$\int_U |\psi(x)|^2 dx.$$

[This explains why ψ must be normalized, i.e. has norm 1 in $L^2(\mathbb{R}^n)$.]

What are the *quantum observables*? They are linear operators A acting on $\mathcal{H}$ which are self-adjoint so that the eigenvalues of A are real numbers. We will assume that the eigenvalues of A are discrete and the corresponding eigenfunctions can be chose to form an orthonormal basis of $L^2(\mathbb{R}^n)$. The *quantum mechanics axiom* states the set of eigenvalues (usually called the *spectrum*) of a quantum observable is exactly the set of possible values that can be obtained in a measurement. More precisely, suppose the eigenvalues of A are λ_j's and the corresponding orthonormal set of eigenfunctions are φ_j's, i.e.

$$A\varphi_j = \lambda_j \varphi_j, \qquad \langle \varphi_k, \varphi_j \rangle = \delta_{kj}.$$

We can express any normalized state $\psi \in L^2(\mathbb{R}^n)$ as a summation

$$\psi = \sum_{j=0}^{\infty} c_j \varphi_j.$$

Note that $|\psi|_{L^2} = 1$ implies

$$\sum_j |c_j|^2 = 1.$$

Then the quantum mechanics axiom claims that

> the result of a quantum observation, A, to a quantum system in the state ψ, is an eigenvalue of A, in the following sense: the result is (again!) not a determined quantity, any eigenvalue might be the result, and the probability that one gets the eigenvalue λ_j is $|c_j|^2$.

As a consequence, we can prove

Proposition 2.1. *The expected value of a measurement of the quantum observable A to a quantum system in the state ψ is*

$$\langle A \rangle_\psi = \langle A\psi, \psi \rangle. \tag{12}$$

Proof. The expected value is

$$\sum_j \lambda_j |c_j^2| = \langle A \sum c_j \varphi_j, \sum c_k \varphi_k \rangle = \langle A\psi, \psi \rangle.$$

□

Remark. Note that if we multiply ψ by a "constant phase" $e^{i\theta/\hbar}$, then $\langle A\rangle_\psi = \langle A\rangle_{e^{i\theta/\hbar}\psi}$. In other words, we can't distinguish ψ and $e^{i\theta/\hbar}\psi$. This, together with the fact $\|\psi\|_{L^2} = 1$, explains why the "true" model should be the projectified Hilbert space $\mathbb{P}\mathcal{H}$ instead of $\mathcal{H}$.

We have just seen that the classical Hamiltonian H determines the behavior of the classical system. What is the *quantum Hamiltonian* that plays the same role for a quantum system? In Schrödinger's picture of quantum mechanics, the quantum mechanical analogue of the Hamiltonian (3) is the time-independent *Schrödinger operator*

$$\hat{H} = -\frac{\hbar^2}{2}\Delta + V(x), \tag{13}$$

and the quantum mechanical analogue of the system of Hamilton's equations (4) is the *Schrödinger equation*

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi, \tag{14}$$

where $h = 6.62607015 \times 10^{-34}$ is the *Planck's constant* and $\hbar = h/2\pi$ is the *reduced Planck's constant*, $\Delta = \sum \frac{\partial^2}{\partial x_k^2}$ is the Laplace operator, and the potential function $V(x) \in C^\infty(\mathbb{R}^n)$ is a real-valued function which acts on $L^2(\mathbb{R}^n)$ by multiplication, and $\psi = \psi(t,\cdot)$ is the quantum mechanical time-evolution of a quantum state ψ at time t. Note that the quantum Hamiltonian $\hat{H}$ arises from the classical Hamiltonian H by replacing the momentum variable ξ_k with the operator $\frac{\hbar}{i}\frac{\partial}{\partial x_k}$. It is very important to notice that $\hat{H}$ is a self-adjoint operator acting on $L^2(\mathbb{R}^n)$.

What is the quantum analogue of the Hamiltonian flow $\rho_t = e^{t\Xi_H}$? Since ρ_t maps an initial classical state γ_0 to its time-t classical state $\gamma(t)$, the quantum analogue must maps the initial quantum state $\psi(0) = \psi_0$ to its time-t quantum state ψ_t, which is the solution to the problem

$$\begin{cases} i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi, \\ \psi(0) = \psi_0. \end{cases}$$

In other words, the quantum analogue of ρ_t has to be solution operator of the Schrödinger equation, which we can formally denoted by

$$U(t) = e^{-it\hat{H}/\hbar} : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n).$$

Note that $U(t)$ maps an L^2-normalized function to an L^2-normalized one (which is what we need), since we have

$$\frac{d}{dt}\langle U(t)\psi_0, U(t)\psi_0\rangle = \langle\frac{\partial\psi}{\partial t},\psi\rangle + \langle\psi,\frac{\partial\psi}{\partial t}\rangle = \frac{1}{i\hbar}\langle\hat{H}\psi,\psi\rangle - \frac{1}{i\hbar}\langle\psi,\hat{H}\psi\rangle = 0.$$

In the language of mathematics, $U(t)$ is a unitary operator[3] acting on $L^2(\mathbb{R}^n)$. As $\rho(t)$, the operator $U(t)$ form a *Schrödinger (semi-)group*

$$U(t)U(s) = U(t+s).$$

It is usually called the *propagator* associated with the quantum Hamiltonian $\hat{H}$.

What is the quantum analogue of the conservation of energy, which tells us that the classical Hamiltonian H is unchanged under the flow ρ_t? It should tell us that the expected value $\langle \hat{H} \rangle_{\psi(t)}$ is unchanged. This can be verified by almost the same computation as above:

$$\begin{aligned}\frac{d}{dt}\langle \hat{H} \rangle_{\psi(t)} = \frac{d}{dt}\langle \hat{H}\psi(t), \psi(t)\rangle &= \langle \hat{H}\frac{1}{i\hbar}\hat{H}\psi, \psi\rangle + \langle \hat{H}\psi, \frac{1}{i\hbar}\hat{H}\psi\rangle \\ &= \frac{1}{i\hbar}\langle \hat{H}\hat{H}\psi, \psi\rangle - \frac{1}{i\hbar}\langle \hat{H}\hat{H}\psi, \psi\rangle = 0.\end{aligned}$$

Finally let's study the equation of motion in a quantum system. Let A be a quantum observable (which is time independent). As we have seen, at time t the result of A to a quantum state $\psi(t) = \psi(t, \cdot)$ is $\langle A \rangle_{\psi(t)}$. By repeating the same computation the third time, we get

$$\begin{aligned}\frac{d}{dt}\langle A \rangle_{\psi(t)} = \frac{d}{dt}\langle A\psi(t), \psi(t)\rangle &= \langle A\frac{1}{i\hbar}\hat{H}\psi, \psi\rangle + \langle A\psi, \frac{1}{i\hbar}\hat{H}\psi\rangle \\ &= \frac{1}{i\hbar}\langle A\hat{H}\psi, \psi\rangle - \frac{1}{i\hbar}\langle \hat{H}A\psi, \psi\rangle \\ &= \frac{1}{i\hbar}\langle [A, \hat{H}]\psi, \psi\rangle,\end{aligned}$$

where

$$[A, \hat{H}] = A\hat{H} - \hat{H}A \tag{15}$$

is the Lie bracket between the operators A and $\hat{H}$, and we have used the facts that $\hat{H}$ is self-adjoint and that the conjugate of i is $-i$. So we end up with

Proposition 2.2. *The equation of motion of a quantum system is*

$$\frac{d}{dt}\langle A \rangle_\psi = \frac{i}{\hbar}\langle [\hat{H}, A] \rangle_\psi. \tag{16}$$

Comparing this with proposition 1.2, we are led to the following principle:

> *The normalized Lie bracket $\frac{i}{\hbar}[\cdot, \cdot]$ is the quantum analogue of the Poisson bracket $\{\cdot, \cdot\}$.*

Remark. As in the classical case where we can replace $\mathbb{R}^{2n}$ by a cotangent bundle T^*X, here in the quantum case we can replace $\mathbb{R}^n$ by a (Riemannian) manifold X.

[3]Being a unitary operator means that $U(t) : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ always preserves the inner product structure. This is the quantum analogue of the fact that $\rho_t : T^*\mathbb{R}^n \to T^*\mathbb{R}^n$ always preserves the symplectic structure.