LECTURE 3 — 09/27/2020
QUANTIZATION V.S. SEMI-CLASSICAL LIMIT

Let's summarize what we did last time:

	Classical world	Quantum world
Space of states	The cotangent bundle $T^*\mathbb{R}^n$ with symplectic structure $\omega = \sum dx_i \wedge d\xi_i$	The function space $L^2(\mathbb{R}^n)$ with Hilbert structure $\langle f, g\rangle = \int_{\mathbb{R}^n} f(x)\overline{g(x)}dx$
State	a point (x, ξ)	a function ψ with $\\|\psi\\| = 1$
Hamiltonian	The energy function $H(x, \xi) = \frac{\\|\xi\\|^2}{2} + V(x)$	The Schrödinger operator $\hat{H} = -\frac{\hbar^2}{2}\Delta + V$
Observables	Real-valued functions $a \in C^\infty(T^*\mathbb{R}^n)$	Self-adjoint operators $A : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$
Result of an observable	The value $a(x, \xi)$	an eigenvalue of A $\rightsquigarrow$expected value $\langle A\rangle_\psi = \langle A\psi, \psi\rangle$
Evolution of a state	Hamilton's equations $\dot{x} = \frac{\partial H}{\partial \xi},\ \dot{\xi} = -\frac{\partial H}{\partial x}$	Schrödinger's equation $i\hbar\frac{\partial \psi}{\partial t} = \hat{H}\psi$
Evolution of the system	The flow (symplectomorphism) $\rho_t = e^{t\Xi_H} : T^*\mathbb{R}^n \to T^*\mathbb{R}^n$	The propagator (unitary) $U(t) = e^{-\frac{it\hat{H}}{\hbar}} : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$
Conservation of energy	$H(\rho_t(x_0, \xi_0)) = H(x_0, \xi_0)$	$\langle \hat{H}\rangle_{U(t)\psi_0} = \langle \hat{H}\rangle_{\psi_0}$
Evolution of observables	$\frac{d}{dt}a = \{H, a\}$	$\frac{d}{dt}\langle A\rangle_{\psi(t)} = \langle \frac{i}{\hbar}[\hat{H}, A]\rangle_{\psi(t)}$

In some sense, one of the major task in this course is to add more classical-quantum correspondence to this list.

1. Quantization

The word "quantization" refers to any systematical way of constructing a quantum mechanical description of a system from its classical mechanical description. In the language of mathematics, it should be a "functor" that gives

$$\text{Symplectic space } (M,\omega) \rightsquigarrow \text{ Hilbert space } (\mathcal{H}, \langle\cdot,\cdot\rangle),$$

$$(C^\infty(M,\mathbb{R}), \{\cdot,\cdot\}) \rightsquigarrow (\text{self-adjoint operators on } \mathcal{H}, \frac{i}{\hbar}[\cdot,\cdot]).$$

At the very beginning of quantum mechanics, Dirac suggested several *natural* axioms that a quantization procedure should satisfy:

Dirac's Axioms. A quantization procedure assigns to any classical observable $a \in C^\infty(M,\mathbb{R})$ a self-adjoint operator $Q(a)$ on some Hilbert space $\mathcal{H}$, such that

- (D1) (linearity) $Q(\mu a + \nu b) = \mu Q(a) + \nu Q(b)$ for any $\mu, \nu \in \mathbb{R}$.
- (D2) (normalization) $Q(1) = \mathrm{Id}$.
- (D3) (quantizaiton condition) $Q(\{a,b\}) = \frac{i}{\hbar}[Q(a), Q(b)]$.
- (D4) (minimality) Any complete family of functions on M passes to a complete family of self-adjoint operators on $\mathcal{H}$.
  - A family of functions on M is complete if they separate points almost everywhere on M.
  - A family of operators on $\mathcal{H}$ is complete if they act irreducibly on $\mathcal{H}$, i.e. no nonzero proper closed subspace of $\mathcal{H}$ is invariant under the family of operators.

Unfortunately, such a quantization does not exists!

Theorem 1.1 (Groenewold-van Hove no-go theorem). *A quantization procedure that satisfies (D1)-(D4) for all $f \in C^\infty(M)$ does not exist.*

In fact, one can not even quantize all polynomials of degree ≤ 4 in $C^\infty(T^*\mathbb{R})$,. To see this one need to observe the following facts:

- The first key ingredient is a Schur-type lemma:

  Lemma 1.2. *Suppose Y is an self-adjoint operator on $\mathcal{H}$ such that*

  $$[Y, Q(x)] = [Y, Q(\xi)] = 0,$$

  then $Y = c \cdot \mathrm{Id}$ for some constant c.

  Proof. We will need some facts from functional analysis:
  - By a theorem in functional analysis (c.f. K. Yosida, *Functional analysis*, 6th ed., page 339), if A is a self-adjoint operator and B is a bounded self-adjoint operator, and A, B commutes, then for any Baire function f, $f(A)$ commutes with B. In particular, B commutes with any spectral projection $\chi_E(A)$ of A onto an interval finite E.

– Conversely, if B commutes with any spectral projection $\chi_E(A)$ of A, then by spectral theorem, B commutes with A.

Note that as a consequence of the first fact, for any finite interval F, $\chi_F(B)$ commutes with $\chi_E(A)$. Then as a consequence of the second fact, $\chi_F(B)$ commutes with A.

Now we start to prove the theorem. First assume Y is a bounded self-adjoint operator. Then as we just argued, for any finite interval $F \subset \mathbb{R}$, the spectral projection $\chi_F(Y)$ commutes with $Q(x)$ and $Q(\xi)$, i.e. the range of the operator $\chi_F(Y)$ is a subspace of $\mathcal{H}$ which is invariant under both $Q(x)$ and $Q(\xi)$. But since the two functions x and ξ from a complete set of functions on $T^*\mathbb{R}$, by (D4) the two operators $Q(x)$ and $Q(\xi)$ act irreducibly on $\mathcal{H}$. As a result, the range of $\chi_F(Y)$ is either 0 or $\mathcal{H}$ for any F. So the spectrum of Y contains only one point.

The case where Y is unbounded is more subtle, because all operators involved are only densely defined. Under some extra assumptions that all computations involved make sense in a dense subspace, we can conclude that Y^2, and thus the operator $Y^2 + \mathrm{Id}$, commutes with $Q(x)$ and $Q(\xi)$. Since $Y^2 + \mathrm{Id}$ is positive and self-adjoint, it is invertible. Moreover, its inverse $(Y^2 + \mathrm{Id})^{-1}$ is a bounded self-adjoint operator which commutes with both $Q(x)$ and $Q(\xi)$. Now we can apply what we just proved to claim that $(Y^2 + \mathrm{Id})^{-1}$ has the form $c\mathrm{Id}$, and the conclusion follows. □

- Using the above lemma one can show $Q(x\xi) = Q(x)Q(\xi) + c\mathrm{Id}$ for some constant c, and then inductively prove
$$Q(x^m) = Q(x)^m \quad \text{and} \quad Q(\xi^m) = Q(\xi)^m.$$
The second key observation is that we have the following two different ways to write a degree 4 polynomial as Poisson brackets of two degree 3 polynomials:
$$\{x^3, \xi^3\} = -9x^2\xi^2 = 3\{x^2\xi, x\xi^2\}.$$
A contradiction will appear if calculate $Q(x^2\xi)$ and $Q(x\xi^2)$ explicitly. We will leave the details as an exercise.

This is both a bad news and a good news for mathematicians: on one hand, there is no "perfect theory" describing every aspect of the classical-quantum correspondence. On the other hand side, by focusing on different aspects of the correspondence, mathematicians and physicists has developed several different theories under the title "quantization". Among these different quantization schemes, three of them are most popular and are widely studied by (different groups of) mathematicians:

(A) Weyl quantization. This is one of the first quantization theory in mathematics (proposed by H. Weyl in 1927). It can be viewed as analysts' quantization method since it mainly uses the language of (Fourier) analysis, but it is also very closely related to representation theory. In Weyl quantization we only quantize cotangent bundles. One start point to understand the theory is the *canonical* *quantization* introduced by P. Dirac in his doctoral thesis in 1926, in which the position functions x_k's and the momentum functions ξ_k's are quantized to the position operators Q_k's and the momentum operators P_k's. The central relation between these operators is the canonical commutative relations[1]

$$[Q_k, Q_k] = 0, \quad [P_k, P_j] = 0, \quad [Q_k, P_j] = \frac{\hbar}{i}\delta_{jk} \cdot \mathrm{Id},$$

which is of course the quantum analogue of the classical facts

$$\{x_k, x_j\} = 0, \quad \{\xi_k, \xi_j\} = 0, \quad \{x_k, \xi_j\} = \delta_{kj}.$$

As we mentioned in lecture 1, in Weyl quantization we take

$$x_k \rightsquigarrow Q_k = \text{multiplicaton by } x_k$$
$$\xi_k \rightsquigarrow P_k = \frac{\hbar}{i}\frac{\partial}{\partial x_k},$$

and as a result we can quantize

$$H = \frac{|\xi|^2}{2} + V(x) \rightsquigarrow \hat{H} = -\frac{\hbar^2}{2}\Delta + V(x).$$

However, it is not clear how to quantize functions in *mixed* variables like $x_1\xi_1 = \xi_1 x_1 = \frac{x_1\xi_1+\xi_1 x_1}{2}$, since the multiplications of functions are commutative, while the compositions of operators are not commutative. [In some sense it is the non-commutativity in the quantum side that makes the whole theory interesting.]H. Weyl had the idea of using Fourier transform to solve this problem: for any *nice* function $a(x,\xi) \in C^\infty(T^*\mathbb{R}^n)$, we can *quantize* it to the operator $A : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ defined via Fourier transform, by

$$(Af)(x) = (a^W f)(x) := \frac{1}{(2\pi)^n}\int e^{i\frac{(x-y)]\cdot\xi}{\hbar}} a(\frac{x+y}{2}, \xi)\psi(y)dyd\xi.$$

Such operators are called *semi-classical pseudodifferential operators*. We will see that the Weyl quantization does not satisfy the quantization condition

$$[a^W, b^W] \neq \frac{\hbar}{i}\{a,b\}^W,$$

but it does satisfy a weakened version of quantization condition:

$$[a^W, b^W] = \frac{\hbar}{i}\{a,b\}^W + O(\hbar^2).$$

We will also quantize *canonical relations* (like the Hamiltonian flow) between cotangent bundles. The resulting operator are called *Fourier integral operators*. Pseudodifferential operators and Fourier integral operators are the major objects of this course.

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[1]In the language of representation, we really get a representation of the Heisenberg Lie group.

(B) Geometric quantization. The theory was introduced by Kostant and Souriau in 1970s, and is mainly studied by geometers. In a future course on symplectic geometry, I will describe in detail how to quantize in the general symplectic setting. In geometric quantization, the Hilbert space will be taken to be the set of smooth sections of some "pre-quantum line bundle" satisfying some extra conditions.

(C) Deformation quantization. The theory was introduced by Flato, Lichnerowicz and Sternheimer in 1976, and has been studied extensively since then mainly by algebraists. In this theory, the main focus is trying to understand quantization as a deformation of the (Poisson) structure of the algebra of classical observables. For example, people want to construct a new noncommutative product $\star$ on $C^\infty(M)[\hbar]$ (whose elements are formal power series in $\hbar$ with coefficients in $C^\infty(M)$, where M is a symplectic or Poisson manifold) such that

$$f \star g - g \star f = \frac{\hbar}{i}\{f, g\} + O(\hbar^2).$$

We will see that in Weyl quantization, such a *star product* can be defined for cotangent bundles.

2. Semiclassical Analysis

Roughly speaking, semiclassical analysis is the reverse of quantization: We would like to get the information about the classical system from the information about the corresponding quantum system. As we mentioned in Lecture 1, the guideline of the subject is the so-called Bohr's correspondence principle:

Bohr's Correspondence Principle. The classical mechanics can be realized as the formal $\hbar \to 0$ limit of the corresponding quantum mechanics.

Remark. When we say $\hbar \to 0$ limit, we don't really evaluate the limit, but instead study the asymptotic behavior of our objects as $\hbar \to 0$.

For example, the three theorems we mentioned in Lecture 1 are all in this spirit:

(1) The Egorov's theorem

$$e^{itQ/\hbar} a^W e^{-itQ/\hbar} = (\rho_t^* a)^W + O(\hbar)$$

is a rigorous mathematical theorem justifying our claim "the propagator $U(t) = e^{-itQ/\hbar}$ is the quantum analogue of the classical geodesic flow ρ_t associated to the Hamiltonian $q(x, \xi)$".

(2) The Weyl law

$$\#\{j \mid \lambda_j \leq \lambda\} = \frac{1}{(2\pi\hbar)^n} \left(\mathrm{Vol}(\{(x, \xi) \mid H(x, \xi) \leq \lambda\}) + O(\hbar)\right)$$

tells us that asymptotically, the number of quantum energy below λ coincides with the measure of the classical region with classical energy below λ.

(3) The quantum ergodicity theorem set up a correspondence between classical ergodicity of the geodesic flow and quantum ergodicity of the Laplacian eigenfunctions, which we will explain later.

As the course goes, you will see many other theorems of this flavor.

We end today's lecture by a classical example for which we can calculate all the eigenvalues explicitly, and verify Weyl's law in this special case.

♠ **Example: the harmonic oscillator**.

Consider the n-dimensional Harmonic oscillator

$$\hat{H} = -\frac{\hbar^2}{2}\sum_{j=1}^{n}\frac{d^2}{dx_j^2} + \frac{|x|^2}{2}.$$

We want to compute all the eigenvalues of $\hat{H}$. To do so we start with the creation operators

$$C_k = \frac{1}{\sqrt{2}}\left(\frac{\hbar}{\sqrt{-1}}\frac{\partial}{\partial x_k} + \sqrt{-1}x_k\right)$$

and the annihilation operator

$$A_k = C_k^* = \frac{1}{\sqrt{2}}\left(\frac{\hbar}{\sqrt{-1}}\frac{\partial}{\partial x_k} - \sqrt{-1}x_k\right).$$

You may feel strange where do the creation and annihilation operators come from. To see this let's first turn to the corresponding classical system of harmonic oscillator, i.e. the system with Hamiltonian $H(x,\xi) = (|\xi|^2+|x|^2)/2$. The system of Hamiltonian equations can be written as

$$\frac{d}{dt}\begin{pmatrix} x_k \\ \xi_k \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} x_k \\ \xi_k \end{pmatrix}$$

This is a coupled system. One way (maybe not the simplest way in this example though) to solve such a coupled system is to decoupling the system via eigenvectors of the coefficient matrix. It is easy to find out the unit eigenvectors, which are

$$v_1 = \frac{1}{\sqrt{2}}(i,1)^T \quad \text{and} \quad v_2 = \frac{1}{\sqrt{2}}(-i,1)^T.$$

It turns out that if we set

$$c_k = \frac{1}{\sqrt{2}}(\xi_k + ix_k) \quad \text{and} \quad a_k = \frac{1}{\sqrt{2}}(\xi_k - ix_k),$$

then the system of Hamiltonian equations is decoupled into two simple equations

$$\dot{c}_k = ic_k, \quad \dot{a}_k = -ia_k$$

which can be solved easily. Now you immediately see that the creation operator C_k and the annihilation operator A_k are merely the "quantizations" of the "decoupled variables" c_k and a_k!

One can easily check by direct computations that

$$[C_j, C_k] = 0 = [A_j, A_k] \quad \text{and} \quad [A_j, C_k] = \hbar\delta_{jk} \cdot \mathrm{Id}.$$

Moreover, since

$$\begin{aligned} C_j A_j &= \frac{1}{2}\left(\frac{\hbar}{\sqrt{-1}}\frac{\partial}{\partial x_j} + \sqrt{-1}x_j\right)\left(\frac{\hbar}{\sqrt{-1}}\frac{\partial}{\partial x_j} - \sqrt{-1}x_j\right) \\ &= -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x_j^2} + \frac{x_j^2}{2} - \frac{\hbar}{2} \end{aligned}$$

we get

$$\hat{H} = \sum_{j=1}^{n} C_j A_j + \frac{n}{2}\hbar \cdot \mathrm{Id} \tag{1}$$

and thus

$$[C_j, \hat{H}] = C_j C_j A_j - C_j A_j C_j = C_j [C_j, A_j] = -\hbar C_j,$$

and by a similar computation one has

$$[A_j, \hat{H}] = \hbar A_j.$$

It follows that if λ is an eigenvalue of $\hat{H}$, i.e.

$$\hat{H}u = \lambda u,$$

then

$$\hat{H}C_j u = C_j(\hat{H}u + \hbar u) = (\lambda + \hbar)C_j u$$

and

$$\hat{H}A_j u = A_j(\hat{H}u - \hbar u) = (\lambda - \hbar)A_j u.$$

In other words, the creation operator C_j maps an eigenfunction u of $\hat{H}$ associated to eigenvalue λ to an eigenfunction $C_j u$ of $\hat{H}$ associated to the eigenvalue $\lambda + \hbar$, while the annihilation operator A_j maps u to an eigenfunction $A_j u$ (if it is nonzero) associated to the eigenvalue $\lambda - \hbar$.

To finish the computation of eigenvalues, we observe from (1) that

$$\langle \hat{H}u, u\rangle = \sum_j \|A_j u\|^2 + \frac{n}{2}\hbar\|u\|^2, \tag{2}$$

from which we see that

(1) if λ is an eigenvalue of $\hat{H}$, then $\lambda \geq \frac{n}{2}\hbar$.
(2) a function u is an eigenfunction associated to $\lambda = \frac{n}{2}\hbar$ if and only if $A_j u = 0$ holds for all $1 \leq j \leq n$.

A direct computation shows that

$$A_j u(x_j) = 0 \Longleftrightarrow u(x_j) = ce^{-x_j^2/2\hbar},$$

As a consequence, we see that $\frac{n}{2}\hbar$ is indeed the smallest eigenvalue of $\hat{H}$ and the associated eigenfunction is

$$u_0(x) = e^{-|x|^2/2\hbar},$$

which is often called the *ground state.*

Starting from the ground state, one can find more eigenvalues using the creation operator (this is why the operator called creation operator): For any multi-index $\alpha = (\alpha_1, \cdots, \alpha_n) \in \mathbb{N}_{\geq 0}^n$, the function[2]

$$u_\alpha = C_1^{\alpha_1} \cdots C_n^{\alpha_n} u_0$$

is an eigenfunction of $\hat{H}$ associated with the eigenvalue

$$\lambda_\alpha = \frac{n}{2}\hbar + |\alpha|\hbar,$$

where as usual we denote $|\alpha| = \alpha_1 + \cdots + \alpha_n$.

Finally we claim that these eigenvalues are all the eigenvalues of $\hat{H}$: If $\lambda > \frac{n}{2}\hbar$ is an eigenvalue of $\hat{H}$ with eigenfunction u, then by (2), there is some j such that $A_j u \neq 0$, and thus $\lambda - \hbar$ is also an eigenvalue of $\hat{H}$ with eigenfunction $A_j u$. As a consequence, we get

- any eigenvalue of $\hat{H}$ with $\lambda > \frac{n}{2}\hbar$ must has the form $\lambda = \frac{n}{2}\hbar + k\hbar$ for some $k \in \mathbb{N}$,
- if u is the corresponding eigenfunction, then there exists $\alpha_1, \cdots, \alpha_n \in \mathbb{N}_{\geq 0}$ with $|\alpha| = k$ such that $A^\alpha u := A_1^{\alpha_1} \cdots A_n^{\alpha_n} u = u_0$.

Now we are ready to prove

Proposition 2.1. *The eigenvalues of* $\hat{H}$ *are*

$$\frac{n}{2}\hbar, \frac{n}{2}\hbar + \hbar, \frac{n}{2}\hbar + 2\hbar, \cdots, \frac{n}{2}\hbar + k\hbar, \cdots.$$

Moreover, for each $k \geq 0$*, the associated eigenspace has a basis*

$$u_\alpha = C^\alpha u_0 := C_1^{\alpha_1} \cdots C_n^{\alpha_n} u_0, \quad |\alpha| = k.$$

Proof. We have already proved the first half of the proposition. We have already seen that u_α's are eigenfunctions associated to the eigenvalues $\frac{n}{2}\hbar + |\alpha|\hbar$. Note that if $|\alpha| = |\beta|$ but $\alpha \neq \beta$, then $u_\alpha \neq u_\beta$, since

$$A^\beta C^\alpha u_0 = 0 \quad \text{ for } |\beta| = |\alpha| \text{ but } \beta \neq \alpha$$

while

$$A^\alpha C^\alpha u_0 = \alpha! u_0.$$

So these u_α's are linearly independent eigenfunctions.

[2]Note that $C_j u = 0$ has no nontrivial L^2 solution. So these u_α's are non-zero functions.

To show that there is no other element in the same eigenspace, we suppose v is an eigenfunction with eigenvalue $\frac{n}{2}\hbar + k\hbar$, and v is L^2-perpendicular to all u_αs with $|\alpha| = k$. We just observed that there exists α with $|\alpha| = k$ such that $A^\alpha v = u_0$. It follows

$$\langle u_0, u_0 \rangle = \langle A^\alpha v, u_0 \rangle = \langle v, C^\alpha u_0 \rangle = 0,$$

a contradiction. □

Remark. There is an explicit formula for these eigenfunctions. In the case of dimension 1, the normalized eigenfunctions associated to the eigenvalue $\frac{1}{2}\hbar + j\hbar$ are

$$\varphi_j(x) = \frac{1}{2^j j!} \frac{1}{(\pi\hbar)^{1/4}} e^{-\frac{x^2}{2\hbar}} H_j(\frac{x}{\sqrt{\hbar}}),$$

where

$$H_j(x) = (-1)^j e^{x^2} \frac{d^j}{dx^j}(e^{-x^2})$$

is a polynomial in x, known as *the Hermite polynomial*. In the higher dimensional case, the eigenfunctions are simply the products of these functions.

Although one can deduce from some general theorems that for the Harmonic oscillator, these eigenfunctions span $L^2(\mathbb{R}^n)$, we can give a direct proof using these explicit expressions. For simplicity we only consider the case $n = 1$, and we take $\hbar = 1$. The key observation is that H_j is a degree j polynomial with nonzero leading term. It follows that the span of $\varphi_0, \cdots, \varphi_m$ are exactly $p(x)e^{-x^2/2}$, where $p(x)$ is any polynomial of degree no more than m. Now we notice that for any complex number c, the series $\sum_{k=0}^\infty \frac{c^k x^k}{k!} e^{-x^2/2}$ converges to $e^{cx}e^{-x^2/2}$ in L^2. Now suppose $\psi(x)$ is orthogonal to all φ_m's. Then by taking $c = -i\xi$ we will get

$$\int_{\mathbb{R}} e^{-ix\xi} e^{-|x|^2/2} \psi(x) dx = 0.$$

Since $e^{-|x|^2/2}\psi(x)$ belongs to $L^2(\mathbb{R})$, using basic theory of Fourier transform (which is our topic of next lecture) we see $e^{-|x|^2/2}\psi(x) = 0$, i.e. $\psi = 0$.

Finally we are ready to check Weyl's law for the Harmonic oscillator: we have

$$\begin{aligned} \#\{j : \ \lambda_j \le \lambda\} &= \{\alpha : \ \frac{n}{2}\hbar + |\alpha|\hbar \le \lambda\} \\ &= \Big\{\alpha : \ |\alpha| \le (\lambda - \frac{n}{2}\hbar)/\hbar\Big\} \\ &= \frac{1}{n!}(\lambda/\hbar)^n + o(\hbar^{-n}) \end{aligned}$$

while

$$\mathrm{Vol}(\{(x,\xi) : \frac{|\xi|^2}{2} + \frac{|x|^2}{2} \le \lambda\}) = (\sqrt{2\lambda})^{2n} \times \text{the volume of unit ball in } \mathbb{R}^{2n},$$

and Weyl's law in this case follows since the volume of unit ball in $\mathbb{R}^{2n}$ is $\frac{\pi^n}{n!}$.