Math 428. lecture 19

Quantum Mechanics

Connect CM ↔ QM, especially via semiclassical limit: in limit $\hbar \to 0$ expect QM → CM.

Introduction: the dictionary

Say we want to quantize a classical system with config. space X.

	Classical	Quantum
state space:	$M = T^*X$	$L^2(X)$
physical state:	$z = (x,p) \in M$	$\Psi \in L^2(X)$ ($\alpha\Psi$ same state $\alpha \in \mathbb{C}^*$)
observables:	$a \in C^\infty(M)$	selfadjoint linear operators $\hat{a} : L^2(X) \circlearrowleft$
warning:	$xp = px$	$\hat{x}\hat{p} \neq \hat{p}\hat{x}$
Algebra:	$\{a, b\}$	$\frac{1}{i\hbar}[\hat{a}, \hat{b}] = \frac{1}{i\hbar}(\hat{a}\hat{b} - \hat{b}\hat{a})$
Time evolution:	$\frac{dz}{dt} = -\omega^{-1}(dH_z)$	$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$. Schrödinger equation

Evolution of states: $z(t) = \Phi_t(z)$ $\qquad$ $\Psi(t) = U(t)\,\Psi(0)$

$i\hbar \frac{d}{dt} U(t) = U(t)\,\hat{H}$

Evolution of observables: $\frac{da}{dt} = \{H, a\}$ $\qquad$ $\frac{dA}{dt} = \frac{1}{i\hbar}[H, A]$

$a_t = a \circ \Phi_t$

Heisenberg picture:
$A(t) = U(-t)\,A\,U(t)$

Ensemble: measure μ on M $\qquad$ Positive selfadjoint trace class operator with trace 1

Remark: treating the Scrödinger equation as an ODE in $L^2(X)$, it's a constant-coeff ODE, so can be solved spectrally. E.g. if have o.n.b. $\{\phi_n\}_{n=0}^{\infty} \subset L^2(X)$ s.t. $H\phi_n = E_n \phi_n$ then the general solution to the equation is

$$\Psi(t) = \sum_{n=0}^{\infty} a_n\, e^{\frac{E_n}{i\hbar} t}\, \phi_n \,, \qquad a_n \in \ell^2(\mathbb{N})$$

$\Rightarrow$ often discussion restricts to time-independent Schrödinger equation $\boxed{H\phi = E\phi}$.

Remark: Measuring observable A in state Ψ has effect (Copenhaven interpretation): say spectral decomposition of A is $\sum_\lambda \lambda \cdot \pi_\lambda$ $\qquad$ π_λ = proj. on eigenspace then the probability of measuring λ is $\frac{\|\pi_\lambda \psi\|^2}{\|\psi\|^2}$

and if we measure λ then ("collapse of wavefunction")
after system in state $\pi_\lambda \psi$. (normalized if want)

$\Rightarrow$ Expected value of measurement is $\sum_\lambda \lambda \cdot \frac{\|\pi_\lambda \psi\|^2}{\|\psi\|^2}$

$$= \sum_\lambda \frac{\langle \psi, \lambda \pi_\lambda \psi \rangle}{\|\psi\|^2} = \frac{\langle \psi | A | \psi \rangle}{\langle \psi | \psi \rangle}.$$

Quantization: $X = E^d$, $T^*X = E^d \times (\mathbb{R}^d)^* = \{(x,p)\}$

classically algebra of observables generated by x_i, p_j
$\mathbb{R}[x_1, .., x_d, p_1, .., p_d]$, $\{x_i, p_j\} = \delta_{ij}$
with $\{ab, c\} = a\{b,c\} + \{a,c\}b$ compute $\{a,b\}$ for all $a, b \in \mathbb{R}[x,p]$.

Take operators $\hat{x}_i, \hat{p}_j$ with $[\hat{x}_i, \hat{p}_j] = i\hbar\, \delta_{ij}$

$[A,B]^\dagger = (AB - BA)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger = -[A,B]$ if $A^\dagger = A$, $B^\dagger = B$

Canonical quantization: take non-commutative alg generated by $\hat{x}_i, \hat{p}_j$ subject to $\frac{1}{i\hbar}[\hat{x}_i, \hat{p}_j] = \delta_{ij}$.

Concretely, take $\hat{x}_i$ = mult by x_i
$\hat{p}_j = -i\hbar \frac{\partial}{\partial x_j}$. } acting on functions on $\mathbb{R}^d$.

check: this works

Theorem: (Groenewold 1946) there is no map $\mathrm{Op}_\hbar$ mapping $\mathbb{R}[x,p]$ to $\mathbb{R}\langle \hat{x}, \hat{p}\rangle$ which is:
(1) linear (2) unital (3) $\mathrm{Op}_\hbar(\{a,b\}) = \frac{1}{i\hbar}[\mathrm{Op}_\hbar(a), \mathrm{Op}_\hbar(b)]$

Problems: is $\widehat{xp} = \hat{x}\hat{p}$? is $\widehat{xp} = \hat{p}\hat{x}$? is it $\frac{\hat{x}\hat{p}+\hat{p}\hat{x}}{2}$?
observation all these choices agree to $O(\hbar^0)$:
$$\hat{x}\hat{p} - \hat{p}\hat{x} = [\hat{x},\hat{p}] = O(\hbar).$$

Calculations:

Example 1: Free particle $H = \frac{p^2}{2m}$, $\hat{H} = -\frac{\hbar^2}{2m}\partial_x^2$

If we take $\Psi(0) = e^{\frac{ip}{\hbar}x}$ $\hat{H}\Psi(0) = \frac{p^2}{2m}$ $(\hat{p}\,\Psi(0) = p\,\Psi(0))$

$\Rightarrow$
$$\Psi(t) = e^{\frac{p^2}{2i\hbar m}t}\, e^{\frac{ip}{\hbar}x}$$

Try instead: $\frac{1}{(\pi\sigma^2)^{1/4}} \exp\left(\frac{ipx}{\hbar} - \frac{(x-q)^2}{2\sigma^2}\right)$

Guess: $\Psi(t) = \frac{1}{(\pi\sigma^2(t))^{1/4}} \cdot \exp\left(\frac{ipx}{\hbar} - \frac{(x-q(t))^2}{2\sigma^2} + i\theta(t)\right)$

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[-\frac{i\hbar}{2}\frac{\dot\sigma}{\sigma} + i\hbar\frac{(x-q)\dot q}{2\sigma^2} + i\hbar\frac{(x-q)^2}{\sigma^3}\dot\sigma - \hbar\dot\theta\right]\Psi$$

$$\partial_x \Psi = \Psi \cdot \left[\frac{ip}{\hbar} - \frac{x-q}{\sigma^2}\right] \Rightarrow \partial_x^2 = \Psi\left[\left(\frac{ip}{\hbar} - \frac{x-q}{\sigma^2}\right)^2 - \frac{1}{\sigma^2}\right]$$

$$\Rightarrow -\frac{i\hbar}{2}\frac{\dot\sigma}{\sigma} + i\hbar\frac{(x-q)\dot q}{2\sigma^2} + i\hbar\frac{(x-q)^2}{\sigma^3}\dot\sigma = -\frac{\hbar^2}{2m}\left[\qquad\right]$$

Try $\Psi(t) = \frac{1}{(\pi\sigma^2)^{1/4}} \exp\left(\frac{ipx}{\hbar} - \frac{(x-q)^2}{2\sigma^2} + i\theta(t)\right)$

where $p = p(t)$, $q = q(t)$

in $\hat H = \frac{1}{2m}\hat p^2 + \frac{1}{2}k\hat x^2$

Get (same calculation):

$$\left(-\frac{\hbar^2}{2m}\partial_x^2 + \frac{1}{2}kx^2\right)\Psi = \left[-\frac{\hbar^2}{2m}\left(\frac{ip}{\hbar} - \frac{(x-q)}{\sigma^2}\right)^2 + \frac{\hbar^2}{2m\sigma^2} + \frac{1}{2}kx^2\right]\Psi$$

$$i\hbar\frac{\partial\Psi}{\partial t} = i\hbar\left[-\frac{1}{2}\frac{\dot\sigma}{\sigma} + i\dot\theta + \frac{i\dot p x}{\hbar} + \frac{(x-q)\dot q}{\sigma^2} + \frac{(x-q)^2}{\sigma^3}\dot\sigma\right]\Psi$$

Matching real, imaginary parts:

$$\begin{cases} \frac{p^2}{2m} - \frac{\hbar^2 (x-q)^2}{2m\sigma^4} + \frac{\hbar^2}{2m\sigma^2} + \frac{1}{2}kx^2 = -\dot{p}x - \hbar\dot{\theta} \\ \frac{p(x-q)}{m\sigma^2} = \frac{\dot{\sigma}}{2\sigma} + \frac{(x-q)\dot{q}}{\sigma^2} + \frac{(x-q)^2}{\sigma^3}\dot{\sigma} \end{cases}$$

From coeff of x^2 in last equation see $\dot{\sigma} = 0$

dividing by $x-q$ get $\boxed{\dot{q} = \frac{p}{m}}$

First equation: coeff of x^2 is $-\frac{\hbar^2}{2m\sigma^4} + \frac{1}{2}k$

$$\Rightarrow \quad \sigma = \left(\frac{\hbar^2}{mk}\right)^{1/4}$$

coeff of x gives:

$$\frac{\hbar^2 q}{m\sigma^4} = -\dot{p} \quad \Rightarrow \quad \boxed{\dot{p} = -kq}$$

const term computes $\dot{\theta}$ as function of p, q, σ.

<u>Conclusion:</u> If $\sigma = \left(\frac{\hbar^2}{mk}\right)^{1/4}$ ("coherent state")
and $(q(t), p(t))$ is a classical solution then

$$\psi(t) = \frac{1}{(\pi\sigma^2)^{1/4}} \exp\left(i\theta + \frac{ip(t)x}{\hbar} - \frac{(x-q(t))^2}{2\sigma^2}\right)$$

solves $i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi$, $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}kx^2$

<u>Textbooks:</u> Physics side: Cohen-Tannoudji.

Math side: Dimassi - Sjöstrand

"spectral asymptotics ..."