Introduction to Quantum Mechanics

Seminar for graduate students in Appl Math

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Scope of the seminar

Classical Mechanics (CM)

- Newton's equation
- Energy conservation

Quantum Mechanics (QM)

- Wavefunction-Schröedinger's equation
- Wavefunction-Interpretation
- Quantization of classical Hamiltonian
- Hilbert space approach
- Uncertainty relations

Scope and style

Brief and informal discussion (non rigorous)
of some mathematical ideas (physical foundations not discussed)
of quantum mechanics

Refs.

(1) S. Gustafson & I.M. Sigal, Mathematical concepts of quantum mechanics, Springer, 2011

(2) S. Trahanas, An Introduction to Quantum Physics, Wiley, 2018

(3) I. Anapolitanos, Lecture notes, www.math.kit.edu/iana1/lehre/quantummech2019w/seite/lecturenotes/

(4) F. Berezin & M. Shubin, The Schrödinger Equation. Kluwer Academic Publishers 1991

CM-Newton's law

▶ Motion of a **Classical Particle** of mass m subjected to force $\boldsymbol{F}(\boldsymbol{x})$, $\boldsymbol{x} \in \mathbb{R}^n$, $n = 1, 2, 3$, is defined by the trajectory $\boldsymbol{x} = \boldsymbol{x}(t)$ which is governed by Newton's law

$$m\ddot{\boldsymbol{x}}(t) = \boldsymbol{F}(\boldsymbol{x}(t)) \ , \quad t > 0 \ ,$$

with initial conditions (position and velocity)

$$\boldsymbol{x}(0) = \boldsymbol{x}_0 \ , \quad \dot{\boldsymbol{x}}(0) = \boldsymbol{v}_0$$

• Assume that the force field is conservative, i.e.,

$$\boldsymbol{F}(\boldsymbol{x}) = -\nabla U(\boldsymbol{x}) \ ,$$

where $U(\boldsymbol{x}) \in C^1(\mathbb{R}^n)$ is the potential function

CM-Energy conservation

- Mechanical energy

$$E = \text{kinetic energy} + \text{potential energy} = \frac{\boldsymbol{p}\cdot\boldsymbol{p}}{2m} + U(\boldsymbol{x})$$

where

$$\boldsymbol{p}(t) = m\dot{\boldsymbol{x}}(t) \quad \text{(momentum of the particle)}$$

- The energy is conserved, since by Newton's law

$$\begin{aligned} \dot{E} &= \frac{1}{m}\boldsymbol{p}\cdot\dot{\boldsymbol{p}} + \nabla U(\boldsymbol{x})\cdot\dot{\boldsymbol{x}} \\ &= \frac{1}{m}m\dot{\boldsymbol{x}}\cdot m\ddot{\boldsymbol{x}} - \boldsymbol{F}(\boldsymbol{x})\cdot\dot{\boldsymbol{x}} \\ &= \dot{\boldsymbol{x}}\cdot\big(m\ddot{\boldsymbol{x}} - \boldsymbol{F}(\boldsymbol{x})\big) = 0 \end{aligned}$$

QM-Schröedinger's equation

▶ Motion of a **Quantum particle** of mass m moving in a potential field $U(\mathbf{x})$ is described by a complex wavefunction $\psi(\mathbf{x}, t; \hbar)$ governed by the Schröedinger's equation (SE)

$$i\hbar \frac{\partial \psi(\mathbf{x}, t; \hbar)}{\partial t} = \Big(-\frac{\hbar^2}{2m}\Delta + U(\mathbf{x})\Big)\psi(\mathbf{x}, t; \hbar)\ , \ \ \psi(\mathbf{x}, t = 0; \hbar) = \psi_0(\mathbf{x}; \hbar)$$

$\hbar$ Planck's constant, small parameter

By (SE) it follows that (Exercise 1: prove)

$$\int_{\mathbb{R}^n} |\psi(\mathbf{x}, t; \hbar)|^2 dx = \int_{\mathbb{R}^n} |\psi_0(\mathbf{x}; \hbar)|^2 dx \text{ (say) } = 1\ , \quad \text{for any } t > 0$$

QM-Interpretation of wavefunction

- Physical interpretation of the wave function ψ

1. Time domain/probabilistic consideration

For any open, non-empty $G \subset \mathbb{R}^n$,

$$\int_G |\psi(\boldsymbol{x}, t; \hbar)|^2 dx = \text{probability of finding the particle in } G \text{ at time } t$$

This models the fact that that in contrary to classical particle, for the quantum particle we know neither the exact position (nor the exact momentum), but only the evolution of the probability density function of its position, which is considered as a random variable (measurement process).

QM-Interpretation of wavefunction

2. Spectral domain/energy consideration

For a stationary state of the particle described by

$$\psi(\boldsymbol{x}, t; \hbar) = \phi(\boldsymbol{x}; \hbar, E) e^{-i \frac{E\, t}{\hbar}}$$

it follows from (SE)

$$E \phi(\boldsymbol{x}; \hbar, E) = \Big(-\frac{\hbar^2}{2m} \Delta + U(\boldsymbol{x}) \Big) \phi(\boldsymbol{x}; \hbar, E)$$

that is, ϕ is an eigenfunction of the stationary Schröedinger operator $-\frac{\hbar^2}{2m}\Delta + U(\boldsymbol{x})$ with corresponding eigenvalue E

The eigenvalue E is interpreted as the energy of the quantum particle in stationary state (bound states/atomic spectra)

QM-Quantization

- Formal quantization of CM

"Def." **Quantization** is the establishment of a correspondence between classical observables (e.g. energy, momentum) and differential operators acting on the wavefunction

- Consider the correspondence

$$E \longleftrightarrow -i\hbar\frac{\partial}{\partial t} \ , \quad \boldsymbol{p} \longleftrightarrow -i\hbar\nabla$$

First, we have the following correspondence between the Hamiltonian function

$$H(\boldsymbol{x},\boldsymbol{p}) = \frac{\boldsymbol{p}\cdot\boldsymbol{p}}{2m} + U(\boldsymbol{x})$$

and the stationary Schröedinger operator

$$\widehat{H} = H(\boldsymbol{x}, -i\hbar\nabla) := -\frac{\hbar^2}{2m}\Delta + U(\boldsymbol{x})$$

QM-Symbols

"Def." we say that the function $H(\boldsymbol{x}, \boldsymbol{p})$ defined on classical phase space $\mathbb{R}^{2n}_{\boldsymbol{x},\boldsymbol{p}}$ (position-momentum) is the symbol of the operator $\widehat{H}$

Important remark: In general, the correspondence between symbols and operators is not unique. For example, if we consider the symbol

$$h_1(\boldsymbol{x}, \boldsymbol{p}) = \boldsymbol{x} \cdot \boldsymbol{p} \equiv h_2(\boldsymbol{x}, \boldsymbol{p}) = \boldsymbol{p} \cdot \boldsymbol{x},$$

the operators

$$\widehat{h_1} = \boldsymbol{x} \cdot (-i\hbar\nabla) \ , \quad \widehat{h_2} = (-i\hbar\nabla)\boldsymbol{x}$$

do not coincide (Exercise 2: compute $\widehat{h_1} u(\boldsymbol{x})$, $\widehat{h_2} u(\boldsymbol{x})$).

QM-Noncommutativity

Example: This non-commutativity issue arises when someone quantizes the motion of a charged particle moving in a non-constant magnetic field. In this case

$$H(\boldsymbol{x}, \boldsymbol{p}) = \frac{\left(\boldsymbol{p} - q\boldsymbol{A}(\boldsymbol{x}, t)\right)^2}{2m} + qU(\boldsymbol{x})$$

where $\boldsymbol{A}(\boldsymbol{x})$ is the magnetic potential. The total electromagnetic force on the charged particle is

$$\boldsymbol{F} = q\left(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}\right)$$

where $\boldsymbol{E} = \nabla U$ is the electric field, U being the electrostatic potential, $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ is the magnetic field, q the charge of the particle and $\boldsymbol{v} = \dot{\boldsymbol{x}}$ its velocity.

QM-Hilbert space approach-1

• complex Hilbert space $X = L_2^{\mathbb{C}}(\mathbb{R}^3)$, $< u, v >= \int_{\mathbb{R}^3} \overline{u} v dx$
identify $\psi(\boldsymbol{x}, t; \hbar)$ with the element $\psi(t) \in X$, $< \psi(t), \psi(t) >= 1$ for any $t \in \mathbb{R}$

• consider the opeartor $\widehat{H} : D(\widehat{H}) \to X$, $\; D(\widehat{H}) := C_0^\infty(\mathbb{R}^3)$ acting by

$$\widehat{H}\phi = \Big(-\frac{\hbar^2}{2m}\Delta + U(\boldsymbol{x})\Big)\phi \ , \quad \phi \in D(\widehat{H})$$

Then, for any $\phi, \psi \in D(\widehat{H})$ we have

$$\int_{\mathbb{R}^3} (\Delta\overline{\phi})\psi dx = \int_{\mathbb{R}^3} \overline{\phi}(\Delta\psi) dx$$

and therefore, for sufficiently smoot U, we get

$$< \phi, \widehat{H}\psi >= \int_{\mathbb{R}^3} \overline{\phi}\widehat{H}\psi) dx = \int_{\mathbb{R}^3} \overline{\widehat{H}\phi}\psi dx =< \widehat{H}\phi, \psi >$$

QM-Hilbert space approach-2

- $\widehat{H}$ is a linear, symmetric operator on X

For the rigorous approach we extend $\widehat{H}$ to a selfadjoint operator (Hamiltonian operator of the particle)

$$\widehat{H} : D(\widehat{H}) \subseteq X \to X$$

and we study its spectrum corresponding to possible energies of the particle

Refs.

1) E. Kreyszig, Introductory Functional Analysis with Applications, Wiley, 1978/ Ch. 11 (basic)

2) M. Schechter, Operator Methods in Quantum Mechnaics, Dover, 2003 (advanced)

QM-Hilbert space approach-3

Standard example: The harmonic oscillator, $n = 1$

- Newton's equation

$$m\ddot{x}(t) = -m\omega^2 x(t), \quad \omega = \text{frequency}$$

harmonic motion of the

$$[mass - sping\ system : m\ddot{x}(t) = -kx(t)\ , k = m\omega^2\ (= \text{spring constant})]$$

- Energy of the classical particle

$$E = H(x,p) = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2, \quad p = m\dot{x}$$

Check $\dot{E} = 0$ (Exercise 3)

QM-Hilbert space approach-4

- Quantum Hamiltonian operator

$$\widehat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2}x^2$$

- The eigenvalue problem $\widehat{H}\phi_n = E_n\phi_n$ $(n = 0, 1, \dots)$ has the solutions

$$E_n = \hbar\omega(n + 1/2)$$

$$\phi_n(x) = u_n\left(\frac{x}{x_0}\right)x_0^{-\frac{1}{2}}, \quad x_0 = \left(\frac{\hbar}{m\omega}\right)^{1/2}$$

where u_n are the Hermite functions

$$u_n(x) = \alpha_n(-1)^n\frac{d^n}{dx^n}e^{-x^2}, \quad \alpha_n = \frac{1}{2^{n/2}\pi^{1/4}(n!)^{1/2}}$$

QM-Hilbert space approach-5

Refs.
1) V. Fock, Fundamentals of quantum mechanics, MIR, 1982/ Part II, Ch. 1

2) E. Kreyszig, Introductory Functional Analysis with Applications, Wiley, 1978/ Sec. 3.7-2 (Hermite functions)

QM-Momentum & position operators-1 ($n = 1$)

- Momentum operator

$$\widehat{A} : D(\widehat{A}) \subseteq X \to X = L_2^{\mathbb{C}}(\mathbb{R})$$

$$(\widehat{A}\phi) = -i\hbar \frac{d}{dx}\phi(x)$$

$$D(\widehat{A}) = \{\phi \in X : \phi' \in X\} \ , \quad \phi' : \text{generalized derivative}$$

QM-Momentum & position operators-2

- Position operator

$$\widehat{B} : D(\widehat{B}) \subseteq X \to X$$

$$\left(\widehat{B}\phi\right) = x\phi(x)$$

$$D(\widehat{B}) = \{\phi \in X : x\phi \in X\}$$

▶ $\widehat{A}, \widehat{B}$ are selfadjoint operators on their domains of definition

Check that $\widehat{A}\widehat{B} \neq \widehat{B}\widehat{A}$ (Exercise 4)

QM-Heizenberg's inequality-1

For $\phi \in X$, $< \phi, \phi >= 1$, we define Mean Values of position and momentum in state ϕ

- Mean position,

$$\overline{x} =< \phi, \widehat{B} >= \int_{-\infty}^{\infty} x|\phi(x)|^2 dx$$

- Mean momentum

$$\overline{p} =< \phi, \widehat{A}\phi >= \int_{-\infty}^{\infty} \overline{\phi(x)}(-i\hbar\phi'(x))dx$$

QM-Heizenberg's inequality-2

- We also define Dispersions Δx, Δp

$$(\Delta x)^2 = ||\widehat{B}\phi - \overline{x}\phi||_{L^2}^2 = \int_{-\infty}^{\infty}(x-\overline{x})^2|\phi(x)|^2 dx$$

$$(\Delta p)^2 = ||\widehat{A}\phi - \overline{p}\phi||_{L^2}^2$$

Then, by

$$\widehat{A}\widehat{B}\phi - \widehat{B}\widehat{A}\phi = i\hbar\Big(x\phi'(x) - (x\phi(x))'\Big) = -i\hbar\phi(x)$$

we get (Exercise 5: use Schwarz inequality)

$$\Delta p \Delta x \geq \frac{1}{2} < (BA - BA)\phi, \phi >= \hbar/2$$

Exercise 5

More generally Schwarz's inequality

quantum system in state ψ

$\hat{A}, \hat{B}$ operators with symbols $A(x,p), B(x,p)$

quantum observables — classical observables

mean values

$\bar{A} = \langle \psi, A\psi \rangle \qquad \bar{B} = \langle \psi, B\psi \rangle$

$\langle (\hat{B}\hat{A} - \hat{A}\hat{B})\psi, \psi \rangle$

$= \langle (\hat{B} - \bar{B})(\hat{A} - \bar{A})\psi, \psi \rangle - \langle (\hat{A} - \bar{A})(\hat{B} - \bar{B})\psi, \psi \rangle$

$= \langle (\hat{B} - \bar{B})(\hat{A} - \bar{A})\psi, \psi \rangle - \langle \psi, (\hat{B} - \bar{B})(\hat{A} - \bar{A})\psi \rangle$

$= 2i \, \mathrm{Im} \langle (\hat{B} - \bar{B})(\hat{A} - \bar{A})\psi, \psi \rangle$

dispersion

$\Delta A = \| \hat{A}\psi - \bar{A}\psi \|, \quad \Delta B = \| \hat{B}\psi - \bar{B}\psi \|$

$\Delta A \cdot \Delta B = \| \hat{A}\psi - \bar{A}\psi \| \, \| \hat{B}\psi - \bar{B}\psi \|$

$\geq | \langle \hat{A}\psi - \bar{A}\psi, \hat{B}\psi - \bar{B}\psi \rangle |$

$\geq | \mathrm{Im} \langle (\hat{B} - \bar{B})(\hat{A} - \bar{A})\psi, \psi \rangle |$

$\geq 2^{-1} | \langle (\hat{B}\hat{A} - \hat{A}\hat{B})\psi, \psi \rangle |$

QM-Heizenberg's inequality-3

- From the last inequality, follows

Heisenberg's uncertainty principle:

it is impossible to measure exactly the momentum and the position at the same time

End!!!

But to learn quantum mechanics someone should start with the fundamentals of the theory

e.g., E. Schröedinger, Collected papers on wave mechanics, AMS Chelsea Publ. 2003

or

P. Dirac, The principles of quantum mechanics, Oxford Science Publ., 1999

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