Quantum Mechanics

Lecture #1: Ch. 1 & 3: Wave function & Formalism

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Outline

Prelude for this course

- Purpose of this course is NOT to teach you how to *understand* quantum mechanics(QM), but to teach you how to *use* QM.
  - "I think I can safely say that nobody understands quantum mechanics." - *Feynman*.
  - (Quasi-)Philosophical questions about QM are left to the end of the semester.
  - Full history of the development of QM will not be introduced.
  - You will learn the framework of QM and some basic techniques for solving (single particle) problems in QM.

- About the textbook ("Introduction to Quantum Mechanics", by Griffiths):
  Part I: covers the basic theoretical framework, and some exactly solvable problems;
  Part II: covers the application of QM, especially approximation schemes.
  - Homework problems will come from the textbook, and you are recommended to also work on some other exercise problems there.

Goals and Requirements: Lecture #1

- The goal of this lecture is for you to become familiar with the following items:
  - basic objects in quantum mechanics: wave functions & operators.
  - basic math structure of quantum mechanics: Hilbert space.
  - measurement postulate, and collapse postulate.
  - uncertainty relation.
  - generic Schrödinger equation and its solutions: stationary states.
- By the end of this lecture, you should master the following skills:
  - computing normalization and superpositions of wave functions.
  - using and understanding the Dirac symbols.
  - applying basic operators (position, momentum) on wave functions.
  - representing states as vectors, operators as matrices, under eigenbasis.
  - computing the measurement result distributions.
  - writing down generic solutions of Schrödinger equation in terms of stationary states.
- "Side remark"s are NOT required.
- References:

  D.J. Griffiths, *Introduction to Quantum Mechanics*, Chapter 1 & 3.

Comparison to classical mechanics

- We summarize the basic frameworks of classical mechanics and QM in following tables.
- Quantities describing the (time evolution of) state of a "particle"

Newtonian mechanics	trajectory $\boldsymbol{r}(t)$
Hamiltonian mechanics	trajectory in phase space $(\vec{q}(t), \vec{p}(t))$
quantum mechanics	"wave function" $\psi(\boldsymbol{r}, t)$

- "Equations of motion": equations governing the time evolution

Newtonian ...	"2[nd] law", $m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\boldsymbol{r} = \boldsymbol{F}(\boldsymbol{r}, \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t})$.
Hamiltonian ...	$\frac{\mathrm{d}\vec{q}}{\mathrm{d}t} = \frac{\partial H}{\partial \vec{p}}$, $\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = -\frac{\partial H}{\partial \vec{q}}$, $H = H(\vec{q}, \vec{p})$ is classical Hamiltonian
quantum ...	"Schrödinger equation" $\mathrm{i}\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi$, $\hat{H}$ is "Hamiltonian operator"

- Why using "wave function"? Justification (not proof): "wave-particle duality", microscopic particles behave like waves, wave function is the amplitude of "matter wave"
  - For example: particles with certain momentum $\boldsymbol{p}$ $\to$ planewaves $\propto e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$ with certain wavevector $\boldsymbol{k} = \boldsymbol{p}/\hbar$ (de Broglie relation)
- A fundamental constant: $\hbar \equiv \frac{h}{2\pi}$, "reduced Planck constant", $= 1.054571817\cdots \times 10^{-34}(J\cdot s)$ (2018 CODATA value, exact value in the new SI units).
  - Side remark: about the new SI units, see *e.g.* *Physics Today 73, 5, 32 (2020).*

Normalization and statistical interpretation

- Wave function $\psi(\boldsymbol{r}, t)$ is complex, not directly observable.
- Most wave functions we'll deal with are *normalizable*, $\int |\psi(\boldsymbol{r}, t)|^2 \, \mathrm{d}^3\boldsymbol{r} < \infty$.
  - non-normalizable wave functions, *e.g.* planewaves in infinite space, may be made normalizable by restricting the coordinates in a finite volume space, then $\frac{1}{\sqrt{\text{volume of space}}} e^{\mathbb{i}\boldsymbol{k}\boldsymbol{r}}$ is normalized, finally infinite volume limit may be taken.
- We will assume ψ is *normalized*, $\int |\psi(\boldsymbol{r}, t)|^2 \, \mathrm{d}^3\boldsymbol{r} = 1$, unless explicitly stated otherwise.
  - If ψ is normalizable, then $A \cdot \psi$ is normalized where $A = [\int |\psi(\boldsymbol{r}, t)|^2 \, \mathrm{d}^3\boldsymbol{r}]^{-1/2}$.
- *Max Born*: $|\psi(\boldsymbol{r}, t)|^2$ is the probability density for particle to be at position $\boldsymbol{r}$ (at time t).
  - ψ is normalized here, otherwise use $\frac{|\psi(\boldsymbol{r},t)|^2}{\int |\psi(\boldsymbol{r},t)|^2 \, \mathrm{d}^3\boldsymbol{r}}$
  - "probability density": probability to be in volume element $\mathrm{d}^3\boldsymbol{r}$ at $\boldsymbol{r}$ is $|\psi(\boldsymbol{r}, t)|^2 \, \mathrm{d}^3\boldsymbol{r}$
- About probability (see textbook Section 1.3):
  - a probability distribution density $\rho(\boldsymbol{r})$ satisfies, $\rho(\boldsymbol{r}) \geq 0$, $\int \rho(\boldsymbol{r}) \, \mathrm{d}^3\boldsymbol{r} = 1$
  - ρ may contain smooth function part(continuous distribution) and Dirac δ-functions(discrete distribution).
  - "average" of function $f(\boldsymbol{r})$, denoted by $\langle f \rangle$ hereafter, is $\int f(\boldsymbol{r}) \, \rho(\boldsymbol{r}) \, \mathrm{d}^3\boldsymbol{r}$.
  - "variance" of $f(\boldsymbol{r})$, denoted by σ_f^2, is $\langle f^2 \rangle - \langle f \rangle^2$.

Hilbert space

- Normalizable wave functions form a complex linear space (Hilbert space, usually $\mathcal{H}$)
  - If $\psi_1(\boldsymbol{r})$ and $\psi_2(\boldsymbol{r})$ are both normalizable, $\int |\psi_{1,2}|^2 \, \mathrm{d}^3\boldsymbol{r} < \infty$, then $c_1\psi_1 + c_2\psi_2$ is also normalizable for any $c_1, c_2 \in \mathbb{C}$.
    Proof: use Cauchy-Schwarz inequality, $|\int \psi_2^* \psi_1 \, \mathrm{d}^3\boldsymbol{r}| \le \frac{1}{2}(\int |\psi_1|^2 \, \mathrm{d}^3\boldsymbol{r} + \int |\psi_2|^2 \, \mathrm{d}^3\boldsymbol{r})$.
- Physical meaning: state of one quantum system can be an arbitrary *superposition* of several other physically allowed states of this system.
  - Side remark: there's no analogue of this in classical physics, the *ensemble* in statistical physics corresponds to the "mixed state" in quantum mechanics, which is different from the "pure state" (described by *one* wave function) here
- Inner product: for $\psi_{1,2} \in \mathcal{H}$, their inner product (overlap) is $(\psi_1, \psi_2) \equiv \int \psi_1^* \psi_2 \, \mathrm{d}^3\boldsymbol{r}$.
  - Hermiticity: $(\psi_2, \psi_1) = (\psi_1, \psi_2)^*$.
  - Linear with respect to(w.r.t.) 2nd argument: $(\phi, \sum_i c_i\psi_i) = \sum_i c_i \cdot (\phi, \psi_i)$, $c_i \in \mathbb{C}$.
  - Positive semi-definiteness: $(\psi, \psi) \ge 0$, [and $\psi \sim 0$ if $(\psi, \psi) = 0$].
  - Derived fact: anti-linear w.r.t. 1st argument $(\sum_i c_i\psi_i, \phi) = \sum_i c_i^* \cdot (\psi_i, \phi)$.
  - Derived fact: Cauchy-Schwarz inequality $(\psi, \phi)(\phi, \psi) \le (\psi, \psi)(\phi, \phi)$.

    Proof: consider $(c_1\psi + c_2\phi, c_1\psi + c_2\phi) = \begin{pmatrix} c_1^* & c_2^* \end{pmatrix} \begin{pmatrix} (\psi,\psi) & (\psi,\phi) \\ (\phi,\psi) & (\phi,\phi) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \ge 0$,

    the 2×2 hermitian matrix is positive semi-definite, so its determinant should ≥ 0.

Dirac symbol

- Dirac "bra-c-ket" symbols are convenient notations for representing the basic objects in Hilbert spaces (vectors, dual vectors, operators, etc.).
- "right Dirac symbol", "ket": $|\psi\rangle$, a vector in a Hilbert space, a (pure) quantum state, described by a wave function ψ.
  - We may also label the state by some "quantum numbers" instead of the wave function, *e.g.* $|n\rangle$, $|L=2, L_z=0\rangle$, etc.
- "left Dirac symbol", "bra": $\langle\psi|$, a *dual* vector in the dual space of a Hilbert space, linear functional $\mathcal{H} \to \mathbb{C}$, $|\phi\rangle \mapsto (\psi, \phi)$.
  - Side remark: (Riesz-Fréchet theorem) Any 'continuous' linear functional $f : \phi \mapsto f(\phi)$, corresponds to a wave function ψ_f so that $f = \langle\psi_f|$, $f(\phi) = (\psi_f, \phi)$.
- Notations (usage of Dirac symbols):
  - Inner product: $\langle\psi|\phi\rangle \equiv (\psi, \phi)$.
  - Certain linear operators, $|\phi\rangle\langle\psi| : |\varphi\rangle \mapsto |\phi\rangle\langle\psi|\varphi\rangle$, maps a wavefunction $|\varphi\rangle$ to another wavefunction $|\phi\rangle$ multiplied by a number $\langle\psi|\varphi\rangle$.
  - Linear superpositions: $c_1|\psi\rangle + c_2|\phi\rangle = |c_1\psi + c_2\phi\rangle$.
    NOTE: $c_1\langle\psi| + c_2\langle\phi| = \langle c_1^*\psi + c_2^*\phi|$. Exercise: check this.
  - Tensor product(direct product), $|\phi\rangle|\psi\rangle$, will be used later in Chapter 5.

Generic linear operators

- We need objects in QM that mimic the classical observable physical quantities, *e.g.* energy, momentum, angular momentum, etc..
- Linear operators: linear mappings on Hilbert spaces, usually denoted by a 'hat', *e.g.* $\hat{O}: \mathcal{H} \to \mathcal{H}$, $|\psi\rangle \mapsto \hat{O}|\psi\rangle$, where $|\psi\rangle, \hat{O}|\psi\rangle \in \mathcal{H}$. The word "linear" is usually omitted.
  - Because wave functions can be arbitrary superpositions, it is natural to request that operations on them are linear, $\hat{O}|\sum_i c_i\psi_i\rangle = \sum_i (c_i \cdot \hat{O}|\psi_i\rangle)$, $\forall c_i \in \mathbb{C}$.
  - Linear superpositions of operators: $(c_1\hat{O}_1 + c_2\hat{O}_2)|\psi\rangle = c_1\hat{O}_1|\psi\rangle + c_2\hat{O}_2|\psi\rangle$.
  - Products of operators: $(\hat{O}_1\hat{O}_2)|\psi\rangle = \hat{O}_1(\hat{O}_2|\psi\rangle)$.
    IMPORTANT: apply the sequence of operators from right to left.
  - Commutator: $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$.
- Hermitian conjugate of an operator $\hat{O}$: denoted by a superscript 'dagger', $\hat{O}^\dagger$, is also a linear operator satisfying $(\hat{O}^\dagger\psi, \phi) = (\psi, \hat{O}\phi)$ for any $\psi, \phi \in \mathcal{H}$.
  - If $\hat{O}^\dagger = \hat{O}$, then $\hat{O}$ is a *hermitian operator*.
- Eigenvalues & eigenstates: if $\hat{O}|\psi\rangle = \lambda|\psi\rangle$, then $\lambda \in \mathbb{C}$ is an eigenvalue of $\hat{O}$, and $|\psi\rangle$ is the eigenstate of $\hat{O}$ corresponding to eigenvalue λ.
  - Exercise: show that eigenvalues of hermitian operators are real.
- Physical observables in QM correspond to hermitian operators.

Momentum operator

- Position operator (1D) $\hat{x}: \psi(x) \mapsto x \cdot \psi(x)$, obviously hermitian.
  - Eigenvalues: all real numbers $x_0 \in \mathbb{R}$.
  - Eigenstates: $\delta(x - x_0)$, a particle exactly at position x_0, NOT normalizable!
- Momentum operator (1D) $\hat{p}: \psi(x) \mapsto -\mathrm{i}\hbar \frac{\partial}{\partial x}\psi(x)$.
  - Justification (not proof): classical particle with momentum p corresponds to planewave $\propto e^{\mathrm{i}kx}$ in QM, $k = p/\hbar$, demand that this is an eigenstate of $\hat{p}$ operator with eigenvalue p (see Measurement postulate[4.1] later).
  - $\hat{p}$ is hermitian. Proof: integration by parts, $(\hat{p}\psi, \phi) = \int_{-\infty}^{\infty}(-\mathrm{i}\hbar\partial_x\psi)^*\phi\,\mathrm{d}x$ $= \mathrm{i}\hbar\big([\partial_x\psi^* \cdot \phi]_{x=-\infty}^{+\infty} - \int_{-\infty}^{\infty}\psi^*\partial_x\phi\,\mathrm{d}x\big) = (\psi, \hat{p}\phi)$, if we omit boundary term.
  - Eigenvalues: all (real?) numbers p.
  - Eigenstates: planewaves $\propto e^{\mathrm{i}px/\hbar}$, NOT normalizable! (see Eigenbasis[3.2] later).
- Canonical commutation relation (1D): $[\hat{x}, \hat{p}] = \mathrm{i}\hbar$.
  Proof: $([\hat{x}, \hat{p}])\psi = x \cdot ((-\mathrm{i}\hbar\partial_x)\psi) - (-\mathrm{i}\hbar\partial_x)(x \cdot \psi) = \mathrm{i}\hbar \cdot \psi$, for any function $\psi(x)$.
- Classical observable $O(x, p)$ corresponds to QM operator $O(\hat{x}, \hat{p})$, generally a differential operator $O(x, -\mathrm{i}\hbar\frac{\partial}{\partial x})$. Example: non-relativistic kinetic energy $\frac{\hat{p}^2}{2m}$, namely $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$.
  - Side remark: classical xp corresponds to $\frac{1}{2}(\hat{x}\hat{p} + \hat{p}\hat{x})$, for more complicated cases, *c.f.* Peskin&Schroeder, "Introduction to Quantum Field Theory", Section 9.1.
- Momentum in 3D space: $\hat{\boldsymbol{p}}$ is a vector $(\hat{p}_x, \hat{p}_y, \hat{p}_z) = -\mathrm{i}\hbar(\partial_x, \partial_y, \partial_z) = -\mathrm{i}\hbar\nabla$.

Eigenbasis

- Eigenstates of a hermitian operator form *complete orthonormal* basis of the Hilbert space.
  - All eigenvalues form "spectrum" of operator $\hat{O}$, may be continuous or discrete.
  - Suppose the eigenstates are non-degenerate, label them by corresponding eigenvalues of $\hat{O}$, like $|\hat{O}=\lambda\rangle$, then $\hat{O}|\hat{O}=\lambda\rangle = \lambda|\hat{O}=\lambda\rangle$.
    - If $\lambda \neq \lambda'$, then $\langle\hat{O}=\lambda|\hat{O}=\lambda'\rangle = 0$. Exercise: prove this.
  - "orthonormal": $\langle\hat{O}=\lambda|\hat{O}=\lambda'\rangle = \begin{cases} \delta_{\lambda,\lambda'}, & \text{discrete } \lambda,\lambda'; \\ \delta(\lambda-\lambda'), & \text{continuous } \lambda,\lambda' \end{cases}$
  - "complete": any state $|\psi\rangle$ is a linear superposition of the eigenbasis, $|\psi\rangle = \text{“}\sum_\lambda\text{''}\psi_\lambda|\hat{O}=\lambda\rangle$. Here "$\sum_\lambda$" may be integral for continuous λ.
    - Expansion coefficient $\psi_\lambda = \langle\hat{O}=\lambda|\psi\rangle$.
      Proof: $\langle\hat{O}=\lambda|\psi\rangle = \text{“}\sum_{\lambda'}\text{''}\psi_{\lambda'}\langle\hat{O}=\lambda|\hat{O}=\lambda'\rangle$, then use the "orthonormal" condition above.
  - Resolution of identity: identity operator $\hat{\mathbb{1}} = \text{“}\sum_\lambda\text{''}|\hat{O}=\lambda\rangle\langle\hat{O}=\lambda|$.
- 'kets' $|\psi\rangle$ are represented as column vectors, $\langle\hat{O}=\lambda|\psi\rangle \equiv \psi_\lambda$, λ is row-index.
- Operators $\hat{A}$ are represented as matrices, with "matrix elements" $A_{\lambda,\lambda'} = \langle\hat{O}=\lambda|\hat{A}|\hat{O}=\lambda'\rangle$. λ,λ' are row-,column-index respectively.
  - $(\hat{A}\psi)_\lambda \equiv \langle\hat{O}=\lambda|\hat{A}|\psi\rangle = \text{“}\sum_{\lambda'}\text{''}A_{\lambda,\lambda'}\cdot\psi_{\lambda'}$, matrix-vector product.
- 'bras' $\langle\phi|$ are represented as row vectors, $\langle\phi|\hat{O}=\lambda\rangle = \phi^*_\lambda$, λ is column-index.
  - $\langle\phi|\psi\rangle = \text{“}\sum_\lambda\text{''}\phi^*_\lambda\cdot\psi_\lambda$, vector inner product.

Eigenbasis (cont'd)

- If the eigenstates of $\hat{O}$ have degeneracy, label the degenerate eigenstates by another index k (discrete or continuous) as $|\hat{O}=\lambda,\ k\rangle$, they can form complete orthonormal basis.
  - $\langle\hat{O}=\lambda',\ k'|\hat{O}=\lambda,\ k\rangle = \left(\left\{\begin{array}{l}\delta_{\lambda',\lambda}\\ \delta(\lambda'-\lambda)\end{array}\right.\right)\times\left(\left\{\begin{array}{l}\delta_{k',k}\\ \delta(k'-k)\end{array}\right.\right).$
    The Kronecker-δ and Dirac-δ should be used for cases with discrete and continuous index respectively.
  - $\hat{\mathbb{1}} = \text{“}\sum_\lambda\text{”}\,\text{“}\sum_k\text{”}|\hat{O}=\lambda,\ k\rangle\langle\hat{O}=\lambda,\ k|.$
  - k may be the eigenvalue of another observable $\hat{Q}$, or the collection of eigenvalues of several observables $\hat{Q}_i$ [then $\delta_{k',k}$ and $\delta(k'-k)$ are higher dimensional Kronecker-δ and Dirac-δ]. $\hat{O}$ and $\hat{Q}$s must mutually commute.
- Position basis (1D): $|\hat{x}=x_0\rangle$ or usually just $|x_0\rangle$, “normalized” wave function $\delta(x-x_0)$.
  - $\hat{x}|x\rangle = x|x\rangle$, $\langle x|x'\rangle = \delta(x-x')$, $\int \mathrm{d}x\,|x\rangle\langle x| = \hat{\mathbb{1}}$.
  - $|\psi\rangle = \int \mathrm{d}x\,|x\rangle\langle x|\psi\rangle$, $\langle x|\psi\rangle = \psi(x)$ is the wave function (in position representation).
- Momentum basis (1D): $|\hat{p}=p_0\rangle$ or just $|p_0\rangle$, “normalized” wave function $\frac{e^{\mathrm{i}p_0\cdot x/\hbar}}{\sqrt{2\pi\hbar}}$
  - $\hat{p}|p\rangle = p|p\rangle$, $\langle p|p'\rangle = \delta(p-p')$, $\int \mathrm{d}p\,|p\rangle\langle p| = \hat{\mathbb{1}}$.
  - $|\psi\rangle = \int \mathrm{d}p\,|p\rangle\langle p|\psi\rangle$, $\langle p|\psi\rangle \equiv \tilde{\psi}(p)$ is wave function in momentum representation.
  - $\tilde{\psi}(p) = \int \mathrm{d}x\,\langle p|x\rangle\langle x|\psi\rangle = \int \mathrm{d}x\,\frac{e^{-\mathrm{i}px/\hbar}}{\sqrt{2\pi\hbar}}\psi(x)$, is the Fourier transform of $\psi(x)$.
- Example: matrix element $\langle x_1|\hat{p}|x_2\rangle = \int \mathrm{d}p\,\langle x_1|\hat{p}|p\rangle\langle p|x_2\rangle = \int \mathrm{d}p\,\langle x_1|p|p\rangle\langle p|x_2\rangle$
  $= \int p\frac{e^{\mathrm{i}p(x_1-x_2)/\hbar}}{2\pi\hbar}\mathrm{d}p = -\mathrm{i}\hbar\frac{\partial}{\partial x_1}\left(\int\frac{e^{\mathrm{i}p(x_1-x_2)/\hbar}}{2\pi\hbar}\mathrm{d}p\right) = -\mathrm{i}\hbar\frac{\partial}{\partial x_1}\left(\delta(x_1-x_2)\right).$
  Exercise: check that $\langle x_1|\hat{p}|\psi\rangle = \int \mathrm{d}x_2\,\langle x_1|\hat{p}|x_2\rangle\langle x_2|\psi\rangle = -\mathrm{i}\hbar\frac{\partial}{\partial x}\psi(x)\Big|_{x=x_1}$.

Measurement postulate

- Measurement postulate: one measurement of observable $\hat{O}$ under state $|\psi\rangle$ will produce one of the eigenvalues λ of $\hat{O}$, with *a priori* probability (density) $|\langle\hat{O}=\lambda|\psi\rangle|^2$.
  - Here $|\hat{O}=\lambda\rangle$ and $|\psi\rangle$ must be "normalized".
  - Consistency check: total probability "$\sum_\lambda$"$|\langle\hat{O}=\lambda|\psi\rangle|^2 =$ "$\sum_\lambda$"$\langle\psi|\hat{O}=\lambda\rangle\langle\hat{O}=\lambda|\psi\rangle = \langle\psi|\hat{\mathbb{1}}|\psi\rangle = 1$.
  - This is called "generalized statistical interpretation" in textbook.
- Collapse postulate: after the above measurement, the state becomes $|\hat{O}=\lambda\rangle$.
- Degenerate eigenstate case: if eigenstates of $\hat{O}$ for eigenvalue λ are degenerate, labeled by another index k, $|\hat{O}=\lambda,\ k\rangle$, the above postulates are modified to:
  - *a priori* probability (density) for measurement result λ is "$\sum_k$"$|\langle\hat{O}=\lambda,\ k|\psi\rangle|^2$.
  - collapsed state is the projection of $|\psi\rangle$ onto the subspace spanned by the degenerate eigenstates, $[$"$\sum_k$"$|\langle\hat{O}=\lambda,\ k|\psi\rangle|^2]^{-1/2}\left(\text{"}\sum_k\text{"}|\hat{O}=\lambda,\ k\rangle\langle\hat{O}=\lambda,\ k|\psi\rangle\right)$.
- The expectation value $\langle\psi|\hat{O}|\psi\rangle$, equals *a priori* average of measurement results.
  - $\hat{O} =$ "$\sum_\lambda$" $\left(|\hat{O}=\lambda\rangle\cdot\lambda\cdot\langle\hat{O}=\lambda|\right)$. Exercise: show this.
    Expectation value $\langle\psi|\hat{O}|\psi\rangle =$ "$\sum_\lambda$" $\left(\langle\psi|\hat{O}=\lambda\rangle\cdot\lambda\cdot\langle\hat{O}=\lambda|\psi\rangle\right) =$ "$\sum_\lambda$" $\left(\lambda\cdot|\langle\hat{O}=\lambda|\psi\rangle|^2\right)$, equals the average of measurement results λ under probability distribution $|\langle\hat{O}=\lambda|\psi\rangle|^2$.
  - The expectation value may also be written as $\langle\hat{O}\rangle_\psi$, or just $\langle\hat{O}\rangle$ if the state ψ is implicitly given.

Uncertainty relation

- Uncertainty relation (by *Heisenberg*): measure observables $\hat{A}$ and $\hat{B}$ under state $|\psi\rangle$, product of their variances are bounded from below, $\sigma^2_{\hat{A}} \cdot \sigma^2_{\hat{B}} \geq \frac{1}{4}\left|\langle[\hat{A},\hat{B}]\rangle_\psi\right|^2$.
  - Variance of observable $\hat{A}$ is $\sigma^2_{\hat{A}} \equiv \langle\hat{A}^2\rangle_\psi - (\langle\hat{A}\rangle_\psi)^2 = \text{“}\sum_\lambda\text{”}\left[(\lambda-\bar{\lambda})^2 \cdot |\langle\hat{A}=\lambda|\psi\rangle|^2\right]$ $= \text{“}\sum_\lambda\text{”}\left(\lambda^2 \cdot |\langle\hat{A}=\lambda|\psi\rangle|^2\right) - \bar{\lambda}^2$, here $\bar{\lambda} = \langle\hat{A}\rangle_\psi = \text{“}\sum_\lambda\text{”}\left(\lambda \cdot |\langle\hat{A}=\lambda|\psi\rangle|^2\right)$.
  - Proof (textbook Section 3.5): Define “inner product” of operators $\hat{A}$, $\hat{B}$ as $(\hat{A},\hat{B}) \equiv \langle\hat{A}^\dagger\hat{B}\rangle_\psi$, then $(\hat{B},\hat{A}) = (\hat{A},\hat{B})^*$, $(\hat{A},\sum_i c_i\hat{B}_i) = \sum_i c_i(\hat{A},\hat{B}_i)$, $(\hat{A},\hat{A}) \geq 0$. (Exercise: check these.) Therefore $(\hat{A},\hat{A})(\hat{B},\hat{B}) \geq |(\hat{A},\hat{B})|^2$ (Cauchy-Schwarz inequality, see Hilbert space[2.2] before).
    Define hermitian operators $\hat{A}' = \hat{A} - \langle\hat{A}\rangle_\psi$, $\hat{B}' = \hat{B} - \langle\hat{B}\rangle_\psi$, for the uncertainty relation, then $\sigma^2_{\hat{A}} = \langle\hat{A}'^2\rangle_\psi = (\hat{A}',\hat{A}')$, $\sigma^2_{\hat{B}} = \langle\hat{B}'^2\rangle_\psi = (\hat{B}',\hat{B}')$, $[\hat{A}',\hat{B}'] = [\hat{A},\hat{B}]$. Finally
    $\sigma^2_{\hat{A}} \cdot \sigma^2_{\hat{B}} = (\hat{A}',\hat{A}')(\hat{B}',\hat{B}') \geq |(\hat{A}',\hat{B}')|^2 = |\langle\hat{A}'\hat{B}'\rangle_\psi|^2 \geq [\mathrm{Im}(\langle\hat{A}'\hat{B}'\rangle_\psi)]^2$
    $= \frac{1}{4}\left|\langle\hat{A}'\hat{B}'\rangle_\psi - \langle\hat{B}'\hat{A}'\rangle_\psi\right|^2 = \frac{1}{4}\left|\langle[\hat{A}',\hat{B}']\rangle_\psi\right|^2 = \frac{1}{4}\left|\langle[\hat{A},\hat{B}]\rangle_\psi\right|^2$.
  - Special case: $\hat{A} = \hat{x}$, $\hat{B} = \hat{p}$, then $\sigma^2_{\hat{x}} \cdot \sigma^2_{\hat{p}} \geq \frac{\hbar^2}{4}$.
  - Example problem: $\psi(x) \propto e^{-ax^2}$, here $a > 0$, compute $\sigma^2_{\hat{x}}$ and $\sigma^2_{\hat{p}}$, check uncertainty relation.
    Solution: $\int_{-\infty}^{+\infty} |e^{-ax^2}|^2\,\mathrm{d}x = \sqrt{\frac{\pi}{2a}}$, so normalized ψ can be $(\frac{2a}{\pi})^{1/4}e^{-ax^2}$; obviously $\langle\hat{x}\rangle_\psi$,$\langle\hat{p}\rangle_\psi$ both vanish (odd function integrands); then $\sigma^2_{\hat{x}} = \langle x^2\rangle_\psi = \int_{-\infty}^{+\infty} x^2\sqrt{\frac{\pi}{2a}}e^{-2ax^2}\,\mathrm{d}x = \frac{1}{4a}$ (Gaussian integrals); $\sigma^2_{\hat{p}} = \langle\psi|\hat{p}^2|\psi\rangle = \langle\hat{p}\psi|\hat{p}\psi\rangle$, here $\hat{p}\psi = -2\mathrm{i}\hbar ax \cdot \psi$, then $\sigma^2_{\hat{p}} = 4\hbar^2a^2\langle\hat{x}^2\rangle_\psi = \frac{\hbar^2 a}{4}$. So $\sigma^2_{\hat{x}}\sigma^2_{\hat{p}} = \frac{\hbar^2}{4}$.

Schrödinger equation

- Schrödinger equation: $\mathbb{i}\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$.
  - The "Hamiltonian" $\hat{H}$ is a hermitian operator.
    - Argument (not proof) about why $\hat{H}$ must be hermitian: normalization $\langle\psi|\psi\rangle$ should be preserved during time evolution for a *closed* quantum system (particles cannot go out of or into the system).
      $\frac{\partial}{\partial t}(\langle\psi|\psi\rangle) = \langle\frac{\partial}{\partial t}\psi|\psi\rangle + \langle\psi|\frac{\partial}{\partial t}\psi\rangle = \langle(-\frac{\mathbb{i}}{\hbar}\hat{H}\psi)|\psi\rangle + \langle\psi|(-\frac{\mathbb{i}}{\hbar}\hat{H}\psi)\rangle$
      $= \frac{\mathbb{i}}{\hbar}\Big(\langle\hat{H}\psi|\psi\rangle - \langle\psi|\hat{H}\psi\rangle\Big)\,\frac{\mathbb{i}}{\hbar}\Big(\langle\psi|\hat{H}^\dagger\psi\rangle - \langle\psi|\hat{H}\psi\rangle\Big) = \frac{\mathbb{i}}{\hbar}\langle\psi|(\hat{H}^\dagger - \hat{H})|\psi\rangle$.
      Therefore, if $\hat{H}$ is hermitian, the normalization of wave function is perserved, $\frac{\partial}{\partial t}(\langle\psi|\psi\rangle) = 0$.
      Exercise: prove the converse statement, if $\langle\psi|(\hat{H}^\dagger - \hat{H})|\psi\rangle = 0$ for any ψ, then $\hat{H}$ must be hermitian.
  - $-\mathbb{i}\hbar\frac{\partial}{\partial t}\langle\psi| = \langle\psi|\hat{H}$, by taking hermitian conjugate.
  - Side remark: *analogy* to Hamilton-Jacobi equation in classical mechanics.
    - For classical mechanics system, with classical Hamiltonian $H(\boldsymbol{p},\boldsymbol{q},t)$, the "action" $S(\boldsymbol{q},t)$ as a function of final coordinate $\boldsymbol{q}$ and final time t satisfies H-J equation, $\frac{\partial S}{\partial t} + H(\boldsymbol{q},\frac{\partial S}{\partial \boldsymbol{q}},t) = 0$. Define $\psi(\boldsymbol{q},t) = \mathrm{Const}\cdot\exp[\frac{\mathbb{i}}{\hbar}S(\boldsymbol{q},t)]$. Then $\mathbb{i}\hbar\frac{\partial}{\partial t}\psi = -\frac{\partial}{\partial t}S\cdot\psi = H\cdot\psi$. This can be more rigorously formulated as "path integral" in QM.
- Hamiltonian for non-relativistic particle in static potential: $\hat{H} = H(\hat{\boldsymbol{p}},\hat{\boldsymbol{r}}) = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{r}})$.
  $\hat{H}\psi(\boldsymbol{r}) = [-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})]\psi(\boldsymbol{r})$.
  - Probability current: $\boldsymbol{J}(\boldsymbol{r}) \equiv \mathrm{Re}[\psi^*(\boldsymbol{r})\frac{\hat{\boldsymbol{p}}}{m}\psi(\boldsymbol{r})]$. Note that $\frac{\hat{\boldsymbol{p}}}{m}$ is "velocity operator".
  - Continuity equation for probability density $\rho(\boldsymbol{r}) \equiv |\psi(\boldsymbol{r})|^2$: $\frac{\partial}{\partial t}\rho(\boldsymbol{r}) + \mathrm{div}[\boldsymbol{J}(\boldsymbol{r})] = 0$.
    - Proof: $\frac{\partial}{\partial t}\rho(\boldsymbol{r}) = (\frac{\partial}{\partial t}\psi^*)\psi + \psi^*(\frac{\partial}{\partial t}\psi) = \frac{\mathbb{i}}{\hbar}(\hat{H}\psi)^*\psi - \frac{\mathbb{i}}{\hbar}\psi^*(\hat{H}\psi)$, [$V$ terms cancel]
      $= \frac{\mathbb{i}}{\hbar}(-\frac{\hbar^2}{2m})[(\nabla^2\psi^*)\psi - \psi^*(\nabla^2\psi)] = \frac{\mathbb{i}\hbar}{2m}\nabla\cdot[(\nabla\psi^*)\psi - \psi^*(\nabla\psi)] = \nabla\cdot\mathrm{Re}[\psi^*(\frac{-\mathbb{i}\hbar}{m}\nabla\psi)]$,
      and $\frac{-\mathbb{i}\hbar}{m}\nabla$ is $\frac{\hat{\boldsymbol{p}}}{m}$.

Some basic properties of Schrödinger equation

- Stationary state: $\psi_E(\boldsymbol{r},t) = e^{-\mathbb{i}E\cdot t/\hbar}\psi_E(\boldsymbol{r})$, where $\hat{H}\psi_E = E\cdot\psi_E$.
  - For *time-independent* $\hat{H}$, *some* solutions to Schrödinger equation can be obtained by "separation of variables", $\psi(\boldsymbol{r},t) = \psi(\boldsymbol{r})\phi(t)$. Then $\phi(t) = e^{-\mathbb{i}E\cdot t/\hbar}$, $\hat{H}\psi(\boldsymbol{r}) = E\cdot\psi(\boldsymbol{r})$. Here real number E is the "energy eigenvalue" of $\hat{H}$, $\psi(\boldsymbol{r})$ is the corresponding eigenstate wave function (labeled by ψ_E hereafter).
  - $\psi_E(\boldsymbol{r},t)$ has definitive energy E (no uncertainty).
  - Expectation value of *time-independent* observable $\hat{O}$ under $\psi_E(\boldsymbol{r},t)$ is independent of time (a.k.a. stationary).
    $\langle\hat{O}\rangle_{\psi_E} \equiv \int \mathrm{d}\boldsymbol{r}\,(e^{-\mathbb{i}Et/\hbar}\psi_E(\boldsymbol{r}))^*\,\hat{O}(e^{-\mathbb{i}Et/\hbar}\psi_E(\boldsymbol{r}))$
    $= \int \mathrm{d}\boldsymbol{r}\, e^{\mathbb{i}Et/\hbar}(\psi_E(\boldsymbol{r}))^* e^{-\mathbb{i}Et/\hbar}\hat{O}\psi_E(\boldsymbol{r}) = \int \mathrm{d}\boldsymbol{r}\,(\psi_E(\boldsymbol{r}))^*\,\hat{O}\psi_E(\boldsymbol{r})$.
  - Generic solution to Schrödinger equation with time-independent $\hat{H}$:
    linear superposition of stationary states, "$\sum_E$" $\left(c_E\cdot e^{-\mathbb{i}Et/\hbar}\cdot\psi_E(\boldsymbol{r})\right)$, $c_E\in\mathbb{C}$.
    Here "$\sum_E$" is "summing" over eigenvalues of $\hat{H}$. Normalization is "$\sum_E$"$|c_E|^2 = 1$.

- (Not required) Heisenberg equations of motion: the expectation value of observable $\hat{O}$ under a solution $\psi(\boldsymbol{r},t)$ to a Schrödinger equation with Hamiltonian $\hat{H}$, satisfies
  $\frac{\mathrm{d}}{\mathrm{d}t}\left(\langle\hat{O}\rangle_\psi\right) = \langle\frac{\partial}{\partial t}\hat{O}\rangle_\psi + \frac{\mathbb{i}}{\hbar}\langle[\hat{H},\hat{O}]\rangle_\psi$.
  - Proof: $\frac{\mathrm{d}}{\mathrm{d}t}\left(\langle\hat{O}\rangle_\psi\right) = \langle\psi|\frac{\partial\hat{O}}{\partial t}|\psi\rangle + \langle\frac{\partial\psi}{\partial t}|\hat{O}|\psi\rangle + \langle\psi|\hat{O}|\frac{\partial\psi}{\partial t}\rangle$
    $= \langle\frac{\partial}{\partial t}\hat{O}\rangle_\psi + \langle\frac{-\mathbb{i}}{\hbar}\hat{H}\psi|\hat{O}|\psi\rangle + \langle\psi|\hat{O}|\frac{-\mathbb{i}}{\hbar}\hat{H}\psi\rangle = \langle\frac{\partial}{\partial t}\hat{O}\rangle_\psi + \frac{\mathbb{i}}{\hbar}\left[\langle\psi|\hat{H}^\dagger\hat{O}|\psi\rangle - \langle\psi|\hat{O}\hat{H}|\psi\rangle\right] = \ldots$
  - Side remark: *analogy* to classical mechanics with classical Hamiltonian $H(\boldsymbol{p},\boldsymbol{q},t)$, $\frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}t} = \frac{\partial H}{\partial\boldsymbol{p}}$, $\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = -\frac{\partial H}{\partial\boldsymbol{q}}$, then $\frac{\mathrm{d}}{\mathrm{d}t}O(\boldsymbol{p},\boldsymbol{q},t) = \frac{\partial O}{\partial t} + \frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}t}\frac{\partial O}{\partial\boldsymbol{q}} + \frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t}\frac{\partial O}{\partial\boldsymbol{p}} = \frac{\partial O}{\partial t} + (\frac{\partial H}{\partial\boldsymbol{p}}\frac{\partial O}{\partial\boldsymbol{q}} - \frac{\partial H}{\partial\boldsymbol{q}}\frac{\partial O}{\partial\boldsymbol{p}}) = \frac{\partial O}{\partial t} + \{O,H\}$. Here $\{f,g\} \equiv \frac{\partial f}{\partial\boldsymbol{q}}\frac{\partial g}{\partial\boldsymbol{p}} - \frac{\partial f}{\partial\boldsymbol{p}}\frac{\partial g}{\partial\boldsymbol{q}}$ is the "Poisson bracket" and corresponds to commutator in QM.

Energy-time uncertainty relation

- Similar to the previous uncertainty relation[4.2], we have $\sigma_E^2 \cdot \sigma_t^2 \geq \frac{\hbar^2}{4}$.
  - σ_E^2 is the variance of energy, corresponding observable is Hamiltonian $\hat{H}$.
  - Time t is not an ordinary "observable". σ_t *may* be defined as follows: consider a time-independent observable $\hat{Q}$, its expectation value $\langle\hat{Q}\rangle$ under a solution to the Schrödinger equation will generically change over time, σ_t is roughly the time scale for the expectation value to change by one standard deviation of $\hat{Q}$, $\sigma_t \sim \frac{\sigma_{\hat{Q}}}{|\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{Q}\rangle|}$.

    Then $\sigma_t^2 \sim \frac{\sigma_{\hat{Q}}^2}{|\frac{\mathrm{i}}{\hbar}\langle[\hat{H},\hat{Q}]\rangle|^2} \geq \frac{\hbar^2}{4} \cdot \frac{\sigma_{\hat{Q}}^2}{\sigma_{\hat{H}}^2 \cdot \sigma_{\hat{Q}}^2} = \frac{\hbar^2}{4}\frac{1}{\sigma_E^2}$. Here we have used the ordinary uncertainty relation between $\hat{H}$ and $\hat{Q}$, $|\langle[\hat{H},\hat{Q}]\rangle|^2 \leq 4 \cdot \sigma_{\hat{H}}^2 \cdot \sigma_{\hat{Q}}^2$.