QM

Five Principles

- Word version
  1. State encoded by a non-zero vector in a Hilbert space
  2. Observables encoded by Hermitian operator : $\hat{A} = \overline{\hat{A}^T}$
  3. Born rule: Possible outcomes of measurements of A are given by eigenvalue of its operator $\hat{A}$
  4. (State collapse postulate)
  5. Dynamic/ Time evolution:$i\hbar|\dot{\psi}\rangle = \hat{H}|\psi\rangle$
- Interpretation
  - State is the raw data of an object, stored in a vector $\varphi \in \mathscr{H}$, $|\varphi| = 1$
  - Observables (e.g. A) are processed data, where the method of processing the data is an Hermitian operator $\hat{A}$
  - $\hat{A}$ and φ admits orthogonal decompositions/eigenvalue decompositions:
    $\hat{A}$ has eigenvalues $\{a_i\}$ and eigenvectors $\{e_i\}$,
    φ can be decomposed as
    $$\varphi = \sum_{i\in I} \langle \varphi, e_i\rangle e_i$$
    Thus
    $$\hat{A}\varphi = \sum_{i\in I} \underbrace{a_i\langle \varphi, e_i\rangle e_i}_{M_i}$$
  - A measurement of A on ϕ is a random variable M on probability space $(\Omega, F, \mathbb{P})$ where
    1. $\Omega = \{a_i\langle\phi, e_i\rangle e_i : i \in I\}$
    2. Since all values of i can be taken, $F = 2^{\Omega}$
    3. $\mathbb{P}(M = M_i) = |\langle \phi_i, e_i\rangle|^2$
       Realisation of M are called results of measurement.
- Operators and quantities
  - Position operator — $\hat{q} : \phi(x) \mapsto x\phi(x)$ — This operator commutes with potential operator!!!
  - Momentum Operator — $\hat{p} : \phi(x) \mapsto -i\hbar\frac{\partial}{\partial x}\phi(x)$
  - Kinetic Energy: $\hat{E}_{kin} = \frac{\hat{p}^2}{2m} : \phi(x) \mapsto -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x)$
  - Expectation (of $\hat{A}$ in state $|\phi\rangle$) — $\langle\hat{A}\rangle = \frac{\langle\phi|\hat{A}|\phi\rangle}{\langle\phi|\phi\rangle}$
  - Uncertainty : $\Delta A = \sqrt{\langle A^2\rangle - \langle A\rangle^2}$ — Thm: If $[\hat{A}, \hat{B}] \neq 0$, then $\Delta A \Delta B \geq \frac{1}{2}|\langle i[A, B]\rangle|$ — $\Delta p \Delta x \geq \frac{\hbar}{2}$
  - Projection Operator — $\hat{P} = \sum_{n=1}^{N} |\phi_n\rangle\langle\phi_n|$ where $\langle\phi_i|\phi_j\rangle = \delta_{ij}$ — Eigenvalues of $\hat{P}$ are either 1 or 0
  - Probability — $p(a_j) = \langle\phi|\hat{P}_j|\phi\rangle$
    - This equation means the probability of obtaining measurement a_j, which has to be an eigenvalue of $\hat{A}$
    - $\hat{P}_j$ is the projection operator onto the subspace associated to the eigenvalue a_j
    - If eigenvalues of $\hat{A}$ are discrete, $p(a_j) = ????$

Mathematical Fundation

- Mathematical Background
  - State and Observables
    1. The state of a quantum system is described by a non-zero vector in a Hilbert space
    2. A measurable quantity is described by a Hermitian operator on the Hilbert space. Both the measurable quantities and the operators representing them are often referred to as observables
  - Dirac Notation
    - $F(\phi) = (f, \phi) = \langle f|\phi\rangle$
    - Bra-vector: $\langle\phi|$
      Ket-vector: $|\psi\rangle$
    - $\langle\phi|\hat{A}^\dagger = \langle\hat{A}\phi|$
    - Conjudgation:
      $\langle\phi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}^\dagger|\phi\rangle^*$
  - Spectrum for Hermitian Operator
    - All eigenvalues re real
    - Eigenvectors are orthogonal
    - All expectations are real — This is also a sufficient condition for Hermcity
    - Eigenvectors span the space

Quantum Harmonic Oscillator

- Algebraic solution of $\hat{H} = \frac{\hat{p}}{2m} + \frac{1}{2}m\omega^2\hat{q}^2$
  - 1.Change of Variable
    - $\begin{cases} \hat{Q} = \sqrt{\frac{m\omega}{\hbar}}\hat{q} \\ \hat{P} = \sqrt{\frac{1}{m\omega\hbar}}\hat{p} \end{cases}$ — $\begin{cases} [\hat{Q}, \hat{P}] = i\hat{I} \\ \hat{H} = \frac{h\omega}{2}(\hat{P}^2 + \hat{Q}^2) \end{cases}$
    - $\begin{cases} \hat{a} = \frac{1}{\sqrt{2}}(\hat{Q} + i\hat{P}) \\ \hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{Q} - i\hat{P}) \\ \hat{N} := \hat{a}^\dagger\hat{a} \end{cases}$ — $\begin{cases} \hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}) \\ [\hat{a}, \hat{a}^\dagger] = \hat{I} \\ [\hat{N}, \hat{a}] = -\hat{a} \\ [\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger \\ \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = \hat{I} + 2\hat{a}\hat{a}^\dagger = -\hat{I} + 2\hat{a}^\dagger\hat{a} \end{cases}$
    - $\hat{a}$: lowering, annihilation operator
      $\hat{a}^\dagger$: raising, creation
  - 2. Consequences
    - a. Eigenvalues of $\hat{N}$ are non-negative
    - b. Eigenvalue shift
    - c. Discrete spectrum
  - Matrix representations
    - $\hat{a}^\dagger : \langle m|\hat{a}^\dagger|n\rangle = \sqrt{n+1}\,\delta_{m,n+1}$
    - $\hat{a} : \langle\hat{a}^\dagger\rangle = \sqrt{n}\,\delta_{m,n-1}$
    - $\hat{H} : \langle\hat{H}\rangle = \hbar\omega(n + \frac{1}{2})\delta_{m,n}$
  - Harmonic Oscillator basis — representing of position

Classic Dynamic Results

- Hamiltonian Mechanics
  - $H(p, q) = \frac{p^2}{2m} + V(q)$
    - $\dot{p} = -\frac{\partial V}{\partial q}$
    - $\dot{q} = \frac{\partial V}{\partial p}$
    - Hamiltonian conserves energy:
      $$\frac{dH}{dt} = 0$$
    - $p^2/2m$: kinetic
      $V(q)$: potential
  - Use $\vec{F}(\vec{r}) = -\vec{\nabla}\vec{V}(q)$ to find sign
  - Scope: only when energy is conserved, systems with **friction** can't work
  - V: potential, $p^2/2m$ kinetic
  - Equation of motion: Equations on $\dot{p}$, $\dot{q}$
- Time-evolution
  - Any quantity $A(p, q)$ are implicitly time dependent.
  - Those quantities with no explicit time dependence is called **Constants of motion**, equivalent to
    $$\{H, A\} = 0$$
  - Poisson Bracket
    $$\{A, B\} = \sum_i \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} - \frac{\partial B}{\partial p_i}\frac{\partial A}{\partial q_i}$$
    - This is a Lie bracket
    - Constant of motion: $\equiv \frac{d}{dt}A = 0 \equiv \{H, A\} = 0$ — Ways to show:
      1. Direct calculation of partial derivative
      2. Compute by commutator with H
      3. Linear combination or Poisson bracket of constants of motion
- Classical Harmonic Oscillator:
  $$\ddot{x} = -\omega^2 x$$
  has solution
  $$x = A\sin(\omega x) + B\cos(\omega x)$$
- Concepts
  - trajectory
    phase-space trajectory
    phase space
    Phase portrait
    Conservative system
    Kinetic/potential energy
  - In **Phase Portrait**
    fixed point
    equilibrium configuration
    classically allowed/forbidden
    turning points
  - Phase portrait: $(\vec{r}(t), \vec{p}(t))$

Spectra

- Models
- Representations

Angular Momentum

- $[\hat{J}_j, \hat{J}_k] = i\hbar\sum_l \epsilon_{jkl}\hat{J}_l$
- $[\hat{J}_1, \hat{J}_2] = i\hbar\hat{J}_3$
- $[\hat{J}^2, \hat{J}_i] = 0$
- $\hat{J}^2 = \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2$
- $|\beta, m\rangle$: Simultaneous eigenvector
- $\hat{J}^2|\beta, m\rangle = \beta|\beta, m\rangle, \quad \hat{J}_3|\beta, m\rangle = \hbar m|\beta, m\rangle$
- Symmetry gives $\hat{J}_1$ and $\hat{J}_2$ same eigenvalues

Dynamics

- Schrodinger dynamics
  - 1-d Model
    - $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$
    - $\langle\hat{H}\rangle = \int_{\mathbb{R}} \phi^*(x, t)(\hat{H}\phi(x))dx$
    - For 1-d, ϕ is a solution $\implies$ ϕ^* is a solution
  - Wave function: ψ
    - ψ interpreted as probability **amplitude**
    - $|\psi|^2$ is probability density, after normalisation
    - ψ can be normalised $\iff$ $\psi \in L^2$
      - All functions are assumed to be L^2 thus decay to zero at infinity
      - Also assumed ϕ twice differentialble.
    - Superposition principle: If ϕ_1 and ϕ_2 are solutions, then $c_1\phi_1 + c_2\phi_2$ is still a solution.
  - Time-independent Schrodinger eq:
    $$i\hbar\dot{\psi}(\vec{r}, t) = \hat{H}\psi(\vec{r}, t)$$
    - Usually $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$
    - For conjugation ψ^*:
      $-i\hbar\dot{\psi}^*(\vec{r}, t) = \hat{H}\psi^*(\vec{r}, t)$
    - $\langle\hat{H}\rangle$: expectation value — $\langle\hat{H}\rangle = \frac{\int_{-\infty}^{\infty}\phi^*(x, t)\hat{H}\phi(x, t)dx}{\int_{-\infty}^{\infty}|\phi(x, t)|^2dx} = \langle\phi, A\phi\rangle$?
  - Eigen decomposition
    - $\bar{H}\phi_E(\vec{r}) = E\phi_E(\vec{r})$
      - Eigenvalues/eigenergies of Hamiltonian: E
      - Eigenvalues/eigenfunctions/engenstates: $\phi_E(\vec{r})$
    - Eigenstates form orthogonal basis:
      $$\int_{whole\ space}\phi_E(\vec{r})\phi_{E'}(\vec{r})dV = \delta_{EE'}$$
    - Stationary solution method for time-independent equation: TBF
  - Stationary States
    - Start with seperable assumption:
      $$\psi(x, t) = \phi(x)\chi(t)$$
      - End up having basis of solutions
        $$\psi(x, t) = \chi(0)e^{-iet/\hbar}\phi_E(x)$$
        where ϕ_E is the eigen function corresponding to value E
        - **All** separable wave functions are linear combination of these states
          $$\phi(t, x) = \sum_n a_n e^{iE_n t/\hbar}\phi_{E_n}(x)$$
- Dynamics of Expectations
  - Heisenberg's equation
  - Ehrenfest theorem
  - Hadamard Lemma
  - Relation with Lie thoery