3. Principles of QM

Axiomatic principles

State vector axiom: State vector at t is ket $\psi(t)$, or $|\psi\rangle$, bra state.
Probability axiom: Given a system in state $|\psi\rangle$, a measurement will find it in state $|\phi\rangle$ with probability amplitude $\langle\phi|\psi\rangle$.
Hermitian operator axiom: Physical observable is represented by a linear and Hermitian operator.
Measurement axiom: Measurement of a physical observable results in eigenvalue of observable. Observable $\widehat{A}$, we have $\widehat{A}|a\rangle = a|a\rangle$, where a is eigenvalue and $|a\rangle$ is eigenvector. Measurement of the physical quantity represented by $\widehat{A}$ collapses the state $|\psi\rangle$ before measurement into an eigenstate $|a\rangle$ of $\widehat{A}$.
Time evolution axiom: $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \widehat{H}|\psi(t)\rangle$, w/o consider x or p.

Vector space

State vector is neither in position nor momentum space.

Basis vectors: $|0\rangle = \begin{bmatrix}1\\0\\\vdots\\0\end{bmatrix}$, $|1\rangle = \begin{bmatrix}0\\1\\\vdots\\0\end{bmatrix}$, $|n\rangle = \begin{bmatrix}0\\0\\\vdots\\1\end{bmatrix}$ (in nth pos).

Linearity: Because the SE is linear, given two states $|\psi_1(t)\rangle$ and $|\psi_2(t)\rangle$, $|\psi(t)\rangle = c_1|\psi_1(t)\rangle + c_2|\psi_2(t)\rangle$ is also a sol. (c's are complex).
Properties of a vector space

Dual vector space $c|\psi\rangle$ is mapped to $c*\langle\psi|$. Given a vector, $|\psi\rangle = \begin{bmatrix}\vdots\\\alpha\\\vdots\end{bmatrix}$, the dual vector is $\langle\psi| = \begin{bmatrix}\cdots & \alpha^* & \cdots\end{bmatrix}$.
Dual basis vectors are $\langle 0| = \begin{bmatrix}1 & 0 & \cdots\end{bmatrix}, \cdots, \langle n|\begin{bmatrix}0 & \cdots & 1\end{bmatrix}$.
Inner product: $\langle\phi|\psi\rangle = c$, where c is complex.
$\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^* \to \langle\psi|\psi\rangle$ is real, positive, and finite for a normalizable ket vector. Can choose $\langle\psi|\psi\rangle = 1$. $\langle\psi_m|\psi_n\rangle = \delta_{mn}$

Operators

A matrix operator $\widehat{A}$ acting on a state vector $|\psi\rangle$ transforms it into another state vector $|\phi\rangle$, $\widehat{A}|\psi\rangle = |\phi\rangle$. It is linear.
Properties of operators
Hermitian conjugate (Hermitian adjoint) operator in the dual space
Hermitian adjoint operator $\widehat{A}^\dagger$ acts on the dual vector $\langle\psi|$ from the right as $\langle\psi|\widehat{A}^\dagger\rangle$, where $\widehat{A}^\dagger = (\widehat{A})^{T*}$.

$$(\widehat{A}|\psi\rangle)^\dagger = |\psi\rangle^\dagger\widehat{A}^\dagger = \langle\psi|\widehat{A}^\dagger \qquad \langle\psi| = |\psi\rangle^\dagger \qquad \langle\psi|^\dagger = |\psi\rangle$$
$$(\widehat{A}\widehat{B})^\dagger = (\widehat{A}\widehat{B})^{T*} = (\widehat{B}^T\widehat{A}^T)^* = \widehat{B}^{T*}\widehat{A}^{T*} = \widehat{B}^\dagger\widehat{A}^\dagger, \quad (c\widehat{A})^\dagger = c^*\widehat{A}^\dagger$$

Outer product operators: $|\psi\rangle\langle\phi| \qquad [|\psi\rangle\langle\phi|]\chi\rangle = |\psi\rangle\langle\phi|\chi\rangle$
Matrix elements of operators

$$\langle\phi|\widehat{A}|\psi\rangle \text{ (complex num)}$$

Hermitian equiv to complex conj $\langle\phi|\widehat{A}|\psi\rangle^\dagger = \langle\psi|\widehat{A}^\dagger|\phi\rangle = \langle\phi|\widehat{A}|\psi\rangle^*$
Hermitian operators: $\widehat{A}^\dagger = \widehat{A}$, so given $\widehat{A}|\phi\rangle$ in the vector space, we have $\langle\psi|\widehat{A}^\dagger = \langle\phi|\widehat{A}$ in the dual vector space.
Matrix elements of a Hermitian operator

$$\langle\phi|\widehat{A}|\psi\rangle^\dagger = \langle\phi|\widehat{A}|\psi\rangle^* = \langle\psi|\widehat{A}^\dagger|\phi\rangle = \langle\psi|\widehat{A}|\phi\rangle$$

Hermitian operator, real expectation vals: $\langle\psi|\widehat{A}|\phi\rangle^* = \langle\psi|\widehat{A}|\phi\rangle \equiv \langle\widehat{A}\rangle$
Same result whether $\widehat{A}$ acts to right or left: $\langle\phi|\widehat{A}|\psi\rangle = \langle\phi|\widehat{A}^\dagger|\psi\rangle$
Eigenvals and eigenvecs of Hermitian operators: $\widehat{A}|a_n\rangle = a_n|a_n\rangle$
Normalized eigvecs $\langle a_m|a_n\rangle = \delta_{mn}$. Gram-Schmidt, degenerate evec.
Completeness of eigenvector of a Hermitian operator Set $|a_n\rangle$ is complete if $\sum_n |\langle a_n|\psi\rangle|^2 = 1$. $\sum_n |a_n\rangle\langle a_n| = 1$ (identity operator)
Continuous spectra of a Hermitian operator
Hermitian operator $\widehat{A}$, $\widehat{A}|a\rangle = a|a\rangle$, where a is continuous.
$\int da'\langle a'|\widehat{A}|a\rangle = a\int da'\langle a'|a\rangle = \int da' a'\langle a'|a\rangle \to \langle a'|a\rangle = \delta(a'-a)$
Continuous condition: $\int da|a\rangle\langle a| = 1$
Gram-Schmidt orthogonalization procedure
Eigval (like energy level) is n-fold degenerate: n states w same eigval.
Orthogonal eigenstates $\to$ no degeneracy.
1. Normalize each state and define $\alpha_i = \frac{\alpha_i}{\sqrt{\langle a_i|a_i\rangle}}$. 2. $|\alpha_1'\rangle = |\alpha_1\rangle$.
3. $|\alpha_2'\rangle = \frac{|\alpha_2\rangle - |\alpha_1\rangle\langle\alpha_1|\alpha_2\rangle}{\sqrt{\langle\alpha_2|\alpha_2\rangle - \langle\alpha_1|\alpha_2\rangle\langle\alpha_2|\alpha_1\rangle}} = \frac{|\alpha_2\rangle - |\alpha_1\rangle\langle\alpha_1|\alpha_2\rangle}{\sqrt{1-\langle\alpha_1|\alpha_2\rangle\langle\alpha_2|\alpha_1\rangle}}$
4. Subtract components of $|\alpha_3\rangle$ along $|\alpha_1\rangle$ and $|\alpha_2\rangle$, $|\alpha_3\rangle - |\alpha_1\rangle\langle\alpha_1|\alpha_3\rangle - |\alpha_2\rangle\langle\alpha_2|\alpha_3\rangle$, normalize and promote to $|\alpha_3'\rangle$. ...

Position and momentum representation

$\widehat{\vec r}|\vec r\rangle = \vec r|\vec r\rangle \quad \langle\vec{r'}|\vec r\rangle = \delta^3(\vec{r'}-\vec r), \int d^3\vec r|\vec r\rangle\langle\vec r| = 1, \langle\vec{r'}|\hat{\vec r}|\vec r\rangle = \vec r\delta^3(\vec{r'}-\vec r)$
$\widehat{\vec p}|\vec p\rangle = \vec p|\vec p\rangle \quad \langle\vec{p'}|\vec p\rangle = \delta^3(\vec{p'}-\vec p), \int d^3\vec p|\vec p\rangle\langle\vec p| = 1$
State vector $|\psi(t)\rangle$ in position space (scalar): $\langle\vec r|\psi(x,t)\rangle \equiv \psi(\vec r,t)$
$\langle\psi|\widehat{\vec p}|\psi\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|\widehat{\vec r}|\psi\rangle m$
Representation of momentum operator in position space: $\widehat{\vec p} = -i\hbar\vec{\boldsymbol\nabla}$.
$\langle x|\widehat p|x'\rangle = -i\hbar\frac{\partial}{\partial x}\delta(x-x') = -i\hbar\frac{\partial}{\partial x}\langle x|x'\rangle$.
$\widehat p = -i\hbar\frac{\partial}{\partial x}$ is Hermitian, $\frac{\partial}{\partial x}$ is not.

$$\langle x|\widehat p|p\rangle = p\langle x|p\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|p\rangle$$

The solution is $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}px}$.
In 3D, $\langle\vec r|\vec p\rangle = \frac{1}{(2\pi\hbar)^{3/2}}e^{\frac{i}{\hbar}\vec p\vec r}$.
We can write the normalized wavefunction of definite position in momentum space, $\langle p|x\rangle = \langle x|p\rangle^*$.
$\widehat{\vec r}$ is Hermitian and $\langle\phi|\widehat{\vec r}^\dagger|\psi\rangle = \langle\phi|\widehat{\vec r}|\psi\rangle$.
Operators and wavefunction in position representation
Position and momentum operators in pos space: $\widehat{\vec r} = \vec r$, $\widehat{\vec p} = -i\hbar\vec{\boldsymbol\nabla}$.
$\widehat O(\widehat{\vec r},\widehat{\vec p}) = \widehat O(\vec r, -i\hbar\vec{\boldsymbol\nabla})$
The expectation val of the observable should be indep of representation. In state $\psi(t)$, $\langle\widehat O\rangle = \langle\psi(t)|\widehat O|\psi(t)\rangle$.
Insert $\int d^2\vec r|\vec r\rangle\langle\vec r| = 1$ to get $\langle\widehat O\rangle = \int d^2\vec r\langle\psi(t)|\vec r\rangle\langle\vec r|\widehat O|\psi(t)\rangle$
$\psi(\vec r,t) = \langle\vec r|\psi(t)\rangle, \qquad \psi(\vec r,t)^* = \langle\vec r|\psi(t)\rangle^* = \langle\psi(t)|\vec r\rangle$,
$\langle\vec r|\widehat O|\psi(t)\rangle = \widehat O(\vec r, -i\hbar\vec{\boldsymbol\nabla})\psi(\vec r,t), \langle\widehat O\rangle = \int d^3\vec r\psi(\vec r,t)^*\widehat O(\vec r,-i\hbar\vec{\boldsymbol\nabla})\psi(\vec r,t)$
Operators and wavefunction in momentum representation

Commuting operators

Non-commuting operators and the general uncertainty principle

Time evolution of expectation value of an operator and Ehrenfest's theorem

The simple harmonic oscillator

Raising and lowering operators
Normalized number state vectors
Wavefunctions in position representation
Classical simple harmonic oscillator
The quantum simple harmonic oscillator and coherent state

4. Three-dimensional systems

Three-dimensional infinite square well

The Schrödinger equation in spherical coordinates

Orbital angular momentum

Spherical harmonics