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 $\langle\psi|\widehat{A}^\dagger$, 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 $\alpha_i = \frac{\alpha_i}{\sqrt{\langle\alpha_i|\alpha_i\rangle}}$. 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

$\widehat{\vec{r}}|\vec{r}\rangle = \vec{r}|\vec{r}\rangle \quad \langle\vec{r'}|\vec{r}\rangle = \delta^3(\vec{r'}-\vec{r}), \int d^3\vec{r}|\vec{r}\rangle\langle\vec{r}| = 1, \langle\vec{r'}|\widehat{\vec{r}}|\vec{r}\rangle = \vec{r}\delta^3(\vec{r'}-\vec{r})$
$\widehat{\vec{p}}|\vec{p}\rangle = \vec{p}|\vec{p}\rangle \quad \langle\vec{p'}|\vec{p}\rangle = \delta^3(\vec{p'}-\vec{p}), \int d^3\vec{p}|\vec{p}\rangle\langle\vec{p}| = 1$
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: $\widehat{\vec{p}} = -i\hbar\vec{\nabla}$.
$\langle x|\widehat{p}|x'\rangle = -i\hbar\frac{\partial}{\partial x}\delta(x-x') = -i\hbar\frac{\partial}{\partial x}\langle x|x'\rangle$.
$\widehat{p} = -i\hbar\frac{\partial}{\partial x}$ 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, $\langle p|x\rangle = \langle x|p\rangle^*$. So, $\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{-\frac{i}{\hbar}px}$ (particle moving to the left, or with momentum $-p$, in the momentum space).
Operators and wavefunction in position representation
Position and momentum operators in pos space: $\widehat{\vec{r}} = \vec{r}$, $\widehat{\vec{p}} = -i\hbar\vec{\nabla}$.
$\widehat{\vec{r}}$ is Hermitian and $\langle\phi|\widehat{\vec{r}}^\dagger|\psi\rangle = \langle\phi|\widehat{\vec{r}}|\psi\rangle$.
$\widehat{O}(\widehat{\vec{r}},\widehat{\vec{p}}) = \widehat{O}(\vec{r}, -i\hbar\vec{\nabla})$
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 $\langle\widehat{O}\rangle = \int d^2\vec{r}\langle\psi(t)|\vec{r}\rangle\langle\vec{r}|\widehat{O}|\psi(t)\rangle$
$\psi(\vec{r},t) = \langle\vec{r}|\psi(t)\rangle, \qquad \psi(\vec{r},t)^* = \langle\vec{r}|\psi(t)\rangle^* = \langle\psi(t)|\vec{r}\rangle$,
$\langle\vec{r}|\widehat{O}|\psi(t)\rangle = \widehat{O}(\vec{r}, -i\hbar\vec{\nabla})\psi(\vec{r},t), \langle\widehat{O}\rangle = \int d^3\vec{r}\psi(\vec{r},t)^*\widehat{O}(\vec{r}, -i\hbar\vec{\nabla})\psi(\vec{r},t)$
Operators and wavefunction in momentum representation
$\widehat{\vec{r}} = i\hbar\vec{\nabla}_{\vec{p}}$, or in 1D, $\widehat{x} = i\hbar\frac{\partial}{\partial p}$, $\widehat{\vec{p}} = \vec{p}$, where $\vec{p}^* = \vec{p}$.
$\widehat{O}(\widehat{\vec{r}},\widehat{\vec{p}}) = \widehat{O}(i\hbar\vec{\nabla}_{\vec{p}}, \vec{p})$
$\langle\widehat{O}\rangle = \langle\psi(t)|\widehat{O}|\psi(t)\rangle \to \langle\widehat{O}\rangle = \int d^2\vec{p}\langle\psi(t)|\vec{p}\rangle\langle\vec{p}|\widehat{O}|\psi(t)\rangle$.
$\psi(\vec{p},t) = \langle\vec{p}|\psi(t)\rangle, \qquad \psi(\vec{p},t)^* = \langle\vec{p}\psi(t)\rangle^* = \langle\psi(t)|\vec{p}\rangle$
$\langle\vec{p}|\widehat{O}|\psi(t)\rangle = \widehat{O}(i\hbar\vec{\nabla}_{\vec{p}}, \vec{p}), \langle\widehat{O}\rangle = \int d^3\vec{p}\psi(\vec{p},t)^*\widehat{O}(i\hbar\vec{\nabla}_{\vec{p}}, \vec{p})\psi(\vec{p},t)$.

$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \widehat{H}|\psi(t)\rangle$, where $\widehat{H} = \frac{\widehat{\vec{p}}^2}{2m} + V(\widehat{\vec{r}},t)$ becomes
$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{r},t) + V(\vec{r},t)\psi(\vec{r},t)$

Commuting operators

If $[\widehat{A},\widehat{B}] = 0$ and the states are nondegenerate, $|\psi\rangle$ is a simultaneous eigenstate of $\widehat{A}$ and $\widehat{B}$.
$|\psi\rangle = |ab\rangle$, and $\widehat{A}|ab\rangle = a|ab\rangle$, $\widehat{B}|ab\rangle = b|ab\rangle$

Non-commuting operators and the general uncertainty principle

$(\Delta A)^2(\Delta B)^2 \geq (\frac{1}{2i}\langle[\widehat{A},\widehat{B}]\rangle)^2$
Cannot construct simultaneous eigenstates (which correspond to definite eigenvalues) of non-commuting observables.

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

Ehrenfest's theorem: how observable $\widehat{O}$'s expectation value in state $|\psi(t)\rangle$ evolves in time, $\frac{\mathrm{d}}{\mathrm{d}t}\langle\widehat{O}\rangle = \langle\frac{\partial\widehat{O}}{\partial t}\rangle + \frac{i}{\hbar}\langle[\widehat{H},\widehat{O}]\rangle$
For $\widehat{O} = \widehat{\vec{p}}$ and a Hamiltonian that is TI, $\frac{\mathrm{d}}{\mathrm{d}t}\langle\widehat{\vec{p}}\rangle = -\langle\vec{\nabla}V(\widehat{\vec{r}})\rangle$, which is just Newton's Second Law! $\to$ QM contains all of classical mech.

The simple harmonic oscillator

$\widehat{H} = \frac{\widehat{p}^2}{2m} + \frac{1}{2}m\omega^2\widehat{x}^2$
Raising and lowering operators
Lowering op: $\widehat{a} = \sqrt{\frac{m\omega}{2\hbar}}(\widehat{x} + \frac{i}{m\omega}\widehat{p})$, Raising op: $\widehat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\widehat{x} - \frac{i}{m\omega}\widehat{p})$.
$[\widehat{a},\widehat{a}^\dagger] = 1 \qquad \widehat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\widehat{a}^\dagger + \widehat{a})$, $\widehat{p} = i\sqrt{\frac{m\omega\hbar}{2}}(\widehat{a}^\dagger - \widehat{a})$
$\widehat{H} = (\widehat{N} + \frac{1}{2})\hbar\omega$, where $\widehat{N} = \widehat{a}^\dagger\widehat{a}$. Now $\widehat{N}$ is Hermitian, and $\widehat{N}|n\rangle = n|n\rangle$
$[\widehat{N},\widehat{a}] = -\widehat{a}$, $[\widehat{N},\widehat{a}^\dagger] = \widehat{a}^\dagger$
$\widehat{N}(\widehat{a}|n\rangle) = (n-1)(\widehat{a}|n\rangle)$, $\widehat{N}(\widehat{a}^\dagger|n\rangle) = (n+1)(\widehat{a}^\dagger|n\rangle)$
Normalized number state vectors Energy levels are not degenerate, so
$|n-1\rangle = c_n\widehat{a}|n\rangle \to c_n = \frac{1}{\sqrt{n}} \to \widehat{a}|n\rangle = \sqrt{n}|n-1\rangle$.
$|n+1\rangle = d_n\widehat{a}^\dagger|n\rangle \to d_n = \frac{1}{\sqrt{n+1}} \to \widehat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$
Ground state: $|0\rangle$, excited state: $|n\rangle = \frac{(\widehat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle$, $n = 0,1,2,\ldots$
$\langle n'|\widehat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle n'|(\widehat{a}^\dagger + \widehat{a})|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1})$
$\langle n'|\widehat{p}|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}\langle n'|(\widehat{a}^\dagger - \widehat{a})|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}(\sqrt{n+1}\delta_{n',n+1} - \sqrt{n}\delta_{n',n-1})$
Wavefunctions in position representation
$E_n = (n + \frac{1}{2})\hbar\omega, n = 0,1,2,\ldots$
The stationary wavefunctions of definite energy: $\psi_n(x) = \langle x|n\rangle$
$\langle x'|\widehat{a}^\dagger|x''\rangle = \delta(x'-x'')\frac{1}{\sqrt{2}\sigma}(x'' - \sigma^2\frac{\partial}{\partial x''})$, where $\sigma \equiv \sqrt{\frac{\hbar}{m\omega}}$
$\xi = \frac{x}{\sigma}, \qquad \langle x|n\rangle = \frac{1}{\sqrt{\sqrt{\pi}n!2^n\sigma}}(\xi - \frac{\partial}{\partial\xi})^n e^{-\frac{1}{2}\xi^2}$
$\langle x|0\rangle = (\frac{m\omega}{\pi\hbar})^{1/4}e^{-\frac{m\omega}{2\hbar}x^2}, \qquad \langle x|1\rangle = \sqrt{2}(\frac{m^3\omega^3}{\pi\hbar^3})^{1/4}xe^{-\frac{m\omega}{2\hbar}x^2}$
Classical simple harmonic oscillator Hamiltonian of a simple harmonic is
$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2. \qquad \dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}, \qquad \dot{p} = -\frac{\partial H}{\partial x} = -m\omega^2x$
Define $\sqrt{\hbar\omega}\alpha = \sqrt{\frac{m\omega^2}{2}}x + \frac{i}{\sqrt{2m}}p$, so $x = \sqrt{\frac{2\hbar}{m\omega}}\alpha_R$ and $p = \sqrt{2m\hbar\omega}\alpha_I$
Rewrite Hamiltonian, $H = \hbar\omega|\alpha|^2, \qquad \dot{\alpha} = -i\omega\alpha$. The sol is $\alpha = \alpha_0e^{-i\omega t}$.
The quantum simple harmonic oscillator and coherent state
Coherent state, superpos of stat states $|n\rangle$: $|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^\infty\frac{\alpha^n}{\sqrt{n!}}|n\rangle$
$P(n) = |\langle n|\alpha\rangle|^2 = |\alpha_n|^2 = \frac{\langle n\rangle^n e^{-\langle n\rangle}}{n!}$, where $\langle n\rangle = \langle\alpha|a^\dagger a|\alpha\rangle = |\alpha|^2$.

4. Three-dimensional systems

Three-dimensional infinite square well

$-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})\phi(x,y,z) = E\psi(x,y,z)$ for $0 \leq x \leq l_x, \ldots$
while $\psi(x,y,z) = 0$ outside.
$\psi(x,y,z) = \psi_1(x)\psi_2(y)\psi_3(z)$
The SE then becomes $-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_1(x) = E_1\psi_1(x), \ldots$, where $E = E_1 + E_2 + E_3$.
$\psi_{n_xn_yn_z}(x,y,z) = \sqrt{\frac{8}{l_xl_yl_z}}\sin\left(\frac{n_x\pi}{l_x}x\right)\sin\left(\frac{n_y\pi}{l_y}z\right)\sin\left(\frac{n_z\pi}{l_z}z\right)$
$E_{n_xn_yn_z} = \frac{\hbar^2\pi^2}{2m}(\frac{n_x^2}{l_x^2} + \frac{n_y^2}{l_y^2} + \frac{n_z^2}{l_z^2})$, with $n_x, n_y, n_z = 1,2,\ldots$.
Wave vector: $\vec{k} = (k_x,k_y,k_z) = (\frac{n_x\pi}{l_x}, \frac{n_y\pi}{l_y}, \frac{n_z\pi}{l_z})$

The Schrödinger equation in spherical coordinates

Orbital angular momentum

Spherical harmonics