1 Mathematics

1.1 Projectors

Let $\{|e_j\rangle\}$ be an **orthonormal** basis for V, and $\{|f_j\rangle\}$ be an **orthonormal** basis for $V^\perp$, then any vector $|\psi\rangle$ in $V \oplus V^\perp$

$$|\psi\rangle = \sum_{j=1}^{\dim V} |e_j\rangle \langle e_j|\psi\rangle + \sum_{k=1}^{\dim V^\perp} |f_k\rangle \langle f_k|\psi\rangle$$

The orthogonal projector associated to V is then

$$\Pi_V = \sum_{j=1}^{\dim V} |e_j\rangle \langle e_j|$$

Through the entire space $W = V \oplus V^\perp$, the sum of projectors on the whole basis

$$\sum_{i=1}^{\dim W} |\psi_i\rangle \langle \psi_i| = \mathbf{I}$$

1.2 Normal Operators

An operator A is *normal* if $[A, A^\dagger] = 0$, or if its eigenvectors from an orthonormal basis of V. It can be written

$$A = \sum_k \lambda_k \Pi_{\lambda_k}$$

Normal operators divides the vector space into eigenspaces. Also functions can be written as

$$f(A) = \sum_k f(\lambda_k) \Pi_{\lambda_k}$$

Two normal operators commute iff they have a common set of eigenvectors.

2 Physics

2.1 Misc

Born's rule:

$$P(\psi_n \mid \psi) = |\langle \psi_n|\psi\rangle|^2 = \langle \psi|\Pi_{\psi_n}|\psi\rangle = \langle \psi_n|\Pi_\psi|\psi_n\rangle = \mathrm{Tr}(\Pi_{\psi_n}\Pi_\psi)$$

Statistics:

$$\langle A^k\rangle_\psi = \sum_n a_n^k P(\psi_n \mid \psi) = \langle \psi|A^k|\psi\rangle$$

Time evolution operator with eigenvector $|n\rangle$ of H corresponding to eigenvalue E_n:

$$U(t) = e^{-iHt/\hbar} = \sum_n e^{-iE_n t/\hbar} |n\rangle \langle n|$$

hence for a state decomposed as $|\psi\rangle = \sum_n C_n |n\rangle$,

$$|\psi(t)\rangle = \sum_n C_n e^{-iE_n t/\hbar} |n\rangle$$

2.2 Position and momentum

1D. In position repr. the operators:

$$X|\psi\rangle = \int_{\mathbb{R}} x\psi(x)\,|x\rangle\,\mathrm{d}x \qquad P|\psi\rangle = \int_{\mathbb{R}} -i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\psi(x)\,|x\rangle\,\mathrm{d}x$$

$$[X, P] = i\hbar\mathbf{I}$$

Hamiltonian after expansion therefore reads

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right)\phi(x) = E\phi(x)$$

Statistics:

$$\langle X^n\rangle_\psi = \int_{\mathbb{R}} |\psi(x)|^2 x^n\,\mathrm{d}x \qquad \langle P^n\rangle_\psi = (-ih)^n \int_{\mathbb{R}} \psi^*(x)\frac{\mathrm{d}^n}{\mathrm{d}x^n}\psi(x)\,\mathrm{d}x$$

Changing repr., the wave function undergoes a Fourier transform:

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{\mathbb{R}} \psi(x)e^{-ipx/\hbar}\,\mathrm{d}x$$

In 3D, X generalises easily, while as shorthand $P = -i\hbar\boldsymbol{\nabla}$. Now

$$[X_i, X_j] = 0 \qquad [P_i, P_j] = 0 \qquad [X_i, P_j] = i\hbar\delta_{ij}\mathbf{I}$$

2.3 Angular momentum

Components of J have to satisfy

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k.$$

With the magnitude $J^2 = J_x^2 + J_y^2 + J_z^2$,

$$[J^2, J_i] = 0$$

Eigenvalues of J^2 are non-negative. To find common eigenvalues of J^2 and J_z, define ladder operators

$$J_\pm = J_x \pm iJ_y$$

They work very much like the harmonic oscillator, see that section. Use these properties

$$J_+J_- = J^2 - J_z^2 + \hbar J_z \qquad J_-J_+ = J^2 - J_z^2 - \hbar J_z$$

$$[J^2, J_-] = 0 \qquad [J_-, J_z] = \hbar J_- \qquad [J_+, J_z] = -\hbar J_+$$

to prove that $-j \le m \le j$, the raising and lowering properties, and j is integer or half integer. The eigenvalues of J^2 are of the form $\hbar^2 j(j+1)$ and those of J_z are $\hbar m$. Also

$$J_\pm |k, j, m\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\,|k, j, m\rangle$$

2.4 Orbital angular momentum

Define $L = X \times P$, so $L_i = \epsilon_{ijk}(X_jP_k - X_kP_j)$. This satisfies the commutator above, so it is an angular momentum. Write

$$L_i|\psi\rangle = \iiint_{\mathbb{R}^3} l_u\psi(r,\theta,\phi)\,|r,\theta,\phi\rangle\,r^2\sin\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi$$

where

$$l_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right)$$
$$l_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \frac{\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right)$$
$$l_z = -i\hbar\frac{\partial}{\partial\phi}$$
$$l^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \csc^2\frac{\partial^2}{\partial\phi^2}\right)$$

The explicit solutions for wave functions are too long to place here.

2.5 Continuity equation

The continuity equation where $j(x)$ is the density of probability current:

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi(x)|^2 + \frac{\mathrm{d}}{\mathrm{d}x}j(x) = 0$$

In 1D:

$$j(x) = \frac{i\hbar}{2m}\,\mathrm{Im}\left(\psi^*(x)\frac{\mathrm{d}}{\mathrm{d}x}\psi(x)\right)$$

In 3D:

$$j(x) = \frac{i\hbar}{2m}(\phi(x)\boldsymbol{\nabla}\phi^*(x) - \phi^*(x)\boldsymbol{\nabla}\phi(x))$$

3 Case studies

3.1 Free particle

Hamiltonian $H = \frac{P^2}{2m}$, $V(x) = 0$. The eigenvalues are positive, and for every E there are two solutions:

$$\psi_\pm(x) = C_\pm e^{\pm ikx} \qquad k = \frac{\sqrt{2mE}}{\hbar} \qquad E = \frac{\hbar^2k^2}{2m}$$

Decomposing the initial state onto eigenvectors and changing variables:

$$\phi(x, t=0) = \int_{\mathbb{R}} \tilde{\phi}(k)e^{ikx}\,\mathrm{d}x$$

Time evolution describes a wave with dispersion relation $\omega(k)$:

$$\phi(x,t) = \int_{\mathbb{R}} \tilde{\phi}(k)e^{i(kx-\omega(k)t)}\,\mathrm{d}k \qquad \omega(k) = \frac{\hbar}{2m}k^2$$

3.2 Piecewise-constant potentials

With $k = \sqrt{2m|V-E|}/\hbar$,

$$E < V \implies \phi(x) = Ae^{kx} + B^{-kx}$$
$$E > V \implies \phi(x) = C\cos(kx) + D\sin(kx)$$

For square wells the solutions depend a little on set-up so they are not written here. For infinite square wells we can however note the quantisation of energy:

$$E_n = \frac{\hbar^2\pi^2}{2ma^2}n^2$$

and the wave functions in infinite square wells look like $\sin\left(n\pi\frac{x}{a}\right)$ but again it will be different depending on configuration of the set-up.

3.3 1D harmonic oscillator

The Hamiltonian is now $H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2X^2$. Annihilation a and creation $A^\dagger$ operator and N:

$$a = \sqrt{\frac{m\omega}{2\hbar}}X + \frac{i}{\sqrt{2m\hbar\omega}}P \qquad N = a^\dagger a$$

Some properties:

$$[a, a^\dagger] = \mathbf{I} \qquad [N, a] = -a \qquad [N, a^\dagger] = a^\dagger \qquad H = \hbar\omega(N + \frac{1}{2}\mathbf{I})$$

$$a\,|n\rangle \propto |n-1\rangle \qquad a^\dagger\,|n\rangle \propto |n+1\rangle$$

From these we can show that eigenvalues of N are $\mathbb{Z}^+$. Hence the eigenvalues of H are

$$E_n = \hbar\omega(n + \frac{1}{2}) \qquad n \in \mathbb{Z}^+$$

The solution:

$$\left|a^\dagger\,|n\rangle\right|^2 = n+1 \implies a^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \implies |n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}\,|0\rangle$$

Where solving the ODE for $n = 0$ gives a Gaussian:

$$\psi_0(x) = \left(\frac{mn}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{\hbar}\frac{x^2}{2}}$$

3.4 Spin 1/2

Here write J as S, j as s, m as m_s. A simple 2-level system for angular momentum mandates $s = \frac{1}{2}$ and $m_s \in \{-\frac{1}{2}, \frac{1}{2}\}$ and therefore

$$S_z\left|s = \frac{1}{2}, m_s = \pm\frac{1}{2}\right\rangle = \pm\frac{\hbar}{2}\left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle$$

Repr. $\left|m_s = +\frac{1}{2}\right\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and $\left|m_s = -\frac{1}{2}\right\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ gives $S = \frac{\hbar}{2}\sigma$.

Rotating by angle θ about axis n:

$$U(\theta, n) = e^{-i\theta n\cdot\sigma/2} = \cos\frac{\theta}{2}\mathbf{I} - i\sin\frac{\theta}{2}n\cdot\sigma$$

3.5 Hydrogen atom

Ordinarily:

$$H = \frac{P_p^2}{2m_p} + \frac{P_e^2}{2m_2} + V(|X_p - X_e|)$$

Centre of mass and relative coordinates:

$$X_{CM} = \frac{m_1X_1 + m_2X_2}{m_1 + m_2} \qquad P_{CM} + P_1 + P_2$$

$$X_r = X_1 - X_2 \qquad P_r = \frac{m_2O_1 - m_1P_2}{m_1 + m_2}$$

Hamiltonian becomes decoupled:

$$H = \frac{P_{CM}^2}{2M} + \frac{P_r^2}{2m} + V(|X_r|)$$

Solutions are skipped. Eigenvalues:

$$E_{kl} = E_n = \frac{E_1}{(k+l)^2} = \frac{E_1}{n^2}$$