Review of Quantum Mechanics

2.1 States and Operators

A quantum mechanical system is defined by a Hilbert space, $\mathcal{H}$, whose vectors, $\big|\psi\big\rangle$ are associated with the states of the system. A state of the system is represented by the set of vectors $e^{i\alpha}\big|\psi\big\rangle$. There are linear operators, $\mathcal{O}_i$ which act on this Hilbert space. These operators correspond to physical observables. Finally, there is an inner product, which assigns a complex number, $\big\langle\chi\big|\psi\big\rangle$, to any pair of states, $\big|\psi\big\rangle$, $\big|\chi\big\rangle$. A state vector, $\big|\psi\big\rangle$ gives a complete description of a system through the expectation values, $\big\langle\psi\big|\mathcal{O}_i\big|\psi\big\rangle$ (assuming that $\big|\psi\big\rangle$ is normalized so that $\big\langle\psi\big|\psi\big\rangle = 1$), which would be the average values of the corresponding physical observables if we could measure them on an infinite collection of identical systems each in the state $\big|\psi\big\rangle$.

The adjoint, $\mathcal{O}^\dagger$, of an operator is defined according to

$$\big\langle\chi\big|\ \left(\mathcal{O}\big|\psi\big\rangle\right) = \left(\big\langle\chi\big|\mathcal{O}^\dagger\right)\ \big|\psi\big\rangle \tag{2.1}$$

In other words, the inner product between $\big|\chi\big\rangle$ and $\mathcal{O}\big|\psi\big\rangle$ is the same as that between $\mathcal{O}^\dagger\big|\chi\big\rangle$ and $\big|\psi\big\rangle$. An Hermitian operator satisfies

$$\mathcal{O} = \mathcal{O}^\dagger \tag{2.2}$$

while a unitary operator satisfies

$$\mathcal{O}\mathcal{O}^\dagger = \mathcal{O}^\dagger\mathcal{O} = 1 \tag{2.3}$$

If $\mathcal{O}$ is Hermitian, then

$$e^{i\mathcal{O}} \tag{2.4}$$

is unitary. Given an Hermitian operator, $\mathcal{O}$, its eigenstates are orthogonal,

$$\left\langle \lambda' \middle| \mathcal{O} \middle| \lambda \right\rangle = \lambda \left\langle \lambda' \middle| \lambda \right\rangle = \lambda' \left\langle \lambda' \middle| \lambda \right\rangle \tag{2.5}$$

For $\lambda \neq \lambda'$,

$$\left\langle \lambda' \middle| \lambda \right\rangle = 0 \tag{2.6}$$

If there are n states with the same eigenvalue, then, within the subspace spanned by these states, we can pick a set of n mutually orthogonal states. Hence, we can use the eigenstates $\left|\lambda\right\rangle$ as a basis for Hilbert space. Any state $\left|\psi\right\rangle$ can be expanded in the basis given by the eigenstates of $\mathcal{O}$:

$$\left|\psi\right\rangle = \sum_\lambda c_\lambda \left|\lambda\right\rangle \tag{2.7}$$

with

$$c_\lambda = \left\langle \lambda \middle| \psi \right\rangle \tag{2.8}$$

A particularly important operator is the Hamiltonian, or the total energy, which we will denote by H. Schrödinger's equation tells us that H determines how a state of the system will evolve in time.

$$i\hbar \frac{\partial}{\partial t}\left|\psi\right\rangle = H\left|\psi\right\rangle \tag{2.9}$$

If the Hamiltonian is independent of time, then we can define energy eigenstates,

$$H\left|E\right\rangle = E\left|E\right\rangle \tag{2.10}$$

which evolve in time according to:

$$\Big|E(t)\Big\rangle = e^{-i\frac{Et}{\hbar}}\Big|E(0)\Big\rangle \tag{2.11}$$

An arbitrary state can be expanded in the basis of energy eigenstates:

$$\Big|\psi\Big\rangle = \sum_i c_i \Big|E_i\Big\rangle \tag{2.12}$$

It will evolve according to:

$$\Big|\psi(t)\Big\rangle = \sum_j c_j e^{-i\frac{E_j t}{\hbar}}\Big|E_j\Big\rangle \tag{2.13}$$

For example, consider a particle in $1D$. The Hilbert space consists of all continuous complex-valued functions, $\psi(x)$. The position operator, $\hat{x}$, and momentum operator, $\hat{p}$ are defined by:

$$\begin{aligned} \hat{x} \cdot \psi(x) &\equiv x\,\psi(x) \\ \hat{p} \cdot \psi(x) &\equiv -i\hbar\frac{\partial}{\partial x}\,\psi(x) \end{aligned} \tag{2.14}$$

The position eigenfunctions,

$$x\,\delta(x-a) = a\,\delta(x-a) \tag{2.15}$$

are Dirac delta functions, which are not continuous functions, but can be defined as the limit of continuous functions:

$$\delta(x) = \lim_{a\to 0}\frac{1}{a\sqrt{\pi}}\,e^{-\frac{x^2}{a^2}} \tag{2.16}$$

The momentum eigenfunctions are plane waves:

$$-i\hbar\frac{\partial}{\partial x}\,e^{ikx} = \hbar k\,e^{ikx} \tag{2.17}$$

Expanding a state in the basis of momentum eigenstates is the same as taking its Fourier transform:

$$\psi(x) = \int_{-\infty}^{\infty} dk\,\tilde{\psi}(k)\,\frac{1}{\sqrt{2\pi}}e^{ikx} \tag{2.18}$$

where the Fourier coefficients are given by:

$$\tilde{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, \psi(x)\, e^{-ikx} \tag{2.19}$$

If the particle is free,

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \tag{2.20}$$

then momentum eigenstates are also energy eigenstates:

$$\hat{H} e^{ikx} = \frac{\hbar^2 k^2}{2m} e^{ikx} \tag{2.21}$$

If a particle is in a Gaussian wavepacket at the origin at time $t = 0$,

$$\psi(x, 0) = \frac{1}{a\sqrt{\pi}}\, e^{-\frac{x^2}{a^2}} \tag{2.22}$$

Then, at time t, it will be in the state:

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \frac{a}{\sqrt{\pi}}\, e^{-i\frac{\hbar k^2 t}{2m}}\, e^{-\frac{1}{2}k^2 a^2}\, e^{ikx} \tag{2.23}$$

2.2 Density and Current

Multiplying the free-particle Schrödinger equation by ψ^*,

$$\psi^*\, i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m}\, \psi^* \frac{\partial^2}{\nabla^2} \psi \tag{2.24}$$

and subtracting the complex conjugate of this equation, we find

$$\frac{\partial}{\partial t} \left(\psi^* \psi\right) = \frac{i\hbar}{2m} \vec{\nabla} \cdot \left(\psi^* \vec{\nabla} \psi - \left(\vec{\nabla} \psi^*\right) \psi\right) \tag{2.25}$$

This is in the form of a continuity equation,

$$\frac{\partial \rho}{\partial t} = \vec{\nabla} \cdot \vec{j} \tag{2.26}$$

The density and current are given by:

$$\rho = \psi^* \psi$$

$$\vec{j} = \frac{i\hbar}{2m}\left(\psi^* \vec{\nabla}\psi - \left(\vec{\nabla}\psi^*\right)\psi\right) \tag{2.27}$$

The current carried by a plane-wave state is:

$$\vec{j} = \frac{\hbar}{2m}\,\vec{k}\,\frac{1}{(2\pi)^3} \tag{2.28}$$

2.3 δ-function scatterer

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\,\delta(x) \tag{2.29}$$

$$\psi(x) = \begin{cases} e^{ikx} + Re^{-ikx} & \text{if } x < 0 \\ Te^{ikx} & \text{if } x > 0 \end{cases} \tag{2.30}$$

$$\begin{aligned} T &= \frac{1}{1 - \frac{mV}{\hbar^2 k}\,i} \\ R &= \frac{\frac{mV}{\hbar^2 k}\,i}{1 - \frac{mV}{\hbar^2 k}\,i} \end{aligned} \tag{2.31}$$

There is a *bound state* at:

$$ik = \frac{mV}{\hbar^2} \tag{2.32}$$

2.4 Particle in a Box

Particle in a $1D$ region of length L:

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \tag{2.33}$$

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{2.34}$$

has energy $E = \hbar^2 k^2/2m$. $\psi(0) = \psi(L) = 0$. Therefore,

$$\psi(x) = A\,\sin\left(\frac{n\pi}{L}x\right) \tag{2.35}$$

for integer n. Allowed energies

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \tag{2.36}$$

In a $3D$ box of side L, the energy eigenfunctions are:

$$\psi(x) = A \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right) \sin\left(\frac{n_z \pi}{L} z\right) \tag{2.37}$$

and the allowed energies are:

$$E_n = \frac{\hbar^2 \pi^2}{2mL^2} \left(n_x^2 + n_y^2 + n_z^2\right) \tag{2.38}$$

2.5 Harmonic Oscillator

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} k x^2 \tag{2.39}$$

Writing $\omega = \sqrt{k/m}$, $\tilde{p} = p/(km)^{1/4}$, $\tilde{x} = x(km)^{1/4}$,

$$H = \frac{1}{2} \omega \left(\tilde{p}^2 + \tilde{x}^2\right) \tag{2.40}$$

$$[\tilde{p}, \tilde{x}] = -i\hbar \tag{2.41}$$

Raising and lowering operators:

$$\begin{aligned} a &= (\tilde{x} + i\tilde{p}) / \sqrt{2\hbar} \\ a^\dagger &= (\tilde{x} - i\tilde{p}) / \sqrt{2\hbar} \end{aligned} \tag{2.42}$$

Hamiltonian and commutation relations:

$$\begin{aligned} H &= \hbar\omega \left(a^\dagger a + \frac{1}{2}\right) \\ [a, a^\dagger] &= 1 \end{aligned} \tag{2.43}$$

The commutation relations,

$$[H, a^\dagger] = \hbar\omega a^\dagger$$

$$[H, a] = -\hbar\omega a \tag{2.44}$$

imply that there is a ladder of states,

$$\begin{aligned} Ha^\dagger|E\rangle &= (E + \hbar\omega)\, a^\dagger|E\rangle \\ Ha|E\rangle &= (E - \hbar\omega)\, a|E\rangle \end{aligned} \tag{2.45}$$

This ladder will continue down to negative energies (which it can't since the Hamiltonian is manifestly positive definite) unless there is an $E_0 \geq 0$ such that

$$a|E_0\rangle = 0 \tag{2.46}$$

Such a state has $E_0 = \hbar\omega/2$.

We label the states by their $a^\dagger a$ eigenvalues. We have a complete set of H eigenstates, $|n\rangle$, such that

$$H|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle \tag{2.47}$$

and $(a^\dagger)^n|0\rangle \propto |n\rangle$. To get the normalization, we write $a^\dagger|n\rangle = c_n|n+1\rangle$. Then,

$$\begin{aligned} |c_n|^2 &= \langle n|aa^\dagger|n\rangle \\ &= n + 1 \end{aligned} \tag{2.48}$$

Hence,

$$\begin{aligned} a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle \\ a|n\rangle &= \sqrt{n}|n-1\rangle \end{aligned} \tag{2.49}$$

2.6 Double Well

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \tag{2.50}$$

where

$$V(x) = \begin{cases} \infty & \text{if } |x| > 2a + 2b \\ 0 & \text{if } b < |x| < a + b \\ V_0 & \text{if } |x| < b \end{cases}$$

Symmetrical solutions:

$$\psi(x) = \begin{cases} A \cos k'x & \text{if } |x| < b \\ \cos(k|x| - \phi) & \text{if } b < |x| < a + b \end{cases} \tag{2.51}$$

with

$$k' = \sqrt{k^2 - \frac{2mV_0}{\hbar^2}} \tag{2.52}$$

The allowed k's are determined by the condition that $\psi(a + b) = 0$:

$$\phi = \left(n + \frac{1}{2}\right)\pi - k(a + b) \tag{2.53}$$

the continuity of $\psi(x)$ at $|x| = b$:

$$A = \frac{\cos(kb - \phi)}{\cos k'b} \tag{2.54}$$

and the continuity of $\psi'(x)$ at $|x| = b$:

$$k \tan\left(\left(n + \frac{1}{2}\right)\pi - ka\right) = k' \tan k'b \tag{2.55}$$

If k' is imaginary, $\cos \to \cosh$ and $\tan \to i \tanh$ in the above equations.

Antisymmetrical solutions:

$$\psi(x) = \begin{cases} A \sin k'x & \text{if } |x| < b \\ \text{sgn}(x)\, \cos(k|x| - \phi) & \text{if } b < |x| < a + b \end{cases} \tag{2.56}$$

The allowed k's are now determined by

$$\phi = \left(n + \frac{1}{2}\right)\pi - k(a + b) \tag{2.57}$$

$$A = \frac{\cos(kb - \phi)}{\sin k'b} \tag{2.58}$$

$$k \tan\left(\left(n+\frac{1}{2}\right)\pi - ka\right) = -\,k' \cot k'b \tag{2.59}$$

Suppose we have n wells? Sequences of eigenstates, classified according to their eigenvalues under translations between the wells.

2.7 Spin

The electron carries spin-1/2. The spin is described by a state in the Hilbert space:

$$\alpha|+\rangle \;\; + \;\; \beta|-\rangle \tag{2.60}$$

spanned by the basis vectors $|\pm\rangle$. Spin operators:

$$\begin{aligned} s_x &= \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ s_y &= \frac{1}{2}\begin{pmatrix} 0 & -\,i \\ i & 0 \end{pmatrix} \\ s_z &= \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -\,1 \end{pmatrix} \end{aligned} \tag{2.61}$$

Coupling to an external magnetic field:

$$H_{\text{int}} = -g\mu_B \vec{s}\cdot\vec{B} \tag{2.62}$$

States of a spin in a magnetic field in the $\hat{\mathbf{z}}$ direction:

$$\begin{aligned} H|+\rangle &= -\frac{g}{2}\mu_B\,|+\rangle \\ H|-\rangle &= \frac{g}{2}\mu_B\,|-\rangle \end{aligned} \tag{2.63}$$

2.8 Many-Particle Hilbert Spaces: Bosons, Fermions

When we have a system with many particles, we must now specify the states of all of the particles. If we have two distinguishable particles whose Hilbert spaces are spanned by the bases

$$\Big|i, 1\Big\rangle \tag{2.64}$$

and

$$\Big|\alpha, 2\Big\rangle \tag{2.65}$$

Then the two-particle Hilbert space is spanned by the set:

$$\Big|i, 1; \alpha, 2\Big\rangle \equiv \Big|i, 1\Big\rangle \otimes \Big|\alpha, 2\Big\rangle \tag{2.66}$$

Suppose that the two single-particle Hilbert spaces are identical, e.g. the two particles are in the same box. Then the two-particle Hilbert space is:

$$\Big|i, j\Big\rangle \equiv \Big|i, 1\Big\rangle \otimes \Big|j, 2\Big\rangle \tag{2.67}$$

If the particles are identical, however, we must be more careful. $\Big|i, j\Big\rangle$ and $\Big|j, i\Big\rangle$ must be physically the same state, i.e.

$$\Big|i, j\Big\rangle = e^{i\alpha}\Big|j, i\Big\rangle \tag{2.68}$$

Applying this relation twice implies that

$$\Big|i, j\Big\rangle = e^{2i\alpha}\Big|i, j\Big\rangle \tag{2.69}$$

so $e^{i\alpha} = \pm 1$. The former corresponds to bosons, while the latter corresponds to fermions. The two-particle Hilbert spaces of bosons and fermions are respectively spanned by:

$$\Big|i, j\Big\rangle + \Big|j, i\Big\rangle \tag{2.70}$$

and

$$\Big|i, j\Big\rangle - \Big|j, i\Big\rangle \tag{2.71}$$

The n-particle Hilbert spaces of bosons and fermions are respectively spanned by:

$$\sum_\pi \Big|i_{\pi(1)}, \ldots, i_{\pi(n)}\Big\rangle \tag{2.72}$$

and

$$\sum_{\pi}(-1)^{\pi}\Big|i_{\pi(1)},\ldots,i_{\pi(n)}\Big\rangle \tag{2.73}$$

In position space, this means that a bosonic wavefunction must be completely symmetric:

$$\psi(x_1,\ldots,x_i,\ldots,x_j,\ldots,x_n)=\psi(x_1,\ldots,x_j,\ldots,x_i,\ldots,x_n) \tag{2.74}$$

while a fermionic wavefunction must be completely antisymmetric:

$$\psi(x_1,\ldots,x_i,\ldots,x_j,\ldots,x_n)=-\psi(x_1,\ldots,x_j,\ldots,x_i,\ldots,x_n) \tag{2.75}$$