Quantum Mechanics Class Notes Week 5

1 The Postulates of QM

Postulate 1.

We call the state of a quantum mechanical system "pure" if we have the maximum possible information about this system, meaning it is uniquely defined within the rules of quantum mechanics. (The state is uniquely defined if we know the probability for each possible measurement result for all observables – see below.)

Such a pure state (at time t) of a system in a Quantum Mechanical system is represented by a vector $|\psi\rangle(t)$ in some appropriate Hilbert Space. The dimension of this Hilbert space is determined by the degrees of freedom we need to both *describe* the outcome of any measurement we may be interested in and to correctly predict the time evolution of the state.

Any multiple $\alpha\psi$ with α from the set of complex numbers refers to the *same* physical state. In the following, we will normally assume that this multiplicative freedom has been used to normalize the state such that $<\psi|\psi>= 1$.

We mention in passing that we can also describe a system that is *not* pure in this sense, meaning there are a number of possible states that it can be in. This will be done in the 2nd semester using the concept of a *density matrix*.

Postulate 2.

The observables Ω of the system are Hermitian operators in the same HS. Only the eigenstates $|\omega\rangle$ of an operator will yield sharp, singular values ω of the observable upon measurement.

Applying the operator to the eigenstate gives a real number ω which can be used to label the basis vectors $|\omega\rangle$

$$\Omega|\omega\rangle = \omega|\omega\rangle$$

The eigenvectors of any observable form a basis for the HS. In general, we may have more than one operator with mutual eigenvectors

$$\Omega,\ \Lambda, \quad with\ eigenvectors\ |\omega,\lambda\rangle$$

that can be labelled by the eigenvalues to form a complete orthonormal basis set.

$$\Omega|\omega,\lambda\rangle = \omega|\omega,\lambda\rangle\ ;\ \Lambda|\omega,\lambda\rangle = \lambda|\omega,\lambda\rangle$$

Note: Two operators have a set of joint eigenvectors if they commute: if $[\Omega, \Lambda] = 0$, then any eigenvector $|\omega_i, j\rangle$ of Ω will be turned into a (possibly different) eigenvector with the *same* eigenvalue ω_i if we apply Λ (here, j is an additional label that may be needed if the eigenvalue is degenerate):

$$\Omega(\Lambda|\omega_i, j\rangle) = \Lambda\Omega|\omega_i, j\rangle = \omega_i\Lambda|\omega_i, j\rangle \tag{1}$$

Therefore, Λ is an operator that acts only *within* a given subspace $\mathbf{V}_\omega$ of eigenvectors of Ω with fixed eigenvalue (it can be written as a "block diagonal" matrix). Thus, there must be a basis of eigenvectors to Λ within each subspace $\mathbf{V}_\omega$. Combining all these basis vectors for all different "eigenspaces" of Ω yields a basis of joint eigenvectors for both Ω and Λ that spans the whole HS.

If we can find a set of, say, two operators that have such a common basis uniquely defined by the eigenvalues for both operators, we can write any state ψ as

$$|\psi\rangle = \sum_{\omega_i,\lambda_i} a_{\omega_i,\lambda_i}|\omega_i,\lambda_i\rangle = \sum_{i,j}\langle\omega_i,\lambda_i|\,|\psi\rangle\,|\omega_i,\lambda_i\rangle$$

(given that the eigenvectors must be orthogonal and can be normalized properly).

Postulate 3.a

The observables and their eigenvalues determine what can be measured for any given system. Measuring the observable Ω on a (normalized) state ψ yields one of the eigenvalues ω with a probability $P(\omega)$ given by $|\mathbf{P}|\psi>|^2$, where $\mathbf{P}$ is the projection operator on the sub-space $\mathbf{V}_\omega$ of all vectors in HS with the same eigenvalue ω under Ω. If ω is a non-degenerate eigenvalue with only one eigen vector $|\omega>$, then $\mathbf{P}|\psi>=|\omega><\omega|\psi>$ and $P(\omega)=|<\omega|\psi>|^2$. In the more general case (several eigenvectors with the same eigenvalue ω), the projection operator can be written as

$$\mathbf{P}_\omega = \sum_j |\omega, j\rangle \langle\omega, j| . \tag{2}$$

To calculate the *expectation value* $<\Omega>$ of the observable for any wave function we can write

$$<\Omega>_\psi = \sum_{\omega_i} \omega_i P(\omega_i) = \sum_{\omega_i, j} \omega_i \left|\langle\omega_i, j|\, \psi\rangle\right|^2 = \sum_{\omega_i, j} \langle\psi|\, \omega_i, j\rangle\, \omega_i \,\langle\omega_i, j|\, \psi\rangle = \sum_{\omega_i, j} \langle\psi|\, \Omega\, |\omega_i, j\rangle \langle\omega_i, j|\, \psi\rangle =$$

$$= \langle\psi|\, \Omega\, |\psi\rangle$$

Note that while the expectation value might be any real number (within the range of eigenvalues of Ω), no single experiment can yield anything but *one of the eigenvalues* of Ω.

The function itself, Ψ, may be completely specified (100% certain) but the outcome of a measurement still cannot be predicted and could in principle yield any ω_i.

Postulate 3.b

A measurement of Ω does not only yield an eigenvalue as result (with probability given above), but it also *changes* the wave function (i.e., our knowledge - because of the new information). Instead of the initial ψ, the new wave function after a measurement that yielded the result ω will be given by

$$|\psi_{new}\rangle = \frac{\mathbf{P}_\omega\, |\psi\rangle}{|\mathbf{P}_\omega\, |\psi\rangle\, |} \tag{3}$$

This is the famous "collapse of the wave function". In reality, the only thing that "collapses" is the information we have about the system and therefore our prediction for any *future* measurement on $|\psi\rangle$. The only circumstance under which the wave function does *not* change upon measurement is when it is already in an eigenstate of the observable being measured. In that case, the measurement will give the corresponding eigenvalue with 100% probability and the state remains unchanged.

Example

Given HS basis vectors

$$|1>= \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |2>= \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and the operator as

$$\Omega = \begin{pmatrix} a & 0 \\ 0 & \mathrm{b} \end{pmatrix}$$

the most general form of the wavefunction is $|\Psi\rangle = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$ normalised by ${c_1}^2 + {c_2}^2 = 1$ where c_1, c_2 are complex numbers..

Any measurement of Ω on the state of Ψ can only give a or b (eigenvalues of Ω) and the state will then collapse into the corresponding eigenstate with this eigenvalue:

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \xrightarrow{\Omega} \begin{cases} a;\ P = |c_1|^2 \rightarrow |\psi_{new}>=|1> \\ b;\ P = |c_2|^2 \rightarrow |\psi_{new}>=|2> \end{cases}$$

Second Example

Assume the operator Ω has several eigenvalues $\omega_1, \omega_2, \omega_3$, ...
For each eigenvalue, you can have several eigenvectors that span a subspace of the full HS. E.g., assume ω_3 has several eigenvectors, $|\omega_{3,j}\rangle$ $(j = 1...n)$.

A measurement of Ω that yields the value ω_3 "collapses" the initial state $|\psi>$ by projecting it onto the vector space $\mathbb{V}_{\omega 3}$ with $\mathbb{P}_{\omega 3} = \sum_j |\omega_{3,j}\rangle \langle\omega_{3,j}|$.
This means that the final state is not uniquely specified by the measurement alone - we also need to know the a priori state. This can be avoided by doing a complete set of measurements with commuting observables.

Continuous set of eigenvalues

In this case, we cannot interpret $|\langle\omega|\,|\psi\rangle\,|^2$ as a probability, but rather as a probability *density*. For instance, if we measure the continuous observable $\mathbf{X}$ with a continuous set of eigenstates $|x\rangle$, $\mathbf{X}\,|x\rangle = x\,|x\rangle$, then the probability of finding the particle at exactly the position x_0 is infinitely small; instead, one can define the probability for finding the particle at a position x within the interval $x_0 \ldots x_0 + \Delta x$ as $P(x_0 \ldots x_0 + \Delta x) = |\langle x_0|\ \Psi\rangle|^2\,\Delta x = \psi^*(x_0)\psi(x_0)\Delta x$ in the limit $\Delta x \to 0$.

Further Points on QM measurements:

- In practice, it is not easy to devise a "perfect quantum measurement" that can give any possible value of an observable. Instead, it is easier to make a "projection measurement" that answers a simple yes-no question, e.g., "is the particle within a box of length L?". In that case, the final "collapsed" wave function is an eigenfunction of the projection operator, or perhaps a statistical ensemble of such eigenfunctions.
- Even if you know the initial state, you cannot predict the result of a measurement unless the initial state is an eigenstate to the observable being measured.
- If you make the same measurements immediately following one another, you keep getting the same answer and the system remains in the same eigen state. However, if you wait awhile, the system evolves with time and may no longer be in an eigenstate of the observable you are measuring.
- You can "prepare" a system in a definite state of HS by making measurements of a complete set of observables (mutually compatible operators). Quantum Mechanics then tells you what the probability of any outcome for any measurement of any observable will be at any later time.

Postulate 4.

Given a generator g, the Poisson bracket of it with any observable ω gives the change $\delta\omega$ of its value under the infinitesimal coordinate transformation (by the small amount ϵ) generated by g:

$$x \to x + \{x, g\}\epsilon$$
$$p \to p + \{p, g\}\epsilon$$

$$\delta\omega = \{\omega, g\}\epsilon$$

As we showed, if the Hamiltonian H is invariant under this transformation,

$$\delta H = 0; \quad \{H, g\} = 0$$

then the observable g is conserved.

In particular, recall that if the generator is the momentum, $g = p$, the infinitesimal transformation described by g is a shift of x by the amount $\epsilon = \delta x$: $x \to x + \{x, p\}\delta x = x + \delta x$ and

$$\delta\omega = \{\omega, p\}\delta x$$

is the change of ω due to this shift. We note that this shift can be interpreted as a *passive* transformation moving the origin of the coordinate system to the *left* by an amount δx, thereby increasing all values of x relative to this new origin. Similarly, taking the Hamiltonian H as the generator, we are describing a (active) transformation by which we simply observe the change of the observable ω after some time $\epsilon = \delta t$ has elapsed:

$$\delta\omega(\delta t) = \{\omega, H\}\delta t.$$

The 4th postulate now stipulates the following: Replacing the Poisson brackets with commutators and substituting in the operators representing the observables and the generator, $\Omega, \mathcal{G}$, the change in the expectation value of Ω is given by

$$i\hbar\delta\langle\Omega\rangle = \langle\Psi|\, [\Omega, \mathcal{G}]\, |\Psi\rangle\, \epsilon$$

where

$$\langle\Omega\rangle = \langle\Psi|\, \Omega\, |\Psi\rangle$$

Schrödinger's Equation

With H as the generator acting on Ω :

$$i\hbar\delta\langle\Omega\rangle = \langle\Psi|\, [\Omega, H]\, |\Psi\rangle\, \delta t$$

$$i\hbar\frac{\partial \langle\Psi|\, \Omega\, |\Psi\rangle}{\partial t} = \langle\Psi|\, [\Omega, H]\, |\Psi\rangle$$

Assuming $|\Psi\rangle \to |\Psi\rangle\,(t)$ (the state depends on time - this is the so-called "Schrödinger picture"):

$$i\hbar\frac{\partial \langle\Psi|\, \Omega\, |\Psi\rangle}{\partial t} = i\hbar\left(\left\langle \frac{\partial\Psi}{\partial t}\right|\Omega\, |\Psi\rangle + \langle\Psi|\, \Omega \left|\frac{\partial\Psi}{\partial t}\right\rangle\right) = \langle\Psi|\, \Omega H\, |\Psi\rangle - \langle\Psi|\, H\Omega\, |\Psi\rangle$$

$$\left\langle -i\hbar\frac{\partial\Psi}{\partial t}\right|\Omega\, |\Psi\rangle + \langle\Psi|\, \Omega \left| i\hbar\frac{\partial\Psi}{\partial t}\right\rangle = \langle\Psi|\, \Omega\, |H\Psi\rangle - \langle H\Psi|\, \Omega\, |\Psi\rangle$$

This implies

$$i\hbar\frac{\partial\, |\Psi\rangle\,(t)}{\partial t} = H\, |\Psi\rangle\,(t)$$

$|\Psi\rangle$ is a vector in HS and describes the state of the system at any given time t. From the Schrödinger Equation, the change in state over time can be predicted if the Hamiltonian H is known. A formal solution of the equation, ignoring the HS and pretending H is "like a number" is given as

$$|\Psi\rangle\,(t) = e^{\frac{-iHt}{\hbar}}\, |\Psi\rangle\,(0)$$

For any observable, the expectation value after Δt can be written

$$\langle O\rangle(t + \Delta t) = \langle O\rangle(t) + \langle\Psi|\, [O, H]\, |\Psi\rangle\, \frac{\Delta t}{i\hbar}$$

The Hamiltonian in $\mathbb{V}$ space depends on the representation of classical observables in the Hilbert space and can be as simple as a 2x2 matrix or as complicated as a differential operator. In the most common case, if the classical Hamiltonian is a function of positions x_i and momenta p_i, we have to find representations of these operators in HS and then write the Hamiltonian as the same function of these operators.

Representation of X and P

If our HS should represent measurements of continuous position (either on an interval or on all real numbers), we have to use the $\aleph_0$ or $\aleph$-dimensional HS of complex-valued functions discussed earlier. In that case, there is no "true" basis of the Hilbert space - instead, we use the "pseudo-basis" $|x\rangle$ which is normalized as $\langle x|\, x'\rangle = \delta(x - x')$. In this basis, $\langle x|\, \psi\rangle = \psi(x)$ and the operator representing position measurements is $X = \int_{-\infty}^{\infty} |x\rangle\, x\, \langle x|\, dx$ with $X\,|x\rangle = x\,|x\rangle$. This agrees with Shankar's version of Postulate II:

$$\langle x|\, X\,|x'\rangle = \int_{-\infty}^{\infty} \langle x|\, x''\rangle\, x''\, \langle x''|\, x'\rangle\, dx'' = \int_{-\infty}^{\infty} \delta(x - x'')x''\delta(x'' - x')dx'' = \delta(x - x')x' = x\delta(x - x') \quad (4)$$

For the representation of momentum P, we return to the 4th postulate: Since P is the generator of a shift of the coordinate system to the *left* by δx, we have

$$i\hbar\delta\langle\Omega\rangle = \langle\Psi|\,[\Omega, P]\,|\Psi\rangle\,\delta x \Rightarrow$$

$$i\hbar\delta\langle\Psi|\,\Omega\,|\Psi\rangle = i\hbar\,\langle\delta\Psi|\,\Omega\,|\Psi\rangle + i\hbar\,\langle\Psi|\,\Omega\,|\delta\Psi\rangle = \langle\Psi|\,\Omega P\,|\Psi\rangle\,\delta x - \langle\Psi|\,P\Omega\,|\Psi\rangle\,\delta x$$

$$-\langle i\hbar\delta\Psi|\,\Omega\,|\Psi\rangle + \langle\Psi|\,\Omega\,|i\hbar\delta\Psi\rangle = \langle\Psi|\,\Omega\,|\delta x P\Psi\rangle - \langle\delta x P\Psi|\,\Omega\,|\Psi\rangle$$

from which we conclude that $\delta x P\,|\Psi\rangle = i\hbar\,|\delta\Psi\rangle$

Now we know that after shifting the coordinate system to the left by δx, the same physical state must be represented by a new function $\bar{\psi}$ of the new variable x' with

$$\langle x'|\, \bar{\psi}\rangle = \bar{\psi}(x') = \psi(x) = \psi(x' - \delta x) = \psi(x') + (-\delta x)\cdot\frac{\partial\psi}{\partial x}(x') = \langle x'|\, \psi\rangle + \langle x'|\, \delta\psi\rangle$$

since $x' = x + \delta x$. From this we conclude

$$(P\,|\psi\rangle)(x') = \langle x'|\, P\,|\psi\rangle = i\hbar\,\langle x'|\, \delta\Psi\rangle\,/\delta x = -i\hbar\frac{\partial\psi}{\partial x}(x')$$

i.e. the action of the operator P on the function $\psi(x)$ is to turn it into $\frac{\hbar}{i}\frac{\partial\psi}{\partial x}$.

We already know (again, from our review of mathematics) what the eigenfunctions $|p\rangle$ of this operator (with $P\,|p\rangle = p\,|p\rangle$) look like:

$$\langle x|\, p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$$

i.e. our "alternative basis" of the same Hilbert Space. In this basis, we can write

$$P = \int_{-\infty}^{\infty} |p\rangle\, p\, \langle p|\, dp$$

which allows us to verify the 2nd part of Shankar's Postulate II:

$$\langle x|\, P\,|x'\rangle = \int_{-\infty}^{\infty} \langle x|\, p\rangle\, p\, \langle p|\, x'\rangle\, dp = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} pe^{ip(x-x')/\hbar}dp = \frac{\hbar}{i}\frac{\partial}{\partial x}\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ip(x-x')/\hbar}dp = \frac{\hbar}{i}\frac{\partial\delta(x - x')}{\partial x}$$