Phys 342 Lecture 37

Welcome to the final ~~#~~ week of lectures for physics 342, Quantum Mechanics. I hope you've had a fun time exploring this crazy world during the semester, even though our time together in class was abruptly ended. Like last week's content, there is no associated homework for this week, but we're just going to have some fun exploring more quantum weirdness.

For the topic of this week, we are going to consider ensembles of quantum mechanical particles and attempt to understand their collective dynamics (or, at least, provide a brief introduction). By "ensemble", I just mean that we are considering a quantum system with more than one particle in it. So, instead of, say, one spin-½ particle, we will consider a collection of N spin-½ particles, or N particles in the infinite square well, or something like that. With this set up, we can immediately see that the quantum description of states on a Hilbert space is insufficient and incomplete for describing this collection of particles.

We have so far described a quantum system by a state in the Hilbert space, which can be represented by a sum over some set of basis states. Let's consider a state $|\psi\rangle \in \mathcal{H}$, the Hilbert space, and we will denote the orthonormal basis states as, say, $|\chi_i\rangle$ so that

$$|\psi\rangle = \sum_{i=0}^{\infty} \beta_i |\chi_i\rangle,$$ and the β_i are some complex coefficients. Such a sum over the basis states is called a <u>coherent</u> <u>sum</u>, because the phase of the coefficients is relevant in the sum. That is, a coherent sum can exhibit constructive or destructive

interference. Indeed, when two waves pass through one another, the resulting wave is a <u>superposition</u> of the initial waves, in which the relative phases of the waves is important. If their phases differ by a multiple of 2π, the waves constructively interfere, and if they differ by an odd multiple of π, they destructively interfere, for example.

Further, this $|\psi\rangle$ is a <u>definite</u> state on the Hilbert space. We happen to express it as a linear combination over some basis states, but that is merely convenience; $|\psi\rangle$ is just state $|\psi\rangle$, independent of basis. We had provided a physical interpretation for the β-coefficients when $|\psi\rangle$ is expanded in some basis: $|\beta_i|^2$ represents the probability for an experiment to return the eigenvalue of the basis state $|x_i\rangle$. We defined this probability by considering N identical systems on which we perform the measurement. Then, as $N \to \infty$, the law of large numbers states that the number of measurements that produce the eigenvalue corresponding to $|x_i\rangle$ is $|\beta_i|^2 N$. Note, however, that in this set up as we have defined it so far, each of these N systems is isolated from the others, and we can unambiguously state that each system is state $|\psi\rangle$. Our "quantum system" is not N particles; we have N quantum systems.

Now, let's consider a system of N particles; for concreteness and say simplicity, we will consider N spin-$\frac{1}{2}$ particles. Now, with the formalism we have currently developed, we would want to write the quantum state of the system as some ket, $|\psi\rangle$, which could be expressed as a coherent linear combination of eigenstates of S_z, say:

$$|\psi\rangle = \beta_\uparrow |\uparrow\rangle + \beta_\downarrow |\downarrow\rangle, \quad \text{where } |\uparrow\rangle \text{ and } |\downarrow\rangle \text{ are}$$

the spin-up $\left(S_z = +\frac{\hbar}{2}\right)$ and spin-down $\left(S_z = -\frac{\hbar}{2}\right)$ eigenstates of S_z. Now, while this linear combination of states may seem to suggest an interpretation for the N particles in our system, we have to be careful. This state does not mean that a fraction $|\beta_\uparrow|^2$ spin-$\frac{1}{2}$ particles have spin-up and $|\beta_\downarrow|^2$ have spin-down. $|\psi\rangle$ is a definite state for spin and the expansion in eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$ just means that the definite spin points in a direction defined by the ratio of $\beta_\uparrow$ to $\beta_\downarrow$. We are representing the state of all N particles in our system by $|\psi\rangle$ and thus all N particles must be in state $|\psi\rangle$. That is, we say that these spin-$\frac{1}{2}$ particles are polarized, ase all of their spins point in the same direction, just like light when it passes through a polarizing filter. Further, because every particle is in the same state $|\psi\rangle$, it is therefore called a pure state. So, formally, the study of quantum mechanics of states in a Hilbert space is restricted to studying the dynamics of pure states.

Why is this restrictive? Well, our N spin-$\frac{1}{2}$ particles clearly do not have to be polarized or all be in the same state. As an extreme example, we can consider an unpolarized collection of N spin-$\frac{1}{2}$ particles. Completely unpolarized means that $N/2$ particles have spin-up and $N/2$ have spin down. Clearly in this case there is no way to write a single state on the Hilbert space $|\psi\rangle$ to represent this collection of particles. It is not correct to express the state of this unpolarized collection of particles as

$|\nearrow\rangle = \frac{1}{\sqrt{2}} |\uparrow\rangle + \frac{1}{\sqrt{2}} |\downarrow\rangle$, as this actually describes a net spin pointed along the x-axis (it's an eigenstate of $\hat{S}_x$). However, for our unpolarized collection of particles, the net spin is 0: there are just as much up as down spinning particles. So, this coherent sum of basis states is clearly the wrong way to express the quantum system. Insted, we must consider an incoherent sum of probabilities of the N particles to be in the spin-up or spin-down state. That is, each particle is in a definite eigenstate of $\hat{S}_z$: it's just that half have spin-up and the other half spin-down. So, if we were to measure the spin of one particle at random, we would indeed find that half the time we find spin-up and ~~there~~ half the time spin-down. However, this would just be like putting your hand in a bag that contains an equal number of red and blue balls. The properties of the balls are fixed before you pull one out (there's no "collapsing" to an eigenstate); you're ignorant of what you pull out simply because you didn't know beforehand. We also call this unpolarized state of N particles "completely random" and it is very similar to classical probability.

Pure states and completely random states of an ensemble of N particles are ends of a spectrum of state configurations. In general, a state of N particles occupies a mixed state, which consists of some amount of polarization and some amount of randomness. More precisely, we can characterize a mixed state by a collection of pure states, which are present in the ensemble with some fraction. Let's call

the collection of pure states present in the ensemble $\{|\psi_i\rangle\}_i$. As pure states, they are represented by an unambiguous ket on Hilbert space. Additionally, these pure states are present in the N particle ensemble with fractions $\{w_i\}_i$. Note that these fractions/ probabilities must sum to unity:

$$\sum_i w_i = 1.$$

Importantly, the pure states that compose our ensemble are _not_ an orthonormal basis, like we discussed for specifying states on the Hilbert space.

Now, with this set up, let's consider an observable A (i.e., a Hermitian operator) and calculate its expectation value or ensemble average on this system. For each pure state, we know the answer:

$$\langle A \rangle_i = \langle \psi_i | A | \psi_i \rangle, \quad \text{and then each of these}$$

pure states are present with a fraction w_i, so we sum the $\langle A \rangle_i$ together, weighted by w_i:

$$\langle A \rangle = \sum_i w_i \langle A_i \rangle = \sum_{i \text{ pure}} w_i \langle \psi_i | A | \psi_i \rangle.$$

To make a bit more sense of this, let's now introduce an orthonormal and complete basis on the Hilbert space in which the pure states live. Let's call this basis $\{|b_n\rangle\}_i$ and completeness means:

$$1 = \sum_n |b_n\rangle\langle b_n|, \quad \text{where the}$$

sum runs over all basis states. Inserting this into the ensemble average for A, we have:

$$\langle A \rangle = \sum_{i\,pure} \sum_{n\,basis} \sum_{m\,basis} w_i \langle \Psi_i | b_n \rangle \langle b_n | A | b_m \rangle \langle b_m | \Psi_i \rangle$$

$$= \sum_{n\,basis} \sum_{m\,basis} \left(w_i \langle b_m | \Psi_i \rangle \langle \Psi_i | b_n \rangle \right) \langle b_n | A | b_m \rangle$$

Now, going way, way back to the beginning of this course, we immediately ~~reg~~ recognize $\langle b_n | A | b_m \rangle$ as the nth row, m^{th} column matrix element of A in the b-basis: A_{nm}. Further, with this same interpretation, we identify

$$\rho_{mn} \equiv w_i \langle b_m | \Psi_i \rangle \langle \Psi_i | b_n \rangle \text{ as the } m^{th} \text{ row, } n^{th} \text{ column}$$

of a matrix we will denote as ρ: ρ_{mn}. That is, we can express the ensemble average of A as:

$$\langle A \rangle = \sum_{n\,basis} \sum_{m\,basis} \rho_{mn} A_{nm} \equiv tr(\rho A) , \text{ where } tr$$

denotes the trace, or sum of diagonal elements of the matrix ρA, where ρ is the <u>density matrix</u>, defined as:

$$\boxed{\rho = \sum_{i\,pure} w_i | \Psi_i \rangle \langle \Psi_i |} .$$

Thus, this density matrix is central for defining the most general state of a collection of quantum particles.

For the remainder of this lecture, we will just enumerate some properties of the density matrix. First it is Hermitian:

$$\rho^\dagger = \sum_{i\,pure} w_i \left(| \Psi_i \rangle \langle \Psi_i | \right)^\dagger = \sum_{i\,pure} w_i | \Psi_i \rangle \langle \Psi_i | = \rho$$

as w_i is a real number (i.e., a fraction in $(0,1]$). Next, the

trace of the density matrix is 1:

$$\text{tr } \rho = \sum_{n\,basis} \sum_{i\,pure} w_i \langle b_n | \Psi_i \rangle \langle \Psi_i | b_n \rangle = \sum_{i\,pure} w_i \langle \Psi_i | \Psi_i \rangle = 1,$$

where we note that $\rho_{nn} = \langle b_n | \Psi_i \rangle \langle \Psi_i | b_n \rangle w_i$, for some basis $\{|b_n\rangle\}_n$ and completeness of the basis: $1 = \sum_{n\,basis} |b_n\rangle \langle b_n|$. $\text{tr } \rho = 1$ is the mixed state formulation of probability conservation.

From the density matrix exclusively, we can define or determine if the system is in a pure state. Let's square ρ:

$$\rho^2 = \sum_{i\,pure} \sum_{j\,pure} w_i w_j |\Psi_i\rangle \langle \Psi_i | \Psi_j \rangle \langle \Psi_j |$$

$$= \sum_{i,j\,pure} \left(w_i w_j \langle \Psi_i | \Psi_j \rangle \right) |\Psi_i\rangle \langle \Psi_j |.$$

Now, for a general mixed state, this is just some other matrix, and in particular, note that the quantity in parentheses has an absolute value less than or equal to 1. It can only equal 1 if $w_i = w_j = 1$ and $\langle \Psi_i | \Psi_j \rangle = 1$, as $0 \le w_i \le 1$. However, because the sum of the w_i is 1, there must be only one non-zero w_i, or that the entire system is in the same pure state. Thus, if one $w_i = 1$, we find

$$\rho^2 = |\Psi_i\rangle \langle \Psi_i | = \rho.$$

So, an ensemble is in a pure state if and only if $\rho^2 = \rho$ or $\text{tr } \rho^2 = 1$.

Finally, let's just quickly derive the time evolution of the density matrix, using the schrödinger equation. Recall that pure states evolve in time with the Schrödinger

equation: $i\hbar \frac{\partial |\psi_i\rangle}{\partial t} = \hat{H} |\psi_i\rangle$,

and so the time derivative of the density matrix is:

$$\frac{\partial \rho}{\partial t} = \sum_{i\,pure} w_i \frac{\partial}{\partial t}\left(|\psi_i\rangle\langle\psi_i|\right) = \sum_{i\,pure} w_i \left[\left(\frac{\partial}{\partial t}|\psi_i\rangle\right)\langle\psi_i| + |\psi_i\rangle\frac{\partial}{\partial t}\langle\psi_i|\right]$$

$$= \sum_{i\,pure} w_i \left[\frac{\hat{H}}{i\hbar}|\psi_i\rangle\langle\psi_i| - |\psi_i\rangle\langle\psi_i|\frac{\hat{H}}{i\hbar}\right]$$

$$= \frac{1}{i\hbar}[\hat{H},\rho], \quad \text{where we note that}$$

$$\left(\frac{\partial|\psi_i\rangle}{\partial t}\right)^\dagger = \frac{\partial}{\partial t}\langle\psi_i| = \left(\frac{\hat{H}}{i\hbar}|\psi_i\rangle\right)^\dagger = -\langle\psi_i|\frac{\hat{H}}{i\hbar}.$$

Thus,

$$\boxed{i\hbar \frac{\partial\rho}{\partial t} = [\hat{H},\rho]}$$, which will be useful in what we do in the next lectures.

More next time...