Lecture 17

Relevant sections in text: §2.2, 2.3

Ehrenfest's Theorem

The Heisenberg equations are appealing because they make formal contact with the Hamilton equations of classical mechanics. In classical mechanics functions on phase space represent the observables, and the time rate of change of an observable A is controlled by the Poisson bracket with the Hamiltonian:

$$\frac{dA}{dt} = \{A, H\}.$$

The formal correspondence with quantum mechanics is made via

$$\{A, B\} \quad \longleftrightarrow \quad \frac{1}{i\hbar}\, [A, B],$$

where the observables are represented by functions on phase space on the left and operators on the right. This formal correspondence implies that expectation values will, in a suitable approximation, follow classical trajectories, a result known as *Ehrenfest's theorem.*

To derive this theorem in the Heisenberg picture is quite easy. Take the expectation value of the quantum form of Newton's second law,

$$\frac{d^2 X^i(t)}{dt^2} = -\frac{\partial V}{\partial x^i}(\mathbf{X}(t)),$$

and use the time independence of the state vector to obtain (exercise)

$$\frac{d^2}{dt^2}\langle \mathbf{X}\rangle(t) = \langle \mathbf{F}\rangle(t),$$

where $\mathbf{F}$ is the force. This result is Ehrenfest's theorem.

Exercise: How would you derive this equation in the Schrödinger picture?

It is often said that Ehrenfest's theorem shows that expectation values obey the classical dynamical laws. This slogan is not quite true. In particular, the expectation value of position does *not* necessarily obey Newton's second law. A true version of Newton's second law for the expectation value would read

$$m\frac{d^2\langle X^i\rangle(t)}{dt^2} = -\frac{\partial V(\langle \vec{X}\rangle(t))}{\partial\langle X^i\rangle}.$$

Of course, this latter equation is *not* what quantum mechanics gives, in general. To get this last result we need

$$\langle\frac{\partial V(\vec{X}(t))}{\partial X^i}\rangle = \frac{\partial V(\langle\vec{X}\rangle(t))}{\partial\langle X^i\rangle},$$

whose validity depends upon the state vector being used as well as on the form of the potential energy operator. A simple example where this equality *does* hold is provided by the harmonic oscillator potential in one dimension (to be discussed below in more detail) for which

$$V(X) = \frac{1}{2}kX^2,$$

so that

$$\frac{\partial V(X(t))}{\partial X} = kX,$$

which satisfies for any state vector

$$\langle kX\rangle(t) = \frac{\partial V(\langle X\rangle(t))}{\partial\langle X\rangle} = k\langle X\rangle(t).$$

The harmonic oscillator example is exceptional. Generally, Ehrenfest's theorem does *not* imply that expectation values obey classical equations of motion. For example, consider the potential

$$V(X) = \frac{1}{3}kX^3.$$

We have in this case

$$\frac{\partial V(\langle X\rangle(t))}{\partial\langle X\rangle} = k\langle X\rangle^2(t),$$

which does not, in general, equal

$$\langle\frac{\partial V(X(t))}{\partial X}\rangle = k\langle X^2\rangle(t).$$

Indeed, these two expressions agree if and only if the dispersion in $X(t)$ vanishes – which it never does, strictly speaking. (On the other hand, one can find states which make the position dispersion arbitrarily small at the expense of a large dispersion in momentum.) Thus, according to Ehrenfest's theorem, the expectation values of position for this cubic potential will only agree with the classical behavior insofar as the dispersion in position is negligible (for all time) in the chosen state. This result illustrates a general rule: classical behavior for particle motion arises when the statistical uncertainties in the basic observables are sufficiently small.

Harmonic Oscillator: Definitions, the Hamiltonian

We now begin a survey of key properties of one of the workhorse models of quantum mechanics: the simple harmonic oscillator (SHO). This model is useful because it is analytically quite tractable, it illustrates a wide variety of quantum mechanical features both

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physically and at the level of the formalism itself, and it provides a very nice first approximation to many simple models of real physical systems in the vicinity of stable equilibrium. It is remarkable how often the idea of a harmonic oscillator appears in physics. For example, the harmonic oscillator illustrates generic features of "bound state behavior", it is used to model the confinement of quarks in nucleons, it is used to model the spectral properties of molecules, it is the elementary building block of the "free quantum field". One can use harmonic oscillators to understand photons!

The SHO can be viewed mathematically as a particle moving in one dimension under the influence of a quadratic potential (although, physically, it doesn't usually arise that way). The position is X, the momentum is P, which we have already defined in some detail (in the Heisenberg pictures these are the position and momentum operators at the initial time). The dynamics are generated by the Hamiltonian (in either the Schrödinger or Heisenberg picture)

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2.$$

Classically, this would be the energy function for a "mass on a spring" dynamical system where m is the mass and ω is the natural frequency of the spring according to Hooke's law. We retain that terminology here.

The position and momentum observables we have studied in some detail. For this simple one-dimensional system, the Hamiltonian is the center of attention. Of course, we would like to understand its spectrum and eigenvectors, since these characterize the possible energies and the states where the energy is known with statistical certainty. Moreover, the spectral properties of H will determine the dynamical evolution of the oscillator in the Schrödinger picture. The algebraic (commutator) properties of H, X and P will control the dynamics in the Heisenberg picture. In fact, as you will see, the algebraic properties of the operators H, X and P essentially tell us everything we want to know.

Spectrum of the SHO Hamiltonian

To analyze H we follow an elegant algebraic approach pioneered (I believe) by Dirac. Rather than working directly with the position and momentum operators, a more convenient set of operators can be defined as follows. Set

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(X + \frac{i}{m\omega}P\right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(X - \frac{i}{m\omega}P\right),$$

so that (exercises)

$$X = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger), \quad P = \frac{1}{i}\sqrt{\frac{\hbar}{2m\omega}}(a - a^\dagger).$$

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Note that a and $a^\dagger$ can be viewed as quantum versions of the complex amplitudes featuring in the general solution of the equations of motion of a classical oscillator (exercise). We will say a little more about this later.

From the CCR for position and momentum, we have (exercise)

$$[a, a^\dagger] = I.$$

A straightforward computation reveals (exercise)

$$H = \frac{1}{2}\hbar\omega(aa^\dagger + a^\dagger a) = \hbar\omega(a^\dagger a + \frac{1}{2}I).$$

Evidently, the gist of the Hamiltonian is to be found in the "number operator"

$$N := a^\dagger a.$$

This operator is self-adjoint, and we denote its eigenvectors, for now, by $|\lambda\rangle$,

$$N|\lambda\rangle = \lambda|\lambda\rangle,$$

so that the energy eigenvectors are $|\lambda\rangle$ with

$$H|\lambda\rangle = E_\lambda|\lambda\rangle, \quad E_\lambda = (\lambda + \frac{1}{2})\hbar\omega.$$

Note that the eigenvalues λ are dimensionless (exercise).

It is not hard to check that*

$$[N, a] = -a, \quad [N, a^\dagger] = a^\dagger.$$

This implies that (exercise)

$$N(a^\dagger|\lambda\rangle) = (\lambda + 1)(a^\dagger|\lambda\rangle),$$

and

$$N(a|\lambda\rangle) = (\lambda - 1)(a|\lambda\rangle).$$

Therefore $a^\dagger$ (a) takes an eigenvector of N and turns it into an eigenvector with eigenvalue raised (lowered) by one unit. Correspondingly, the action of $a^\dagger$ (a) on an energy eigenvector yields an eigenvector with energy raised (lowered) by one "quantum", $\hbar\omega$. For this reason

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* One way to check this is to use the identity

$$[AB, C] = A[B, C] + [A, C]B,$$

which you should prove as an exercise.

$a^\dagger$ and a are often called "creation and annihilation operators", or "ladder operators" or "raising and lowering operators". So, if one has a single eigenvector of N (or H), then one will have an infinity of such eigenvectors with eigenvalues all differing by integers (or by integer multiples of $\hbar\omega$). This result follows merely from the commutation relations for position and momentum (or a and $a^\dagger$).

It is shown in detail in the text that the eigenvalues of N are non-degenerate and are non-negative integers,

$$\lambda \equiv n = 0, 1, 2, \ldots.$$

The essence of the proof is to note that the number operator must have a non-negative expectation value:

$$\langle\psi|N|\psi\rangle = \langle\psi|a^\dagger a|\psi\rangle = ((\langle\psi|a^\dagger)(a|\psi\rangle)) \geq 0,$$

where

$$\langle\psi|N|\psi\rangle = 0 \quad \Longleftrightarrow \quad a|\psi\rangle = 0.$$

On the other hand, since a lowers the eigenvalue of N by one unit, there must be a unique (up to normalization) lowest-eigenvalue eigenvector $|0\rangle$ such that

$$a|0\rangle = 0.$$

One then easily infers that the spectrum of N is non-degenerate, consisting of the non-negative integers:

$$N|n\rangle = n|n\rangle, \quad n = 0, 1, 2, \ldots .$$

Therefore, the energy spectrum is purely discrete:

$$E_n = (n + \frac{1}{2})\hbar\omega, \quad n = 0, 1, 2, \ldots$$

and the energy eigenvectors are labeled $|n\rangle$. These results arise from the assumption that X and P are self-adjoint operators on a Hilbert space (or, equivalently, that a and $a^\dagger$ are adjoints of each other with respect to the Hilbert space scalar product).

Finally, it is shown in the text that we have

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \quad \langle n|m\rangle = \delta_{nm}.$$

Note that the "ground state" $|0\rangle$ has energy $\frac{1}{2}\hbar\omega$ and satisfies

$$a|0\rangle = 0.$$