

## Lecture 11

Relevant sections in text: §1.7, 2.1

### Gaussian state

Here we consider the important example of a Gaussian state for a particle moving in 1-d. Our treatment is virtually identical to that in the text, but this example is sufficiently instructive to give it again here.

We define this state by giving its components in the position basis, *i.e.*, its wave function:

$$\psi(x) = \langle x|\psi\rangle = \left(\frac{1}{\pi^{1/4}\sqrt{d}}\right) \exp\left(ikx - \frac{x^2}{2d^2}\right).$$

You can check as a good exercise that this state/wave function is normalized:

$$1 = \langle\psi|\psi\rangle = \int_{-\infty}^{\infty} dx \langle\psi|x\rangle\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx |\psi(x)|^2.$$

The wave function is oscillatory with wavelength  $\frac{2\pi}{k}$  but the oscillations are in a Gaussian envelope centered at the origin. The probability density for position is thus a Gaussian centered at the origin with width determined by  $d$ . Thus this state represents a particle “localized” near the origin within a statistical uncertainty specified by  $d$ .

Let us make this more precise and exhibit some properties of this state. As an exercise you can check the following results.

$$\langle X\rangle = \langle\psi|X|\psi\rangle = \int_{-\infty}^{\infty} dx x |\psi(x)|^2 = 0.$$

so that the mean location of the particle is at the origin in this state. Next we have

$$\langle X^2\rangle = \langle\psi|X^2|\psi\rangle = \int_{-\infty}^{\infty} dx x^2 |\psi(x)|^2 = \frac{d^2}{2}.$$

Thus the dispersion in position is

$$\langle\Delta X^2\rangle = \frac{d^2}{2},$$

*i.e.*,  $\frac{d}{\sqrt{2}}$  is the standard deviation of the probability distribution for position. Next we have

$$\langle P\rangle = \langle\psi|P|\psi\rangle = \int_{-\infty}^{\infty} dx \psi^*(x) \frac{\hbar}{i} \frac{d}{dx} \psi(x) = \hbar k,$$

telling us that, on the average, this state is one in which the particle is moving with momentum  $\hbar k$ , and

$$\langle P^2\rangle = \langle\psi|P^2|\psi\rangle = \int_{-\infty}^{\infty} dx \psi^*(x) (-\hbar^2) \frac{d^2}{dx^2} \psi(x) = \frac{\hbar^2}{2d^2} + \hbar^2 k^2,$$

so that the momentum uncertainty is

$$\langle \Delta P^2 \rangle = \frac{\hbar^2}{2d^2}.$$

Thus the momentum uncertainty varies reciprocally with  $d$  relative to the position uncertainty. The product of position and momentum uncertainties is as small as allowed by the uncertainty relation:

$$\langle \Delta X^2 \rangle \langle \Delta P^2 \rangle = \frac{\hbar^2}{4}.$$

One sometimes calls the Gaussian state a *minimum uncertainty state*.

Because the Fourier transform of a Gaussian function is another Gaussian, it happens that the momentum probability distribution is a Gaussian:

$$\begin{aligned} \tilde{\psi}(p) &= \langle p | \psi \rangle = \int_{-\infty}^{\infty} dx \langle p | x \rangle \langle x | \psi \rangle \\ &= \int_{-\infty}^{\infty} dx \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}px} \psi(x) \\ &= \sqrt{\frac{d}{\hbar\sqrt{\pi}}} \exp \left\{ -\frac{1}{2\hbar^2} (p - \hbar k)^2 d^2 \right\}. \end{aligned}$$

You can see that this Gaussian is peaked about the expected momentum value, as it should be, and that its width varies like  $1/d$ , *i.e.*, reciprocal to the position uncertainty, as expected.

In summary, the Gaussian state we have defined corresponds to a particle which (on the average) is moving, and has a Gaussian spread of position and momentum values such that the uncertainty product is minimized. One can use such states to model macroscopic objects. Just put in reasonable values for  $d$  and  $k$  and you will find that the quantum uncertainties are sufficiently small to be negligible.

## Dynamics: the Schrödinger picture

We now have enough tools to formulate quantum dynamics. Dynamics are characterized by the final postulate: *Time evolution is a continuous unitary transformation*. We have, of course, just studied an example of a continuous unitary transformation: Translation by an amount  $a$ . In that application  $a$  is not identified with time, though. The idea of dynamical evolution is that measurable aspects of the system are changing in time.\*

\* For us, time will be modeled in its Newtonian form as a non-dynamical, *a priori* way of ordering events, valid in any inertial reference frame. In particular, in this framework time is not treated as an observable whose value depends upon the state of the quantum system, but instead as a special kind of parameter. Of course, there are many interesting issues here associated with the physical meaning of time in quantum mechanics, but we will not be able to explore them further in this course. We simply assume that some suitable standard of temporal reference has been chosen once and for all.

In quantum mechanics the state of the system at any given time can be identified with the totality of probability distributions for all observables at that time. Time evolution, therefore, ought to correspond to a time varying change in the probability distributions. As we have noted already, all probability distributions can be computed by taking expectation values of suitable observables (*e.g.*, characteristic functions, *etc.*). Therefore, time evolution can be defined in terms of the evolution of expectation values. The rules of the game say that given an observable  $A$  the expectation value is to be computed via

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

where  $|\psi\rangle$  is a unit vector in Hilbert space and  $A$  is the operator representing the observable. We now consider this definition as time varies. At each instant of time we need to have a system of vectors and operators that can be used to make physical predictions via, say, expectation values. Our strategy will be to assume we have a single Hilbert space for all time, but we allow the mathematical identification of states and observables to vary in time. To describe mathematically how expectation values change in time we then have a number of options. Two such options are often the most convenient. First, we can let the operator representing the observable change in time, with the vector  $|\psi\rangle$  fixed for all time:

$$\langle A \rangle(t) = \langle \psi | A(t) | \psi \rangle.$$

This point of view of dynamics is called the *Heisenberg picture*, and will be discussed later. Another way of viewing dynamics, known as the *Schrödinger picture*, is based upon letting the vector  $|\psi\rangle$  change in time while holding the operator representatives of the observables fixed in time:

$$\langle A \rangle(t) = \langle \psi, t | A | \psi, t \rangle.$$

There are infinitely many different “pictures” intermediate to these two. We shall look first at the postulate on dynamics from the point of view of the Schrödinger picture.

### **The Schrödinger picture: The time evolution operator**

Much as we did with spatial translations, we assume that the state vector at time  $t$ , denoted by  $|\psi, t\rangle$ , is related by a continuous, unitary transformation from the state at any earlier time  $t_0$ . Therefore we write

$$|\psi, t\rangle = U(t, t_0) |\psi, t_0\rangle.$$

Here  $|\psi, t_0\rangle$  can in principle be any unit vector.  $U$  is unitary so that the state vector remains normalized as time progresses:

$$\langle \psi, t | \psi, t \rangle = \langle \psi, t_0 | U^\dagger U | \psi, t_0 \rangle = \langle \psi, t_0 | \psi, t_0 \rangle = 1.$$

(It is not hard to show that a (bounded) operator on a complex Hilbert space vanishes if and only if all its diagonal matrix elements vanish (exercise). Since  $|\psi, t_0\rangle$  is arbitrary we see that the state vector remains normalized if and only if  $U^\dagger = U^{-1}$ , that is,  $U$  is unitary.) Given,

$$U^\dagger(t, t_0) = U^{-1}(t, t_0),$$

we naturally associate the inverse transformation as time evolution from  $t$  back to  $t_0$ , so that

$$U^\dagger(t, t_0) = U^{-1}(t, t_0) = U(t_0, t).$$

Finally, we assume that time evolution from  $t_0$  to  $t$  can be viewed as time evolution from  $t_0$  to  $t_1$  and then from  $t_1$  to  $t$ , so that

$$U(t, t_1)U(t_1, t_0) = U(t, t_0).$$

The operator  $U$  is called the *time evolution operator*. The principal issue when studying dynamics using quantum mechanics is to uncover the nature of the time evolution operator for the given system. Generally speaking, this is not easy to do if one proceeds in a direct fashion. After all, the time evolution operator has to be a pretty complicated object, given that it knows how to evolve any initial state. A deep principle of physics/mathematics going back to Lie is the following. When considering continuous transformations it is always easier to work with infinitesimal transformations. This is because the finite transformation is completely characterized by the infinitesimal transformation, which is a much simpler structure than the finite transformation. This is one of the reasons that you usually find dynamical evolution (whether in Newtonian dynamics, fluid dynamics, electrodynamics, etc.) expressed in terms of differential equations.

Thus we consider the infinitesimal generator of time evolution, much as we did previously with translations. The infinitesimal generator of the unitary time evolution will be an observable called the *Hamiltonian* (in analogy with classical mechanics where the Hamiltonian is the generating function of a canonical transformation corresponding to motion in time). Normally, the Hamiltonian represents the energy, which is conserved provided  $H$  does not depend upon the time. Indeed, just as we defined the momentum as the generator of spatial translations, we *define* the Hamiltonian/energy as the generator of time translations. One subtlety which occurs here, unlike what occurs with spatial translations, is that the Hamiltonian may be time dependent, that is, it may be a family of operators parameterized by the time. This demands a slightly more sophisticated analysis than we used for the spatial translations.