After the energy measurement

After the energy measurement with outcome \( E_i \), the particle will be in the energy eigenstate \( u_i \), and all subsequent energy measurements will yield the energy \( E_i \).

What is the energy before measurement is made?

If \( \psi(x) \) is not an eigenstate, the energy is “uncertain”. A measurement can yield different energy values, only probabilities can be predicted. However, an average value of the energy can be calculated:

\[
\langle E \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n \rightarrow \text{generally valid} \quad (12-1)
\]

Using the definition of the expansion coefficients \( c_n \), we can also write this as

\[
\begin{align*}
\langle E \rangle &= \sum_{n=1}^{\infty} |c_n|^2 E_n \\
&= \sum_{n=1}^{\infty} c_n \left( \int dx u_n^*(x) \psi(x) \right)^* E_n \\
&= \sum_{n=1}^{\infty} c_n \int dx \psi^*(x) E_n u_n(x) \\
&= \sum_{n=1}^{\infty} c_n \int dx \psi^*(x) \hat{H} u_n(x) \\
&= \int dx \psi^*(x) \hat{H} \left( \sum_{n} c_n u_n(x) \right) \\
&= \int dx \psi^*(x) \hat{H} \psi(x)
\end{align*}
\]

Expectation value of energy in state \( \psi(x) \):

\[
\langle E \rangle = \int dx \psi^*(x) \hat{H} \psi(x) \rightarrow \text{valid for any potential, not only box potential} \quad (12-2)
\]

Hamiltonian operator and energy

If we postulate that a particle of momentum \( p \) is associated with a deBroglie wavelength \( \lambda_{dB} = \frac{\hbar}{p} \), then it is represented by a plane wave \( e^{ikx} \) with a wavevector
The quantum physics equation:

\[ k = \frac{2\pi}{\lambda} = \frac{\pi p}{\hbar} = \frac{p}{\hbar}, \text{ or } p = \hbar k. \]

Then, since the Fourier transform \( \phi(k) \) of \( \psi(x) \) gives the probability amplitude for the plane wave with wavevector \( k \rightarrow \)

\[ \psi(x) = \frac{1}{\sqrt{2\pi}} \int dk \phi(k) e^{i k x}, \]

the expectation value of momentum is given by

\[ \langle p \rangle = \int dk \hbar k |\phi(k)|^2 \]
\[ \langle p^2 \rangle = \int dk (\hbar k)^2 |\phi(k)|^2 \]

Note. In PS5 you show using the properties of Fourier transforms that these expectation values can also be expressed as

\[ \langle p \rangle = \int dx \psi^*(x) \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \psi(x) \]
\[ \langle p^2 \rangle = \int dx \psi^*(x) \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right)^2 \psi(x) \]

It follows that the expectation value of the KE is

\[ \langle T \rangle = \langle \frac{p^2}{2m} \rangle = \int dx \psi^*(x) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \psi(x) \]

How large is the expectation value of the potential energy?

Potential \( V(x) \) should be weighted by probability to find particle between \( x \) and \( x + dx \), hence

\[ \langle V \rangle = \int dx V(x) |\psi(x)|^2 = \int dx \psi^*(x) V(x) \psi(x) \]

Since \( \langle E \rangle = \langle V \rangle + \langle T \rangle \) it follows that

\[ \langle E \rangle = \int dx \psi^*(x) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi(x) \]
\[ = \int dx \psi^*(x) \hat{H} \psi(x) \]

This is the so-called “sandwich form” for calculating the mean value (expectation value) of the energy. If \( \psi(x) \) is an energy eigenfunction with eigenvalue \( E_0 \), i.e. if
\[ \hat{H} \psi_{E_0}(x) = E_0 \psi_{E_0}(x), \]

then

\[
\langle E \rangle = \int dx \psi_{E_0}^*(x) \hat{H} \psi_{E_0}(x) \\
= \int dx \psi_{E_0}^*(x) E_0 \psi_{E_0}(x) \\
= E_0 \int dx |\psi_{E_0}(x)|^2 \\
= E_0,
\]

(12-12)

where we have used the fact that the wavefunction is normalized. This shows that the constant \( E_0 \) appearing when we make the product ansatz \( \Psi(x, t) = T(t)\psi(x) \) to solve the SE is really the energy of the system. We define the expectation value \( \langle \hat{O} \rangle \) of an operator \( \hat{O} \) acting on a wavefunction \( \psi(x) \) via the sandwich form

\[
\langle \hat{O} \rangle = \int dx \psi^*(x) \hat{O} \psi(x)
\]

(12-13)

Then we have

\[
\langle E \rangle = \langle \hat{H} \rangle = \int dx \psi^*(x) \hat{H} \psi(x)
\]

(12-14)

The mean energy of the state described by the wave-function \( \psi(x) \) is the expectation value of the Hamiltonian operator \( \hat{H} \). We say that the Hamiltonian \( \hat{H} \) is the operator associated with the measurable quantity energy. The operator \( \hat{T} \) associated with the kinetic energy is

\[
\hat{T} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}
\]

(12-15)

with \( \langle T \rangle = \langle \hat{T} \rangle = \int dx \psi^*(x) \hat{T} \psi(x) \), while the operator \( \hat{V} \) for the potential energy is simply a multiplicative factor

\[
\hat{V} = V(x)
\]

(12-16)

with \( \langle V \rangle = \langle \hat{V} \rangle = \int dx \psi^*(x) \hat{V} \psi(x) \)

Why is potential energy associated with a simple multiplicative factor while kinetic energy is associated with a second derivative?

Because we are working with wavefunctions in real space \( \psi(x) \). We say that we are working with wavefunctions in position space or in the position representation.
Another possibility is to work in momentum space (the momentum representation). Then the wavefunction should be the probability amplitude in momentum space, which is just the Fourier transform $\phi(p)$ of $\psi(x)$. Then to calculate the KE we have to weigh $\frac{p^2}{2m}$ for each $p$ with the probability to find the particle momentum between $p$ and $p + dp$:

$$\left\langle \frac{p^2}{2m} \right\rangle = \int dp \frac{p^2}{2m} |\phi(p)|^2 \quad (12-17)$$

$$= \int dp \phi^*(p) \frac{p^2}{2m} \phi(p) \quad (12-18)$$

We see that in momentum space the KE operator is simply a multiplicative factor

$$\hat{T} = \hat{p}^2 = \frac{p^2}{2m} \quad \text{→ in momentum space} \quad (12-19)$$

**How to calculate the potential energy $V(x)$ in terms of the wavefunctions in momentum space $\phi(p)$?**

*Note.* In PS5, you have shown that

$$\langle x \rangle = \int dp \phi^*(p) \left( i\hbar \frac{\partial}{\partial p} \right) \phi(p) \quad (12-20)$$

$$\langle x^n \rangle = \int dp \phi^*(p) \left( i\hbar \frac{\partial}{\partial p} \right)^n \phi(p) \quad (12-21)$$

Consequently, for any potential function

$$V(x) = \sum_{n=0}^{\infty} a_n x^n \quad (12-22)$$

we can calculate the expectation value $\langle V \rangle$ as

$$\langle V \rangle = \int dp \phi^*(p) V \left( i\hbar \frac{\partial}{\partial p} \right) \phi(p)$$

$$= \int dp \phi^*(p) \hat{V} \phi(p) \quad (12-23)$$

Consequently, the representation of the operator for the PE in momentum space is

$$\hat{V} = V \left( i\hbar \frac{\partial}{\partial p} \right) \quad (12-24)$$
where a function $V$ of an operator is defined in terms of its Taylor expansion, Eq. (12-22). It follows that the Hamiltonian is

$$\hat{H} = \hat{T} + \hat{V}$$  \hspace{1cm} (12-25)

$$= \frac{1}{2m} \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right)^2 + V(x) \hspace{1cm} \text{in position space} \hspace{1cm} (12-26)$$

$$= \frac{p^2}{2m} + V \left( i\hbar \frac{\partial}{\partial p} \right) \hspace{1cm} \text{in momentum space} \hspace{1cm} (12-27)$$

The SE equation is always the same:

$$ih\frac{\partial}{\partial t} \Psi(x,t) = \hat{H} \Psi(x,t) \hspace{1cm} \text{time-dependent SE} \hspace{1cm} (12-28)$$

$$ih\frac{\partial}{\partial t} \Phi(p,t) = \hat{H} \Phi(p,t) \hspace{1cm} \text{time-dependent SE} \hspace{1cm} (12-29)$$

$$\hat{H} \psi(x) = E \psi(x) \hspace{1cm} \text{time-independent SE} \hspace{1cm} (12-30)$$

$$\hat{H} \phi(p) = E \phi(p) \hspace{1cm} \text{time-independent SE} \hspace{1cm} (12-31)$$

**Example.** For the harmonic oscillator, the SE (in appropriately chosen units) looks the same in position and momentum space:

1. **linear potential** $V(x) = Ax$

   $$-\frac{\hbar^2}{2m} \psi''(x) + Ax \psi(x) = E \psi(x) \hspace{1cm} \text{in position space} \hspace{1cm} (12-32)$$

   $$\frac{p^2}{2m} \phi(p) + i\hbar A \phi'(p) = E \phi(p) \hspace{1cm} \text{simpler equation in momentum space} \hspace{1cm} (12-33)$$

2. **harmonic oscillator**: $V(x) = \frac{1}{2}m\omega^2x^2$

   $$-\frac{\hbar^2}{2m} \psi''(x) + \frac{1}{2}m\omega^2x^2 \psi(x) = E \psi(x) \hspace{1cm} (12-34)$$

   $$\frac{p^2}{2m} \phi(p) - \frac{1}{2}\hbar^2m\omega^2 \phi''(p) = E \phi(p) \hspace{1cm} (12-35)$$

   If we know the solutions in one space, we know the solutions in the other. The HO is symmetric in position and momentum.
8.04 Quantum Physics Lecture XII

Time evolution of the wave function

Consider a particle in the infinite box with a wavefunction at \( t = 0 \), \( \Psi(x, t = 0) \). Expansion into eigenstates \( \Psi(x, t = 0) = c_1 u_1(x) + c_2 u_2(x) + \cdots = \sum_{n=1}^{\infty} c_n u_n(x) \).

Since each eigenstate \( u_n(x, t) \) evolves at a rate given by its eigenenergy \( E_n \),

\[
\Psi(x, t) = \sum_{n=1}^{\infty} c_n u_n(x)e^{-iE_n t/\hbar}
\]

the wavefunction \( \Psi(x, t) \) at later time \( t \) is simply given by the linear superposition

where the expansion coefficients \( c_n \) are calculated at \( t = 0 \):

\[
c_n = \int_{-\infty}^{\infty} dx u_n^*(x) \Psi(x, t = 0)
\]

Hence the importance of energy eigenstates and eigenvalues: The eigenvalues represent not only the only possible outcomes of individual energy measurements, but the combination of eigenstates and eigenvalues allows one to write down the time evolution of an arbitrary initial state.

How does a particle move?

**Example.** \( \Psi(x, t = 0) = \frac{1}{\sqrt{2}}(u_1(x) + u_2(x)) \). Particle in equal superposition of ground and first excited state.

\[
\Psi(x, t) = \frac{1}{\sqrt{2}} \left[ u_1(x)e^{-iE_1 t/\hbar} + u_2(x)e^{-iE_2 t/\hbar} \right]
\]

\[
= \frac{1}{\sqrt{2}} e^{-iE_1 t/\hbar} \left[ u_1(x) + u_2(x)e^{i(E_2-E_1)t/\hbar} \right]
\]

\[
|\Psi(x, t)|^2 = \frac{1}{2} |u_1(x) + u_2(x)e^{-i(E_2-E_1)t/\hbar}|^2
\]

At any fixed position, interference term between \( u_1 \) and \( u_2 \) oscillates from constructive to destructive interference with angular frequency

\[
\omega_{21} = \frac{E_2 - E_1}{\hbar}
\]

The energy difference determines the oscillation of the particle between the halves of the box.
Figure I: A particle in a superposition of the ground state an the first excited state oscillates from left to right at the frequency corresponding to the energy difference between the two states.

*Note.* If \( \Psi(x, t = 0) \) is an eigenstate, \( \Psi(x, t = 0) = u_n(x) \), then \( |\Psi(x, t)|^2 = |\Psi(x, 0)|^2 \), i.e. the probability density does not change in time: Bohr’s *stationary states* are energy eigenstates.

An oscillating electron (particle) is in a superposition of at least two energy eigenstates. An electron in a Bohr atom that emits a Lyman \( \alpha \) photon is in a superposition of the ground \( (E_1) \) and the first excited state \( (E_2) \). It oscillates in space at the frequency \( \frac{E_2 - E_1}{\hbar} \), exactly the frequency of the emitted Lyman \( \alpha \) photon.

Our box example also shows: The more localized the initial spatial distribution \( \Psi(x, 0) \), the more eigenstates are involved, and the more complicated the time evolution will be (there will be interference terms oscillating at \( \frac{E_2 - E_1}{\hbar}, \frac{E_3 - E_1}{\hbar}, \frac{E_3 - E_2}{\hbar}, \ldots \)) All motion of particles involves oscillating interference.

**What is the relation between the SE and CM**

**QM should reproduce CM as limiting case**

- **CM** \( p = mv = m\frac{dx}{dt} \)

- We expect this (and other) classical equation(s) to hold for the QM expectation values (average position, momentum), at least in some limiting case.

- Calculate \( m \langle \frac{dx}{dt} \rangle \): the only time variation arises from the time variation of wave function, \( x \) is coordinate, not particle position in the SE.
\[
m\left\langle \frac{dx}{dt} \right\rangle = \frac{d}{dt} \langle x \rangle \tag{12-44}
\]
\[
= m \frac{d}{dt} \int dx \Psi^*(x,t)x\Psi(x,t) \tag{12-45}
\]
\[
= m \int dx \left\{ \frac{\partial \Psi^*}{\partial t} x \Psi + \Psi^* x \frac{\partial \Psi}{\partial t} \right\} \tag{12-46}
\]
\[
= \frac{\hbar}{2i} \int_{-\infty}^{\infty} dx \left[ \frac{\partial^2 \Psi^*}{\partial x^2} x \Psi - \Psi^* x \frac{\partial^2 \Psi}{\partial x^2} \right] - \frac{1}{i\hbar} \int dx \left[ \Psi^* V(x)x\Psi - \Psi^* xV(x)\Psi \right] \tag{12-47}
\]

The second term is zero, the first term can be integrated by parts:

\[
\frac{\partial^2 \Psi^*}{\partial x^2} x \Psi = \frac{\partial}{\partial x} \left( \frac{\partial \Psi^*}{\partial x} x \Psi \right) - \frac{\partial \Psi^*}{\partial x} \frac{\partial}{\partial x} (x \Psi) \tag{12-49}
\]
\[
= \frac{\partial}{\partial x} \left( \frac{\partial \Psi^*}{\partial x} x \Psi \right) - \frac{\partial \Psi^*}{\partial x} x \Psi - \frac{\partial \Psi^*}{\partial x} x \frac{\partial \Psi}{\partial x} \tag{12-49}
\]

Similarly,

\[
\Psi^* x \frac{\partial^2 \Psi}{\partial x^2} = \left( \frac{\partial^2 \Psi^*}{\partial x^2} x \Psi \right)^* \tag{12-50}
\]

\[
A = \frac{\partial}{\partial x} \left( \frac{\partial \Psi^*}{\partial x} x \Psi - \Psi^* x \frac{\partial \Psi}{\partial x} \right) - \frac{\partial \Psi^*}{\partial x} x \Psi \tag{12-51}
\]
\[
= \frac{\partial}{\partial x} \left( \frac{\partial \Psi^*}{\partial x} x \Psi - \Psi^* x \frac{\partial \Psi}{\partial x} \right) - \frac{\partial}{\partial x} \left( \Psi^* \Psi \right) + 2\Psi^* \frac{\partial \Psi}{\partial x} \tag{12-52}
\]

\[
\boxed{\frac{i\hbar}{\partial t} \frac{\partial \Psi}{\partial t} = \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi \rightarrow \text{SE} \tag{12-53}}
\]

For the wavefunction to be normalizable, it has to vanish at ±∞ faster than \( \frac{1}{\sqrt{x}} \). Consequently, the integral over the first two terms in A yields zero and we are left
with

\[ m \frac{d}{dt} \langle x \rangle = \frac{\hbar}{2i} \int_{-\infty}^{\infty} dx 2\Psi^* \frac{\partial \Psi}{\partial x} \]

\[ = \int_{-\infty}^{\infty} dx \Psi^*(x,t) \left( \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi(x,t) \]  

\[ = \int_{-\infty}^{\infty} dx \Psi^*(x,t) \hat{p} \Psi(x,t) = \langle p \rangle \]

So it follows from the SE that the expectation value of momentum is equal to the particle mass times the rate of change of the expectation value of particle position:

\[ m \frac{d}{dt} \langle x \rangle = \langle p \rangle \]  

This equation follows from the SE in combination with the position representation of the momentum operator \( \hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x} \). Does the appearance of \( \frac{1}{i} \) mean that momentum is complex (imaginary)? Let us calculate the complex conjugate \( \langle p \rangle^* \) of the expectation values of \( \langle p \rangle \) in some arbitrary state \( \Psi(x,t) \) ...