

Thurs: Seminar WS 2023

Fri: MW 5pm

Tues: Read 153-160 (my notes)

Text: Ch 6.1, 6.2

Infinite well kets + wavefunctions

Consider a particle in an infinite well for which

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & \text{otherwise} \end{cases}$$

Then the energy eigenstates $|\phi_n\rangle$ satisfy

$$\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$$

where $n = 1, 2, 3, \dots$. Solving the TISE gives possible energy eigenvalues:

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2}$$

and also the wavefunctions associated with the energy eigenstates:

$$|\phi_n\rangle \rightsquigarrow \phi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & 0 \leq x \leq L \\ 0 & \text{otherwise} \end{cases}$$

These states are orthonormal. Thus

$$\langle \phi_m | \phi_n \rangle = \delta_{mn}.$$

The energy eigenstates are special states - each will give a single outcome with certainty when energy is measured. There must clearly be more general states.

Quantum theory allows for states which are superpositions. Thus we can form:

State

$$|\Psi\rangle = \sum_{n=1}^{\infty} c_n |\phi_n\rangle \quad \rightsquigarrow$$

for complex c_n

Note that in the wavefunction representation

$$\Psi(0) = \sum_{n=1}^{\infty} c_n \underbrace{\phi_n(0)}_0 = 0$$

$$\Psi(L) = \sum_{n=1}^{\infty} c_n \underbrace{\phi_n(L)}_0 = 0$$

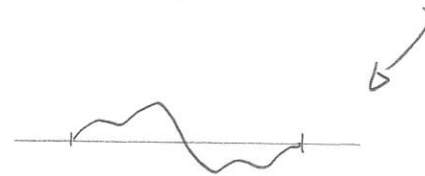
Wavefunction

$$\Psi(x) = \sum_{n=1}^{\infty} c_n \phi_n(x)$$


 $\phi_1(x) \times c_1$


 $\phi_2(x) \times c_2$


 $\phi_3(x) \times c_3$



Demo: Falstad Infinite Well

Note that we can use the ket/state formalism to describe:

- * how the coefficients are constrained.
- * how the coefficients related to measurements
- * how to extract coefficients.

First consider normalization. We show that

$$\left. \begin{array}{l} |\Psi\rangle = \sum_{n=1}^{\infty} c_n |\phi_n\rangle \text{ is normalized} \\ \Psi(x) = \sum_{n=1}^{\infty} c_n \phi_n(x) \text{ is normalized} \end{array} \right\} \Leftrightarrow \sum_{n=1}^{\infty} |c_n|^2 = 1$$

Proof: We require

$$\langle \Psi | \Psi \rangle = 1$$

$$\text{Then } |\Psi\rangle = \sum_{m=1}^{\infty} c_m |\phi_m\rangle \Rightarrow \langle \Psi | = \sum_{m=1}^{\infty} c_m^* \langle \phi_m |$$

$$\begin{aligned} \text{and } \langle \Psi | \Psi \rangle &= \sum_{m=1}^{\infty} c_m^* \langle \phi_m | \sum_{n=1}^{\infty} c_n |\phi_n\rangle \\ &= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_m^* c_n \underbrace{\langle \phi_m | \phi_n \rangle}_{\delta_{mn}} = \sum_{n=1}^{\infty} c_n^* c_n \end{aligned}$$

$$\Rightarrow \sum_{n=1}^{\infty} |c_n|^2 = 1$$

Then the comparable statement for wavefunctions follows in the same way. This requires

$$\langle \phi_m | \phi_n \rangle = \int_{-\infty}^{\infty} \phi_m^*(x) \phi_n(x) dx = \int_0^L \frac{2}{L} \sin\left(\frac{m\pi x}{L}\right) \sin\left(\frac{n\pi x}{L}\right) dx$$

and direct integration shows this is equal to δ_{mn} . \square

Next we can show how to extract coefficients in a superposition.

Thus

$$\text{If } |\Psi\rangle = \sum_{n=1}^{\infty} c_n |\phi_n\rangle \text{ then } c_n = \langle \phi_n | \Psi \rangle$$

$$\text{and if } \Psi(x) = \sum c_n \phi_n(x) \text{ then } c_n = \int_{-\infty}^{\infty} \phi_n^*(x) \Psi(x) dx$$

Proof: $|\Psi\rangle = \sum_{m=1}^{\infty} c_m |\phi_m\rangle$, Then $\langle \phi_n | \Psi \rangle = \sum_{m=1}^{\infty} c_m \underbrace{\langle \phi_n | \phi_m \rangle}_{\delta_{nm}} = c_n$

$$\text{Now } \langle \phi_n | \Psi \rangle = \int_{-\infty}^{\infty} \phi_n^*(x) \Psi(x) dx = c_n \quad \square$$

1 Localized particle in an infinite well

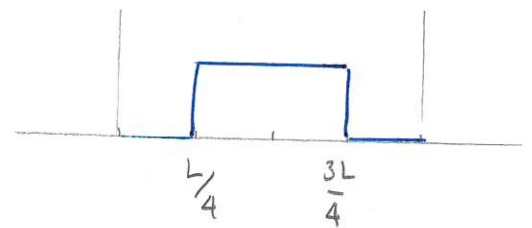
Consider a particle in an infinite well running in the range $0 \leq x \leq L$. Suppose that the wavefunction of the particle is

$$\Psi(x, 0) = \begin{cases} \sqrt{\frac{2}{L}} & \text{if } \frac{L}{4} \leq x \leq \frac{3L}{4} \\ 0 & \text{otherwise.} \end{cases}$$

Determine the coefficients in the expansion of this in terms of the energy eigenstates.

Answer: $\Psi(x) = \sum_{n=1}^{\infty} C_n \Phi_n(x)$

$$C_n = \int_{-\infty}^{\infty} \Phi_n^*(x) \Psi(x) dx$$



and $\Phi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & 0 \leq x \leq L \\ 0 & \text{otherwise} \end{cases}$

So $C_n = \int_{L/4}^{3L/4} \sin\left(\frac{n\pi x}{L}\right) \sqrt{\frac{2}{L}} dx = -\frac{2}{L} \frac{L}{n\pi} \cos\left(\frac{n\pi x}{L}\right) \Big|_{L/4}^{3L/4}$

$$C_n = \frac{2}{n\pi} \left[\cos\left(\frac{n\pi}{4}\right) - \cos\left(\frac{3n\pi}{4}\right) \right]$$

We can compute these:

n=0	C _n
1	$\frac{2}{\pi} \frac{2}{\sqrt{2}}$
2	0
3	$-\frac{2}{3\pi} \frac{2}{\sqrt{2}}$
4	0
5	$\frac{2}{5\pi} \frac{2}{\sqrt{2}}$

$$C_n = \begin{cases} \frac{4}{\sqrt{2}\pi n} (-1)^{(n-1)/2} & n \text{ odd} \\ 0 & n \text{ even} \end{cases}$$

General systems in one dimension

The same process applies to any system in one dimension.

Solve TISE to obtain energy states / wavefunctions

$$\hat{H} |\phi_E\rangle = E |\phi_E\rangle$$

$$\leadsto -\frac{\hbar^2}{2m} \frac{\partial^2 \phi_E}{\partial x^2} + V(x) \phi_E = E \phi_E(x)$$

↓

energy eigenstates and wavefunctions

$$|\phi_E\rangle \text{ for allowed } E \quad \leadsto \quad \phi_E(x) \text{ for allowed } E$$

∑
↓

An arbitrary state can be represented as a superposition of energy eigenstates:

$$|\Psi\rangle = \sum_E c_E |\phi_E\rangle$$

$$\leadsto \Psi(x) = \sum_E c_E \phi_E(x)$$

↓

Obtain coefficients via

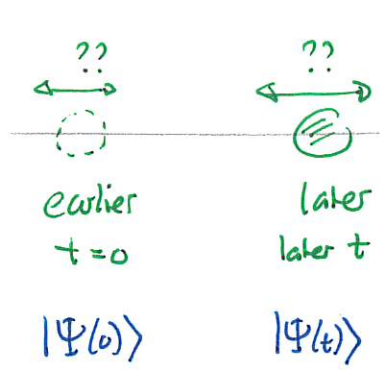
$$c_E = \langle \phi_E | \Psi \rangle$$

$$c_E = \int_{-\infty}^{\infty} \phi_E^*(x) \Psi(x) dx$$

Demo: QuVis Expansion in eigenstates

Time evolution for systems in one dimension

The state of a particle in one dimension will typically change as time passes. Thus in general we expect the wavefunction to display time evolution. The formalism is then that the ket depends on time



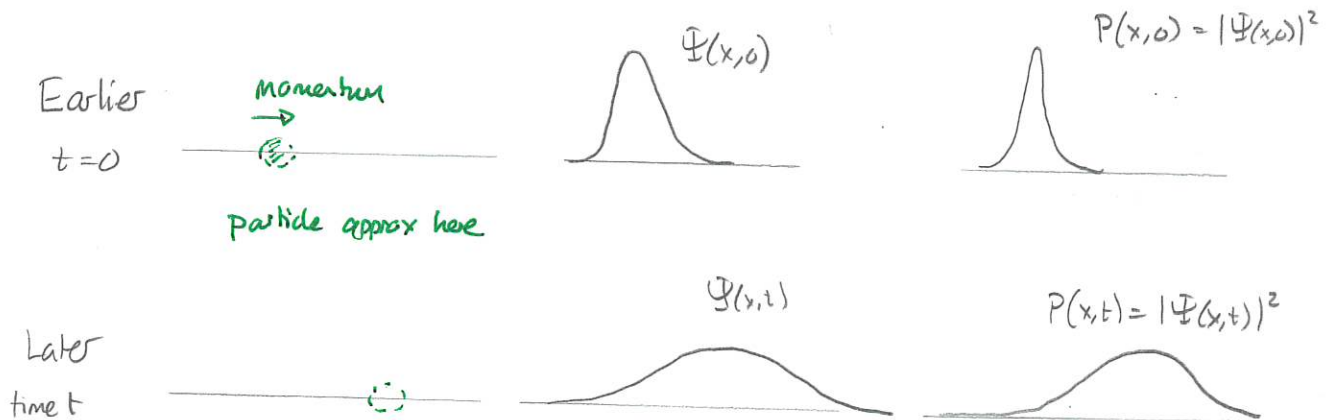
$$|\Psi(t)\rangle$$

The corresponding wavefunction will also depend on time since $\Psi(x) = \langle x | \Psi(t) \rangle$. Thus we get an associated wavefunction

$$\Psi(x, t)$$

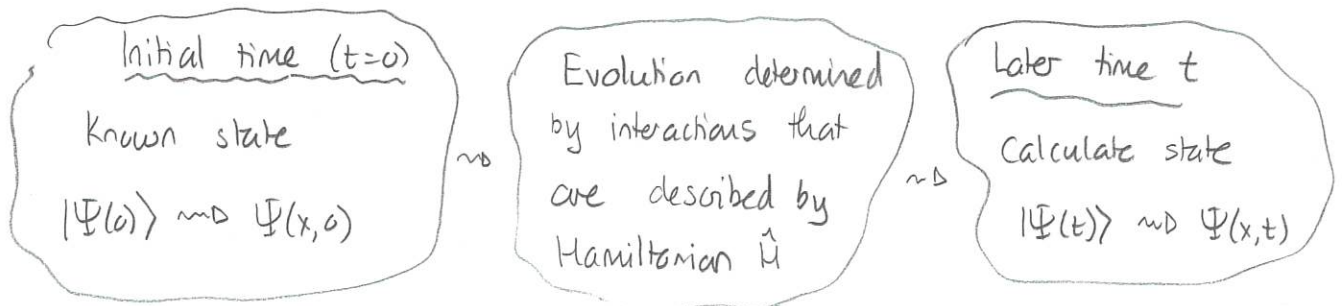
that is a complex valued function of position and time. Similarly for the probability density

So we have



Demo: QnV's Gaussian Wave Packet

The issue is then to determine how the wavefunction evolves so that we can determine statistics of measurements at later times. Thus



The evolution of the state will follow the general rule encountered previously:

$$|\Psi(t)\rangle = \hat{U}(t) |\Psi(0)\rangle \quad \text{where } \hat{U}(t) \text{ is a unitary evolution operator determined by the Hamiltonian}$$

The evolution operator can be determined indirectly by solving the Schrödinger equation:

$$i\hbar \frac{d|\Psi(t)\rangle}{dt} = \hat{H} |\Psi(t)\rangle \quad \text{where } \hat{H} \text{ is the Hamiltonian}$$

It is then straightforward algebra to show that

$$\text{If the Hamiltonian is time-independent then} \\ \hat{U}(t) = e^{-i\hat{H}t/\hbar}$$

However, actually exponentiating the Hamiltonian is usually not feasible or can be difficult. There are alternatives that use energy eigenstates. We will see that

Determine how any single energy eigenstate evolves

Determine how superposition evolves

Express initial state as superposition of energy eigenstates

This will use the following:

$$\text{For any integer } m \quad \underbrace{\hat{H}^m}_{\text{operator}} |\phi_E\rangle = \underbrace{E^m}_{\text{number}} |\phi_E\rangle$$

$$\begin{aligned} \text{Proof: } \hat{H}^m |\phi_E\rangle &= \hat{H}^{m-1} \underbrace{\hat{H} |\phi_E\rangle}_{E |\phi_E\rangle} = E \hat{H}^{m-1} |\phi_E\rangle \\ &= E \underbrace{E \hat{H}^{m-2} |\phi_E\rangle}_{\text{number}} \\ &= E^2 \hat{H}^{m-2} |\phi_E\rangle \\ &\quad \vdots \\ &= E^m |\phi_E\rangle \quad \square \end{aligned}$$

For any energy eigenstate $|\phi_E\rangle$ with eigenvalue E

$$\underbrace{e^{-i\hat{H}t/\hbar}}_{\text{operator}} |\phi_E\rangle = e^{-iEt/\hbar} \underbrace{|\phi_E\rangle}_{\text{number}}$$

$$\begin{aligned} \text{Proof: } e^{-i\hat{H}t/\hbar} |\phi_E\rangle &= \sum_{m=0}^{\infty} \frac{1}{m!} \left(\frac{-i\hat{H}t}{\hbar}\right)^m |\phi_E\rangle \\ &= \sum_{m=0}^{\infty} \frac{1}{m!} \left(\frac{-it}{\hbar}\right)^m \underbrace{\hat{H}^m |\phi_E\rangle}_{E^m |\phi_E\rangle} \\ &= \underbrace{\sum_{m=0}^{\infty} \frac{1}{m!} \left(\frac{-itE}{\hbar}\right)^m}_{e^{-iEt/\hbar}} |\phi_E\rangle \\ &= e^{-iEt/\hbar} |\phi_E\rangle \quad \square \end{aligned}$$

2 Evolution of wavefunctions for a particle in one dimension

Let $|\phi_E\rangle$ be the eigenstate of \hat{H} with energy E .

a) Suppose that at $t = 0$ the state of the system is

$$|\Psi(0)\rangle = |\phi_E\rangle \leftrightarrow \phi_E(x).$$

Determine an expression for the wavefunction and the position probability density at all later times. Does the position probability density depend on time?

b) Suppose that at $t = 0$ the state of the system is an arbitrary superposition

$$|\Psi(0)\rangle = \sum_E c_E |\phi_E\rangle$$

Show that

$$|\Psi(t)\rangle = \sum_E c_E e^{-iEt/\hbar} |\phi_E\rangle.$$

How does this translate into a statement involving wavefunctions?

Answer: $|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\Psi(0)\rangle$

a) Here

$$|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\phi_E\rangle = e^{-iEt/\hbar} |\phi_E\rangle$$

$$\Rightarrow \Psi(x,t) = e^{-iEt/\hbar} \phi_E(x)$$

$$P(x,t) = |\Psi(x,t)|^2 = |e^{-iEt/\hbar} \phi_E(x)|^2 = |\phi_E(x)|^2$$

This does not depend on time.

$$b) |\Psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\Psi(0)\rangle = e^{-i\hat{H}t/\hbar} \sum_E c_E |\phi_E\rangle$$

$$= \sum_E c_E e^{-i\hat{H}t/\hbar} |\phi_E\rangle$$

$$= \sum_E c_E e^{-iEt/\hbar} |\phi_E\rangle$$

$$\Rightarrow \Psi(x,t) = \sum_E c_E e^{-iEt/\hbar} \phi_E(x)$$

Thus

Given initial state
 $|\Psi(0)\rangle \rightsquigarrow \Psi(x,0)$

Decompose into superposition of
energy eigenstates

$$|\Psi(0)\rangle = \sum C_E |\phi_E\rangle \quad C_E = \langle \phi_E | \Psi \rangle$$

\Downarrow

$$\Psi(x,0) = \sum_E C_E \phi_E(x)$$

$$C_E = \int_{-\infty}^{\infty} \phi_E^*(x) \Psi(x) dx$$

Under Hamiltonian \hat{H}
the state at a later time is

$$|\Psi(t)\rangle = \sum_E C_E e^{-iEt/\hbar} |\phi_E\rangle$$

\Downarrow

$$\Psi(x,t) = \sum_E C_E e^{-iEt/\hbar} \phi_E(x,t)$$

where C_E are obtained from
state at $t=0$ as above

We see that a special case is that where the initial state is
an energy eigenstate.

If the initial state of the system is an energy eigenstate

$$|\Psi(0)\rangle = |\phi_E\rangle$$

for some E then the later state is

$$|\Psi(t)\rangle = e^{-iEt/\hbar} |\phi_E\rangle = e^{-iEt/\hbar} |\phi_E\rangle$$

and this only differs from the initial state by an irrelevant
global phase.

Thus energy eigenstates do not produce meaningful time-evolution. However,
superpositions of energy eigenstates do produce meaningful time evolution.

3 Time-evolution for a particle in an infinite well

A particle in an infinite well is initially in the state

$$|\Psi(0)\rangle = \frac{1}{\sqrt{2}} |\phi_1\rangle + \frac{1}{\sqrt{2}} |\phi_2\rangle$$

where $|\phi_1\rangle$ are energy eigenstates. Determine the state at a later time and use this to determine an expression for the position probability density at a later time, in terms of $\phi_1(x)$ and $\phi_2(x)$.

Answer: $|\Psi(t)\rangle = \frac{1}{\sqrt{2}} e^{-iE_1 t/\hbar} |\phi_1\rangle + \frac{1}{\sqrt{2}} e^{-iE_2 t/\hbar} |\phi_2\rangle$

where $E_n = m^2 \frac{\pi^2 \hbar^2}{2mL^2}$

Then the wavefunction is

$$\Psi(x,t) = \frac{1}{\sqrt{2}} \left[e^{-iE_1 t/\hbar} \phi_1(x) + e^{-iE_2 t/\hbar} \phi_2(x) \right]$$

and the position probability density is

$$\begin{aligned} P(x,t) &= |\Psi(x,t)|^2 = \frac{1}{2} \left[e^{-iE_1 t/\hbar} \phi_1(x) + e^{-iE_2 t/\hbar} \phi_2(x) \right]^* \\ &\quad \left[e^{-iE_1 t/\hbar} \phi_1(x) + e^{-iE_2 t/\hbar} \phi_2(x) \right] \\ &= \frac{1}{2} \left[e^{iE_1 t/\hbar} \phi_1^*(x) + e^{iE_2 t/\hbar} \phi_2^*(x) \right] \left[\dots \right] \\ &= \frac{1}{2} \left[\phi_1^*(x) \phi_1(x) + \phi_2^*(x) \phi_2(x) + \phi_1^*(x) \phi_2(x) e^{i(E_1 - E_2)t/\hbar} \right. \\ &\quad \left. + \phi_1(x) \phi_2^*(x) e^{-i(E_1 - E_2)t/\hbar} \right] \end{aligned}$$

But ϕ_1, ϕ_2 are real. Thus

$$\begin{aligned} P(x,t) &= \frac{1}{2} \left[\phi_1^2(x) + \phi_2^2(x) + \phi_1(x) \phi_2(x) 2 \cos\left(\frac{(E_1 - E_2)t}{\hbar}\right) \right] \\ &= \frac{1}{2} \left[\phi_1^2(x) + \phi_2^2(x) + 2\phi_1(x) \phi_2(x) \cos\left(\frac{(E_2 - E_1)t}{\hbar}\right) \right] \end{aligned}$$

Thus for this superposition, the position probability density oscillates with frequency

$$\omega = \frac{E_2 - E_1}{\hbar} \quad \Rightarrow \quad \Delta E = \hbar \omega$$

This oscillatory behavior is typical of superposition states.

Demo: QnVis - Superposition in an infinite square well.