Tues: HW 5pm

Thurs: Seminar

Thurs: Read pg 142-153

Fri: HW 5pm

Kronecker delta review

Recall that the Kronecker delta has two integer indices and

$$\delta_{mn} = \begin{cases} 0 & m \neq n \\ 1 & m = n \end{cases}$$

This frequently occurs in orthonormality relations. Thus for normalized energy eigenstates $|\phi_n\rangle$,

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

and this results in the delta function appearing in summations.

1 Kronecker delta and summation

In the following consider arbitrary complex numbers $\{a_n | n = 1, 2, \ldots\}$ and $\{b_n | n = 1, 2, \ldots\}$.

a) Simplify $\sum_n a_n \delta_{n2}$.

b) Simplify $\sum_n a_n \delta_{n3}$.

c) Consider $\sum_n a_n \delta_{nm}$ for any integer m. Would n remain after this is simplified?

d) Expand $\sum_{n=1}^{2} a_n b_n$. Does this equal $b_n \sum_{n=1}^{2} a_n$?

e) Expand $\sum_{n=1}^{2} a_n \sum_{m=1}^{2} b_m$. Does this equal $\sum_{n=1}^{2} a_n b_n$?

f) Expand $\sum_{n=1}^{2} a_n \sum_{m=1}^{2} b_m \delta_{mn}$. Does this equal $\sum_{n=1}^{2} a_n b_n$?

Answer:

a) $\sum_n a_n \delta_{n2} = a_1 \overset{0}{\cancel{\delta_{12}}} + a_2 \overset{1}{\cancel{\delta_{22}}} + a_3 \overset{0}{\cancel{\delta_{32}}} + \ldots = a_2$

b) $\sum_n a_n \delta_{n3} = a_1 \overset{1}{\cancel{\delta_{13}}} + a_2 \overset{0}{\cancel{\delta_{23}}} + a_3 \overset{1}{\cancel{\delta_{33}}} + a_4 \overset{0}{\cancel{\delta_{34}}} + \ldots = a_3$.

c) The only term in the sum that gives non-zero is when $n = m$.

Thus

$\sum_n a_n \delta_{nm} = a_m \overset{1}{\cancel{\delta_{mm}}} = a_m$ (n does not remain)

d) $a_1 b_1 + a_2 b_2$. $b_n \sum_{n=1}^{2} a_n = b_n (a_1 + a_2)$ not the same.

e) $(a_1 + a_2)(b_1 + b_2) = a_1 b_1 + a_1 b_2 + a_2 b_1 + a_2 b_2$

$\sum_{n=1}^{2} a_n b_n = a_1 b_1 + a_2 b_2$ not equal

f) $\sum_{n=1}^{2} a_n \sum_{m=1}^{2} b_m \delta_{mn} = \sum_{n=1}^{2} a_n (b_1 \delta_{1n} + b_2 \delta_{2n})$

$= a_1 (b_1 \overset{1}{\cancel{\delta_{11}}} + b_2 \overset{0}{\cancel{\delta_{21}}}) + a_2 (b_1 \overset{0}{\cancel{\delta_{12}}} + b_2 \overset{1}{\cancel{\delta_{22}}})$

$= a_1 b_1 + a_2 b_2$

$= \sum_{n=1}^{2} a_n b_n$

States and wavefunctions for particles moving in one dimension

Consider a particle moving in one dimension. Such a particle could be subjected to various measurements and the same general formalism for quantum theory applies

particle

state

$|\Psi\rangle$

$\boxed{\text{Measure position}}$

possible outcomes

- any $x \in \mathbb{R}$ (could be constrained depending on system)

can **calculate**

- probability that outcome is in range $x \to x + dx$.

OR

$\boxed{\text{Measure momentum}}$

possible outcomes

- any $p \in \mathbb{R}$.

can **calculate**

- probability that outcome is in range $p \to p + dp$.

OR

$\boxed{\text{Measure energy}}$

possible outcomes

- depends on system
  - e.g. for free particle any $E > 0$
  - e.g. for particle in well one of $E_1, E_2, E_3, \ldots$

- can **calculate**
  - probability for each outcome.

Although the state formalism can be used it is often converted into a wavefunction formalism for purposes of calculating probabilities. Thus we find that:

Given that the state of the particle is $|\Psi\rangle$ there is an associated complex-valued wavefunction $\Psi(x)$.

$\downarrow$

Given two states with associated wavefunctions

$$|\Psi\rangle \rightsquigarrow \Psi(x)$$

$$|\Phi\rangle \rightsquigarrow \Phi(x)$$

then the inner product of $|\Phi\rangle$ with $|\Psi\rangle$ is

$$\langle\Phi|\Psi\rangle = \int_{-\infty}^{\infty} \Phi^*(x)\,\Psi(x)\,dx$$

$\downarrow$

The probability density for position measurements for a particle in state $|\Psi\rangle$ is:

$$P(x) = |\Psi(x)|^2$$

and thus, for a position measurement,

$$\text{Prob}\,(a \leq x \leq b) = \int_a^b |\Psi(x)|^2\,dx$$

Actually finding the wavefunction from the state $|\Psi\rangle$ requires particular detailed knowledge about the construction of the state and will vary depending on the circumstances

Explanation in terms of the general framework

The position states $\{|x\rangle\}$ satisfy two crucial rules:

1) $\langle x'|x\rangle = \delta(x'-x)$ (orthonormality)

2) $\displaystyle\int_{-\infty}^{\infty} |x\rangle\langle x|\, dx = \hat{I}$ (completeness).

Then the meaning of the wavefunction is

$$\Psi(x) = \langle x|\Psi\rangle.$$

Thus

$$\int_{-\infty}^{\infty} \Psi(x)\, |x\rangle\, dx = \int_{-\infty}^{\infty} \langle x|\Psi\rangle\, |x\rangle dx = \int_{-\infty}^{\infty} |x\rangle\langle x| dx\, |\Psi\rangle = |\Psi\rangle.$$

So

$$|\Psi\rangle = \int_{-\infty}^{\infty} \Psi(x)|x\rangle\, dx$$

Then $|\Phi\rangle = \displaystyle\int_{-\infty}^{\infty} \Phi(x')\, |x'\rangle dx' \Rightarrow \langle\Phi| = |\Phi\rangle^{\dagger} = \int_{-\infty}^{\infty} \Phi^*(x')\langle x'|\, dx'$

$$\Rightarrow \langle\Phi|\Psi\rangle = \int_{-\infty}^{\infty} dx'\, \Phi^*(x')\langle x'| \int_{-\infty}^{\infty} \Psi(x)\, |x\rangle dx = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx'\, \Phi^*(x')\, \Psi(x) \langle x'|x\rangle$$

$$= \int_{-\infty}^{\infty} dx \int dx'\, \Phi^*(x')\, \Psi(x)\, \delta(x'-x)$$

$$= \int_{-\infty}^{\infty} dx\, \Psi(x)\, \Phi^*(x) \Rightarrow \langle\Phi|\Psi\rangle = \int_{-\infty}^{\infty} \Phi^*(x)\, \Psi(x)\, dx.$$

The measurement result comes from. The measurement operator for outcome x is

$$\hat{P}_x = |x\rangle\langle x|.$$

Then the operator for outcomes $a \le x \le b$ is $\displaystyle\int_a^b |x\rangle\langle x|\, dx$ (sum of all meas ops in range)

Thus

$$\text{Prob}(a \leq x \leq b) = \langle \Psi | \int_a^b |x\rangle\langle x| \, dx \, |\Psi\rangle$$

$$= \int_a^b \langle \Psi(x)\rangle\langle x|\Psi\rangle \, dx$$

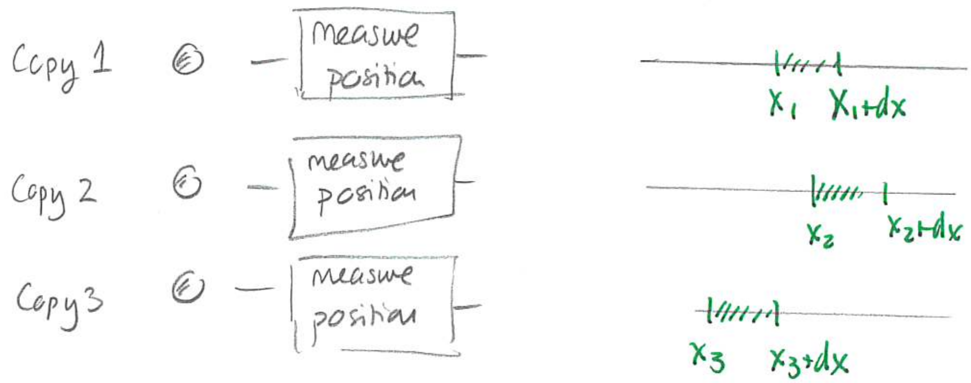
$$= \int_a^b \Psi^*(x)\,\Psi(x)\, dx$$

$$= \int_a^b |\Psi(x)|^2 \, dx$$

Thus the position probability density is $P(x) = |\Psi(x)|^2$. $\boxtimes$

Statistics of position measurement outcomes.

Suppose that we have an ensemble of particles each in state $|\Psi\rangle$ and that we measure the position of each ensemble member



We could average the outcomes giving

$$\text{sample average} = \frac{x_1 + x_2 + \dots}{\text{total number particles}}$$

Given that the particles are all in the same state, we should be able to approximate the sample average via an expectation value calculated from $|\Psi\rangle$. We will show that.

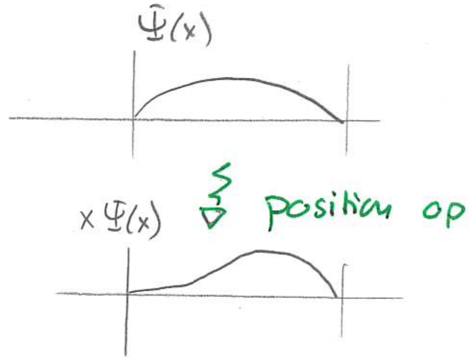
> For a system in state $|\Psi\rangle$, the expectation value of position measurement outcomes is
>
> $$\langle x\rangle = \langle \Psi|\hat{x}|\Psi\rangle$$
>
> where $\hat{x}$ is a position operator (observable) and this gives
>
> extra factor of x
>
> $$\langle x\rangle = \int \Psi^*(x)\, x\, \Psi(x)\, dx$$

In general the expectation value of any power of x is:

$$\boxed{\begin{aligned} \langle x^n \rangle &= \int_{-\infty}^{\infty} \Psi^*(x)\, x^n\, \Psi(x)\, dx \\ &\text{or} \\ \langle x^n \rangle &= \langle \Psi | \hat{x}^n | \Psi \rangle \end{aligned}}$$

We can also represent the position operator in terms of its actions on wave functions

$$\begin{array}{ccc} |\Psi\rangle & \rightsquigarrow & \Psi(x) \\ \big\downarrow \text{position op} & & \big\Downarrow \\ \hat{x}|\Psi\rangle & \rightsquigarrow & x\,\Psi(x) \end{array}$$



Explanation in terms of the general framework.

The position operator satisfies an eigenvalue equation for the position states.

For any $x \in \mathbb{R}$: $\hat{x}|x\rangle = x|x\rangle$

label number label

Thus

$$\langle x \rangle = \langle \Psi | \hat{x} | \Psi \rangle = \langle \Psi | \hat{x} \underbrace{\int_{-\infty}^{\infty} |x\rangle\langle x|\, dx}_{\hat{I}} |\Psi\rangle$$

$$= \langle \Psi | \int_{-\infty}^{\infty} \underbrace{\hat{x}|x\rangle}_{x|x\rangle} \underbrace{\langle x | \Psi\rangle}_{\Psi(x)}\, dx$$

and

$$\langle x \rangle = \int_{-\infty}^{\infty} x \langle \Psi | x \rangle \langle x | \Psi \rangle \, dx$$

$$= \int_{-\infty}^{\infty} x \, \Psi^*(x) \Psi(x) \, dx \quad = \int_{-\infty}^{\infty} \Psi^*(x) \, x \, \Psi(x) \, dx$$

The x^n rule follows by iteration

2 Expectation value of position

Suppose that a particle is in the state

$$|\Psi\rangle \leftrightarrow \Psi(x) = Ae^{-x^2/2\alpha^2}$$

where $\alpha > 0$. Determine $\langle x \rangle$.

Answer:

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^*(x)\, x\, \Psi(x)\, dx$$

$$= \int_{-\infty}^{\infty} |A|^2 e^{-x^2/\alpha^2}\, x\, dx = |A|^2 \underbrace{\int x e^{-x^2/\alpha^2} dx}_{=0}$$

since function is antisymmetric about $x=0$

$$\Rightarrow \langle x \rangle = 0.$$

Momentum operator

There is an observable associated with momentum measurements. Denote momentum by p and the associated observable $\hat{p}$. We need to represent the action of this as an action on wavefunctions.

$$
\begin{tikzcd}
|\Psi\rangle \arrow[r, rightsquigarrow] \arrow[d, "\hat{p}"] & \Psi(x) \arrow[d, "\hat{p}"] \\
\hat{p}|\Psi\rangle \arrow[r, rightsquigarrow] & -i\hbar\dfrac{\partial\Psi}{\partial x}
\end{tikzcd}
$$

The latter is an assumption which must eventually be used to make predictions about observable quantities. One way that is is done is to incorporate it into energy expressions. These will involve terms such as

$$\hat{p}^2|\Psi\rangle \rightsquigarrow -i\hbar\frac{\partial}{\partial x}\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$$

Successive actions with the momentum operator map wavefunctions into new wavefunctions.

3 Momentum operator and wavefunctions

Suppose that a particle is in the state

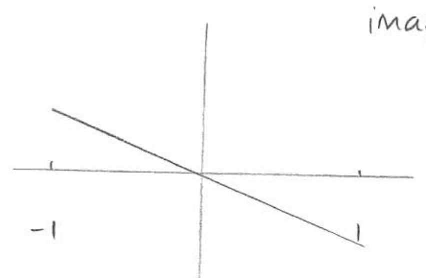
$$|\Psi\rangle \leftrightarrow \Psi(x) := \begin{cases} \sqrt{\dfrac{15}{16}}\,(x^2-1) & \text{if } -1 \leqslant x \leqslant 1 \\ 0 & \text{if } |x| \geqslant 1. \end{cases}$$

a) Determine the wavefunction representing $\hat{p}\,|\Psi\rangle$. Sketch this qualitatively.

b) Determine the wavefunction representing $\hat{p}^2\,|\Psi\rangle$. Is this wavefunction normalized? Sketch this qualitatively.

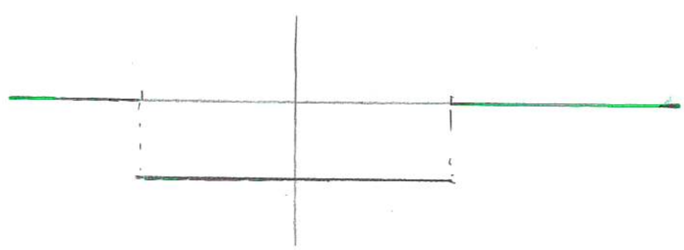
Answer: a) $\hat{p}|\Psi\rangle \rightsquigarrow -i\hbar \frac{\partial \Psi}{\partial x} = \begin{cases} -i\hbar \sqrt{\frac{15}{16}} \frac{\partial}{\partial x}(x^2-1) & -1 \leq x \leq 1 \\ 0 & \text{otherwise} \end{cases}$

$$= \begin{cases} -i\hbar \sqrt{\frac{15}{16}}\, 2x & |x| \leq 1 \\ 0 & \text{otherwise} \end{cases}$$



b) $\hat{p}^2|\Psi\rangle \rightsquigarrow -i\hbar\frac{\partial}{\partial x}\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi = \begin{cases} -i\hbar \frac{\partial}{\partial x}\left(-i\hbar\sqrt{\frac{15}{16}}\,2x\right) & |x| \leq 1 \\ 0 & |x| \geq 1 \end{cases}$

$$= \begin{cases} -\hbar^2 \sqrt{\frac{15}{16}}\, 2 & |x| \leq 1 \\ 0 & |x| \geq 1 \end{cases}$$



then labeling this $\Phi(x)$

$$\int_{-\infty}^{\infty} |\Phi(x)|^2 dx = \int_{-1}^{1} \hbar^4 \frac{15}{4}\, dx$$

$$= \hbar^4 \frac{15}{2} \quad \text{not normalized.}$$

Energy operator

We can construct the energy observable, Hamiltonian, for a particle moving in one dimension that is the analog of a classical particle. To do this we use the scheme

Construct the energy for the classical system in terms of p, x.

$$E_{classical} = \frac{p^2}{2m} + V(x)$$

where $V(x)$ is a potential energy that only depends on x

$\longrightarrow$

Construct a Hamiltonian by replacing

$p \rightsquigarrow \hat{p}$ observable

$x \rightsquigarrow \hat{x}$ observable

$\downarrow$

Hamiltonian

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{x})$$

Note that $V(x)$ could be a complicated function of x but as long as it has a converging Taylor series we can construct an operator

$$V(x) = \sum_{n=0}^{\infty} a_n x^n \quad \rightsquigarrow \quad V(\hat{x}) = \sum_{n=0}^{\infty} a_n \hat{x}^n$$

real

same real

well defined.

Energy eigenstates: Time-independent Schrödinger equation

The energy eigenstates satisfy the usual eigenvalue equation:

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

where E is a real eigenvalue and $|\phi_E\rangle$ is the energy eigenstate associated with eigenvalue E. This can be expressed as

$$\boxed{\left[\frac{1}{2M}\hat{p}^2 + V(\hat{x})\right]|\phi_E\rangle = E|\phi_E\rangle}$$

and can be converted into an equation for the wavefunction associated with $|\phi_E\rangle$:

$$|\phi_E\rangle \rightsquigarrow \phi_E(x)$$

Then

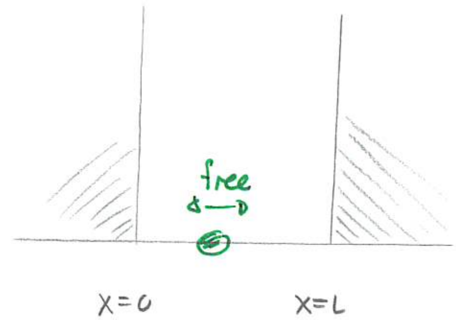
$$(-i\hbar)^2 \frac{\partial^2\phi_E}{\partial x^2} + V(x)\,\phi_E(x) = E\,\phi_E(x)$$

$$\Rightarrow \boxed{-\hbar^2 \frac{\partial^2\phi_E}{\partial x^2} + V(x)\,\phi_E(x) = E\,\phi_E(x)}$$

This is the time-independent Schrödinger equation. So it gives a scheme

Provide potential $V(x)$ → Solve TISE for energy eigenstate function $\phi_E(x)$ → This gives the wavefunction that represents the state and can be used in probability and other calculations

Example: Particle in an infinite well



In an infinite well, a particle is restricted to a finite range ($0 \leq x \leq L$) but is free within that range. Within this range the particle is free. The potential is

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

The only permissible solutions to the TISE have $\phi(x) = 0$ outside the well and

$$\phi(0) = \phi(L) = 0 \qquad \text{Boundary conditions}$$

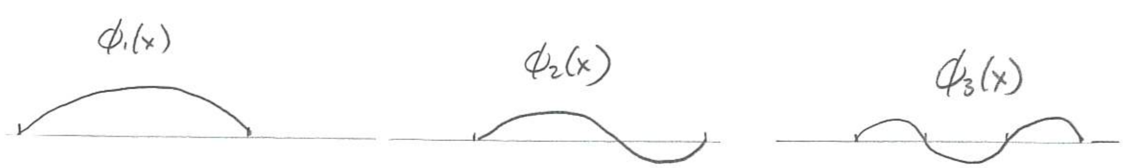
Then, inside the well the TISE gives

$$-\frac{\hbar^2}{2m}\frac{d^2\phi_E}{dx^2} = E\,\phi_E(x) \qquad \text{Differential equation}$$

Solving the TISE gives:

> The possible energy eigenvalues and states are labeled by
> $n = 1, 2, 3, \ldots$
>
> and the energy eigenvalues are
>
> $$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$
>
> and the associated wavefunctions are
>
> $$\phi_n(x) = \sqrt{\frac{2}{L}}\,\sin\left(\frac{n\pi x}{L}\right)$$

The lowest three are plotted:



$$E_1 = \frac{\pi^2\hbar^2}{2mL^2} \qquad E_2 = 4\,\frac{\pi^2\hbar^2}{2mL^2} \qquad E_3 = 9\,\frac{\pi^2\hbar^2}{2mL^2}$$