Phys 321 2023

Lecture 15

Fri: HW by 5pm

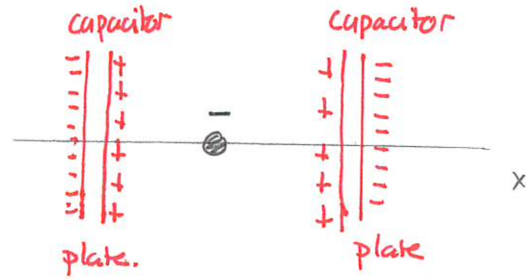
Tues: March 28 – HW 5pm

– Read ... Text 5.3, 5.4.

My notes 1.3, 2.0.1.

Position and momentum measurements

We will need to consider particles which can move in one or more spatial dimension. A charged particle trapped in an infinite well could be an example. In this case we could



* measure the particle's energy
* measure the " position
* measure the " momentum

...

In order to answer questions about the energy we would need to construct the Hamiltonian. A further question would be

* how can one construct the Hamiltonian from the comparable classical energy

$$E = \frac{p^2}{2m} + V(x).$$

In order to answer these we will need to describe

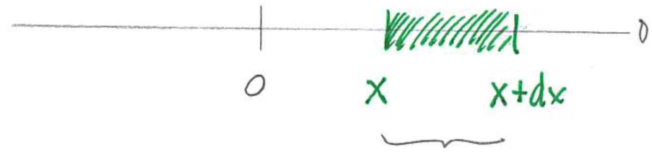
* position states + measurement outcomes
* position observable
* momentum states + measurement outcomes
* momentum observable

The first complication here is that the measurement outcome possibilities are continuous. This means that we cannot make any statement about the probability of a particular outcome, e.g

$$\text{Prob}\,(x = 6.3) = ?$$

or $\text{Prob}(x = -12.6) = ?$

Rather we can describe the probability of an outcome in a given range. So we can get



what is probability that measurement gives outcome here?

$$\text{Prob}\left(\begin{array}{l}\text{position is in}\\ \text{range } x \to x+dx\end{array}\right)$$

or

$$\text{Prob}\,(a \leq x \leq b)$$

The route to answering these questions is via a probability density $P(x)$. This is a quantity that roughly means

$$\text{Prob}\left(\begin{array}{l}\text{position outcome in}\\ \text{range } x \to x+dx\end{array}\right) = P(x)\,dx$$

or more precisely

$$\boxed{\text{Prob}\,(a \leq x \leq b) = \int_a^b P(x)\,dx}$$

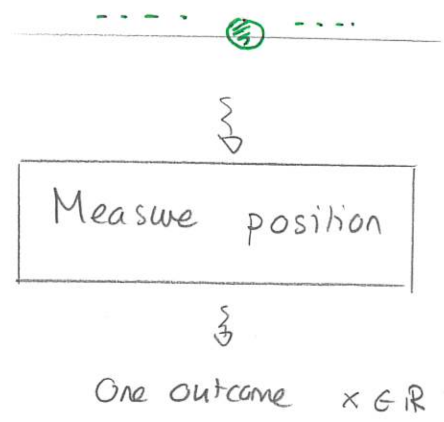
What quantum theory will do is.

Provide state of system $|\Psi\rangle$ ⟶ Construct wavefunction from state $\Psi(x)$ ⟶ Construct probability density for position measurements $P(x) = |\Psi(x)|^2$

Process takes state + produces prob density

⟶ Determine probabilities and statistics of measurement outcomes

Position "states" and measurements



Consider a particle restricted to one spatial dimension. In an idealized situation, a position measurement would yield one outcome with perfect precision. We must then have a table

outcome	associated state
$\vdots$	$\vdots$
x	$\lvert x\rangle$
$\vdots$	$\vdots$

any real number

Then the set of associated states is

$$\{ \lvert x\rangle : \text{all real } x \}$$

These must be orthogonal for different outcomes. Thus

$$\boxed{\text{If } x \neq x' \text{ then } \langle x' \vert x\rangle = 0}$$

We will consider $x = x'$ in a while. These states form a basis and thus we expect that for any state

$$\lvert\Psi\rangle = \sum \Psi_x \lvert x\rangle$$

where Ψ_x are real. However the range of x is continuous and the sum must be replaced by an integral. The subscript will be replaced by a functional variable. So

sum.

$$\boxed{\lvert\Psi\rangle = \int_{-\infty}^{\infty} \underbrace{\Psi(x)}_{\text{coefficient}} \underbrace{\lvert x\rangle}_{\text{basis}} \, dx}$$

where $\Psi(x)$ is a complex valued function (with units m^{-1}) called a wavefunction

Then we obtain a bra via

$$\langle\Psi| = |\Psi\rangle^{\dagger}$$

$$= \left[\int_{-\infty}^{\infty}\Psi(x)|x\rangle\, dx\right]^{\dagger} = \int_{-\infty}^{\infty}\left(\Psi(x)|x\rangle\, dx\right)^{\dagger}$$

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

So

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

As before the probabilities of measurement outcomes will require inner products. This will require $\langle x'|x\rangle$ for $x' = x$.

Dirac delta function

Recall the Kronecker delta function that has two integer arguments

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

This was useful for certain basis states $\{|n\rangle : n = 1, 2, \ldots\}$ where

$$\langle m|n\rangle = \delta_{mn}$$

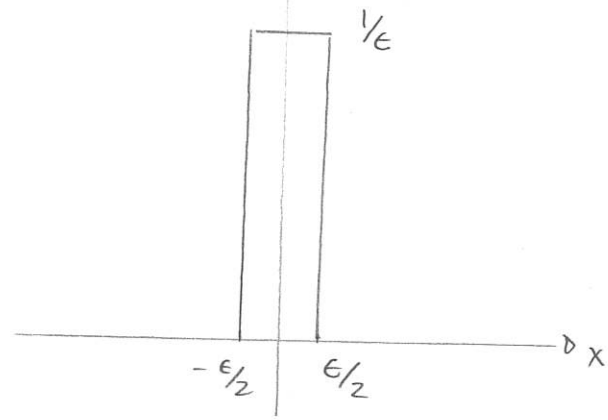
This can be extended to continuous variable labels/indices,... via the <u>Dirac delta function:</u>

$$\delta(x) = \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases}$$

is defined so that for any function $f(x)$,

$$\int_{-\infty}^{\infty} f(x)\,\delta(x)\, dx = f(0)$$

One graphical way to represent uses



$$\delta_\epsilon(x) := \begin{cases} \frac{1}{\epsilon} & -\frac{\epsilon}{2} \leq x \leq \epsilon/2 \\ 0 & \text{otherwise} \end{cases}$$

as $\epsilon \to 0$.

Then definitely

$$\int_{-\infty}^{\infty} \delta_\epsilon(x)\,dx = \int_{-\infty}^{\infty} \delta_\epsilon(x)\, 1 \,dx = 1 = \int_{-\infty}^{\infty} \delta(x)\,dx$$

and so this at least works for a constant function. For a general function

$$\delta_\epsilon(x) f(x) \to \frac{1}{\epsilon} f(0) \quad \text{as } \epsilon \to \infty$$

$$\Rightarrow \int_{-\infty}^{\infty} \delta_\epsilon(x) f(x)\,dx = \int_{-\epsilon/2}^{\epsilon/2} \frac{1}{\epsilon} f(0)\,dx \to f(0) \quad \text{as } \epsilon \to 0$$

1 Dirac delta function: basic rules

a) Show that

$$\delta(x - x') := \begin{cases} 0 & \text{if } x \neq x' \\ \infty & \text{if } x = x'. \end{cases}$$

and

$$\int_{-\infty}^{\infty} f(x')\, \delta(x - x')\, \mathrm{d}x' = f(x).$$

b) Evaluate

$$\int_{-\infty}^{\infty} x' e^{-x'\lambda} \delta(x - x')\, \mathrm{d}x'.$$

c) Show that

$$\int_{-\infty}^{\infty} \delta(x - x')\, \mathrm{d}x' = 1.$$

Answer: a) If $x \neq x'$ then $\delta(\text{argument} \neq 0) = 0$

If $x = x'$ then $\delta(x-x') = \delta(0) = \infty$

$$\int_{-\infty}^{\infty} f(x')\, \delta(x-x')\, dx' = \int_{\infty}^{-\infty} f(x+u)\, \delta(u)\, (-du) \qquad u = x - x'$$

$$= \int_{-\infty}^{\infty} f(x+u)\, \delta(u)\, du = f(x+0) = f(x)$$

b) Here $f(x') = x' e^{-x'\lambda}$, So

$$\int_{-\infty}^{\infty} x' e^{-x'\lambda} \delta(x-x')\, dx' = f(x) = x e^{-x\lambda} \Rightarrow \int_{-\infty}^{\infty} x' e^{-x'\lambda} \delta(x-x')\, dx' =$$

c) Here $f(x') = 1$. So

$$\int_{-\infty}^{\infty} \delta(x-x')\, dx' = f(x) = 1 \qquad \Rightarrow \int_{-\infty}^{\infty} \delta(x-x')\, dx' = 1$$

With similar derivations:

$$\boxed{\begin{aligned} \int_{-\infty}^{\infty} f(x')\,\delta(x-x')\,dx' &= f(x) \\ \int_{-\infty}^{\infty} f(x')\,\delta(x'-x)\,dx' &= f(x) \\ \int_{-\infty}^{\infty} \delta(x'-x)\,dx &= 1 \end{aligned}}$$

Wavefunctions and position states

We now complete the definition of the inner product of position states:

$$\boxed{\langle x|x'\rangle = \delta(x-x')}.$$

Then we can extract, formally, the wavefunction from the state.

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

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

Thus

$$\boxed{\Psi(x) = \langle x|\Psi\rangle}$$

A related useful identity is the completeness relation

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

Proof: $\left[\int_{-\infty}^{\infty} |x\rangle\langle x|\,dx\right]|\Psi\rangle = \int_{-\infty}^{\infty} |x\rangle\underbrace{\langle x|\Psi\rangle}_{\Psi(x)}\,dx = \int_{-\infty}^{\infty} \Psi(x)\,|x\rangle\,dx = |\Psi\rangle = I|\Psi\rangle.$ ∎

The completeness relation often appears in the midst of calculations and derivations

States, inner products and wavefunctions.

An essential computational requirement is calculating the inner product of two states. We want:

Given states $|\Psi\rangle, |\Phi\rangle$ $\rightarrow$ Associated wavefunctions $\Psi(x), \Phi(x)$ $\rightarrow$ How to express $\langle\Psi|\Phi\rangle$ in terms of $\Psi(x), \Phi(x)$

First recall the basic association:

Given ket $|\Psi\rangle$ $\rightarrow$ Wavefunction is $\Psi(x) = \langle x|\Psi\rangle$

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

Then

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

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

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

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

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

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

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

Thus we have

Given

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

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

Then

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

Note that this gives the normalization requirement

Given

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

then

$$\langle \Psi | \Psi \rangle = 1 \iff \int_{-\infty}^{\infty} \Psi^*(x)\, \Psi(x)\, dx = 1$$

$$\iff \int_{-\infty}^{\infty} |\Psi(x)|^2\, dx = 1.$$

Also note that for a bra:

$$\boxed{\langle \Phi | x \rangle = \Phi^*(x)}$$

since

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

$$= \Phi^*(x)$$

Measuements: Position

If we were able to measue position with perfect precision then we could determine

$$\text{Prob}(\text{position meas} \to x) = |\langle x|\Psi\rangle|^2 = \langle\Psi|\underbrace{|x\rangle\langle x|}_{\text{position meas. operator}}|\Psi\rangle$$

However we will only be able to do this over a range $a \le x \le b$. So

$$\text{Prob}(a \le x \le b) = \langle\Psi|\Big[\sum_{a \le x \le b} |x\rangle\langle x|\Big]|\Psi\rangle$$

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

$$= \int_a^b \underbrace{\langle\Psi|x\rangle}_{\Psi^*(x)}\underbrace{\langle x|\Psi\rangle}_{\Psi(x)}\, dx \qquad = \int_a^b \Psi^*(x)\Psi(x)\, dx.$$

Thus:

> If a system is in state $|\Psi\rangle$ with corresponding wavefunction $\Psi(x)$ then
>
> $$\text{Prob}\big[\text{position measuement gives } a \le x \le b\big] = \int_a^b |\Psi(x)|^2\, dx$$

So the probability density for position measuement outcomes is:

$$\boxed{P(x) = |\Psi(x)|^2}$$

2 Wavefunction mathematics

Consider the states

$$|\Psi_1\rangle \leftrightarrow \Psi_1(x) = Ae^{-|x|/2\alpha^2}$$
$$|\Psi_2\rangle \leftrightarrow \Psi_2(x) = Be^{-|x|/2\beta^2}$$

where $\alpha, \beta > 0$.

a) Determine A and B.

b) Determine $\langle\Psi_1|\Psi_2\rangle$.

Answer: a) $\langle \Psi_1 | \Psi_1 \rangle = 1$

$$\Rightarrow |A|^2 \int_{-\infty}^{\infty} e^{-|x|/2\alpha^2} e^{-|x|/2\alpha^2} dx = 1$$

$$\Rightarrow |A|^2 \int_{-\infty}^{\infty} e^{-|x|/\alpha^2} dx = 1$$

$$\Rightarrow 2|A|^2 \int_{0}^{\infty} e^{-|x|/\alpha^2} dx = 1$$

$$\Rightarrow 2|A|^2 \left[e^{-|x|/\alpha^2} (-\alpha^2) \Big|_0^\infty \right] = 1$$

$$\Rightarrow 2|A|^2 \alpha^2 = 1 \Rightarrow A = \frac{1}{\sqrt{2}\,\alpha}$$

Similarly $B = \frac{1}{\sqrt{2}\,\beta}$.

b) $$\langle \Psi_1 | \Psi_2 \rangle = \int_{-\infty}^{\infty} A^* e^{-|x|/2\alpha^2} B e^{-|x|/2\beta^2} dx = \frac{2}{2\alpha\beta} \int_0^\infty e^{-|x|\gamma} dx$$

where $$\gamma = \frac{1}{2\alpha^2} + \frac{1}{2\beta^2} = \frac{2\alpha^2 + 2\beta^2}{4\alpha^2\beta^2} = \frac{\alpha^2+\beta^2}{2\alpha^2\beta^2}$$

$$\Rightarrow \langle \Psi_1 | \Psi_2 \rangle = \frac{-1}{\alpha\beta} \frac{1}{\gamma} e^{-|x|\gamma} \Big|_0^\infty = \frac{1}{\alpha\beta}\frac{1}{\gamma} = \frac{2\alpha^2\beta^2}{\alpha\beta(\alpha^2+\beta^2)} = \frac{2\alpha\beta}{\alpha^2+\beta^2}$$