Phys 321 2023

Lecture 19

Fri: HW by 5pm

Tues: Read 9.1, 9.2

HW by 5pm

Free particles

Consider a particle that can move in one dimension free of any interaction. We can ask

mass M

* what are possible energy eigenstates and eigenvalues for this particle?
* are there states such that the particle is localized?
* how will the state of such a particle evolve with time?

The crucial starting point, that eventually answers questions about energy and time evolution, is to describe the Hamiltonian. Classically the energy is

$$E_{classical} = \frac{1}{2} M v^2 = \frac{p^2}{2M}.$$

Thus, for a free particle, the Hamiltonian is

$$\boxed{\hat{H} = \frac{1}{2M} \hat{p}^2 \qquad \text{Free particle}}$$

where $\hat{p}$ is the momentum operator. We can then answer questions about energy measurements.

1 Free particle energies

Consider a free particle with mass m.

a) Determine the position wavefunction, $\Psi(x)$, associated with any energy eigenstate of the particle.

b) What are the possible outcomes of an energy measurement?

Answer: a) We need $|\Psi\rangle$ that satisfied

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

$$\Rightarrow \frac{1}{2m}\hat{p}^2|\Psi\rangle = E|\Psi\rangle$$

Consider a momentum state, $|p\rangle$. Then

$$\underbrace{\hat{p}^2}_{\text{operator.}}|p\rangle = \hat{p}\,\hat{p}|p\rangle = \hat{p}\,p|p\rangle = p\,\hat{p}|p\rangle = p\,p|p\rangle = \underbrace{p^2}_{\text{number}}|p\rangle$$

Thus a possible energy eigenstate is $|\Psi\rangle = |p\rangle$. In this case

$$\hat{H}|\Psi\rangle = \frac{p^2}{2m}|\Psi\rangle$$

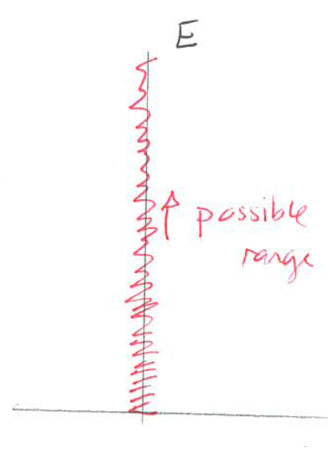
$\hookrightarrow$ the wavefunction is

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$$

and the energy is:

$$E = \frac{p^2}{2m}$$

b) Any real p is possible. Thus any $E > 0$ is possible.



So we have that

The energy eigenvalues, eigenstates and wavefunctions for a free particle are indexed by $p \in \mathbb{R}$.

energy	state	wavefunction
$\vdots$	$\vdots$	$\vdots$
$E = \frac{p^2}{2m}$	$\vert p\rangle$	$\Psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$
$\vdots$	$\vdots$	$\vdots$

Time evolution for a free particle

Suppose that the initial state and wavefunction for a free particle are known:

$$|\Psi(0)\rangle \rightsquigarrow \Psi(x,t)$$

We would like to be able to determine the state at any later time. We can use a general scheme:

Known initial state $|\Psi(0)\rangle$ $\longrightarrow$ Expand in terms of energy eigenstates $|\phi_E\rangle$

$$|\Psi(0)\rangle = \sum_{\substack{\text{energies}\\ E}} C_E |\phi_E\rangle$$

$\longrightarrow$ Later state

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

In this case the "summation index" is p and the summation must be replaced by an integral.

Thus

$$|\Psi(0)\rangle = \int_{-\infty}^{\infty} \underset{\text{coefficient}}{C(p)}\,\underset{\text{energy eigenstate}}{|p\rangle}\, dp \qquad \text{where} \qquad C(p) = \langle p|\Psi(0)\rangle$$

$$\Rightarrow C(p) = \tilde{\Psi}(p,0)$$

$$\downarrow$$

$$|\Psi(t)\rangle = \int_{-\infty}^{\infty} C(p)\, e^{-ip^2t/2m\hbar}\, |p\rangle\, dp$$

$$= \int_{-\infty}^{\infty} \tilde{\Psi}(p,0)\, e^{-ip^2t/2m\hbar}\, |p\rangle\, dp$$

So

$$\Psi(x,t) = \langle x|\Psi(t)\rangle$$

$$= \int_{-\infty}^{\infty} \tilde{\Psi}(p,0)\, e^{-ip^2t/2m\hbar}\, \underbrace{\langle x|p\rangle}_{e^{ipx/\hbar}\frac{1}{\sqrt{2\pi\hbar}}}\, dp$$

Thus the procedure is: FREE PARTICLE ONLY

1) Determine the initial position space wavefunction $\Psi(x,0)$

2) Determine the initial momentum space wavefunction

$$\tilde{\Psi}(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar}\, \Psi(x,0)\, dx$$

3) Then at a later time:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \tilde{\Psi}(p,0)\, e^{-ip^2t/2m\hbar}\, e^{ipx/\hbar}\, dp$$

2 Free particle evolution: Gaussian wavefunction

A particle is initially in the state corresponding to the wavefunction

$$\Psi(x,0) = \left(\frac{1}{\pi a^2}\right)^{1/4} e^{-x^2/2a^2}$$

where $a > 0$. This is normalized.

a) What type of function will represent the momentum wavefunction at $t = 0$? What type of function will represent the momentum wavefunction at any later time? What type of function will represent the position wavefunction at a later time?

The initial momentum wavefunction is

$$\tilde{\Psi}(p,0) = \left(\frac{a^2}{\pi \hbar^2}\right)^{1/4} e^{-p^2a^2/2\hbar^2}.$$

b) Determine the position wavefunction and position probability density at any later time.

Note the following integrals, all true if the real part of α is positive.

$$\int_{-\infty}^{\infty} e^{-\alpha x^2+\beta x+\gamma} dx = e^{\gamma}\, e^{\beta^2/4\alpha} \sqrt{\frac{\pi}{\alpha}}$$

$$\int_{-\infty}^{\infty} x e^{-\alpha x^2+\beta x+\gamma} dx = e^{\gamma}\, e^{\beta^2/4\alpha} \frac{\beta}{2}\sqrt{\frac{\pi}{\alpha^3}}$$

$$\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2+\beta x+\gamma} dx = e^{\gamma}\, e^{\beta^2/4\alpha} \frac{\beta^2+2\alpha}{4}\sqrt{\frac{\pi}{\alpha^5}}.$$

Answer: a)
$$\tilde{\Psi}(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x,0)\, e^{-ipx/\hbar}\, dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \left(\frac{1}{\pi a^2}\right)^{1/4} \int e^{-x^2/2a^2}\, e^{-ipx/\hbar}\, dx$$

This is a Gaussian integral. The result will be another Gaussian function of p. At a later time

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \underbrace{\tilde{\Psi}(p,0)}_{\text{Gaussian}}\, e^{ipx/\hbar} e^{-ip^2t/2m\hbar}\, dp$$

will also be Gaussian.

b) $$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \tilde{\Psi}(p,0)\, e^{ipx/\hbar}\, e^{-ip^2t/2m\hbar}\, dp$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \left(\frac{a^2}{\pi\hbar^2}\right)^{1/4} \int_{-\infty}^{\infty} e^{-p^2a^2/2\hbar^2}\, e^{-ip^2t/2m\hbar}\, e^{ipx/\hbar}\, dp.$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \left(\frac{a^2}{\pi\hbar^2}\right)^{1/4} \int_{-\infty}^{\infty} e^{-p^2\left(\frac{a^2}{2\hbar^2}+\frac{it}{2m\hbar}\right) + p\left(\frac{ix}{\hbar}\right)}\, dp$$

The integral has form

$$\int_{-\infty}^{\infty} e^{-p^2\alpha + p\beta + \gamma}\, dp$$

where $\alpha = \left(\frac{a^2}{2\hbar} + \frac{it}{2m\hbar}\right) = \frac{ma^2 + it\hbar}{2m\hbar^2}$

$\beta = \frac{ix}{\hbar}$

$\gamma = 0$

Since $Re(\alpha) > 0$ the formulas apply. Then

$$\int_{-\infty}^{\infty} e^{-p^2\alpha + p\beta + \gamma}\, dp = e^{\beta^2/4\alpha} \sqrt{\frac{\pi}{\alpha}}$$

So $$\frac{\beta^2}{4\alpha} = \frac{-x^2}{4\hbar^2} \frac{(2m\hbar^2)}{(ma^2+it\hbar)} = -\frac{mx^2}{2} \frac{1}{ma^2+it\hbar}$$

But $$\frac{1}{ma^2+it\hbar} = \frac{ma^2-it\hbar}{ma^2-it\hbar} \frac{1}{ma^2+it\hbar} = \frac{ma^2-it\hbar}{m^2a^4+t^2\hbar^2}$$

So

$$\frac{\beta^2}{4\alpha} = -\frac{mx^2}{2}\;\frac{ma^2 - i\hbar t}{m^2a^4 + t^2\hbar^2} = \underbrace{\frac{-i\hbar m x^2 t}{2(\ldots)}}\; - \;\frac{m^2a^2}{2(m^2a^4+t^2\hbar^2)}\,x^2$$

Thus:

$$\Psi(x,t) = \frac{1}{\sqrt{\cancel{2\pi\hbar}}}\left(\frac{a^2}{\pi\hbar^2}\right)^{1/4} \underbrace{e^{-i(\ldots)}}_{\text{overall phase}}\; e^{-x^2\frac{m^2a^2}{2(m^2a^4+t^2\hbar^2)}}\sqrt{\frac{\cancel{2\pi\hbar}\hbar\, m}{ma^2+it\hbar}}$$

$$= \left(\frac{a^2}{\pi}\right)^{1/4}\sqrt{\frac{m}{ma^2+it\hbar}}\; e^{-i(\ldots)}\; e^{-x^2 m^2a^2/2(m^2a^4+t^2\hbar^2)}$$

$$= \left(\frac{a^2}{\pi}\right)^{1/4}\sqrt{\frac{m}{ma^2+it\hbar}}\; \underbrace{e^{-i(\ldots)}}_{\text{phase}}\; \underbrace{e^{-x^2/2a^2\left(1+\frac{t^2\hbar^2}{m^2a^2}\right)}}_{\text{Gaussian.}}$$

Then the position probability density is:

$$P(x,t) = |\Psi(x,t)|^2 = \sqrt{\frac{a^2}{\pi}}\;\frac{m}{\sqrt{(ma^2+it\hbar)(ma^2-it\hbar)}}\; e^{-x^2/a^2\left(1+\frac{t^2\hbar^2}{m^2a^2}\right)}$$

This describes a Gaussian with width

$$a\sqrt{1+\frac{t^2\hbar^2}{m^2a^2}}$$

We see that as time passes the width of the distribution increases

Demo: QuVis Gaussian Wave Packet

Note that for the free particle

$$\tilde{\Psi}(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx'/\hbar}\, \Psi(x',0)\, dx'$$

gives:

$$\Psi(x,t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dx'\; \Psi(x',0)\, e^{-ipx'/\hbar}\, e^{ipx/\hbar}\, e^{-ip^2 t/2m\hbar}$$

$$\underbrace{\Psi(x,t)}_{\text{later wavefunction}} = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx' \underbrace{\int_{-\infty}^{\infty} dp\, e^{ip(x-x')/\hbar}\, e^{-ip^2 t/2m\hbar}}_{\text{amounts to evolution operator}} \underbrace{\Psi(x',0)}_{\text{initial wavefunction}}$$

later wavefunction

* can be integrated
* function of x, x'

amounts to <u>evolution operator</u>

~~initi~~ initial wavefunction