Time Development, Conservation Theorems, Parity

Liboff, chap. 6

In this chapter we're going to consider the time development of arbitrary wave fns – given a wave fn $\psi(x,0)$, what does the wave fn look at for later times? Then we'll consider quantities that don't change w/ time – i.e. conserved quantities. We'll talk about what that means in quantum mechanics (i.e. in what sense something can be said to be conserved in a non-deterministic system) and we'll see that conservation theorems result from symmetries of systems. Finally, we'll talk about parity, or space reflection.

Time development of state functions

How does an arbitrary wave function $\psi(x,0)$ evolve with time? We already know enough from previous chapters to answer this explicitly. We know in general

$$\psi(x,t) = \exp\left(\frac{-i\overset{\text{operator}}{\hat{H}}t}{\hbar}\right)\psi(x,0)$$

and recall that the exponential of the operator is understood in terms of a power series expansion.

We also know that for an eigenfunction of $\hat{H}$, $\hat{H}\psi_n = E_n\psi_n$, the operator in the exponential just gets replaced with →

the corresponding eigenvalue:

$$e^{\left(-i\hat{H}t/\hbar\right)}\varphi_n = e^{-iE_nt/\hbar}\varphi_n$$

But we can write any wave function $\psi(x,0)$ as a superposition of energy eigenstates

$$\psi(x,0) = \sum_n b_n \varphi_n(x) \qquad \text{with} \quad b_n = \langle \varphi_n | \psi(x,0)\rangle$$

(this is discrete case; see below for continuous) so we have

$$\psi(x,t) = e^{-i\hat{H}t/\hbar}\psi(x,0) = \sum_n b_n e^{-i\hat{H}t/\hbar}\varphi_n$$

$$= \sum_n b_n e^{-iE_nt/\hbar}\varphi_n$$

$$= \sum_n b_n e^{-i\omega_n t}\varphi_n \qquad (\omega_n = E_n/\hbar)$$

$$\equiv \sum_n \bar{b}_n(t)\varphi_n(x) \qquad \left(\bar{b}_n(t) \equiv b_n e^{-i\omega_n t}\right)$$

$\Rightarrow$ The contribution to ψ of each energy eigenstate evolves according to $e^{-iE_nt/\hbar}$ where E_n is the corresponding eigenvalue, i.e. each amplitude oscillates w/ frequency corresponding to the energy eigenvalue.

What about energy measurements, & in particular, probabilities for measuring specific energies? (5.3)

We have

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

$\bar{b}_{n'}, \bar{b}_n$ include time dependence

$$= \sum_{n'} \sum_{n} \bar{b}_{n'}^{*} \bar{b}_n \langle \varphi_{n'} | \hat{H} | \varphi_n \rangle$$

$$= \sum_{n'} \sum_{n} \bar{b}_{n'}^{*} \bar{b}_n E_n \delta_{n'n}$$

$$= \sum_{n} |\bar{b}_n(t)|^2 E_n$$

So the prob. for measuring a given E_n is

$$P(E) = |\bar{b}_n(t)|^2 = e^{+i\omega_n t} e^{-i\omega_n t} b_n^* b_n$$

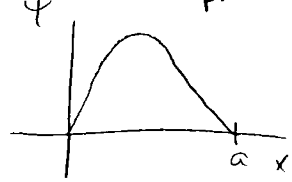
$$= |b_n|^2 = \text{constant in time}$$

$$\therefore \quad \langle E \rangle = \sum |\bar{b}_n(t)|^2 E_n = \sum |b_n|^2 E_n = \text{constant in time}$$

So although the wave function changes w/ time, the expectation value of the energy does not, and the prop. of finding a specific energy also does not change w/ time

Ex Consider a superposition of the first two eigenstates of a particle in a box, $\psi_1 + \psi_2$ s.t. (5.4)

fig 6.1 p. 154



$$\psi(x,0) = \sqrt{\frac{2}{a}}\left[\frac{2\sin(\pi x/a) + \sin\left(\frac{2\pi x}{a}\right)}{\sqrt{5}}\right]$$

This is normalized, w/ $b_1 = \frac{2}{\sqrt{5}}$, $b_2 = \frac{1}{\sqrt{5}}$, $b_n = 0$ all other n

At later times t the wave fn becomes

$$\psi(x,t) = \sqrt{\frac{2}{a}}\left[\frac{2e^{-i\omega_1 t}\sin\left(\frac{\pi x}{a}\right) + e^{-i\omega_2 t}\sin\left(\frac{2\pi x}{a}\right)}{\sqrt{5}}\right]$$

standing waves

What is the prob. for finding the various energies?

$$P(E_1) = |b_1(t)|^2 = \frac{4}{5}$$

$$P(E_2) = |b_2|^2 = \frac{1}{5}$$

$$P(E_n) = 0 \qquad n > 2$$

and

$$\langle E \rangle = \frac{4}{5}E_1 + \frac{1}{5}E_2$$

but for part. in box, $E_n \propto n^2$ so $E_2 = 4E_1$

$$= \frac{8}{5}E_1$$

<u>Continuous</u> case: We can extend this in the usual way to the case of continuous eigenfns. Write $\psi(x,0)$ as an integral over plane wave states, and let each one evolve according to its eigenfrequency:

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k)\, e^{ikx}\, dk$$

and as usual $\quad b(k) = \langle \varphi_k | \psi(x,0)\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,0)\, e^{-ikx}\, dx$

For $t > 0$ we have

$$\psi(x,t) = \left(e^{-i\hat{H}t/\hbar}\right) \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k)\, e^{ikx}\, dk$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k)\, e^{-iE_k t/\hbar}\, e^{ikx}\, dk$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k)\, e^{i(kx-\omega t)}\, dk \qquad \hbar\omega = E_k = \frac{\hbar^2 k^2}{2m}$$

Note that each component here is a traveling wave.

Recall that the phase is constant for $x = \frac{\omega}{k} t$

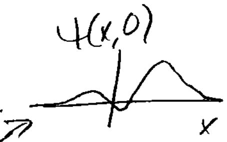
$\Rightarrow$ phase velocity is $\bar{v} = \frac{\omega}{k} = \frac{\hbar k}{2m}$

$\Rightarrow$ large wave numbers propagate faster. So the components don't stay in phase with each other.

The phase velocity being different for different k means that the initial wave fn doesn't keep its shape; in general it disperses.

In what sense can we describe the wave as a whole moving, even if it changes shape? That would be a propagating wave packet (and that's what we need to approximate a classical particle).

e.g.



We need two conditions. ① We want the packet to be localized in space: $|\psi(x,0)| \neq 0$ in small region, and ② the average momentum of the particle in the initial state must be nonzero; $\langle p \rangle_{t=0} \neq 0$.

As we discussed earlier, this packet's velocity is the group velocity

$$v_g = \frac{\partial \omega}{\partial k}\bigg|_{k_{max}}$$ group velocity

where k_{max} means k at which $|b(k)|^2$ is maximum, in which case $\hbar k_{max} \simeq \langle p \rangle = \int_{-\infty}^{\infty} |b(k)|^2 \hbar k \, dk$

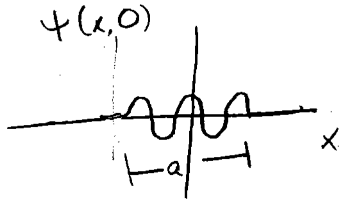
So evaluating the group velocity,

$$v_g = \frac{\partial \omega}{\partial k}\bigg|_{k_{max}} = \frac{\partial (\hbar k^2/2m)}{\partial k}\bigg|_{k_{max}} = \frac{\hbar k_{max}}{m} \simeq \frac{\langle p \rangle}{m} = v_{cl}$$

So the packet moves with the classical velocity

Now let's consider two examples; ① A pulse of particles w/ a fixed momentum; ② a Gaussian wave packet

① Pulse. Let's take a beam of particles, neutrons say, all w/ a fixed momentum $\hbar k_0$. But truncate the beam to get a pulse of length a:



$$\psi(x,0) = \begin{cases} \frac{1}{\sqrt{a}} e^{ik_0 x} & -\frac{a}{2} \le x \le +\frac{a}{2} \\ 0 & |x| > a/2 \end{cases}$$

What happens to this pulse at time $t>0$? Decompose into plane wave components, i.e. find $b(k)$. [Note: it's tempting to say $b(k) = \delta(k-k_0)$ but that would only be true if the plane wave extended to ∞ in x. Because the pulse is truncated, other contributions come in from other k's.]

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}}\int b(k) e^{ikx} dk$$

So
$$b(k) = \frac{1}{\sqrt{2\pi a}} \int_{-a/2}^{+a/2} e^{ik_0 x} e^{-ikx} dx$$

$$= \frac{1}{\sqrt{2\pi a}} \frac{1}{i(k_0-k)} \left[e^{i(k_0-k)a/2} - e^{-i(k_0-k)a/2} \right]$$

$$= \sqrt{\frac{2}{\pi a}} \frac{1}{k-k_0} \sin[(k-k_0)a/2]$$

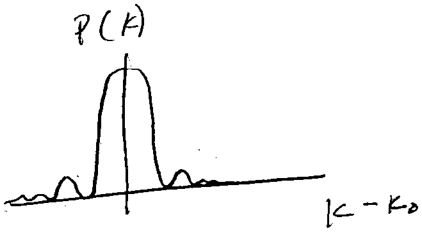
So for $\Psi(t)$, each component evolves according to its eigenfrequency $\omega = \frac{\hbar k^2}{2m}$:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k)\, e^{i(kx-\omega t)}\, dk$$

$$= \frac{1}{\pi\sqrt{a}} \int_{-\infty}^{\infty} \frac{\sin\{(k-k_0)a/2\}}{(k-k_0)}\, e^{i(kx-\omega t)}\, dk$$

and the momentum prob. density looks like

$$P(k) = |b(k)|^2 = \frac{2}{\pi a} \frac{\sin^2[(k-k_0)a/2]}{(k-k_0)^2}$$



and is indep. of time

Most likely momentum is

$$p = \hbar k_{max} = \hbar k_0 = \text{only momentum before beam chopped}$$

(+ in general you find this from $\frac{d}{dk} P(k) = 0$)

and $P(k) = 0$ for momenta

$$\hbar k = \hbar k_0 + \frac{2n\pi\hbar}{a} \quad n = 1, 2, 3 \ldots$$

$\Rightarrow$ these have 0 prob. of being found

Note similarity to square wave.

Now how many neutrons w/ momentum interval? (5.9)

$$\Delta N = N \int_{k_1}^{k_2} |b(k)|^2 dk \qquad \text{indep. of time}$$

Now compare to square wave packet, chap. 5. Same mom. dist, but centered at $k=0$, not $k=k_0$. Packet has mean momentum $p=0$, so it doesn't propagate, it just diffuses

(2) Gaussian wave packet. Remember we discussed a Gaussian wave packet

$$\psi(x,0) = \frac{1}{\sqrt{a}\,(2\pi)^{1/4}} e^{ik_0 x} e^{-x^2/4a^2}$$

It has initial prob density

$$P(x,0) = |\psi|^2 = \frac{1}{a\sqrt{2\pi}} e^{-x^2/2a^2} \qquad \text{(already normalized)}$$

with mean $x = 0$, $\Delta x = a$, and minimum uncertainty product $\Delta x \Delta p = \hbar/2$.

Now the $e^{ik_0 x}$ means it has avg momentum

$$\langle p \rangle = \hbar k_0 \qquad \text{(exercise: verify this)}$$

So physically, this is a particle (or packet) w/ wave fn spread a about origin and avg momentum $\hbar k_0$

(5.10)

Q: What's the corresponding momentum amplitude?

A: It's also a Gaussian! The Fourier transform of a Gaussian is another Gaussian:

$$b(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,0)\, e^{-ikx}\, dx$$

$$= \frac{1}{\sqrt{a}(2\pi)^{3/4}} \underbrace{\int_{-\infty}^{\infty} e^{-x^2/4a^2}\, e^{ix(k_0-k)}\, dx}_{\equiv I}$$

To evaluate this we have to complete the square in the exponent, to get a form $\int_{-\infty}^{\infty} e^{-y^2} dy = \sqrt{\pi}$

So write $\frac{x^2}{4a^2} - x[i(k_0-k)] =$

$$= \left[\frac{x}{2a} - i(k_0-k)a\right]^2 + (k_0-k)^2 a^2$$

$$= \frac{x^2}{4a^2} - \frac{2i(k_0-k)a}{2a} - (k_0-k)^2 a^2 + (k_0-k)^2 a^2$$

OK

$$\Rightarrow \quad I = \int_{-\infty}^{\infty} dx\, e^{-\left[\frac{x}{2a} - i(k_0-k)a\right]^2} e^{-(k_0-k)^2 a^2}$$

$$= e^{-(k_0-k)^2 a^2}\, 2a \underbrace{\int_{-\infty}^{\infty} e^{-y^2} dy}_{\sqrt{\pi}}$$

So $b(k) = \frac{2a\,\pi^{1/2}}{a^{1/2}(2\pi)^{3/4}} e^{-(k_0-k)^2 a^2} = \frac{\sqrt{2a}\,\sqrt{2}}{\sqrt{2}\,(2\pi)^{1/4}} e^{-(k_0-k)^2 a^2} = \sqrt{\frac{2a}{\sqrt{2\pi}}}\, e^{-a^2(k_0-k)^2}$

also a Gaussian

and momentum probability density is

$$|b(k)|^2 = \frac{2a}{\sqrt{2\pi}} e^{-2a^2(k_0-k)^2}$$

mean $k = k_0$, $\Delta k = \frac{1}{2a}$ and $\Delta x \Delta p = \frac{\hbar}{2}$

Q: So all this was at $t=0$. What happens at later times?

A: Since different components have different momenta + therefore propagate at different speeds, it follows that the wave fn must get distorted with time. In fact, we'll see that it remains a Gaussian, but it gets spread out over time.

To show this explicitly we're going to introduce a function called the free-particle propagator. (It's an example of a more general function called a Green's function.) The propagator will give the probability that a particle propagates from one point to another in some time.

Let's be more explicit. To find $\psi(x,t)$ we do the usual thing: expand $\psi(x,0)$ in terms of energy eigenfunctions (this is the integral over k) and let each eigenfn evolve according to e^{-iEt}.

So $\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} b(k)\, e^{i(kx-\omega t)}\, dk$

Now we could go ahead and evaluate this directly by substituting the expression for $b(k)$ from the bottom of page 5.10, but let's keep things more general. In particular, let's substitute the general expression for $b(k)$ + save the specifics of this case for later.

$$b(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x',0)\, e^{-ikx'}\, dx'$$

So $$\psi(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dk\, dx'\, \psi(x',0)\, e^{-ikx'}\, e^{i(kx-\omega t)}$$

and to make the k dependence explicit

note $\omega = \frac{\hbar k^2}{2m}$

also, let's pull out the k dependence as much as we can and rearrange:

$$\psi(x,t) = \int_{-\infty}^{\infty} dx'\, \psi(x',0) \underbrace{\left[\frac{1}{2\pi}\int_{-\infty}^{\infty} dk\; e^{i\left[k(x-x') - \frac{\hbar k^2 t}{2m}\right]}\right]}_{\equiv K(x',x;t)}$$

$\equiv K(x',x;t)$ a function of x', x, t only

So we can write

$$\boxed{\psi(x,t) = \int_{-\infty}^{\infty} dx' \; \psi(x',0) \; K(x',x;t)} \qquad (**)$$

What does this mean? $\psi(x,t)$ is prob. amplitude for finding particle at position x at time t, given initial prob. amplitude $\psi(x,0)$. So the integral adds up the contributions to ψ at the value x from all possible positions in the initial state. The function $K(x',x;t)$ gives the weight that $\psi(x',0)$ contributes to $\psi(x,t)$.

In other words,

$$\boxed{K(x',x;t) = \text{prob amplitude that particle initially at } x' \text{ propagates to } x \text{ in the interval } t}$$

Now let's evaluate $K(x',x;t)$.

$$K(x',x;t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \; e^{i\left[k(x-x') - \frac{\hbar k^2 t}{2m}\right]}$$

and now define $\tau \equiv \frac{2ma^2}{\hbar}$, which has dimensions of time and will turn out to be a characteristic time scale for this problem. Note in the process we've introduced length scale a.

So

$$K(x', x; t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{i\left[k(x-x') - \frac{k^2 a^2 t}{\tau}\right]}$$

This integral too can be solved by completing the square (cf p. 5.10 or problem 6.5 on p. 167) and we get

$$\boxed{K(x', x; t) = \sqrt{\frac{\tau}{i 4\pi a^2 t}}\; e^{\left[i(x-x')^2 \tau / 4a^2 t\right]}}$$

free particle propagator

[and substituting back in for τ we get

$$K(x', x; t) = \sqrt{\frac{m}{2\pi i \hbar t}}\; e^{\left[i m (x-x')^2 / 2\hbar t\right]}$$]

Note this K is specific to free particles only; K has a slightly different form when we include interactions.

Finally, let's plug $\psi(x', 0)$ (p. 5.9) $+ K$ back into eqn (**) on p. 5.13 to get explicitly the time evolution of the Gaussian:

$$\psi(x, t) = \int_{-\infty}^{\infty} dx'\, \psi(x', 0)\, K(x', x; t)$$

$$= \frac{1}{(2\pi)^{1/4}} \sqrt{\frac{\tau}{i 4\pi a^3 t}} \int_{\infty}^{\infty} dx'\, e^{\left[i k_0 x' - x'^2/4a^2 + i(x-x')^2 \tau / 4a^2 t\right]}$$

Integrate over x' by again completing the square and find ⟶

$$\Psi(x,t) = \frac{1}{\sqrt{a}\,(2\pi)^{1/4}\sqrt{1+it/\tau}}\, e^{i\frac{\tau}{t}\left(\frac{x}{2a}\right)^2}$$

$$* \; e^{\left[\frac{-\frac{i\tau}{4a^2 t}\left(x - \frac{\hbar k_0 t}{m}\right)^2}{1+it/\tau}\right]}$$

and this has seemingly bizarre x + t dependence, and though the exponentials look on the surface like they might be straight complex exponentials, the denominator shows that it's really more complicated than that.

Things make more sense when we look at the probability density:

$$P(x,t) = |\Psi(x,t)|^2 = \frac{1}{a\sqrt{2\pi}\sqrt{1+t^2/\tau^2}}\, e^{-\frac{\left(x - \hbar k_0 t/m\right)^2}{2a^2(1+t^2/\tau^2)}}$$

Now compare to $P(x,0)$ on p. 5.9. This $P(x,t)$ is still a Gaussian, albeit with a modified width, mean, and normilization:

- width $a \to a\sqrt{1+t^2/\tau^2}$

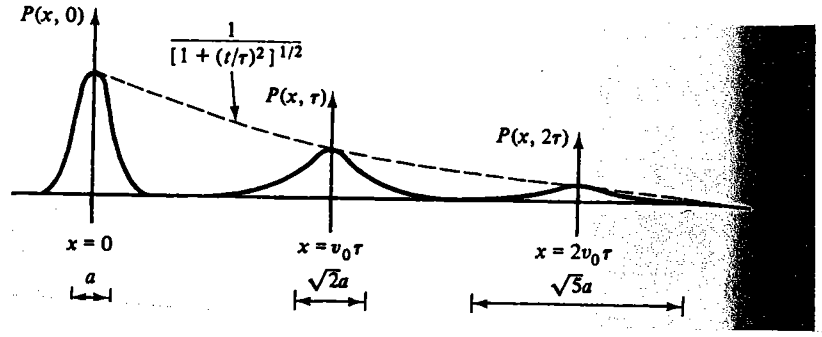
  It's becoming wider with increasing time.

- mean $\bar{x}=0 \to \bar{x} = \frac{\hbar k_0 t}{m} = v_0 t$ with $v_0 = \frac{\hbar k_0}{m}$

  The whole thing is moving to the right (as it's spreading out) with velocity corresponding to the mean initial momentum

- Normalization $\frac{1}{a\sqrt{2\pi}} \to \frac{1}{a\sqrt{2\pi}\sqrt{1+t^2/\tau}}$ decreases to preserve area

So the Gaussian wave packet remains a Gaussian but it spreads out as it propagates:



and we can see from this that the time τ represents the time after which the wave packet is significantly distorted.

Reality check: If the wave fn is distorted after time τ, then ultimately this description of a classical particle breaks down. Why don't we see evidence of this in the world?

Consider a wave packet representing a piece of chalk, say: $a \sim 1\,cm$, $m \sim 1\,g$

$$\Rightarrow \tau = \frac{2ma^2}{\hbar} \sim 10^{27}\,sec \sim 10^{20}\,yr$$

$\Rightarrow$ 10 orders of magnitude bigger than the age of the universe! The bigger and more massive the object, the longer the time. So the timescale for dissipation of the wave packet for macroscopic objects is so long that you never see it.

Let's take this discussion one better and take (5.17)
the classical limit of the probability density
on p. 5.15. This means taking $\hbar \to 0$
(except in $\hbar k_0 = p_0$ = initial momentum: that's fixed).

Now $\hbar$ appears in $\tau = 2ma^2/\hbar$ so $\hbar \to 0$

$\Rightarrow \tau \to \infty$, $\Rightarrow 1 + t^2/\tau^2 \to 1$

$$\lim_{\hbar \to 0} P(x,t) = \frac{1}{a\sqrt{2\pi}} e^{-(x - p_0 t/m)^2/2a^2}$$

Now, classically we're interested in a point particle,
so we also want $a \to 0$. But $\lim_{a \to 0}$ of turns
out to be one representation of a Dirac δ-fn!

So $$\lim_{a \to 0} P(x,t) = \delta(x - p_0 t/m)$$

and this is just the classical trajectory

$$x = \frac{p_0}{m} t$$

Time development of expectation values

Now that we know how the wave function evolves, let's look at how expectation values of operators evolve. As we'll see, there's a connection between an operator's time evolution and it's commutator with the Hamiltonian.

Let A be an observable. We want

$$\frac{d\langle A\rangle}{dt} = \frac{\partial \langle A\rangle}{\partial t}$$

since $\langle A\rangle$ has all space dependence integrated out already.

In a state $\psi(x,t)$ we have

$$\frac{d\langle\psi|\hat{A}\psi\rangle}{dt} = \int dx \, \underbrace{\frac{\partial}{\partial t}(\psi^* \hat{A}\psi)}$$

$$= \left(\frac{\partial\psi^*}{\partial t}\right)\hat{A}\psi + \psi^*\hat{A}\frac{\partial\psi}{\partial t} + \psi^*\left(\frac{\partial\hat{A}}{\partial t}\right)\psi$$

But the time dep- Schr. eq'n tells us that

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi \Rightarrow \frac{\partial\psi}{\partial t} = \frac{-i}{\hbar}\hat{H}\psi$$

& by taking the complex conjugate (and since H is hermitian)

$$\frac{\partial\psi^*}{\partial t} = \frac{i\hat{H}}{\hbar}\psi^*$$

Then substituting

$$\frac{d}{dt}\langle A\rangle = \frac{i}{\hbar}\int dx\left[\hat{H}\psi^*\hat{A}\psi - \psi^*\hat{A}\hat{H}\psi + \frac{\hbar}{i}\psi^*\frac{\partial\hat{A}}{\partial t}\psi\right]$$

Now we can write the first term on the RHS as $\langle\hat{H}\psi|\hat{A}\psi\rangle = \langle\psi|\hat{H}\hat{A}\psi\rangle$ since $\hat{H}$ is hermitian

$$\Rightarrow \quad \frac{d}{dt}\langle A\rangle = \frac{i}{\hbar}\int dx\left\{\psi^*(\hat{H}\hat{A}-\hat{A}\hat{H})\psi + \frac{\hbar}{i}\psi^*\frac{\partial\hat{A}}{\partial t}\psi\right\}$$

or equivalently

$$\boxed{\frac{d\langle\hat{A}\rangle}{dt} = \left\langle\frac{i}{\hbar}[\hat{H},\hat{A}] + \frac{\partial\hat{A}}{\partial t}\right\rangle}$$

Now many operators don't depend explicitly on time, in which case

$$\frac{d\langle A\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H},\hat{A}]\rangle$$

and if $\hat{A}$ commutes w/ $\hat{H}$, then $\langle\hat{A}\rangle$ is constant in time & the observable A is called a "constant of the motion." Examples include the momentum and energy of a free particle.

Now we can use this to derive the classical eq'ns of motion for a particle - it turns out they hold in QM as long as we're talking about expectation values.

We'll consider a particle moving in one dim, with potential $V(x)$. We have

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

1) $p = mv$:

$$\frac{d\langle x\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H}, \hat{x}]\rangle$$ + since $\hat{x}$ commutes w/ $V(x)$

$$= \frac{i}{2m\hbar}\langle \underbrace{[\hat{p}^2, \hat{x}]}_{\hat{p}[\hat{p},\hat{x}] + [\hat{p},\hat{x}]\hat{p} = -2i\hbar\hat{p}} \rangle$$

$$= \frac{i}{2m\hbar}(-2i\hbar)\langle\hat{p}\rangle$$

$$= \frac{1}{m}\langle\hat{p}\rangle$$

Or $\langle p\rangle = m\dfrac{d\langle x\rangle}{dt}$

2) $F = ma = \dfrac{dp}{dt}$ Ehrenfest's Theorem

$$\frac{d\langle p\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H}, \hat{p}]\rangle$$

5.21

and $[\hat{H}, \hat{p}] = [V(x), \hat{p}]$ since $\hat{p}$ commutes w/ $\hat{p}^2/2m$

$$[V(x), \hat{p}]\, g(x) = -i\hbar \left[V(x) \frac{\partial g}{\partial x} - \left(\frac{\partial V}{\partial x}\right) g(x) - V(x) \frac{\partial g}{\partial x} \right]$$

$$= i\hbar \frac{\partial V}{\partial x} g(x)$$

$$\Rightarrow [V(x), \hat{p}] = i\hbar \frac{\partial V}{\partial x}$$

so $$\frac{d\langle p \rangle}{dt} = \frac{i}{\hbar}\, i\hbar \left\langle \frac{\partial V}{\partial x} \right\rangle$$

$$= -\left\langle \frac{\partial V}{\partial x} \right\rangle$$

but $\vec{F} = -\vec{\nabla} V$, so $\dfrac{d\langle p_x \rangle}{dt} = F_x$

$\Rightarrow$ The averages of x + p follow the laws of classical mechanics.

Symmetry + Conservation of Energy, Momentum, Ang. Mom.

What does conservation of energy (or momentum, or...) mean in Quantum mechanics? What does it mean for something to be a constant of the motion?

Take conservation of energy. In classical mechanics energy is conserved in an isolated or a conservative (describable by a potential) system.

Ex In QM, the particle in a 1-D box is conservative. Suppose we have a wave fn

$$\Psi(x,0) = \frac{3}{5}\varphi_1 + \frac{4}{5}\varphi_5$$

Then at $t=0$ (and at any subsequent t), if we measure the energy we don't get a definite value; we get either E_1 or E_5, with probabilities $\frac{9}{25}$ and $\frac{16}{25}$, respectively. So in what sense can we say that energy is conserved? In the expectation value sense: $\frac{d\langle E\rangle}{dt} = 0$

We already saw that if an operator doesn't depend explicitly on time, it is a constant of the motion if it commutes with the Hamiltonian (cf p. 5.19). Now we'll show that symmetries of a system lead directly to conserved quantities.

We'll consider 3 cases:

(1) Homogeneity of time + conservation of energy:

For any isolated system, the laws of physics don't depend on when they're applied, i.e. the physics is homogeneous in time.* (Another way to say this is that it doesn't matter when you define $t=0$.) It follows that the Hamiltonian does not depend explicitly on time, so $\frac{\partial \hat{H}}{\partial t}=0$. And since $[H,H]=0$ (the Hamiltonian commutes with itself), then $\frac{d\langle E\rangle}{dt}=0$

$$\boxed{\begin{aligned}\text{Homogeneity of time} &\Rightarrow \langle E\rangle \text{ is constant}\\ &\Rightarrow \text{energy is conserved}\end{aligned}}$$

(2) Homogeneity of space and conservation of momentum.

Now if a system is isolated, it doesn't matter where it is in space - its physical behavior is the same. We say that the system is translation invariant - the physics doesn't change if we shift or translate the whole system.

When we have translation invariance, momentum is conserved. Let's show this explicitly.

* Note this says the laws don't change over time. It does not say wave functions don't change over time.

Suppose we have translation invariance. Then if $\varphi(x)$ is an eigenfn of H, so is $\varphi(x+b)$ for the same energy:

$$\hat{H}\varphi(x) = E\varphi(x) \qquad (1)$$

same E

$$\hat{H}\varphi(x+b) = E\varphi(x+b) \qquad (2)$$

Now let's expand $\varphi(x+b)$ about $\varphi(x)$ in a Taylor series:

$$\varphi(x+b) = \varphi(x) + b\frac{\partial \varphi(x)}{\partial x} + \frac{1}{2!}b^2\frac{\partial^2\varphi(x)}{\partial x} + \cdots$$

Now b is arbitrary; i.e. we can pick any value for it. Let's let it be infinitessimal, so we can neglect terms of order b^2 and higher. Then

$$\varphi(x+b) \simeq \varphi(x) + b\frac{\partial \varphi(x)}{\partial x} \qquad \hat{p}_x = -i\hbar\frac{\partial}{\partial x}$$

$$= \varphi(x) + \frac{i}{\hbar}b\,\hat{p}\varphi(x)$$

Substituting this back into eq'n (2) we have

cancel

$$\hat{H}\varphi(x) + \frac{i}{\hbar}b\,\hat{H}\hat{p}\varphi(x) = E\varphi(x) + \frac{i}{\hbar}b\hat{p}\underbrace{E\varphi(x)}_{=\hat{H}\varphi(x)}$$

$$\Rightarrow \frac{ib}{\hbar}\hat{H}\hat{p}\varphi(x) = \frac{i}{\hbar}b\,\hat{p}\hat{H}\varphi(x)$$

$\longrightarrow$

or $(\hat{H}\hat{p} - \hat{p}\hat{H})\,\psi(x) = 0$

$$\Rightarrow [\hat{H}, \hat{p}] = 0 \quad \Rightarrow \quad \frac{d\langle p\rangle}{dt} = 0$$

Homogeneity of space (= translation invariance)
$\Rightarrow \langle p\rangle$ is constant
$\Rightarrow$ momentum is conserved

Aside: If we kept all terms in the Taylor expansion we would find

$$\psi(x+b) = e^{\left(\frac{ib\hat{p}_x}{\hbar}\right)}$$

and our argument would show $[\hat{H}, e^{(ib\hat{p}_x/\hbar)}] = 0$ from which momentum conservation would follow.

Aside #2: We could use this same method — Taylor expansion of the wave function — to show the time-homogeneity — conservation of energy connection.

③ Isotropy of space and conservation of angular momentum

The physics of an isolated system — i.e. the results of an experiment — cannot depend on the orientation in space. In other words, if we rotate the whole system in space it cannot change the physics. Under these circumstances, space is said to be isotropic and we have rotational invariance. This invariance leads to conservation of angular momentum. (5.26)

We can show this in much the same way we did for linear momentum, but for rotations we have to work in 3-D.

Suppose we have rotational invariance. Let's consider a rotation about the z axis by an angle θ. Then if $\psi(x,y,z)$ is an eigenfn of H, then so is $\psi(x',y',z)$ for the same energy, where x' and y' are the rotated coordinates.

So $$\hat{H}\,\psi(x,y,z) = E\,\psi(x,y,z) \quad (3)$$
$\updownarrow$ same
$$\hat{H}\,\psi(x',y',z) = E\,\psi(x',y',z) \quad (4)$$

Now we'll do a Taylor expansion as for $\hat{p}$ above, but we need explicit expressions for x' & y'.

For a rotation about z by angle θ, we have

$$x' = x\cos\theta - y\sin\theta$$
$$y' = x\sin\theta + y\cos\theta$$

Now θ is arbitrary, so we are free to take it to be infinitessimal. Then $\cos\theta \simeq 1$ and $\sin\theta \simeq \theta$

So

$$x' \simeq x - \theta y$$
$$y' \simeq y + \theta x$$

and $\varphi(x', y', z) = \varphi(x - \theta y,\ y + \theta x,\ z)$

$$= \varphi(x,y,z) - \theta y \frac{\partial \varphi(x,y,z)}{\partial x} + \theta x \frac{\partial \varphi(x,y,z)}{\partial y} + \text{terms of order } \theta^2$$

$$= \varphi(x,y,z) + \frac{i}{\hbar} \underbrace{\left[x \hat{p}_y - y \hat{p}_x \right]}_{\hat{L}_z} \varphi(x,y,z)$$

$$= \varphi(x,y,z) + \frac{i}{\hbar} \hat{L}_z \varphi(x,y,z)$$

Now substitute $\varphi(x', y', z)$ into eq'n 4 (p. 5.26):

cancel (eq'n (3))

$$\hat{H}\varphi(x,y,z) + \frac{i}{\hbar} \hat{H}\hat{L}_z \varphi(x,y,z) = E\varphi(x,y,z) + \frac{i}{\hbar} \hat{L}_z \underbrace{E\varphi(x,y,z)}_{= \hat{H}\varphi(x,y,z)}$$

Rearranging,

$$\frac{i}{\hbar} \left[\hat{H}\hat{L}_z - \hat{L}_z \hat{H} \right] \varphi(x,y,z) = 0$$

$$\Rightarrow \left[\hat{H}, \hat{L}_z \right] = 0$$

Now there's nothing special about the z axis; what we just did works equally well for rotations about the x and y axes. So we can conclude

$$[\hat{H}, \vec{L}] = 0 \quad \Rightarrow \quad \frac{d\langle \vec{L} \rangle}{dt} = 0$$

Isotropy of space (= rotation invariance)
$\Rightarrow$ $\langle \vec{L} \rangle$ is constant
$\Rightarrow$ angular momentum is conserved

Aside: If we kept all the terms in the Taylor expansion for $\psi(x', y', z)$ we would have

$$\psi(x', y', z) = e^{i\theta \hat{L}_z/\hbar}\, \psi(x, y, z)$$

Note the similarity to linear momentum, p. 5.25. The linear and angular momenta are said to be "generators" of translations and rotations, respectively.

Parity conservation

The symmetries we've discussed so far — time invariance, translation invariance, and rotation invariance are called continuous symmetries because the associated transformations are continuous. But there is another class of symmetries called discrete symmetries where the associated transformations are discrete. We'll discuss one such symmetry:

Parity, or space reflection: $x \to -x$

(Another example is time reversal, $t \to -t$.)

As we'll see, discrete symmetries also lead to conservation.

First, recall what we said about parity in P237:

1. A function is said to have definite parity if

$$f(-x) = \pm f(x)$$

and $f(-x) = f(x)$ = "even parity"

$f(x) = -f(x)$ = "odd parity"

2. If the potential is symmetric about $x=0$, i.e,

$V(-x) = V(x)$

then the corresponding Hamiltonian eigenfunctions have definite parity.

We can promote this to a conservation principle if we define the parity operator $\hat{\mathcal{P}}$

$$\hat{\mathcal{P}} f(x) = f(-x)$$

This operator has eigenvalues ± 1:

let $\hat{\mathcal{P}} f(x) = \alpha f(x)$

then $\hat{\mathcal{P}}\hat{\mathcal{P}} f(x) = \alpha^2 f(x) = f(-(-x)) = f(x)$

$\Rightarrow \alpha^2 = 1 \Rightarrow \alpha = \pm 1$

so even parity is $\hat{\mathcal{P}} f(x) = + f(x)$, i.e. $\mathcal{P} = +1$

odd parity $\hat{\mathcal{P}} f(x) = - f(x)$ $\quad \mathcal{P} = -1$

and the eigenfunctions of $\hat{\mathcal{P}}$ are all the even and odd functions.

Now what about conservation? There's a hint in #2 on p. 5.29: When $V(x) = V(-x)$, the eigenfunctions of the Hamiltonian are also eigenfunctions of parity. The existence of common eigenfunctions suggests that $\hat{H}$ and $\hat{\mathcal{P}}$ commute, and since $\mathcal{P}$ doesn't depend explicitly on time, then <u>that</u> suggests that parity is conserved.

(5.31)

We need only show that $[\hat{H}, \mathcal{P}] = 0$ when $V(-x) = V(x)$.

$$[\hat{H}, \hat{\mathcal{P}}] = \frac{1}{2m}[\hat{p}^2, \hat{\mathcal{P}}] + [V(x), \mathcal{P}]$$

$[\hat{p}^2, \hat{\mathcal{P}}]$: We can write $[p^2, \mathcal{P}] = p[\mathcal{P}, p]_+ - [\mathcal{P}, p]_+ p$

where $[\mathcal{P}, p]_+ = \mathcal{P}p + p\mathcal{P}$ = "anticommutator"

$$[\mathcal{P}, p]_+ g(x) = \frac{-i}{\hbar}\left[\mathcal{P}\frac{\partial g(x)}{\partial x} + \frac{\partial}{\partial x}\mathcal{P}g(x)\right]$$

$$= -\frac{i}{\hbar}\left[\frac{\partial g(-x)}{\partial(-x)} + \frac{\partial g(-x)}{\partial x}\right]$$

$$= 0$$

$$\therefore [\hat{p}^2, \hat{\mathcal{P}}] = 0$$

$$[V(x), \mathcal{P}]g(x) = V(x)\mathcal{P}g(x) - \mathcal{P}V(x)g(x)$$

$$= V(x)g(-x) - \underbrace{V(-x)}_{=V(x)}g(-x)$$

$$= 0$$

$\therefore [H, \mathcal{P}] = 0$ and $\frac{d\langle\mathcal{P}\rangle}{dt} = 0 \Rightarrow$ parity conserved

$$\boxed{\text{Reflection symmetry} \Rightarrow \langle\mathcal{P}\rangle = \text{constant} \Rightarrow \text{parity conserved}}$$

Ex Consider a particle in a 1-D box, $-\frac{a}{2} < x < \frac{a}{2}$.

Energy eigenstates are

$$\psi_n = \begin{cases} \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} & n \text{ even} \\ \sqrt{\frac{2}{a}} \cos \frac{n\pi x}{a} & n \text{ odd} \end{cases}$$

and these are also parity eigenstates,

Supose $\Psi(x,0) = \frac{1}{\sqrt{45}} (3\psi_1 + 6\psi_2)$

Then at $t=0$ and all subsequent t,

$$\langle P \rangle = \langle \Psi(x,0) | \hat{P} \Psi(x,0) \rangle$$

$$= \frac{1}{45} \langle 3\psi_1 + 6\psi_2 | 3\psi_1 - 6\psi_2 \rangle$$

$$= \frac{1}{45} (9 - 36) = -\frac{27}{45}$$