Lecture 12 – 13

Examples

1) : Free particles

wave number $k = \frac{2\pi}{\lambda}$

frequency ω $= \frac{2\pi}{T}$

$$\mathbb{H} = \frac{\mathbb{P}^2}{2m} \Rightarrow \psi_p(x,t) = A e^{i\boxed{\frac{p}{\hbar}}x} e^{-i\left(\frac{p^2}{2m\hbar}\right)t}$$

is a possible solution of $i\hbar \frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi$

In fact, there is such a solution for every value of p $(-\infty \dots \infty)$. This makes sense because classically, if we know p we know $E = \frac{p^2}{2m}$, and of course ψ_p is an ES to $\mathbb{P}$ with eigenvalue p for each t.

a) important point: This particular form of a solution to S.E. is called "separable", since the dependence of ψ_p on x is "separate" from its dependence on t → it's just the product of 2 different functions, one of x (only) and one of t (only): $\psi_p(x,t) = \varphi_p(x) \cdot e^{-iE/\hbar\, t}$ with $E =$

Such solutions are especially important, since the spatial part is an ES to $\mathbb{H}$ with eigen~~state~~value E. So we solved S.E. in 2 parts:

i) first, find solution to $\mathbb{H}\varphi_E(x) = E\varphi$

ii) write full solution as $\psi_E(x,t) = \varphi_E(x) \cdot e^{-\frac{iE}{\hbar}}$

Clearly, such solutions (often called "stationary" which only makes sense for bound states → see later) play an especially important role:

iii) They are states with DEFINITE ("∞ sharp") values of energy, E (since they are eigenstates to H). If we prepare a system in such a state, we will know with certainty what energy we will measure: E.

iv) Expectation values of all operators (that act only on the ~~[illegible]~~ x-coordinate and are time-independent) will be constant with time:

$$\int_{-\infty}^{\infty} \psi^*(x,t)\, O\, \psi(x,t)\, dx = \int_{-\infty}^{\infty} \overbrace{\boxed{e^{i\frac{E}{\hbar}t}}\, \varphi_E^*(x)\, O\, \varphi_E(x)\, \boxed{e^{-i\frac{E}{\hbar}t}}}^{=1} dx$$

→ "Nothing ever happens", the state is totally frozen ("stationary"). These states tend to be stable (at least stable enough to observe) because they do not emit radiation (no varying dipole moments) (except when coupled to an external field → no longer eigenstates). In particular, E = const. and "∞ sharp". If we find the ES to H with the lowest possible E, we have the "ground state" which should be absolutely stable (energy conservation).

v) Of course not <u>all</u> solutions to S.E. look like that (are separable), but (THEOREM) we can build up all possible solutions as linear superpositions of such solutions:

$$\Psi(x,t) = \sum\!\!\!\!\!\!\int C_E\, \varphi_E(x)\, e^{-i\frac{E}{\hbar}t}\, dx .$$

1) We realize that in our special case (free particle), the separable solution is NOT a "real" solution, since $\psi_p(x) = e^{i\frac{p}{\hbar}x}$ is not normalizable (not a "real state").

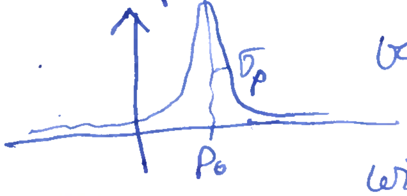
But we can build up <u>all</u> true solution from these special ones:

$$\psi(x,t) = \int_{-\infty}^{\infty} c(p)\, e^{i\frac{p}{\hbar}x}\, e^{-i\frac{E_p t}{\hbar}}\, dp \quad \text{w/} \quad E_p = \frac{p^2}{2m}$$

Special case: Gaussian distribution $c(p) = \sqrt{\frac{1}{\sqrt{2\pi}\,\sigma_p}}\, e^{-\frac{(p-p_0)^2}{4\sigma_p^2}}$

→ G. "Wave Packet" that moves along x with average momentum p_0.

→ if σ_p is <u>small</u>:



very similar to classical particle with fixed momentum p_0

HERE: it so happens that $\sigma_x \cdot \sigma_p = \frac{\hbar}{2}$ (not $\geq \frac{\hbar}{2}$)

$\Rightarrow \sigma_x = \frac{\hbar}{2\sigma_p}$; the closer we get to a true ES of H, the less well we know position, and vice versa.

Example: 1µg dust speck moving with $1000 \pm 0.001 \frac{mm}{s}$ (10^{-6} precision) $\Rightarrow \sigma_p = 10^{-15}$ kg m/s $\Rightarrow \Delta x = \frac{\hbar}{2\sigma_p} = 0.5 \cdot 10^{-19}$ m ($\hbar = 10^{-34}$ Js). $\Rightarrow$ reason classical mechanics (point particle w/ known position + momentum) works.

electron: $m \approx 10^{-30}$ kg, assume $\Delta v \simeq 1000 \frac{m}{s} \Rightarrow \Delta x = 50$ nm

NOT negligible (1000 x atomic diameter).

[<u>NOTE</u>: over time, σ_x increases bc. of σ_p → smearing out of W.P.

Now we apply this method of solving SE to some BOUND states.

2) well with ∞ high walls (Tipler 237–245)

Simplemost case of a binding potential

$$V(x) = \begin{cases} 0, & 0 \le x \le L \\ \infty & \text{else} \end{cases}$$

Classical solution: pick arbitrary initial speed, position
→ keeps bouncing back and forth forever.

Qu.M.: Have to solve $H\varphi_E(x) = E\varphi_E(x)$ with $H = \frac{p^2}{2m} + V(x)$
$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

⇒ a) for $x < 0$, $x > L$: $V(x) = \infty$
cannot work unless $\varphi_E(x) = 0$ there ($V(x)\varphi(x)$ blows up,

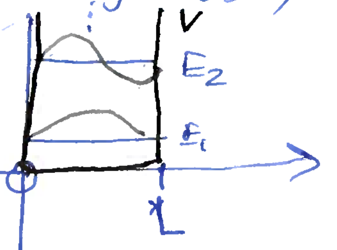
b) for $0 \le x \le L$: equal to <u>FREE</u> particle!
Solutions: $\varphi_p(x) = A\, e^{i\frac{p}{\hbar}x}$ for <u>any</u> p, $-\infty \le p \le \infty$

BUT: need <u>continuous</u> solution at $x = 0, L$!
Can't work with just ~~one~~ φ_p. Note: classical bouncing back and forth → maybe need to combine 2 φ's with p and $-p$? Yes! if we pick
$\frac{1}{2i}\left(e^{i\frac{p}{\hbar}x} - e^{-i\frac{p}{\hbar}x}\right) \Rightarrow \sin\frac{p}{\hbar}x \Rightarrow = 0$ for $x = 0$!

BUT: also need 0 @ $x = L$ ⇒ $\sin\frac{p}{\hbar}L = 0$!

⇒ <u>cannot</u> accept <u>all</u> possible p, only those with
$\frac{pL}{\hbar} = n \cdot \pi$ or $p_n = \frac{n\pi\hbar}{L}$ (waves of $\lambda = \frac{L}{2}, L, \frac{3}{2}L \ldots$
→ standing waves?)

⇒ $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$, $n = 1, 2, \ldots$



<u>Energy is quantized!</u>

+ lowest (ground state) E is NOT 0!
Discuss features of solutions, in particular $|\varphi(x)|^2$, $\langle x\rangle$, $\langle p\rangle$, $\langle p^2\rangle$ etc

3) Harmonic Oscillator (Tipler 253 – 257 and <u>online</u> : Schrödinger's trick)

Physicists LOVE the H.O. It's probably the only bound state system that you have <u>really</u> solved in PHYS 231 (planetary orbits are <u>so much</u> harder, so probably the solution was just handed down to you). There are very good reasons for this love:

a) HO is "simple" (at least in CM)

b) oscillations are (some of the) most fundamental features of the world → basis for all waves

c) Most realistic potentials look like H. O. close to equilibrium point:

$$V(x) = V(x_0) + \underbrace{\cancel{\frac{dV}{dx}(x_0)\cdot(x-x_0)}}_{=0 \text{ because force}=0 \text{ @ equilibrium}} + \frac{1}{2}\frac{d^2V}{dx^2}(x_0)\,(x-x_0)^2 + \dots$$

compare to mass on spring: $F = -kx$ $\quad \Delta W = \int_0^x F\,dx = -\frac{1}{2}kx^2$

$V(x) = -\Delta W = \frac{1}{2}kx^2$ $\quad$ ($x=0$ is equilibrium here!).

Solution : $m\ddot{x}(t) = -kx(t) \Rightarrow x(t) = A\sin\omega t + B\cos\omega t$ with $\omega^2 = \frac{k}{m}$

Hamiltonian : $\frac{p^2}{2m} + \frac{k}{2}x^2 = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}x^2$

Stationary Solution: $\frac{1}{2m}\left(-\hbar^2\right)\frac{\partial^2\varphi_E}{\partial x^2} + \frac{m\omega^2}{2}x^2\varphi_E(x) = E\varphi_E(x)$

Looks scary! Won't be able to solve in general (but: see "Schrödinger's trick" in online companion to Tipler's book → posted on website)

But: we can make it look a bit more symmetric in x:

divide both sides by $\hbar\omega$ $\Rightarrow -\frac{1}{2}\frac{1}{m\omega/\hbar}\frac{\partial^2\varphi_E}{\partial x^2} + \frac{1}{2}\,m\omega/\hbar\; x^2\varphi_E = \frac{E}{\hbar\omega}$

Call $y = x\cdot\sqrt{\frac{m\omega}{\hbar}}$, $e = \frac{E}{\hbar\omega}$ (note: all dimensionless variables!)

$$\Rightarrow -\frac{1}{2}\frac{\partial^2}{\partial y^2}\varphi_E + \frac{1}{2}y^2\varphi_E = e\,\varphi_E .$$

strategy: Solve for $\varphi_E(y)$, then replace $y \to x\sqrt{m\omega/\hbar}$

Possible solutions? (ask for suggestions)

a) e^{ikx} → no, don't fall off @ large $|x|$

→ must find something that falls off a lot faster than $\frac{1}{x^2}$ to keep $V\varphi$ finite!

b) $e^{-\kappa x}$? only works for $x > 0$

$e^{-\kappa|x|}$? unpleasant kink @ $x=0$ (whereas solutions should be smooth in $\frac{\partial^2}{\partial x^2}$)

c) ⇒ maybe Gaussian? Why not → solution SHOULD be well-localized (not ~~go~~ on to large x)

let's try it: $\varphi_E(y) = e^{-\alpha \cancel{x} y^2} \Rightarrow \frac{\partial \varphi_E}{\partial y} = -2\alpha y e^{-\alpha y^2}$

$\Rightarrow \frac{\partial^2 \varphi_E}{\partial y^2} = (4\alpha^2 y^2 - 2\alpha) e^{-\alpha y^2} \quad = y^2 e^{-\alpha y^2} - 2e\, e^{-\alpha y^2}$

⇒ compare: works (only!) if $\alpha = \frac{1}{2}$ and $e = \alpha = \frac{1}{2}$

⇒ found $\underline{\underline{I}}$ solution: $\varphi_{E_0}(x) = A \cdot e^{-\frac{m\omega}{2\hbar}x^2} \qquad E_0 = \frac{1}{2}\hbar\omega$

→ Gaussian wave packet again; but NO motion (centered at $x=0$) and NO "spreading" ($\sigma_x = \frac{\hbar}{\sqrt{2m\omega}}$ for all times)

Some bookkeeping

a) Normalization? $\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{2\pi}\boxed{\frac{1}{\sqrt{2a}}} = \sigma$

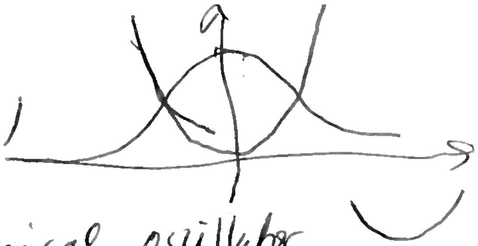
$|\varphi_E(x)|^2 = A^2 e^{-\frac{m\omega}{\hbar}x^2}$

$\Rightarrow A^2 \cdot \sqrt{2\pi}\sqrt{\frac{\hbar}{2m\omega}} \overset{!}{=} 1 \Rightarrow A = \sqrt{\frac{1}{\sqrt{2\pi}\,\sigma_x}}$

b) Full solution: $\varphi(x,t) = \varphi_{E_0}(x)\, e^{-i\frac{\omega}{2}t}$ ← curiously, only $\frac{1}{2}$ of classical frequency

c) Is this the ground state? YES! We already know that ~~the~~ Gaussian distribution is the ONLY example where $\sigma_p \cdot \sigma_x = \frac{\hbar}{2}$, since $H \sim ax^2 + bp^2$, $\langle H \rangle = a\sigma_x^2 + b\sigma_p^2$, To lower E (and therefore $\langle H \rangle$) would require to lower either σ_x^2 or σ_p^2 → but the other one would blow up!

NOTE: "zero-point energy", $E_0 \neq 0$!



d) Properties of the solution: (Probability density)

i) Centered/ ~~at~~ ~~or~~ maximum at origin ~~as~~ (different from classical oscillator which has highest probability at turning points

ii) Classical turning points: $E = \frac{1}{2} k x_{max}^2$

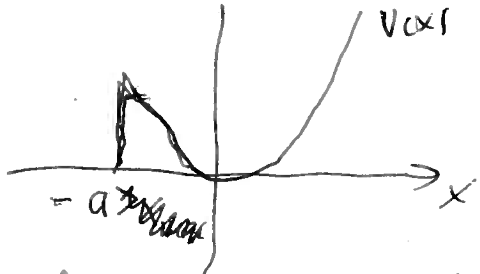
$$\Rightarrow x_{max} = \sqrt{2E/k} = \sqrt{2E/m\omega^2}$$

Solution $E = \frac{1}{2}\hbar\omega \Rightarrow x^{cl}_{max} = \sqrt{\frac{\hbar}{m\omega}}$

which is $\sqrt{2} \cdot \sigma_x$ → not unreasonable.

BUT: $|\psi_E(x)|^2 \neq 0$ even for $x > x^{cl}_{max}$!

Typical feature of QM: "leaking out" or "tunneling". E.g. if potential stops ~~rising~~ rising and falls back to zero for $|a| > x^{cl}_{max}$), the classical oscillator would never "know"



and stay confined in region $-x^{cl}_{max} \le x \le x^{cl}_{max}$ "forever". QM oscillator can "leak ~~off~~ out" or tunnel through energy barriers and then become a free particle within a finite time!

example: α-decay, fission

HO continued

Are there **more** eigenstates / energy eigenvalues ? $\varepsilon_0\hbar\omega = E_0 = \frac{1}{2}\hbar\omega$

Remember : $H = \frac{1}{2}\left(-\frac{\partial^2}{\partial y^2}\right) + \frac{1}{2}y^2$; $H\varphi_{E_0} = \varepsilon_0\varphi_{E_0} = \frac{1}{2}\varphi_{E_0}$

Let's try $\varphi'(y) = y\cdot\varphi_{E_0}(y) \Rightarrow H\varphi' = -\frac{1}{2}\frac{\partial^2}{\partial y^2}y\varphi_{E_0} + \frac{1}{2}y^3 \cancel{\varphi_{E_0}}$

$$= -\frac{1}{2}\frac{\partial}{\partial y}\left(\underbrace{\frac{\partial}{\partial y}y\varphi_{E_0}}_{\varphi_{E_0} + y\frac{\partial}{\partial y}\varphi_{E_0}}\right) + \frac{1}{2}y^2\varphi'$$

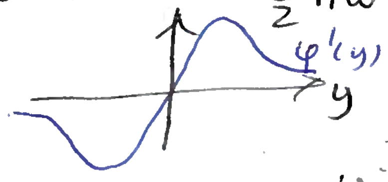
$$= -\frac{1}{2}\left(\frac{\partial}{\partial y}\varphi_{E_0} + \cancel{\left(\frac{\partial y}{\partial y}\right)}\frac{\partial}{\partial y}\varphi_{E_0} + y\frac{\partial^2}{\partial y^2}\varphi_{E_0}\right) + \frac{1}{2}y\left(y^2\varphi_{E_0}\right)$$

$$= (y)\underbrace{\frac{1}{2}\left(-\frac{\partial^2}{\partial y^2}\varphi_{E_0} + y^2\varphi_{E_0}\right)}_{y\cdot E_0\varphi_{E_0}} \underbrace{-\frac{\partial}{\partial y}\varphi_{E_0}}_{=\frac{1}{2}2y\varphi_{E_0}} \Bigg\} = (E_0+1)\,y\,\varphi_{E_0}$$

$\frac{\partial}{\partial y}e^{-\frac{1}{2}y^2} = -\frac{1}{2}2y\,e^{-\frac{1}{2}y^2}$

$\Rightarrow$ EV $E = (\varepsilon_0+1)\hbar\omega = \frac{3}{2}\hbar\omega$

interesting shape :



Flips sign for $x \to -x$

zero (probability) @ $x = 0$!

wider distribution in x

$\Rightarrow$ larger amplitude

↓ leave out if time doesn't permit ↓

Note: ~~in general~~, Could have also used $\varphi' = -\frac{\partial}{\partial y}\varphi_{E_0}$ (same result)

In general, define $a^+ = y - \frac{\partial}{\partial y} \Rightarrow$

$$H(a^+\varphi_E) = yH\varphi_E - \frac{\partial}{\partial y}\varphi_E - \frac{1}{2}\left(\underbrace{\frac{\partial^2}{\partial y^2}\frac{\partial}{\partial y}\varphi_E}_{=\frac{\partial^3}{\partial y^2} = \frac{\partial}{\partial y}\left(\frac{\partial^2}{\partial y^2}\right)} + y^2\frac{\partial}{\partial y}\varphi_E\right)$$

$$y^2\frac{\partial}{\partial y}\varphi_E = \frac{\partial}{\partial y}y^2\varphi_E - 2y\varphi_E$$

⊛

⊛ $= \frac{\partial}{\partial y}H\varphi_E + y\varphi_E \Rightarrow H(a^+\varphi_E) = \left(y - \frac{\partial}{\partial y}\right)H\varphi_E + \left(y - \frac{\partial}{\partial \varphi}\right)\varphi_E = a^+(\varepsilon+1)\varphi_E$

It follows that if φ_E is eigenstate with EV ε then $a^\dagger \varphi_E$ is ES w/ EV $\varepsilon + 1$ $\Rightarrow$ $a^\dagger$ "increases energy by $1\hbar\omega$" → ladder operator.

Can generate all eigenstates using repeatedly $(a^\dagger)^n \varphi_{E_0}$ just need to normalize.

Higher energy eigenstates:

0 : $e^{-\frac{1}{2}y^2}$

1 : $y e^{-\frac{1}{2}y^2}$

2 : $(2y^2-1)e^{-\frac{1}{2}y^2}$ etc.

with energies $\frac{1}{2}\hbar\omega$, $\frac{3}{2}\hbar\omega$, $\frac{5}{2}\hbar\omega$ etc. (equidistant – any 2 states ~~are~~ $\Delta E = \hbar\omega$ apart).

Polynomials times exponent $-\frac{1}{2}y^2$ (Gaussian)

↳ called "Hermite polynomials"