412-1, Week 2, Day 1/2

(Complex math, Graphical solutions to Schr.; Stürm Liouville)

Interference, thinking some in complex plane

$$P_{x,x+\Delta x} = \psi^*(x)\psi(x)\Delta x$$

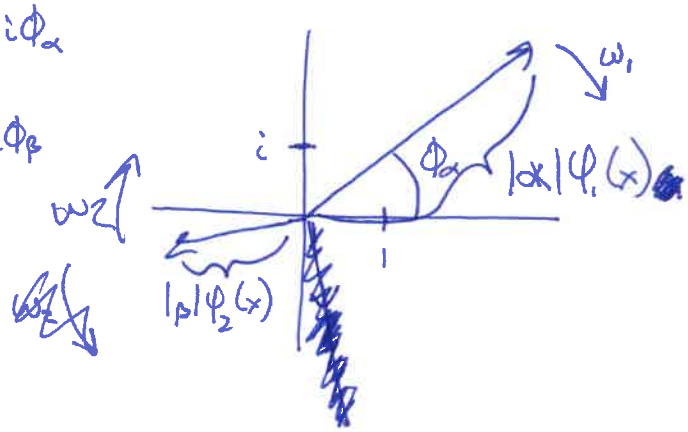
$$\frac{\partial P}{\partial x} = \psi^*(x)\psi(x)$$

$$\psi_{(x)} = \alpha\,\varphi_1(x)e^{-i\omega_1 t} + \beta\,\varphi_2(x)e^{-i\omega_2 t}$$

(Not separable)

$\alpha = |\alpha|e^{i\phi_\alpha}$

$\beta = |\beta|e^{i\phi_\beta}$



- Constructive interference (Max probability) when these vectors align, regardless of particular angle.
- Min prob. when they anti-align

$\Delta\omega = \omega_1 - \omega_2$

$\Delta\phi = \phi_\alpha - \phi_\beta$

$$\psi^*\psi = |\alpha|^2\varphi_1^2 + |\beta|^2\varphi_2^2 + \underbrace{\left(\alpha e^{-i\omega_1 t}\beta^* e^{i\omega_2 t} + \text{c.c.}\right)}_{2\,\mathrm{Re}\left[\alpha\beta^* e^{-i\Delta\omega t}\right]}\varphi_1\varphi_2$$

$$= 2|\alpha||\beta|\,\mathrm{Re}\left[e^{i\Delta\phi}e^{-i\Delta\omega t}\right]$$

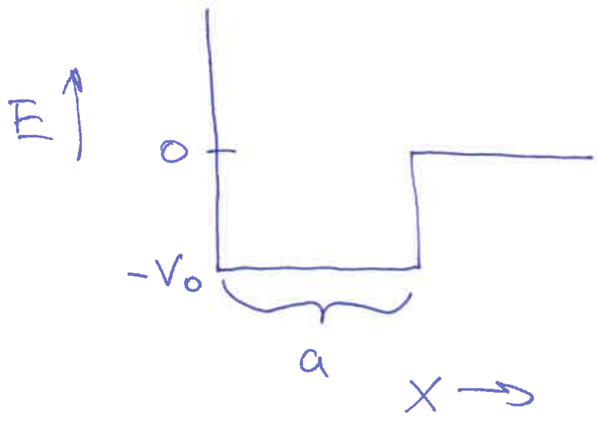
$$= 2|\alpha\beta|\cos(\Delta\omega t - \Delta\phi)$$

$\Rightarrow$ Only $\Delta\phi$ matters. Not $\phi_1 + \phi_2$. Arbitrary choice for overall ϕ offset.

$\Rightarrow$ Cannot turn off interference by adjusting $\Delta\phi$. Why? Can only change time of 1st beat

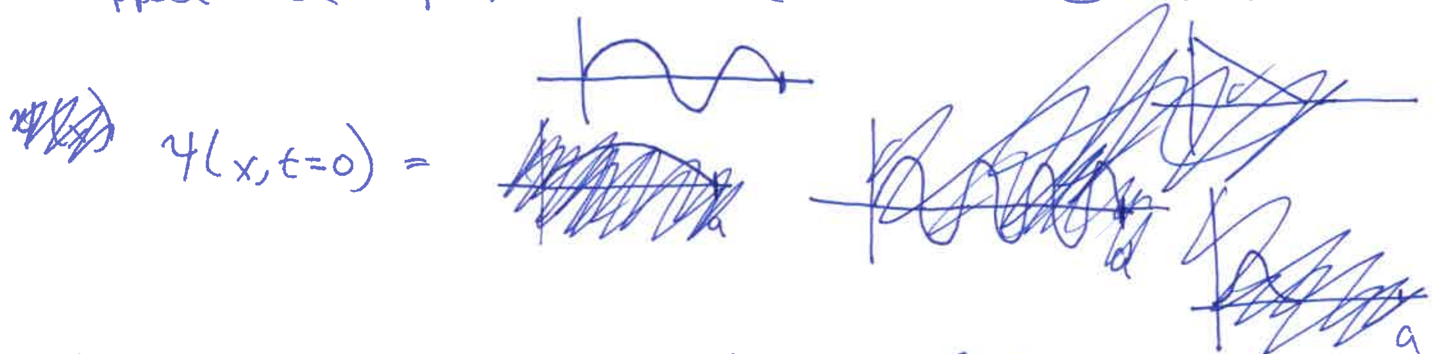
1/3

(Finite Square Well, Graphical Solution)



Suppose I prepare state s.t. @ $t=0$

$\psi(x,t=0) =$



$\boxed{Q}$ How do I find $\psi(x,t)$? ~~Will particle have chance of escaping well?~~

$\boxed{A}$ (Should know this without needing to think.)

1) Find solutions of T.I. Schr eqn $\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\varphi_n(x) + V(x)\varphi_n(x) = E_n\varphi_n(x)$

2) Find coefficients s.t. $\psi(x,t=0) = \sum_n c_n \varphi_n(x)$

(or integral if continuous states involved)

2.5) Normalize

(Easy part)

$\boxed{C}$ 3) $\psi(x,t) = \sum c_n \varphi_n(x) e^{-i\frac{E_n}{\hbar}t}$

$\boxed{Q}$ So, qualitatively, what will $\Psi(x,t)$ look like for our example?

$\boxed{A}$ - Well, ~~it~~ it definitely does more than oscillate. If ∞ square well, it would just oscillate with $e^{-i\omega_3 t}$. But $V(x)$ here is different + that w.f. is not an eigenfunction of ~~the~~ T. I. Schr. with this $V(x)$.

- But ~~not~~ we don't know yet whether probability all stays in well or leaks out. Depends on whether we need any $E>0$ solutions to represent ~~Ψ~~ $\Psi(t=0)$.

$\Rightarrow$ Find solutions of T.I. Schr ~~,~~, i.e. eigenfunctions for this $V(x)$

$x>a$ (Outside well), if $E>0$

$$\frac{d^2}{dx^2}\varphi_E(x) + k^2\varphi_E(x) = 0 \quad , \quad k^2 = \frac{2mE}{\hbar^2}$$

$0<x<a$ (Inside well):

$$\frac{d^2}{dx^2}\varphi_E(x) + k_v^2\varphi_E(x) = 0 \quad , \quad k_v^2 = \frac{2m(E+V_0)}{\hbar^2}$$

(Just for convenience, rewrite ...)

For case of $x>a$ $E<0$

$$\frac{d^2}{dx^2}\varphi_E(x) - \lambda^2\varphi_E(x) = 0 \quad , \quad \lambda^2 = -\frac{2mE}{\hbar^2}$$

Eigenfunctions, ~~Sturm-Liouville Theorem~~ Numerical Solutions ~~Part~~ I

Let's look at a different approach to finding eigenfunctions of Schr.

Previous

① Specify 2 B.C.s for $\varphi_E(x)$, typically @ $x=0$ & $x=\infty$

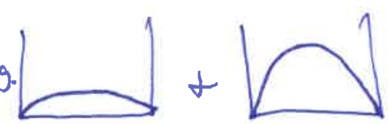
② Find solutions $\varphi_E(x)$ in each region $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi_E(x)+V(x)\varphi_E(x)=E\varphi_E(x)$

③ ~~Require continuity + smoothness (if V(x) finite)~~

Alternative

① Specify 2 B.C.'s by $\varphi(x=0)$ & $\varphi'(x=0)$

Specifying this is equivalent to normalizing, since e.g.



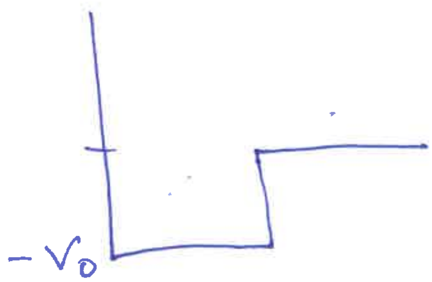
are same solution.

② Try some arbitrary E & integrate Schr eqn vs. x (Diff.eq. specifies precise curvature, so if I know $\varphi(x)$ & $\varphi'(x)$, then I know how it must change as I step away by Δx)

③ Find E that localizes particle, e.g. $\varphi(x=\infty)=0$

Examples with finite square well

Try $E = -V_0$



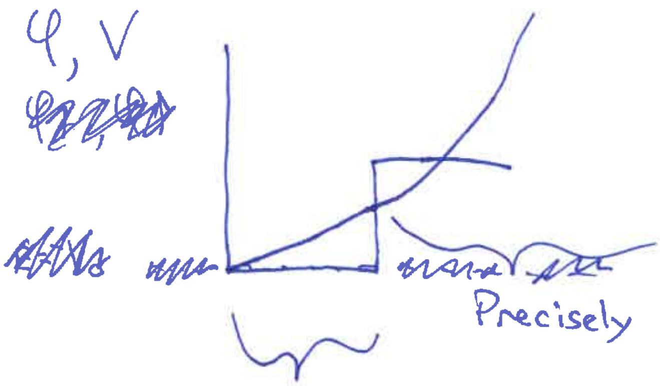
$$\frac{d^2}{dx^2}\varphi_E(x) = \frac{2m}{\hbar^2}\left(V(x) - E\right)\varphi_E(x)$$

$$= 0$$

$\Rightarrow$ straight line.

Pick arbitrary slope.

~~Will not be~~



Precisely $Ae^{-\lambda x} + Be^{\lambda x}$

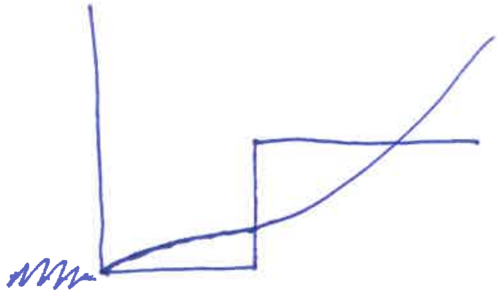
Precisely sines + cosines

- This technically solves T.I. Schr eqn, but not in any useful way. Particle is not localized – all weight is at ∞.

- Note that we didn't need to think about ~~match~~ continuity + smoothness at boundary. Those requirements are just consequences of obeying the diff. eq., and they fall out automatically in this integration approach

- Raise E a bit more, same $\psi'(0)$

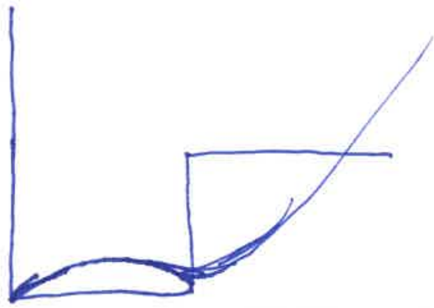
$E = E_a > V_0$



(Will not offset ψ axis on these)

Still doesn't work

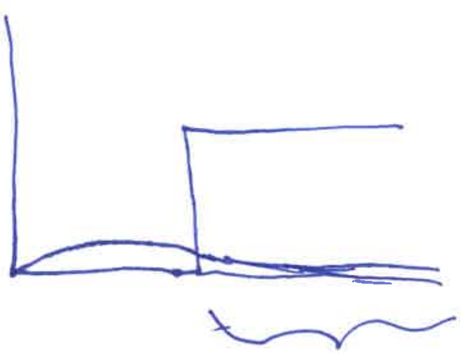
- More:



$\boxed{Q}$ What is going on here? How can RHS of w.f. start going down then reverse?

$\boxed{A}$ $\psi(x) = Ae^{-\lambda x} + Be^{+\lambda x}$. $A > B \Rightarrow$ decaying term dominates at first

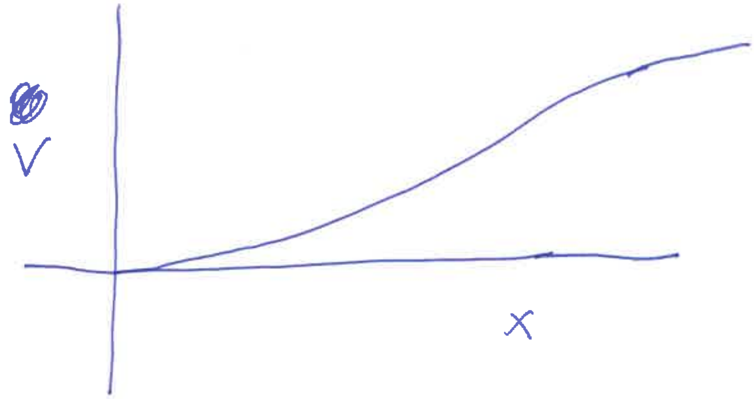
- More



At just the right energy, the integrated solution just settles to 0 @ $x = \infty$

$\underbrace{\qquad\qquad}_{\text{Precisely } Ae^{-\lambda x}}$ $(B = 0)$

More general potential



For $E > V(x)$

$$\frac{d^2}{dx^2}\psi + k^2(x)\psi = 0, \quad k(x) > 0$$

$\Rightarrow$ Positive $\psi \to$ negative 2nd deriv. ~~curvature~~

(oscillations)

sine-like but not exactly b/c $V(x)$ not flat

For $E < V(x)$

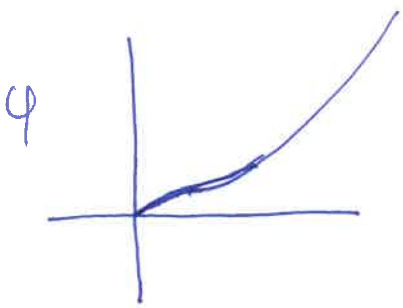
$$\frac{d^2}{dx^2}\psi - \lambda^2(x)\psi = 0, \quad \lambda(x) > 0$$

$\Rightarrow$ Positive $\psi \to$ positive 2nd deriv ~~curvature~~

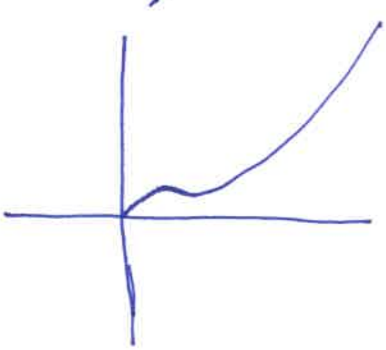
(exp. decay + runaway both work)

exp.-like

Guess some E:

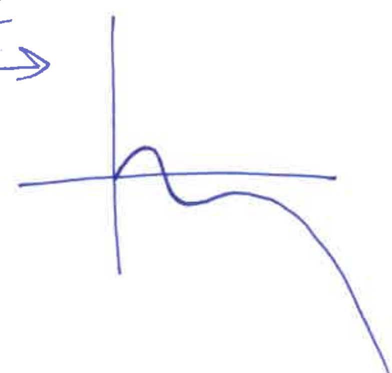


Raise E ↓

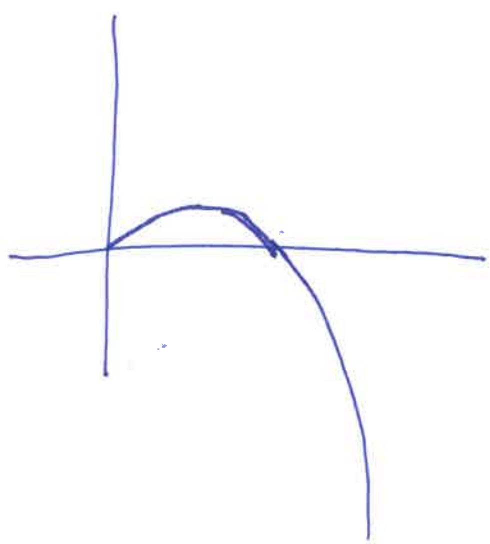


Raise E →

Raise E →



More



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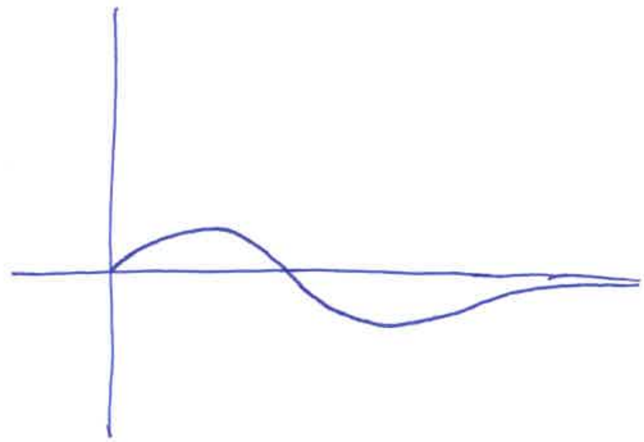
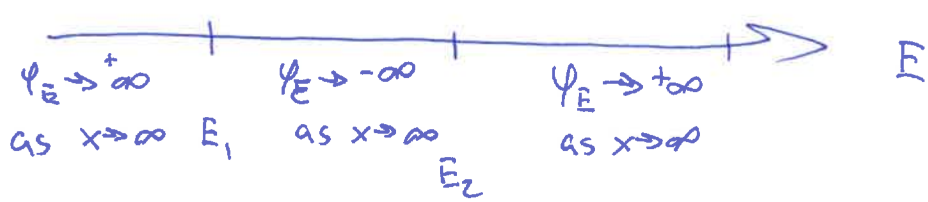


(Note: we should draw transition from sine-like to exp-like behavior happening farther to right as $E\uparrow$. Also $\lambda\downarrow$ as $E\uparrow$.)

Pattern:

- Discrete energies $(E_1, E_2, E_3, \ldots)$ which are well behaved at $x = \infty$.
- As $E\uparrow$, $\varphi_E(x)$ oscillates faster in interior & has more zeroes.
-



- Each successive special function has one more zero, i.e. "node".
- $$\underbrace{\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]}_{\text{operator } \mathcal{O}} \varphi_E(x) = E\,\varphi_E(x)$$

$$\mathcal{O}\varphi_E(x) = E\,\varphi_E(x)$$

- Operator $\mathcal{O}$ has special functions "eigenfunctions"
- "Eigen" means "characteristic of", or "belonging to" in German
- Corresponding E are "eigenvalues"

Schr Eqn

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = H\psi(x,t) \quad , \quad H = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

- $\psi(x,t)$ solves T.D. Schr.

Q Is $\psi(x,t)$ factorable ~~separable~~ into $f(x)g(t)$?

A Only for special cases $f(x) = \varphi_E(x)$

If spatial part only one e.f., then yes.

General solution is

$$\psi(x,t) = \sum_n c_n \varphi_n(x) e^{-i\omega_n t}$$

which is not factorable $\Rightarrow$ interesting spatial & temporal behavior

- But how do we know that sum is really the most general solution?

Stürm-Liouville Theorem

We have found solutions to the Schrodinger equation, both analytically and numerically. But who says that the most general solution can be ~~ep~~ expressed in terms of the eigenfunctions?

Stürm-Liouville Theorem

Let $\mathcal{O}$ be a differential operator on a ~~s~~ space of functions $f(x)$ satisfying B.C.s, such that $\mathcal{O}$ is

(a) Positive: for any $f(x)$
$$\int dx\, f^*(x)\,\mathcal{O}\, f(x) > 0$$

(b) Self-adjoint: for any $f(x), g(x)$
$$\int dx\, g^*(x)\,\mathcal{O}\, f(x) = \int dx\, (\mathcal{O} g(x))^* f(x)$$

$\boxed{E}$ (Think of this as an operator acting either backwards or forwards. This is a rule for how they relate to each other.)

- Then eigenfunctions of $\mathcal{O}$

$$\mathcal{O}\,\varphi_n(x) = \lambda_n \varphi_n(x)$$

form a complete set of functions.

$\Rightarrow$ Any $f(x)$ satisfying the B.C.'s can be approximated by

$$g_M(x) = \sum_{n=1}^{M} c_n \varphi_n(x)$$

s.t. $\int dx\,(f(x) - g_M(x))^2 \to 0$ as $M \to \infty$

$\uparrow$ sum of disagreements ^2 at each point along x ~~in space~~

(Don't want to just consider $\int (f(x) - g(x))$ b/c we don't want to be fooled by + errors at dif points in space cancelling − errors)

Schr eqn $\mathcal{O} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ satisfies the conditions of this theorem for space of fns for ~~which~~ which $f(x) \to 0$ as $x \to \pm\infty$

Positive :

$$\int dx\, f^*\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]f \quad > 0 \quad (?)$$

Well, we know that $f f^* = |f|^2 \geq 0$ for all x

$(f^*(x) f(x) \geq 0) \rightarrow \int \ldots > 0$

And $f^{*\prime} f' \geq 0$ for all x, where $f' = \frac{df(x)}{dx}$

$\downarrow$

$\int \ldots > 0$

So, we need to move one of those derivitives left.

remove a prime — move a prime

Can write down immediately

$$\int_{-\infty}^{\infty} \underbrace{f^*}_{u}\, \underbrace{f''\, dx}_{dv} = \underbrace{f^*}_{u}\underbrace{f'}_{v}\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \underbrace{f'}_{v}\, \underbrace{f^{*\prime}\, dx}_{du}$$

(Cheat to set a prime on f^* & remove one from f)

$u = f^*$ $\Rightarrow du = \frac{df^*}{dx}dx = f^{*\prime}dx$

$dv = f'' dx = \frac{df'}{dx}dx = df' \Rightarrow v = f'$

$$\int u\,dv = uv\Big| - \int v\,du$$

$$\int_{-\infty}^{\infty} f^* f'' dx = \underset{\text{by B.C.'s}}{0} - \underbrace{\int_{-\infty}^{\infty} f^{*\prime} f'\, dx}_{>0}$$

$$\int dx\ f^* H f$$

$$= +\underbrace{\frac{\hbar^2}{2m}\int f'^* f'\,dx}_{>0} + \underbrace{\int V(x)\, f^* f}_{>0 \text{ if } V(x)>0}$$

Energy can always be offset, so for trivial offset of any $V(x)$ with a minimum, we see that H is positive. ✓

<u>Self-adjoint</u> $\int dx\ g^* H f(x)$

$$\int dx\ g^*(x)\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right] f(x)$$

First $\int g^* f''\,dx = g^* f'\Big| - \int g^{*\prime} f'$ but here want that last prime off f

$$= \underbrace{g^* f'\Big| - g^{*\prime} f\Big|}_{=0 \text{ if } f,g\to 0 \text{ at } \infty} + \int g^{*\prime\prime} f$$

$$= \int dx\left[\frac{-\hbar^2}{2m}\frac{d^2 g^*}{dx^2} + V(x)\, g^*\right] f$$

$$= \int dx\ [H g(x)]^* f(x) \quad ✓$$

~~integral be taken to H can't act forward on f or on g first, according to this procedure involving c.c.~~

$\Rightarrow$ So, S-L theorem says that we can always expand $\psi(x,t=0) = \sum_n c_n \varphi_n(x)$

where $H\varphi_n(x) = E_n \varphi_n(x)$.

- If we take enough n, we can reproduce initial state to arb. precision.

$$\Rightarrow \psi(x,t) = \sum_n c_n \varphi_n(x) e^{-i\omega_n t}$$

General set-up of S-L th. implies some properties of eigenfunctions / values.

① λ_n (here E_n) are real numbers

Proof:

$$\mathcal{O}\varphi_n(x) = \lambda_n \varphi_n(x) \Rightarrow \underbrace{\int dx\, \varphi_n^* \mathcal{O} \varphi_n}_{\text{For } \mathcal{O}=H,\text{ this is real (+ also positive if } v(x)>0)} = \lambda_n \underbrace{\int dx\, \varphi_n^* \varphi_n}_{\text{(real) positive}}$$

That's important part

eigenvalues of a positive operator are $\boxed{\text{real}}$ (+ positive if it's really positive i.e. if $V(x)>0$)

If $v(x)<0$ in places, λ_n can be <0

$\Downarrow$

λ_n is ratio of two real #'s $\Rightarrow$ λ_n is real $\Rightarrow E_n$ real

② Orthogonality

$$\int dx\, \varphi_n^*(x)\, \varphi_m(x) = \begin{cases} N_{n,m} & \lambda_n = \lambda_m \\ 0 & \lambda_n \neq \lambda_m \end{cases}$$

If ① non-degenerate (i.e. each λ_n is unique to a single φ_n)

② we normalize φ_n s.t. $\int dx\, \varphi_n^* \varphi_n = 1$

Orthogonality means

$$\Rightarrow \int dx\, \varphi_n^* \varphi_m = \begin{cases} 1 & n=m \\ 0 & n \neq m \end{cases} = \delta_{nm}$$

Degenerate: 2 or more distinct e.f. have same e.v.

Non-deg: E.V.'s are all unique & each corresponds to a single e.f.

Proof:

$$\int dx\, \varphi_n^* \mathcal{O} \varphi_m = \lambda_m \left(\int dx\, \varphi_n^* \varphi_m \right)$$

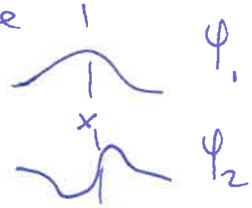
$$= \int dx\, (\mathcal{O}\varphi_n)^* \varphi_m = \lambda_n \left(\int dx\, \varphi_n^* \varphi_m \right)$$

(since $\lambda_n = \lambda_n^*$)

If $\lambda_m \neq \lambda_n$ this is a contradiction, unless

$$\int dx\, \varphi_n^* \varphi_m = 0 \quad \text{for } \lambda_m \neq \lambda_n$$

$\Rightarrow$ Successive φ_n had better get additional nodes so that $\int$ has positive & negative parts cancelling, like



$$\Rightarrow \int dx\, \varphi_1 \varphi_2 = 0$$