Ch. 6 Position & Momentum

- Start with particle moving in one dimension:
- classically position given by $-\infty < x < \infty$ $x \in \mathbb{R}$.
- Ignore spin (will come back next semester)
- Experimentally, we seem to find we can measure a particle's position (e.g., by scattering light off it) and find any value $x \in \mathbb{R}$. I.e., position does not seem to be quantized.

- So posit: exists a position operator

$$\hat{X} = \hat{X}^{+} \quad \text{with eigenvalues} = \mathbb{R}. \quad (*)$$

Note: $(*)$ is an idealization/simplification:

- In reality can only ever measure to some finite precision δx (e.g. wavelength of light), and also $\exists$ max. extent L (e.g. size of lab), so

$$x \in \left\{ n \cdot \delta x \, , \quad n = 0, 1, 2, \ldots, \frac{L}{\delta x} \right\}$$

finite set, so $\dim \mathcal{H} = \frac{L}{\delta x} < \infty$.

- Only get $x \in \mathbb{R}$ as limits $\delta x \to 0$, $L \to \infty$.
- Even <u>in principle</u> we don't think these limits exist:

{ form black hole

$\delta x_{min} \simeq \ell_{Planck} \doteq \sqrt{\hbar G/c^3} \approx 10^{-35}\,m$ {that size & can't see inside

$L_{max} \simeq \frac{c}{H_0} \simeq \frac{1}{\sqrt{\Lambda_{cc}}} \approx 10^{26}\,m$ {size of universe "causal horizon"

$\therefore \dim \mathcal{H}_{universe} \approx \left(\frac{L_{max}}{\delta x_{min}}\right)^3 \approx 10^{180}.$

(b/c 3 dimensions)

Position operator $\hat{X}$

- Eigenvalues $x \in \mathbb{R}$ $\Rightarrow$ $\boxed{\hat{X}|x\rangle = x|x\rangle}$

where $\{|x\rangle, x \in \mathbb{R}\}$ is o-n eigenbasis:

$\langle x|y\rangle = \delta_{x,y}$ $\qquad$ $\sum_x |x\rangle\langle x| = 1$

?? $\qquad$??

- Completeness $\boxed{\int_{-\infty}^{\infty} dx\, |x\rangle\langle x| = 1}$

$\Rightarrow |\psi\rangle = \int_{-\infty}^{\infty} dx\, |x\rangle\langle x|\psi\rangle \equiv \int_{-\infty}^{\infty} dx\, \psi(x)\, |x\rangle$

$\boxed{\psi(x) \doteq \langle x|\psi\rangle = \text{"wave function"}}$

= components of $|\psi\rangle$ in $\{|x\rangle\}$ basis.

- $\psi(x) = \langle x|\psi\rangle = \langle x|\left(\int_{-\infty}^{\infty} dy\, |y\rangle\langle y|\right)|\psi\rangle$

$$= \int_{-\infty}^{\infty} dy\, \langle x|y\rangle\langle y|\psi\rangle = \int_{-\infty}^{\infty} dy\, \langle x|y\rangle\, \psi(y)$$

$\Rightarrow$ call $\boxed{\langle x|y\rangle \doteq \delta(x-y) \quad \text{"Dirac delta function"}}$

and <u>define</u> it by property

$$\boxed{\int_{-\infty}^{\infty} dy\, \delta(x-y)\,\psi(y) = \psi(x) \quad \text{for all } \psi}$$

- Implies:

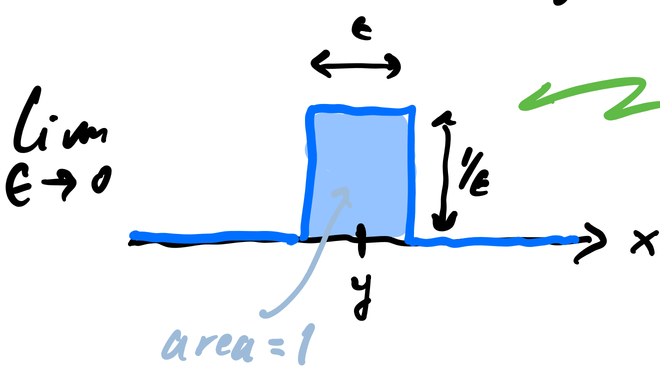
real: $\delta(x-y)^* = \delta(x-y)$

even: $\delta(x-y) = \delta(y-x)$

support @0: $\delta(x-y) = 0$ if $x \neq y$.

& "$\delta(0) = \infty$"

- $\delta(x-y)$ not really a function ("generalized func" or "distribution")



any other shape with area = 1 & max $\to \infty$ works

- $\langle\psi|\varphi\rangle = \left(\int dx\, \psi^*(x)\langle x|\right)\left(\int dy\, \varphi(y)\,|y\rangle\right)$

$$= \iint dx\,dy\, \psi^*(x)\,\varphi(y)\,\langle x|y\rangle$$

$$= \iint dx\, dy\; \psi^*(x)\, \varphi(y)\, \delta(x-y)$$

$$\therefore \quad \boxed{\langle \psi | \varphi \rangle = \int dx\; \psi^*(x)\, \varphi(x)}$$

- $1 = \| |\psi\rangle \|^2 \doteq \langle \psi | \psi \rangle = \int dx\; \psi^*(x)\psi(x) = \int dx\, |\psi(x)|^2$

$$\Rightarrow \quad \boxed{1 = \int dx\, |\psi(x)|^2} \quad \Rightarrow \quad \lim_{|x|\to\infty} |\psi(x)| = 0.$$

Note: $|\psi\rangle$ dimensionless (pure number $\sim \sqrt{\text{probability}}$)
but $\psi(x)$ has dimension : $\frac{1}{\sqrt{\text{length}}}$

- $|x\rangle$ is not normalized! (Not physical state!)

$$\langle x | x \rangle = \delta(x-x) = \delta(0) = \infty$$

General rule: eigenstates corresponding to continuous eigenvalues have "δ-function normalization" $\langle x | y \rangle = \delta(x-y)$.

- Born's rule:

$$\text{Prob}(x_0 \le \hat{x} \le x_1) = \langle \psi | \hat{P}_{x_0 \le x \le x_1} | \psi \rangle$$

$$= \langle \psi | \left(\int_{x_0}^{x_1} dx\, |x\rangle\langle x| \right) | \psi \rangle = \int_{x_0}^{x_1} dx\, |\psi(x)|^2$$

$$\boxed{\text{Prob}(x_0 \leq \hat{x} \leq x_1) = \int_{x_0}^{x_1} dx\, |\psi(x)|^2}$$

$$\therefore \quad |\psi(x)|^2 dx = \text{Prob}(x \leq \hat{x} \leq x+dx)$$

$$\therefore \quad \boxed{|\psi(x)|^2 = \frac{\text{Prob}(x \leq \hat{x} \leq x+dx)}{dx} \doteq \mathcal{P}(x)}$$

"Probability density"

- Expectation values:

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle = \int dx\,dy\, \psi^*(x) \langle x | \hat{A} | y \rangle \psi(y)$$

$$\doteq \int dx\,dy\, \psi^*(x) A(x,y) \psi(y)$$

$$\boxed{A(x,y) \doteq \langle x | \hat{A} | y \rangle}$$

matrix elements of $\hat{A}$ in position basis

[Compare $\langle A \rangle = \sum_{i,j} c_i^* A_{ij} c_j$

$c_i \doteq \langle i | \psi \rangle$

$A_{ij} \doteq \langle i | \hat{A} | j \rangle$

$$= (c_1^* \cdots c_n^*) \begin{pmatrix} A_{11} & \cdots & \\ \vdots & & \\ & \cdots & A_{nn} \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix}$$]

• Example: $\hat{A} = \hat{X}$ $\langle x | \hat{X} | y \rangle = y \langle x | y \rangle = y\, \delta(x-y)$
$= x \langle x | y \rangle = x\, \delta(x-y)$

$$\Rightarrow \langle X \rangle = \int dx\, dy\ \psi^*(x)\ x\ \delta(x-y)\, \psi(y)$$

$$= \int dx \cdot x \cdot |\psi(x)|^2 = \int dx \cdot x \cdot P(x) . \checkmark$$

• Example: $\hat{A} = \hat{X}^n$ $\langle x | \hat{X}^n | y \rangle = x^n\, \delta(x-y)$

$$\Rightarrow \langle X^n \rangle = \int dx \cdot x^n \cdot |\psi(x)|^2 = \int dx \cdot x^n \cdot P(x) .$$

• $\hat{A} = f(\hat{X})$ . . .

$$\Rightarrow \langle f(X) \rangle = \int dx \cdot f(x) \cdot |\psi(x)|^2$$

Momentum Operator $\hat{P}$

- Just like $\hat{X}$: $\hat{P}^\dagger = \hat{P}$ & $\mathrm{spec}(\hat{P}) = \mathbb{R}$
  $\Rightarrow$ δ-fnc o-n basis $\{ |p\rangle,\ p \in \mathbb{R} \}$
  s.t.

$$\hat{P} |p\rangle = p |p\rangle , \quad \langle p | q \rangle = \delta(p-q), \quad \int dp\, |p\rangle\langle p| = 1 .$$

- $|p\rangle$ has dimension $\dfrac{1}{\sqrt{\text{momentum}}} = \sqrt{\dfrac{T}{ML}} = \sqrt{\dfrac{L}{\hbar}}$

  b/c $\delta(p-q)$ " $\dfrac{1}{\text{mom.}} = \dfrac{T}{ML} = \dfrac{L}{\hbar}$

- Relation of $\hat{X}$ to $\hat{P}$ bases

- $\hat{P}$ is generator of translations:

$$\hat{T}(a) \doteq e^{-ia\hat{P}/\hbar} \quad \text{shifts } x \to x+a$$

$$\Rightarrow |x+a\rangle = \hat{T}(a)|x\rangle = \left(1 - \frac{ia}{\hbar}\hat{P} + O(a^2)\right)|x\rangle$$

$$= |x\rangle - \frac{ia}{\hbar}\hat{P}|x\rangle + O(a^2)$$

$$\Rightarrow \hat{P}|x\rangle = i\hbar \frac{|x+a\rangle - |x\rangle}{a} + O(a)$$

$$\lim_{a\to 0} \Rightarrow \quad \boxed{\hat{P}|x\rangle = i\hbar \frac{d}{dx}|x\rangle} \quad \star$$

adj. $\langle x|\hat{P} = -i\hbar \frac{d}{dx}\langle x|$

- $$\hat{P}|\psi\rangle = \hat{P}\int dx\, \psi(x)\,|x\rangle = \int dx\, \psi(x)\, \hat{P}|x\rangle$$

$$= i\hbar \int dx\, \psi(x) \frac{d}{dx}|x\rangle$$

"integration by parts" (IBP) *

$$= -i\hbar \int dx \left(\frac{d\psi(x)}{dx}\right)|x\rangle$$

$$\Rightarrow \quad \boxed{\langle x|\hat{P}|\psi\rangle = -i\hbar \frac{d\psi(x)}{dx}}$$

Note: Townsend & others say:

" $\hat{p} = -i\hbar \frac{d}{dx}$ in position basis"

" $\hat{p}|\psi\rangle = -i\hbar \left|\frac{d\psi}{dx}\right\rangle$ "

This is confusing and wrong!

* I.B.P.

$$\int_a^b dx\, f(x)\, \frac{dg(x)}{dx} = -\int_a^b dx\, \frac{df(x)}{dx} \cdot g(x) + \underbrace{f(b)g(b) - f(a)g(a)}$$

If $a, b \to \pm\infty$ & f or $g \to 0$ $\Rightarrow$ drop boundary terms $\Rightarrow 0$

$$\Rightarrow \qquad \int dx\, f \cdot \frac{dg}{dx} = -\int dx\, \frac{df}{dx}\, g \,.$$

- Matrix elements of $\hat{P}$ in x-basis.

$$\langle y|\hat{P}|x\rangle = \langle y|\, i\hbar \frac{d}{dx} |x\rangle = i\hbar \frac{d}{dx} \langle y|x\rangle$$

$$= i\hbar \frac{d}{dx} \delta(y-x) = i\hbar \frac{d}{dx} \delta(x-y)$$

Check: $i\hbar \frac{d}{dy} \delta(x-y) = \langle x|\hat{P}|y\rangle = \langle y|\hat{P}|x\rangle^* = -i\hbar \frac{d}{dx} \delta(x-y)$

$$\Rightarrow \quad \boxed{\frac{d}{dy} \delta(x-y) = -\frac{d}{dx} \delta(x-y)}$$

Proof:

$$\int dy\ \varphi(y) \frac{d}{dy}\delta(x-y) = -\int dy\ \frac{d\varphi(y)}{dy}\delta(x-y) = -\frac{d\varphi(x)}{dx}$$

$\parallel$? $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \parallel$ ✓

$$-\int dy\ \varphi(y) \frac{d}{dx}\delta(x-y) = -\frac{d}{dx}\left(\int dy\ \varphi(y)\delta(x-y)\right) = -\frac{d\varphi(x)}{dx}$$

- Heisenberg algebra $[\hat{X}, \hat{P}] = ?$

~ Act on any state

$$[\hat{X},\hat{P}]|\psi\rangle = (\hat{X}\hat{P} - \hat{P}\hat{X})|\psi\rangle$$

$$= \int dx\ (\hat{X}\hat{P} - \hat{P}\hat{X})|x\rangle \psi(x)$$

$$= \int dx\ \psi(x)\left(\hat{X}\, i\hbar \frac{d}{dx}|x\rangle - \hat{P}\, x|x\rangle\right)$$

$$= \int dx\ \psi(x)\left\{ i\hbar \frac{d}{dx}(\hat{X}|x\rangle) - x(\hat{P}|x\rangle) \right\}$$

$$= \int dx\ \psi(x)\left\{ i\hbar \frac{d}{dx}(x|x\rangle) - x\, i\hbar \frac{d}{dx}|x\rangle \right\}$$

$$= i\hbar \int dx\ \psi(x)\left\{ |x\rangle + \cancel{x\frac{d}{dx}|x\rangle} - \cancel{x\frac{d}{dx}|x\rangle} \right\}$$

$$= i\hbar \int dx\ \psi(x)|x\rangle = i\hbar|\psi\rangle$$

True for all $|\psi\rangle$ $\therefore$

$$\boxed{[\hat{x}, \hat{p}] = i\hbar}$$

$$\Rightarrow \quad \boxed{\Delta x \cdot \Delta p \geq \frac{\hbar}{2}}$$

"Heisenberg uncertainty relation"

- $\{|x\rangle\} \leftrightarrow \{|p\rangle\}$ change of basis:

What is $|p\rangle$ in terms of $|x\rangle$?

$$|p\rangle = \int dx\, |x\rangle \underbrace{\langle x|p\rangle}_{?}$$

$\langle x|\hat{p} = -i\hbar \frac{d}{dx}\langle x|$

$$p\langle x|p\rangle = \langle x|\hat{p}|p\rangle = -i\hbar \frac{d}{dx}\langle x|p\rangle$$

$$\Rightarrow \quad \langle x|p\rangle = N e^{ipx/\hbar}$$

- Find N by

$$\delta(p-q) = \langle q|p\rangle = \int dx\, \langle q|x\rangle\langle x|p\rangle = \int dx\, N^* e^{-iqx/\hbar} N e^{+ipx/\hbar}$$

$$= |N|^2 \int_{-\infty}^{\infty} dx\, e^{ix(p-q)/\hbar} = |N|^2 (2\pi\hbar)\,\delta(p-q).$$

(useful math identity: $\boxed{\int dx\, e^{ixp/\hbar} = 2\pi\hbar\,\delta(p)}$)

$$\Rightarrow \quad \boxed{\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{ixp/\hbar}}$$

- Momentum-space wave function

$$|\psi\rangle \doteq \int dp\, \tilde{\psi}(p)\, |p\rangle$$

$$\tilde{\psi}(p) = \langle p|\psi\rangle = \int dx\, \langle p|x\rangle\langle x|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int dx\, e^{-ipx/\hbar}\,\psi(x)$$

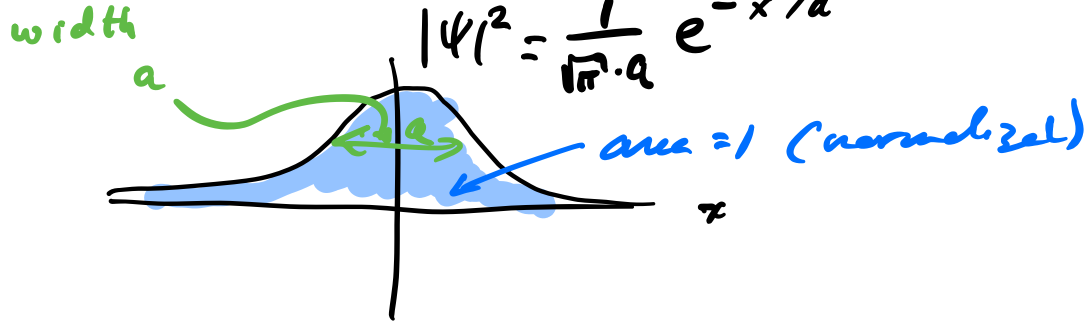
$\Rightarrow$ Fourier transform!

$$\boxed{\begin{aligned} \tilde{\psi}(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int dx\, e^{-ipx/\hbar}\,\psi(x) \\ \psi(x) &= \frac{1}{\sqrt{2\pi\hbar}}\int dp\, e^{+ipx/\hbar}\,\tilde{\psi}(p) \end{aligned}}$$

- Gaussian wave function:

$$\psi(x) = \langle x|\psi\rangle \doteq \frac{1}{\pi^{1/4}\sqrt{a}}\, e^{-x^2/2a^2}$$

$$|\psi|^2 = \frac{1}{\sqrt{\pi}\cdot a} e^{-x^2/a^2}$$



Compute: $\langle x \rangle = 0$ $\quad \langle x^2 \rangle = \frac{1}{2} a^2$

$$\Rightarrow \quad \Delta X = \frac{a}{\sqrt{2}}.$$

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

$$= \sqrt{\frac{a}{\hbar}} \frac{1}{\pi^{1/4}} e^{-a^2p^2/2\hbar^2}$$ Also Gaussian

$$\Rightarrow \quad \Delta P = \frac{\hbar}{a\sqrt{2}}$$

$\therefore \quad \Delta X \cdot \Delta P = \frac{\hbar}{2}$ = minimum allowed by uncertainty relation

Time evolution

- $i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$ Schrö Eqn.

$$\Rightarrow \quad i\hbar \frac{d}{dt} \langle x|\psi(t)\rangle = \langle x| \hat{H} |\psi(t)\rangle$$

Say: $\hat{H} = \underbrace{\frac{1}{2m}\hat{P}^2}_{\text{kinetic energy}} + \underbrace{V(\hat{x})}_{\text{potential energy}}$ particle moving in a potential

particle mass

$$\langle x|\hat{H}|\psi(t)\rangle = \frac{1}{2m}\langle x|\hat{P}^2|\psi(t)\rangle + \langle x|V(\hat{x})|\psi(t)\rangle$$

$$= \frac{1}{2m}(-i\hbar)\frac{d}{dx}\langle x|\hat{P}|\psi(t)\rangle + \langle x|V(x)|\psi(t)\rangle$$

$$= \frac{1}{2m}\left(-i\hbar\frac{d}{dx}\right)^2\langle x|\psi(t)\rangle + V(x)\langle x|\psi(t)\rangle$$

$$= \frac{-\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\,\psi(x,t) \qquad (*)$$

where $\psi(x,t) \doteq \langle x|\psi(t)\rangle$.

Plug into $(*)$ gives diff. eq. for $\psi(x,t)$:

$$\boxed{i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\,\psi(x,t)} \qquad (1)$$

2^{nd}-order, linear, partial differential equation.

- Since $\hat{H}$ is t-independent, we can solve (1) for its time dependence of $\psi(x,t)$ once & for all if we can solve the energy eigenvalue problem:

$$\hat{H}\,|n\rangle = E_n\,|n\rangle \qquad (2)$$

since then

$$|\psi(t)\rangle = \sum_n e^{-iE_n t/\hbar}\,|n\rangle\langle n|\psi(0)\rangle \qquad (3)$$

- Write (2) & (3) in position basis:

$\langle x|n\rangle \doteq \varphi_n(x)$ "energy eigenfunction." Then (2) $\Rightarrow$

$$E_n\varphi_n(x) = E_n\langle x|n\rangle = \langle x|\hat{H}|n\rangle$$

$$= -\frac{\hbar^2}{2m}\frac{d^2\varphi_n(x)}{dx^2} + V(x)\varphi_n(x)$$

using (*). So "time-indep't Schr. eqn":

$$\boxed{-\frac{\hbar^2}{2m}\varphi_n''(x) + V(x)\varphi_n(x) = E_n\varphi_n(x)}$$

$\left(\varphi'' \doteq \frac{d^2}{dx^2}\varphi\right)$.

- (3) $\Rightarrow$ $\boxed{\Psi(x,t) = \sum_n e^{-iE_n t/\hbar}\,\varphi_n(x)\,\langle n|\Psi(0)\rangle}$

where $\boxed{\langle n|\Psi(0)\rangle = \int dy\,\langle n|y\rangle\langle y|\Psi(0)\rangle = \int dy\,\varphi_n^*(y)\,\Psi(y,0)}$

• So, we want to solve 2^{nd}-order, linear ODE:

$$\boxed{-\frac{\hbar^2}{2m}\varphi'' + V(x)\,\varphi = E\,\varphi} \qquad (*)$$

$(\varphi_n \to \varphi;\ E_n \to E)$ for E & $\varphi(x)$

= energy eigenvalue equation!

General solution of a 2^{nd} order ODE is

$$\varphi(x) = A\,\varphi_1(x) + B\,\varphi_2(x) \qquad (**)$$

for arbitrary $A, B \in \mathbb{C}$ & where $\varphi_{1,2}$ are two linearly-independent solutions

In other words, for each value of the eigenvalue E there is potentially a 2-dimensional eigenspace with basis wavefunctions $\{\varphi_1, \varphi_2\}$ (which depend on the value of E).

But this 2-d space of solutions (**) for each E is <u>not</u> in general allowed! This is because (*) is not complete: we need to specify Boundary Conditions (BC's)

The basic BCs come from demanding that states be normalizable, so

$$1 = \langle \varphi | \varphi \rangle = \int dx \, |\varphi|^2 \Rightarrow \boxed{\lim_{x \to \pm\infty} |\varphi| = 0}$$ BC1

- We will see that BC's are actually a bit more subtle. The rule is:

→ Exists BC $\lim_{x \to -\infty} |\varphi| = 0$ only if

$$E < \lim_{x \to -\infty} V(x)$$

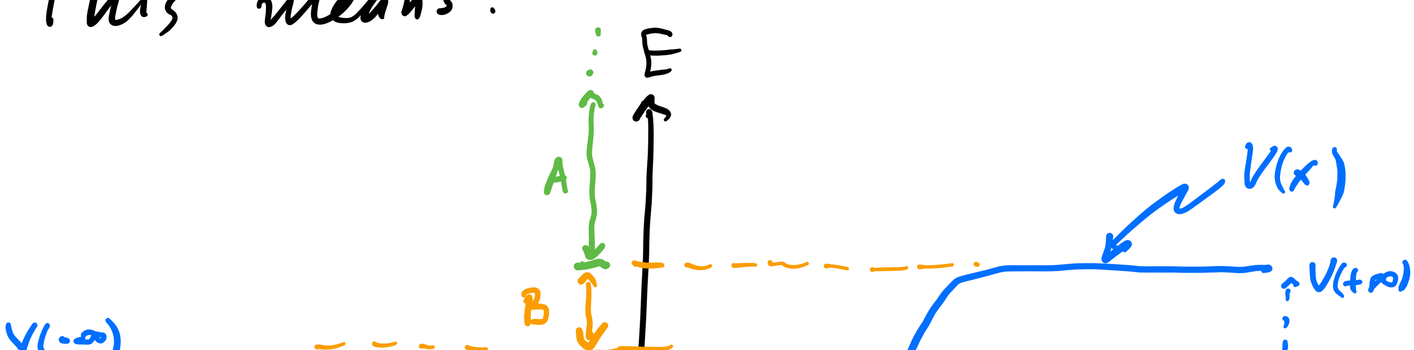
→ Exists BC $\lim_{x \to +\infty} |\varphi| = 0$ only if

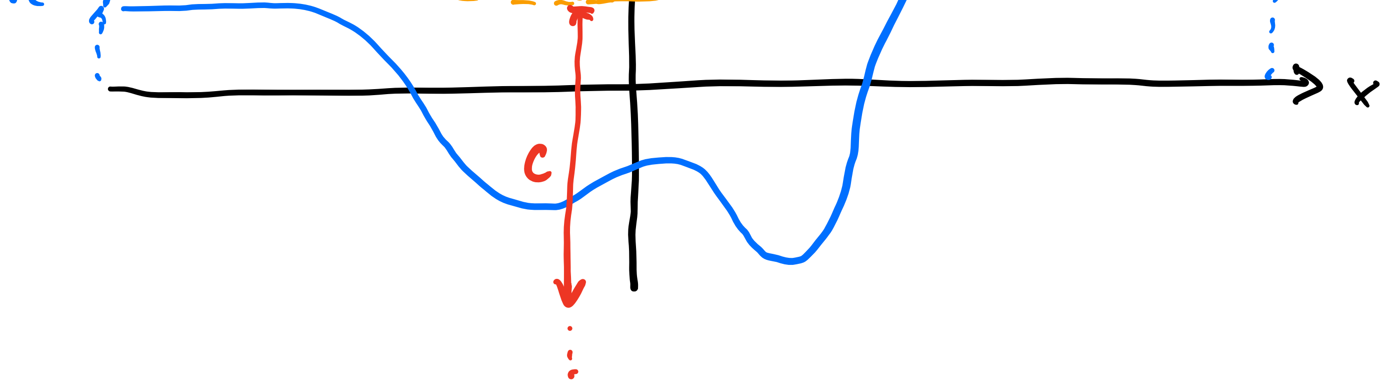
$$E < \lim_{x \to +\infty} V(x)$$

→ Otherwise no BC

BC2

This means:





If $E > V(+\infty)$ (region A):

no BC's, $\therefore$ 2-dim'l eigenspace each E

If $V(+\infty) > E > V(-\infty)$ (region B):

one BC, $\therefore$ 1-dim'l eigenspace each E

"scattering states" $\updownarrow$ continuum spectrum

If $V(-\infty) > E$ (region C):

two BCs, $\therefore$ generically 0-dim'l eigenspace ea. E

$\Rightarrow$ generically E is not an eigenvalue!

But in region C there may be <u>special</u> <u>values</u> of E for which exists a special linear combination of $\varphi_1(x)$ & $\varphi_2(x)$ such that both BC's are satisfied.

For this <u>discrete</u> <u>set</u> of E's, each has a 1-dimensional eigenspace. These are called the "bound states" of the system.

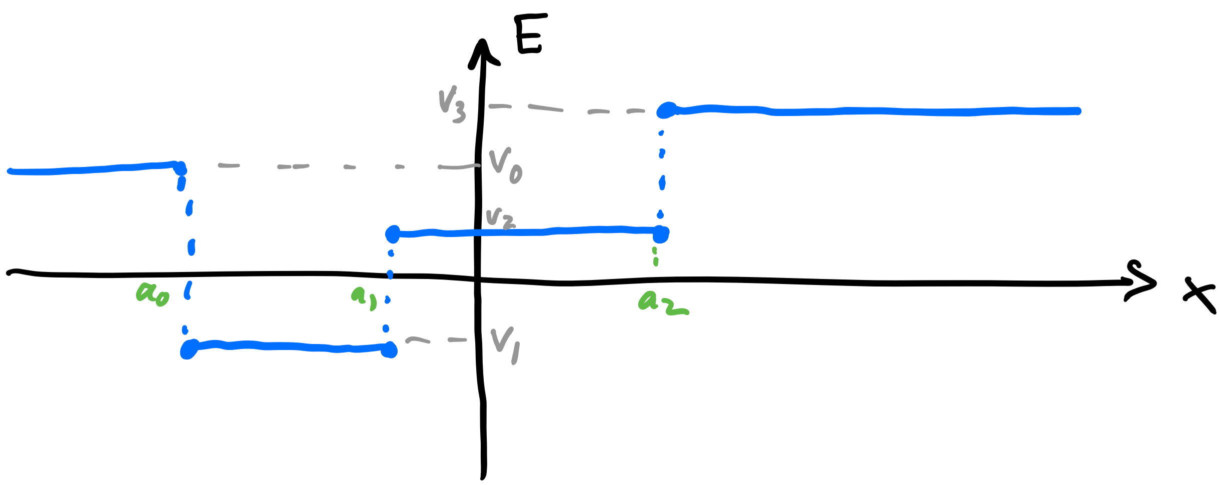
Simple potentials

- There is no closed-form solution for general $V(x)$.
  So focus, to start, on special simple potentials:

(1) Constant: $V(x) = V_0$ (indep't of x)

(2) Piece-wise constant:

$$V(x) = \begin{cases} V_0 & x < a_0 \\ V_1 & a_0 < x < a_1 \\ V_2 & a_1 < x < a_2 \\ & \vdots \\ V_n & a_{n-1} < x \end{cases}$$



(1) Constant potential

$V(x) = V_0 = \text{constant}$ $\Rightarrow$ Free particle (no forces)

$\Rightarrow \quad \hat{H} = \frac{1}{2m}\hat{P}^2 + V_0\,\hat{1}$

$\Rightarrow [\hat{P}, \hat{H}] = 0$, so can simultaneously diagonalize $\hat{P}$ & $\hat{H}$

$\Rightarrow$ p-basis = energy eigenbasis!

$$\hat{H}|p\rangle = \left(\frac{1}{2m}p^2 + V_0\right)|p\rangle \doteq E_p|p\rangle$$

$$E_p \doteq \frac{p^2}{2m} + V_0. \iff \boxed{p \doteq \sqrt{2m(E_p - V_0)}}$$

- $E_p \geq V_0$, so all $E \geq V_0$ are energy eigenvalues
  $\Rightarrow$ continuous energy spectrum.
- $E_{-p} = E_p$, so $\hat{H}|-p\rangle = E_p|-p\rangle$
  $\Rightarrow$ each $E_p > V_0$ is doubly degenerate.

- General sol'n of Schrö. Eqn.

$$|\Psi(t)\rangle = \int dp\, e^{-iE_p t/\hbar}\, |p\rangle \underbrace{\langle p|\Psi(0)\rangle}_{\equiv \tilde{\Psi}(p,0)}$$

$$= \int dp\, e^{-\frac{ip^2 t}{2m\hbar}}\, e^{-iV_0 t/\hbar}\, \tilde{\Psi}(p,0)\, |p\rangle$$

$$= \underbrace{e^{-iV_0 t/\hbar}}\left[\int dp\, e^{-\frac{ip^2 t}{2m\hbar}}\, \tilde{\Psi}(p,0)\, |p\rangle\right]$$

overall phase = unobservable $\rightarrow$ drop!
(reflects fact that overall zero of energy is unobservable)

$$\therefore \quad \boxed{\tilde{\Psi}(p,t) \doteq \langle p|\Psi(t)\rangle = e^{-\frac{ip^2 t}{2m\hbar}}\, \tilde{\Psi}(p,0)}$$

- This is solution in momentum basis.
  What is it in position basis?

$$\hat{H}|\varphi\rangle = E|\varphi\rangle \Rightarrow -\frac{\hbar^2}{2m}\varphi''(x) + V_0\varphi(x) = E\varphi(x)$$

$$\Rightarrow \quad \varphi'' = -\frac{2m}{\hbar^2}(E - V_0)\,\varphi \qquad (*)$$

Recall simple diff. eqns:

$$\varphi'' = -k^2\varphi \Rightarrow \left.\begin{array}{l}\varphi = Ae^{ikx} + Be^{-ikx} \\ (= \tilde{A}\cos kx + \tilde{B}\sin kx)\end{array}\right\} \text{oscillatory}$$

$$\varphi'' = +\kappa^2\varphi \Rightarrow \varphi = Ae^{\kappa x} + Be^{-\kappa x} \Big\} \text{ exponential}$$

$\therefore$ 2 cases for $(*)$:

① $\underline{E > V_0}$ $\Rightarrow$ $k \doteq \frac{1}{\hbar}\sqrt{2m(E - V_0)}$ & $\varphi = Ae^{ikx} + Be^{-ikx}$

② $\underline{E < V_0}$ $\Rightarrow$ $\kappa \doteq \frac{1}{\hbar}\sqrt{2m(V_0 - E)}$ & $\varphi = Ae^{\kappa x} + Be^{-\kappa x}$

In case ②, $\lim_{x\to+\infty} |\varphi| \sim |A| e^{\kappa x} \to \infty$ unless $A=0$

&

$\lim_{x\to-\infty} |\varphi| \sim |B| e^{-\kappa x} \to \infty$ unless $B=0$.

$\therefore$ $|\varphi| \to \infty$ unless $A=B=0 \Rightarrow$ no solution.

$\therefore$ No normalizable solutions for $E < V_0$. ✓

In case ①, $\lim_{x\to\pm\infty} |\varphi|$ oscillates between $\pm(|A|+|B|)$

$\therefore$ does not diverge, but still get $\int dx\, |\varphi|^2 = \infty$

so not normalizable. !?

Compare to momentum space solution: found

$$|\varphi\rangle = A|p\rangle + B|-p\rangle \quad \text{w/ } p = \hbar k.$$

$$\Rightarrow \langle\varphi|\varphi\rangle = \left(A^*\langle p| + B^*\langle -p|\right)\left(A|p\rangle + B|-p\rangle\right)$$

$$= |A|^2 \delta(p-p) + (AB^* + BA^*)\,\cancel{\delta(p+p)}^{\,0} + |B|^2\delta(p-p)$$

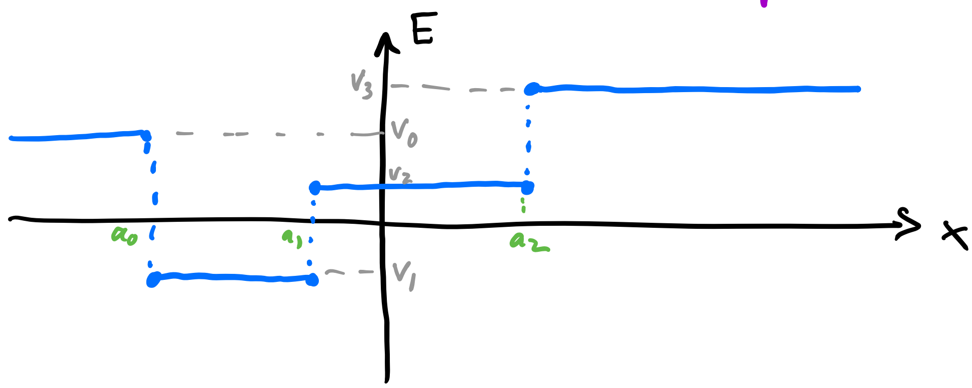
$$= (|A|^2 + |B|^2)\,\delta(0) = \infty,$$

also not normalizable.

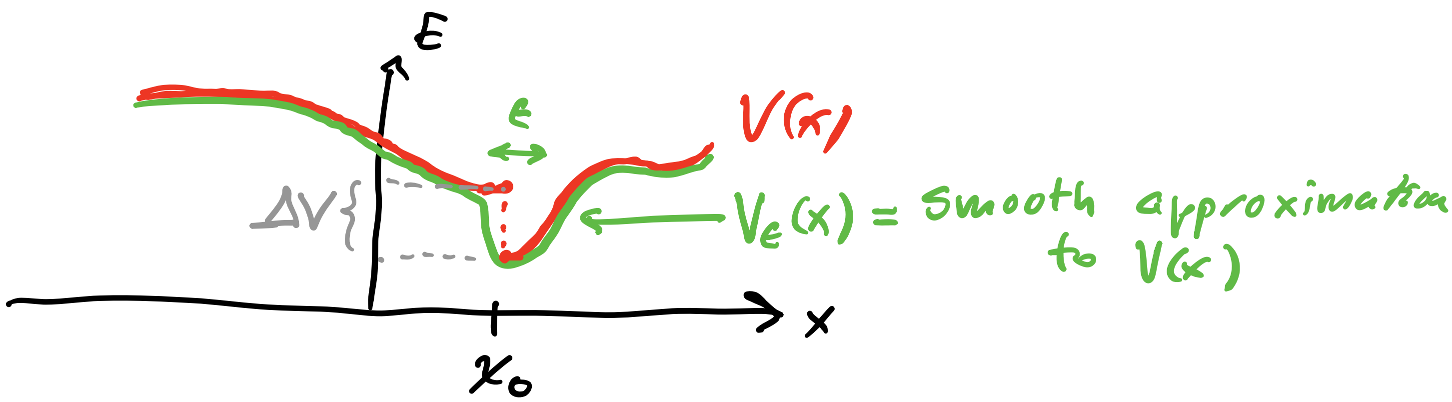
$$\boxed{\text{Math rule: if } \varphi \text{ oscillates @ } \pm\infty \text{ but does not grow, then } \varphi \text{ is } \delta\text{-function normalizable.}}$$

So we allow all $E > V_0$ as doubly-degenerate eigenvalues. ✓

(2) Piece-wise constant potentials



So need to figure out what happens at a discontinuity in $V(x)$:



Look at $\lim\limits_{\varepsilon\to 0}\left(-\frac{\hbar^2}{2m}\varphi'' + (V_\varepsilon(x) - E)\varphi = 0\right).$ (*)

$$\int_{x_0-\varepsilon}^{x_0+\varepsilon} dx \,(*) \Rightarrow 0 = \lim_{\varepsilon\to 0}\left[-\frac{\hbar^2}{2m}\left(\varphi'(x_0+\varepsilon) - \varphi'(x_0-\varepsilon)\right) + \int_{x_0-\varepsilon}^{x_0+\varepsilon} dx\,(V_\varepsilon(x) - E)\,\varphi(x)\right]$$

$$\Rightarrow \lim_{\varepsilon\to 0}\left|\varphi'(x_0+\varepsilon) - \varphi'(x_0-\varepsilon)\right| = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\left|\int_{x_0-\varepsilon}^{x_0+\varepsilon} dx\,(V_\varepsilon(x) - E)\,\varphi(x)\right|$$

$$< \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0} 2\varepsilon\cdot\left|\Delta V\cdot\varphi(x_0)\right| = 0$$

$$\Rightarrow \boxed{\varphi'(x) \;\&\; \therefore\; \varphi(x) \text{ are continuous for finite } \Delta V}$$ MC

"Matching Condition"

- But, if $\Delta V \to \infty$, can get

$$\lim_{\epsilon \to 0} \underset{\downarrow\, 0}{\epsilon} \, |\underset{\downarrow\, \infty}{\Delta V} \cdot \varphi(x_0)| > 0$$

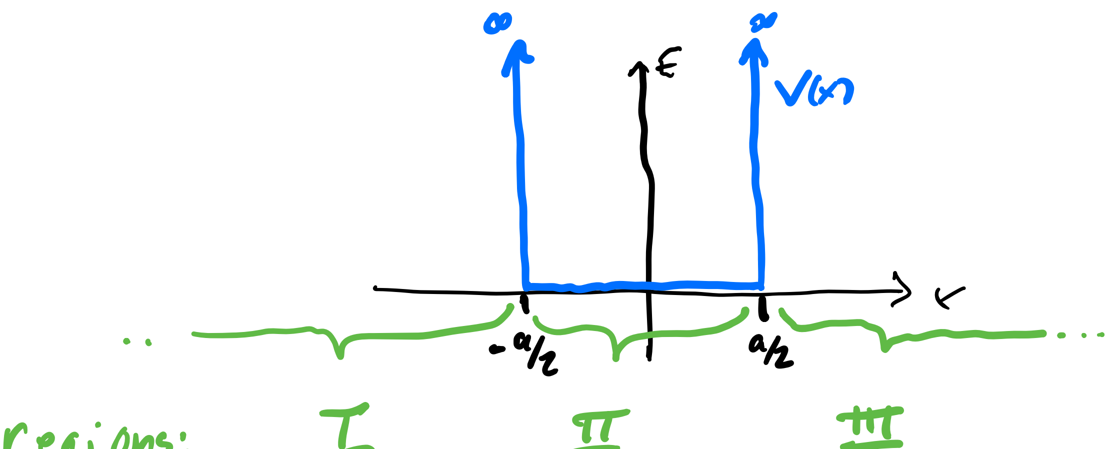
so find

$$\boxed{\varphi(x) \text{ continuous, but } \varphi'(x) \text{ can have finite jump at } \Delta V = \infty \text{ discontinuity.}}$$

MC_∞

(2a) Particle in a box

$$V(x) = \begin{cases} 0 & |x| < a/2 \\ \infty & |x| > a/2 \end{cases}$$



$$\hat{H} = \begin{cases} \frac{1}{2m}\hat{P}^2 & \text{in region II} \\ \infty & \text{in regions I \& III.} \end{cases}$$

so, energy eigenvalue problem

$$\hat{H}|n\rangle = E_n|n\rangle \quad \text{w/} \quad |n\rangle := \int dx\, \varphi_n(x)\,|x\rangle \quad \Rightarrow$$

I: $\quad \infty \cdot \varphi_n(x) = E_n\, \varphi_n(x) \qquad x < -a/2$

II: $\quad -\frac{\hbar^2}{2m}\varphi_n''(x) = E_n\, \varphi_n(x) \qquad -a/2 < x < a/2$

III: $\quad \infty \cdot \varphi_n(x) = E_n\, \varphi_n(x) \qquad a/2 < x$

- In regions I & III, for any E_n only solution is

$$\boxed{\varphi_n(x) = 0 \qquad x < -a/2 \;\;\&\;\; x > a/2}$$

(Matches classical expectation.)

- In region II ($|x| < a/2$) :

$$\varphi_n'' = -\frac{2m}{\hbar^2}E_n\,\varphi_n \equiv \begin{cases} -k^2\varphi_n & \text{if } E_n > 0 \\ +\kappa^2\varphi_n & \text{if } E_n < 0 \end{cases}$$

with $k \doteq \frac{1}{\hbar}\sqrt{2mE_n}$ & $\kappa \doteq \frac{1}{\hbar}\sqrt{2m(-E_n)}$.

$\therefore$ If $E_n > 0 \Rightarrow \varphi_n^{(II)} = Ae^{ikx} + Be^{-ikx}$

$$\boxed{\text{If } E_n<0 \Rightarrow \varphi_n^{(II)} = Ae^{\kappa x} + Be^{-\kappa x}}$$

- Now use matching condition:

MC$_\infty$: $\boxed{\begin{aligned} &\varphi_n^{(II)}(-\tfrac{a}{2}) = \varphi_n^{(I)}(-\tfrac{a}{2}) = 0 \\ &\varphi_n^{(II)}(+\tfrac{a}{2}) = \varphi_n^{(III)}(+\tfrac{a}{2}) = 0 \end{aligned}}$

- If $E_n<0$: MC $\Rightarrow$

$$\begin{cases} Ae^{\kappa(-\frac{a}{2})} + Be^{-\kappa(-\frac{a}{2})} = 0 \\ Ae^{\kappa(\frac{a}{2})} + Be^{-\kappa(\frac{a}{2})} = 0 \end{cases} \Rightarrow \begin{cases} A + Be^{\kappa a} = 0 \\ A + Be^{-\kappa a} = 0 \end{cases}$$

$$\Rightarrow B(e^{\kappa a} - e^{-\kappa a}) = 0 \Rightarrow B = 0 \Rightarrow A = 0.$$

$\therefore$ $\boxed{\text{No solution!}}$ $\Rightarrow$ No eigenenergies <0.

(Makes sense classically.)

- If $E_n>0$: MC $\Rightarrow$

$$\begin{cases} Ae^{ik(-\frac{a}{2})} + Be^{-ik(-\frac{a}{2})} = 0 \\ Ae^{ik(\frac{a}{2})} + Be^{-ik(\frac{a}{2})} = 0 \end{cases} \Rightarrow \begin{cases} B = -Ae^{-ika} \\ B = -Ae^{+ika} \end{cases}$$

$$\Rightarrow A(e^{ika} - e^{-ika}) = 0.$$

$\Rightarrow$ Either $A=0 \Rightarrow B=0 \Rightarrow$ no solution, or $\boxed{A \neq 0 \ \& \ e^{2ika} = 1.}$ (★)

- $e^{i\theta} = 1$ iff $\theta = 2\pi n$, $n \in \mathbb{Z}$, therefore

(★) $\Rightarrow$ $\boxed{k = k_n \doteq \frac{\pi}{a} n, \quad n \in \mathbb{Z}.}$ $\Rightarrow$ $\boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2ma^2}}$

& $B = -A e^{i\pi n} = (-)^{n+1} A$

$$\Rightarrow \boxed{\varphi_n(x) = \begin{cases} A\left(e^{ik_n x} - (-)^n e^{-ik_n x}\right) & |x| < a/2 \\ 0 & |x| > a/2 \end{cases}.}$$

Solution!

- Actually, we have over-counted the solutions

$\varphi_n = (-)^{n+1} \varphi_{-n}$ since $k_{-n} = -k_n$.

So we only have independent solutions for

$n \in \{1, 2, 3, \dots\}$.

$(\varphi_{n=0} \equiv 0)$.

- Note that:

$$\varphi_n(x) = \begin{cases} 2iA \cdot \sin(k_n x) & n \text{ even} \\ 2A \cdot \cos(k_n x) & n \text{ odd.} \end{cases}$$

- Note also that solving the eigenvector equation does not determine the overall normalization "A" of $|n\rangle$ or $\varphi_n(x)$.

- To fix A, note that we have found a discrete set of eigenvalues, so we should normalize the eigenvectors using
$$\delta_{n,m} = \langle n|m\rangle = \int dx\, \varphi_n^*(x)\, \varphi_m(x).$$

In particular

$$1 = \int dx\, |\varphi_n(x)|^2 = \int_{-a/2}^{a/2} dx\, |\varphi_n|^2$$

$$= |A|^2 \int_{-a/2}^{a/2} dx\, \left| e^{ik_n x} - (-)^n e^{-ik_n x} \right|^2$$

$$= |A|^2 \int_{-a/2}^{a/2} dx \left(2 - (-)^n \left[e^{2ik_n x} + e^{-2ik_n x} \right]\right)$$

$$= 2|A|^2 \cdot a - 2(-)^n |A|^2 \cancelto{0}{\int_{-a/2}^{a/2} \cos\left(2\pi n \frac{x}{a}\right)}$$

$$\therefore \quad |A| = \frac{1}{\sqrt{2a}} \quad \&$$

$$\Rightarrow \varphi_n(x) = \sqrt{\frac{2}{a}} \begin{cases} \sin\left(\frac{n\pi x}{a}\right) & n = 2, 4, 6, \ldots \\ \cos\left(\frac{n\pi x}{a}\right) & n = 1, 3, 5, \ldots \end{cases}$$

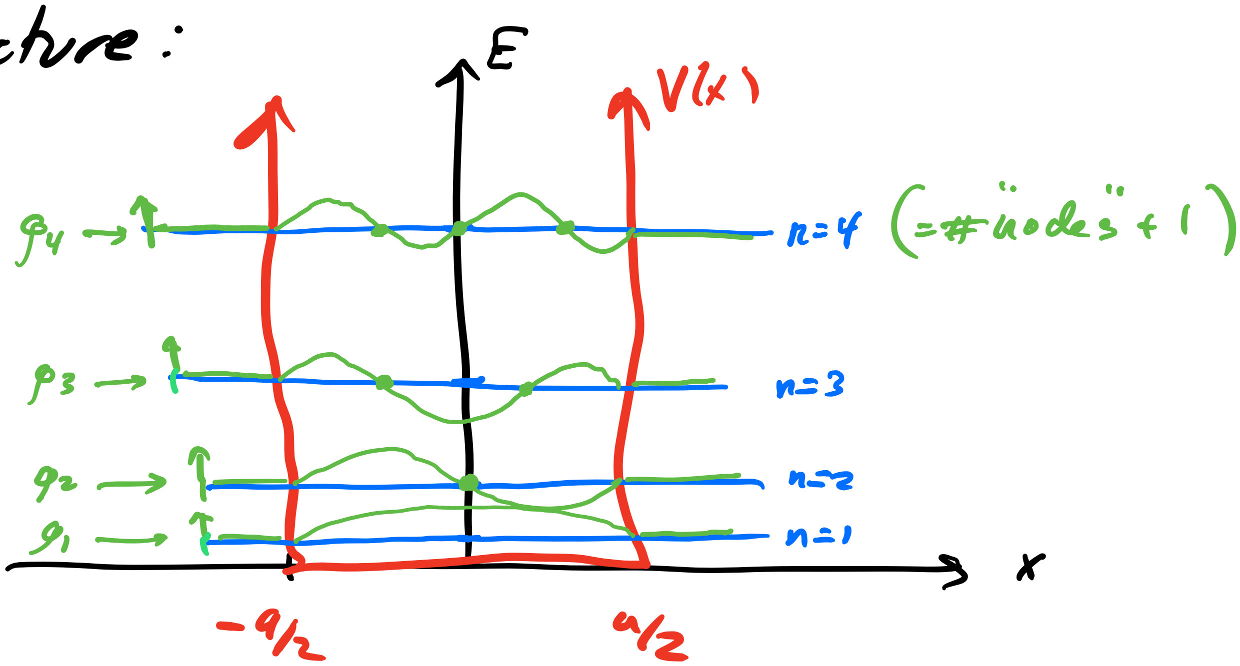
- As a check, the must automatically be orthogonal: for $n \neq m$:

$$0 = \langle n | m \rangle = \int dx\, \varphi_n^* \varphi_m$$

$$\propto \int_{-a/2}^{a/2} dx \left(e^{-ik_n x} - (-)^n e^{ik_n x}\right)\left(e^{ik_m x} - (-)^m e^{-ik_m x}\right)$$

$$= \dots = 0 \checkmark$$ check!

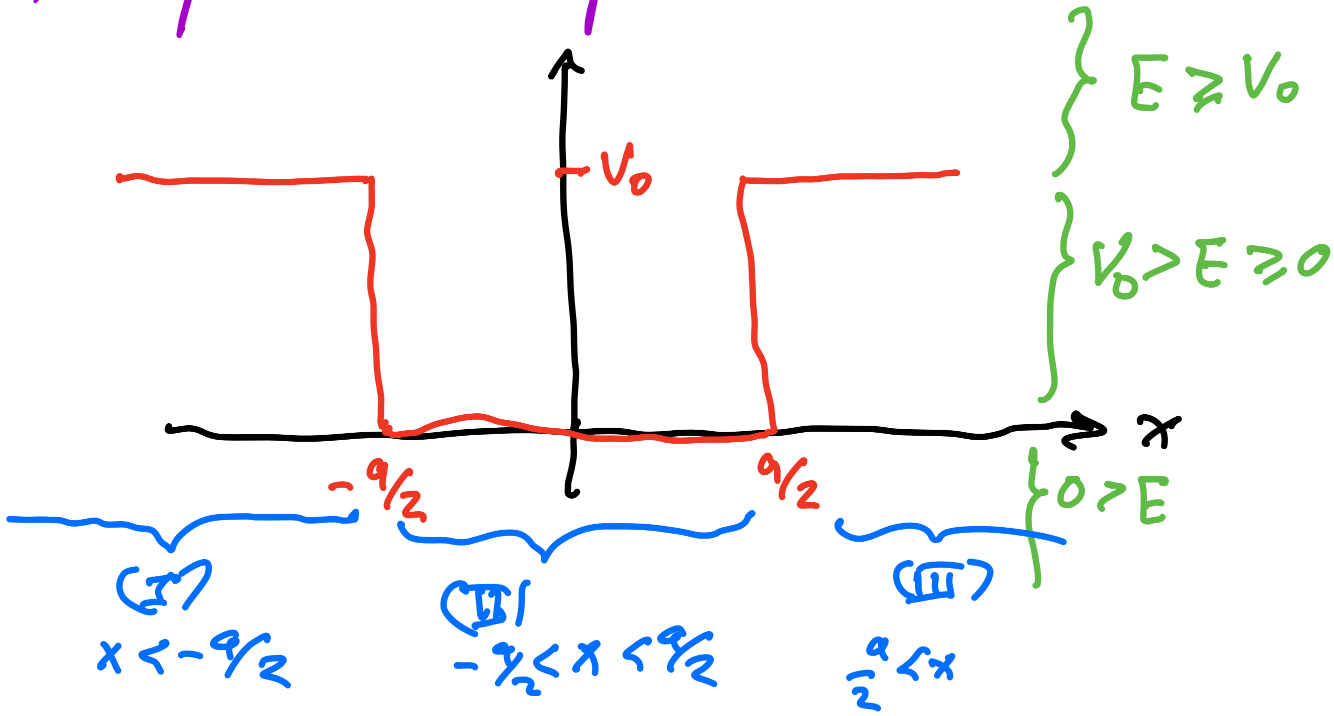
- Picture:



- Question from class: exist infinitely many more normalizable orthogonal wavefunctions in 1-particle Hilbert space than are in the energy eigenbasis!

Example: $\varphi_n(x + ma) \quad |m| > 1$.

(2b) Square-well potential



$$V(x) = \begin{cases} 0 & |x| < a/2 \\ V_0 & |x| > a/2 \end{cases}$$

Set up problem (will not solve; see problem set...)

a) $0 \leq E < V_0$ (Bound states)

$$\hat{H}|\varphi\rangle = E|\varphi\rangle \qquad \langle x|\varphi\rangle = \varphi(x)$$

$$-\frac{\hbar^2}{2m}\varphi'' + V(x)\varphi = E\varphi$$

$$\varphi \doteq \begin{cases} \varphi_I & x < -a/2 \\ \varphi_{II} & -a/2 < x < a/2 \\ \varphi_{III} & a/2 < x \end{cases}$$

- $-\frac{\hbar^2}{2m}\varphi''_{I,III} + V_0\varphi_{I,III} = E\varphi_{I,III}$

$$\Rightarrow \varphi''_{I,III} = \kappa^2\varphi_{I,III} \qquad \boxed{\kappa^2 \doteq \frac{2m(V_0-E)}{\hbar^2}} \quad (\kappa>0)$$

$$\Rightarrow \left.\begin{aligned} \varphi_I &= \mathcal{A}e^{\kappa x} + \mathcal{B}e^{-\kappa x} \\ \varphi_{III} &= \mathcal{E}e^{\kappa x} + \mathcal{F}e^{-\kappa x} \end{aligned}\right\}$$

(not energy!)

- $-\frac{\hbar^2}{2m}\varphi''_{II} + 0\cdot\varphi_{II} = E\varphi_{II}$

$$\Rightarrow \varphi''_{II} = -k^2\varphi_{II} \qquad \boxed{k^2 \doteq \frac{2mE}{\hbar^2}} \quad (k>0)$$

$$\Rightarrow \varphi_{II} = \mathcal{C}e^{ikx} + \mathcal{D}e^{-ikx} \}$$

- To solve, need BCs & MCs:

<u>BCs</u>: $\lim_{|x|\to\infty}\varphi(x) = 0$

$$\Rightarrow \lim_{x\to-\infty}\varphi_I(x) = 0 \Rightarrow \boxed{\mathcal{B}=0}$$

$$\Rightarrow \lim_{x\to+\infty}\varphi_{III}(x) = 0 \Rightarrow \boxed{\mathcal{E}=0}$$

<u>MCs</u>: φ & φ' continuous @ $x = \pm\frac{a}{2}$

$$x = -a/2 \Rightarrow \begin{cases} \varphi_I(-a/2) = \varphi_{II}(-a/2) \\ \varphi_I'(-a/2) = \varphi_{II}'(-a/2) \end{cases}$$

$$\Rightarrow \begin{cases} \mathcal{A} e^{-\kappa a/2} + \cancel{\mathcal{B}}^{0} e^{\kappa a/2} = \mathcal{C} e^{-ika/2} + \mathcal{D} e^{ika/2} \\ \mathcal{A} \kappa e^{-\kappa a/2} - \kappa \cancel{\mathcal{B}}^{0} e^{\kappa a/2} = \mathcal{C} ik e^{-ika/2} - \mathcal{D} ik e^{ika/2} \end{cases}$$

$$\Rightarrow \boxed{2 \text{ lin. equs. for } (\mathcal{A}, \mathcal{C}, \mathcal{D})} \quad MC(-a/2)$$

$$x = +a/2 \Rightarrow \varphi_{II}(a/2) = \varphi_{III}(a/2) \ \& \ \cdots$$

$$\Rightarrow \boxed{2 \text{ lin. equs for } (\mathcal{C}, \mathcal{D}, \mathcal{F})} \quad MC(a/2)$$

Solve $MC(-a/2)$ for $\mathcal{C}, \mathcal{D}$ i.t.o. $\mathcal{A}$:

$$\Rightarrow \begin{cases} \mathcal{C} = \mathcal{A} \cdot a(E) \\ \mathcal{D} = \mathcal{A} \cdot b(E) \end{cases}$$

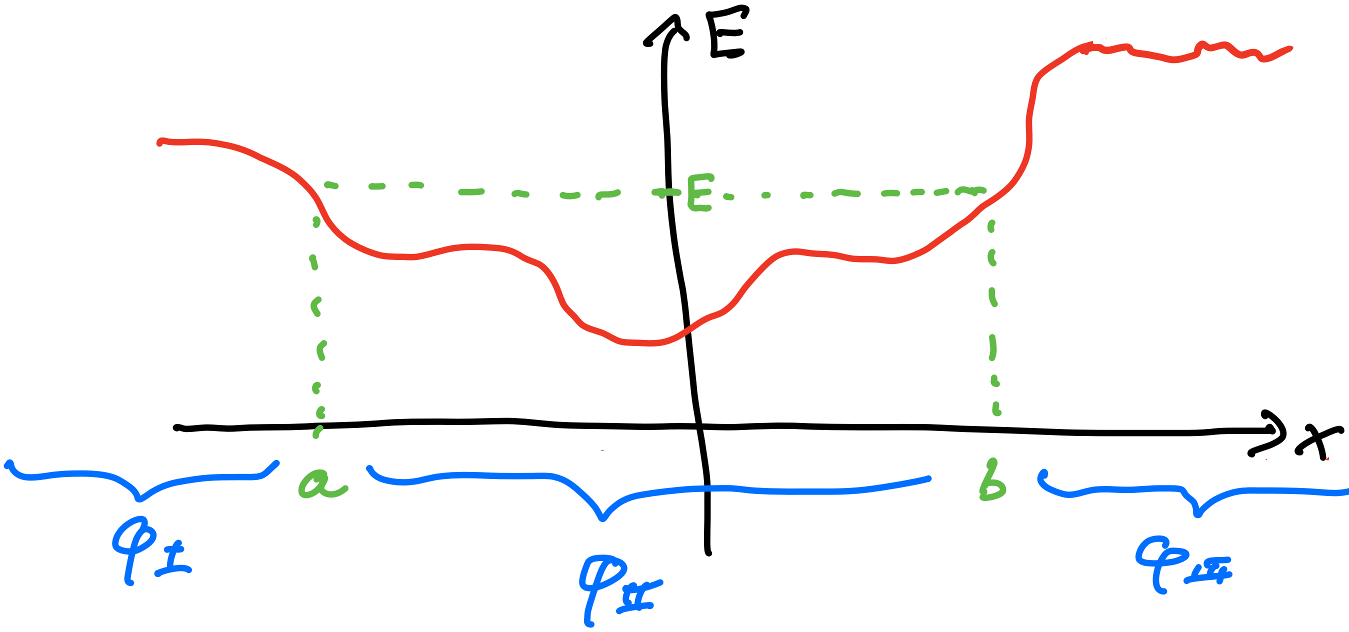
Solve $MC(+a/2)$ for $\mathcal{C}, \mathcal{D}$ i.t.o. $\mathcal{F}$:

$$\Rightarrow \begin{cases} \mathcal{C} = \mathcal{F} \cdot c(E) \\ \mathcal{D} = \mathcal{F} \cdot d(E) \end{cases}$$

$$\Rightarrow \frac{\mathcal{A}}{\mathcal{F}} = \boxed{\frac{c(E)}{a(E)} = \frac{d(E)}{b(E)}} \quad (*)$$

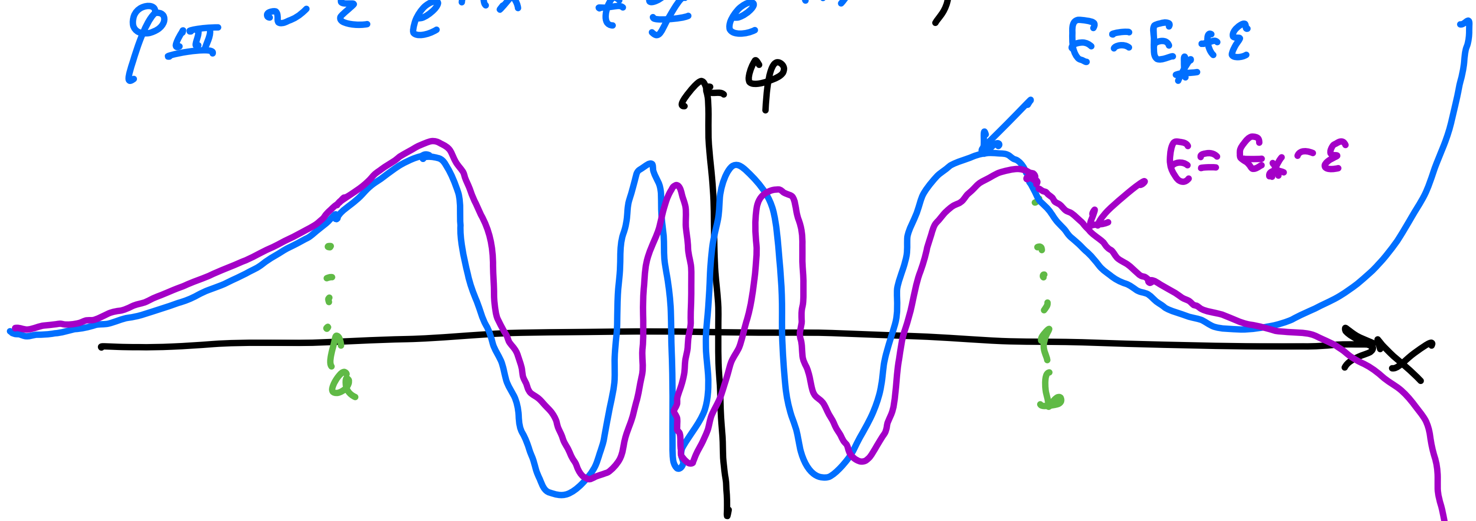
Only at special values of E satisfying $(*)$ are there solutions $\Rightarrow$ discrete eigenenergies.

a') General potential



$$\varphi_I \sim \mathcal{A} e^{\kappa x} + \mathcal{B} e^{-\kappa x}$$
$$\varphi_{II} \sim \mathcal{C} e^{ikx} + \mathcal{D} e^{-ikx}$$
$$\varphi_{III} \sim \mathcal{E} e^{\tilde{\kappa} x} + \mathcal{F} e^{-\tilde{\kappa} x}$$

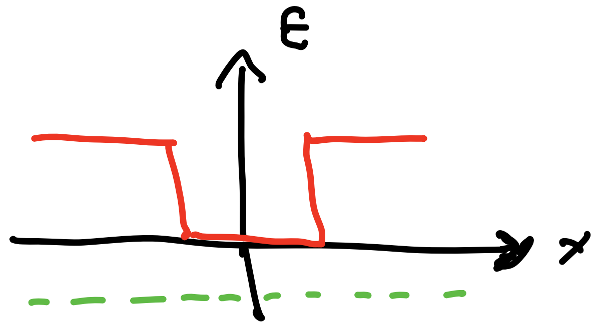
(Really: $\mathcal{A} \cdots \mathcal{F}$ are functions of x)



Exactly at $E = E_*$, $\varepsilon \to 0 \Rightarrow E_* =$ eigenvalue

$\Rightarrow$ $\boxed{\text{Discrete spectrum of bound state energies "in potential well"}}$

b) <u>$E < 0$</u>



$$\Rightarrow \begin{cases} \varphi_I \sim A e^{\kappa x} \\ \varphi_{II} \sim C e^{\kappa' x} + D e^{-\kappa' x} \\ \varphi_{III} \sim \qquad\qquad F e^{-\kappa x} \end{cases}$$

$\Rightarrow$ No solutions to MCs (except $\varphi \equiv 0$) b/c for real exponentials

$$\varphi_I' > 0 \Rightarrow \varphi_{II}' > 0 \ @ \ x = -\frac{a}{2}$$

$$\Rightarrow \varphi_{II}' > 0 \ @ \text{ all } x$$

$$\Rightarrow \varphi_{III}' > 0 \ @ \ x = \frac{a}{2}$$

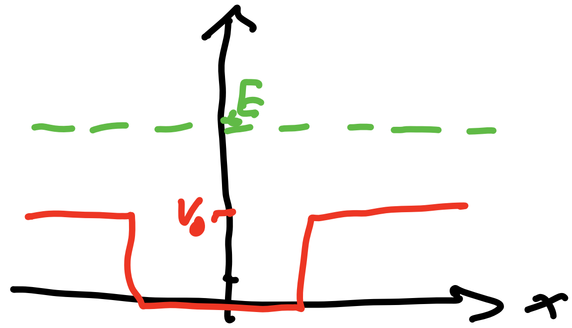
$$\Rightarrow \varphi_{III}' > 0 \ @ \text{ all } x$$

$$\Rightarrow \lim_{x\to\infty} \varphi_{III} = \infty \ . \ \#$$

$\therefore$ $\boxed{\text{No solutions for } E < V_{min}.}$

c) $E \geq V_0$ (scattering states)

$$\Rightarrow \begin{cases} \varphi_I = \mathcal{A} e^{ik_1 x} + \mathcal{B} e^{-ik_1 x} \\ \varphi_{II} = \mathcal{C} e^{ik_2 x} + \mathcal{D} e^{-ik_2 x} \\ \varphi_{III} = \mathcal{E} e^{ik_3 x} + \mathcal{F} e^{-ik_3 x} \end{cases}$$



MCs $\Rightarrow \ldots \Rightarrow \quad \varphi = \alpha \varphi_1 + \beta \varphi_2$

w/ $\varphi_i \sim$ "$e^{\pm i k x}$" ← oscillatory everywhere

$\therefore \lim_{|x| \to \infty} |\varphi| \neq 0$.

But in free case found that we should

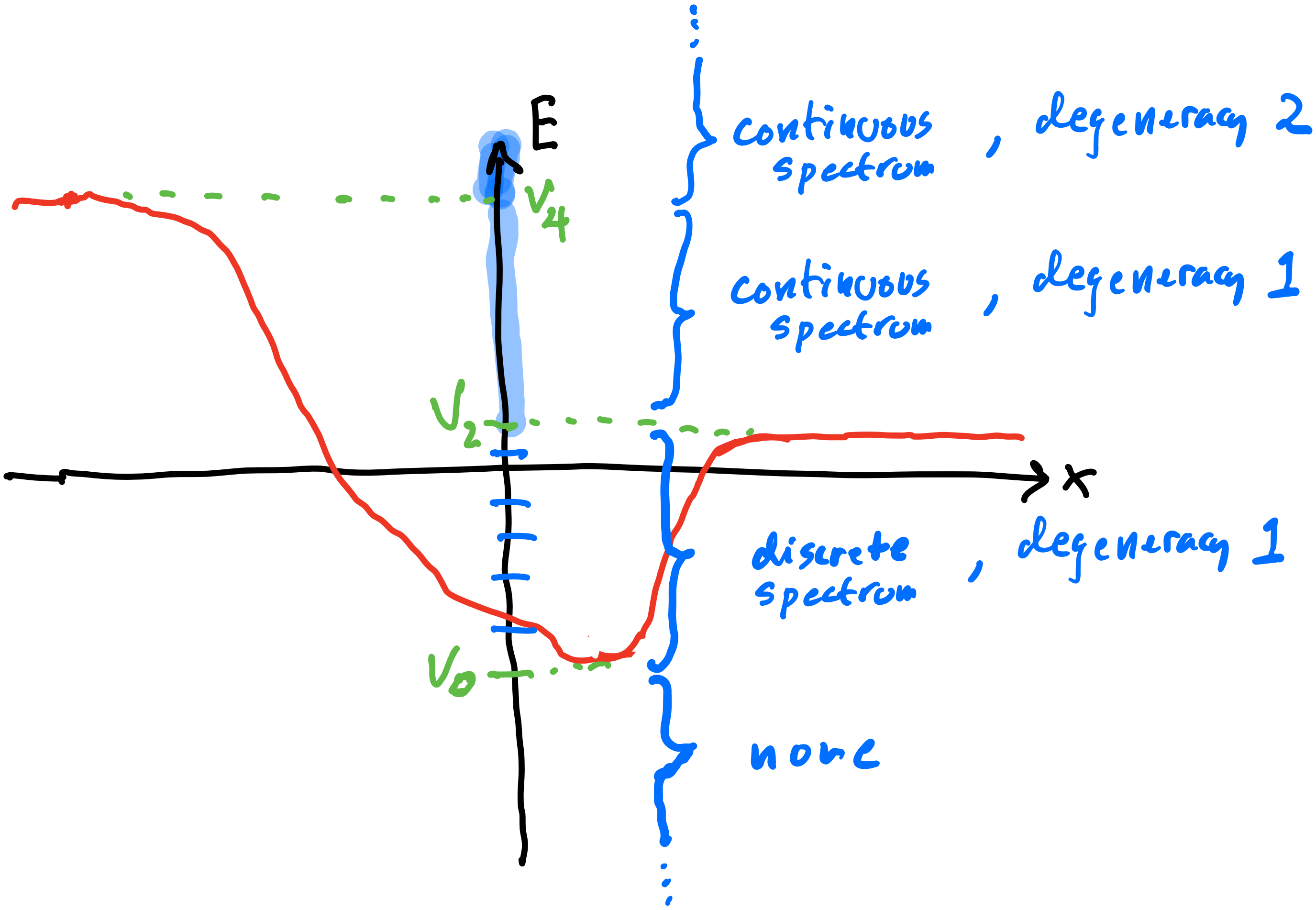
$$\boxed{\text{allow plane wave states, i.e., oscillatory wave functions with } \lim_{|x|\to\infty} |\varphi(x)| = \text{const.} > 0.}$$

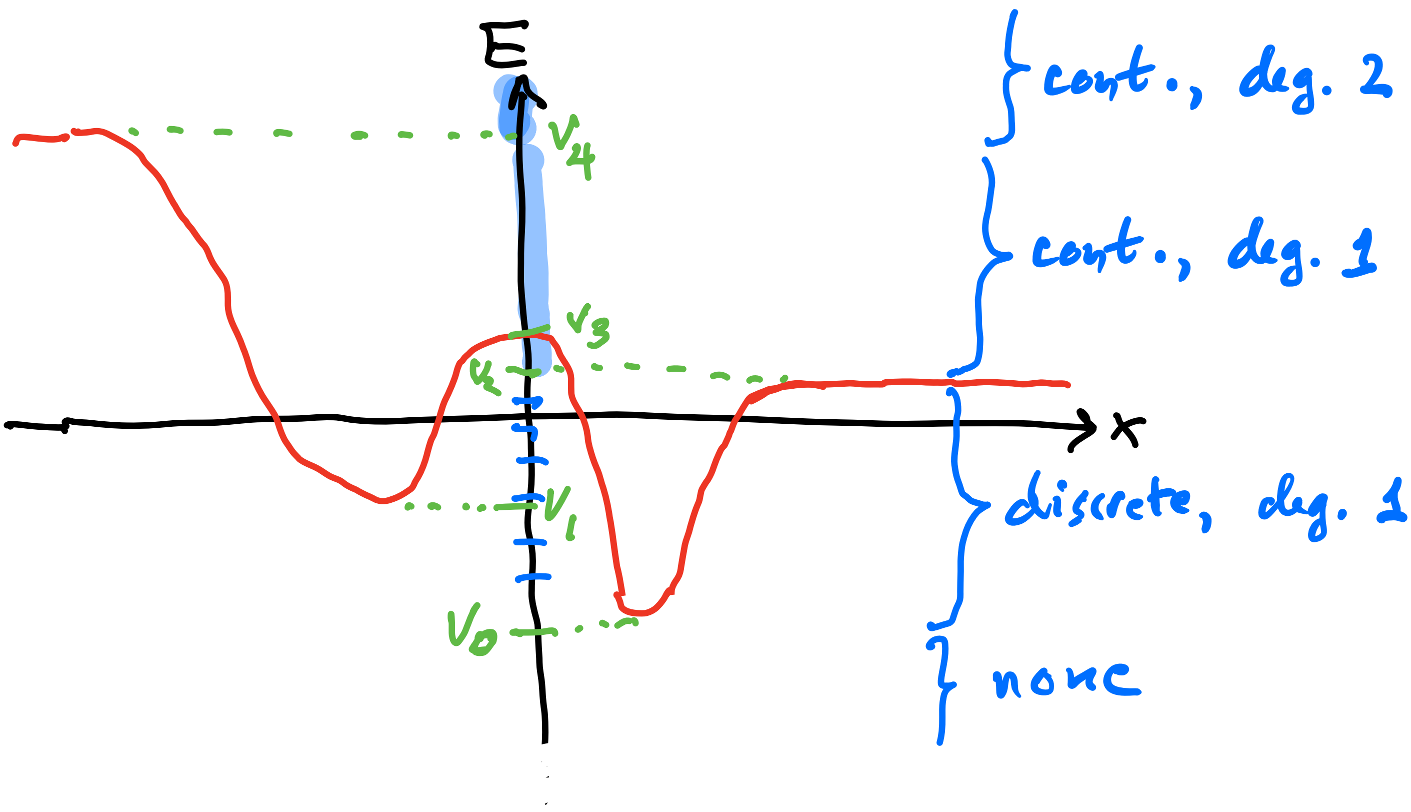
(We will interpret them later as scattering states).

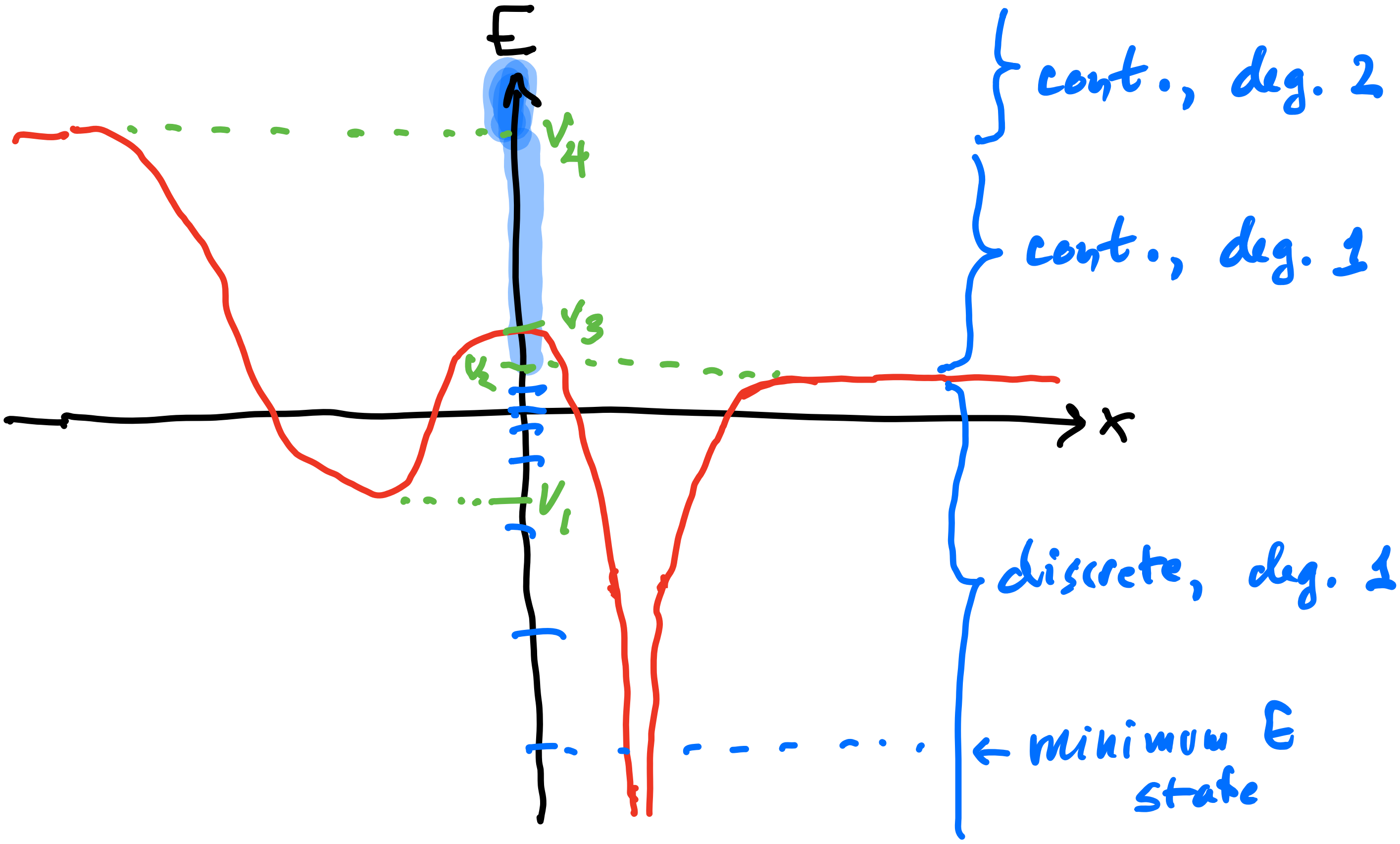
$\Rightarrow$ 2 lin. indep't sol'ns allowed for <u>any</u> E

$\Rightarrow$ "continuous spectrum w/ degeneracy 2"

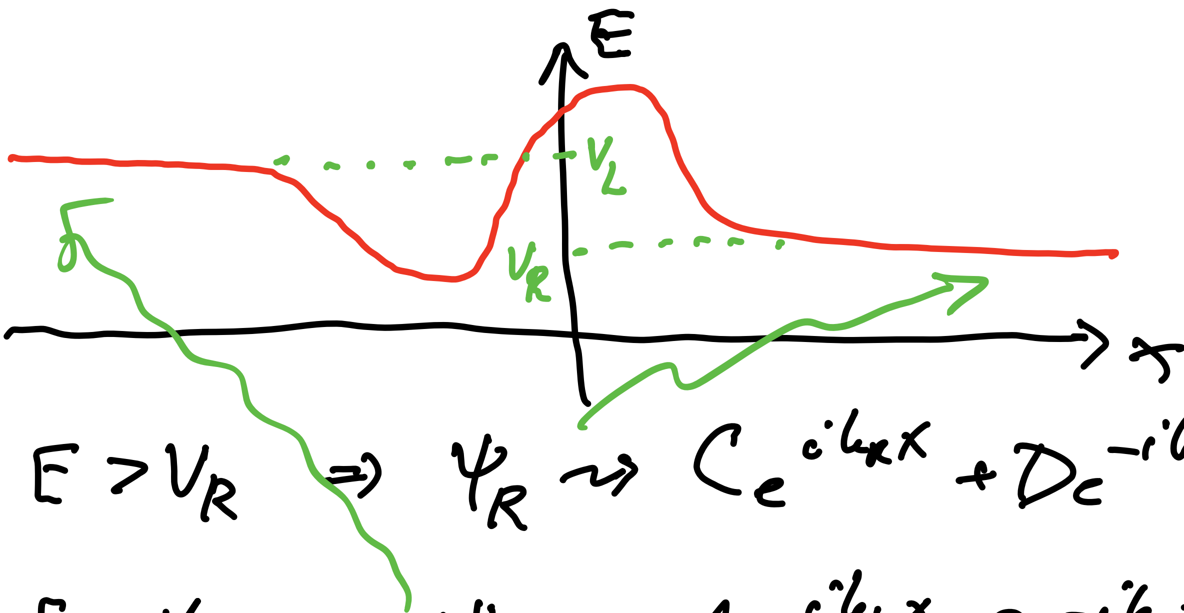
SUMMARY: General picture of spec($\hat{H}$)







Scattering States



$$E > V_R \Rightarrow \psi_R \rightsquigarrow C e^{ik_R x} + D e^{-ik_R x}$$

$$E > V_L \Rightarrow \psi_L \rightsquigarrow A e^{ik_L x} + B e^{-ik_L x}$$

where $\quad k_{L,R} \doteq \frac{1}{\hbar}\sqrt{2m(E - V_{L,R})}$

- Recall $\langle x|p\rangle \sim e^{ixp/\hbar}$

$$\therefore \quad \psi_R \sim C\langle x|\hbar k_R\rangle + D\langle x|-\hbar k_R\rangle$$
$$\psi_L \sim A\langle x|\hbar k_L\rangle + B\langle x|-\hbar k_L\rangle$$

$\Rightarrow$ $\psi_{L,R}$ are $\sim$ superposition of left- & right-moving states of **definite momentum** $(\Delta P = 0)$

$$p_R = \pm\hbar k_R \quad \text{etc.}$$

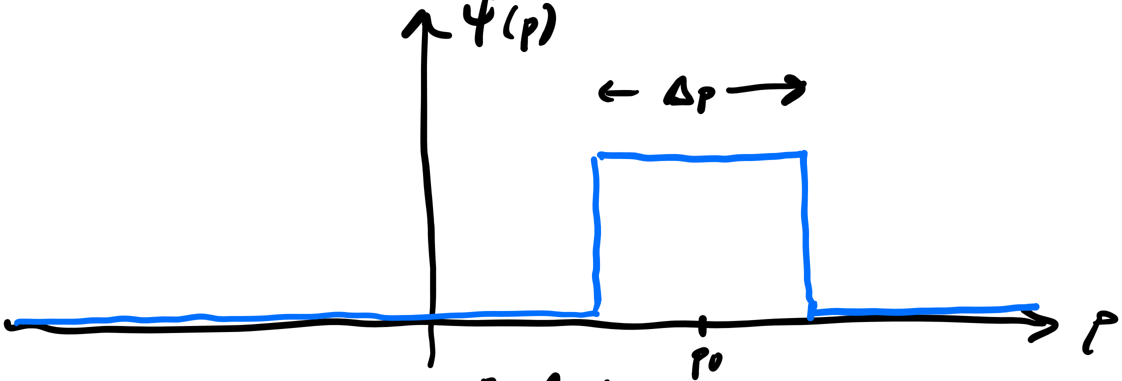
- Non-normalizable just like $|p\rangle$ states:

$$\langle p|p'\rangle = \delta(p-p') \Rightarrow \langle p|p\rangle = \delta(0) = \infty.$$

But, can make normalizable "**wave packets**" which are superpositions of an infinite number of momentum eigenstates

E.g.

$$|p_0, \Delta p\rangle \doteq N\int_{p_0-\frac{1}{2}\Delta p}^{p_0+\frac{1}{2}\Delta p} dp\; |p\rangle$$



$$\langle p_0,\Delta p | p_0,\Delta p\rangle = |N|^2 \iint_{p_0-\Delta p/2}^{p_0+\Delta p/2} dp\, dq\, \underbrace{\langle p | q\rangle}_{\delta(p-q)}$$

$$= |N|^2 \int_{p_0-\Delta p/2}^{p_0+\Delta p/2} dp \;=\; \Delta p \cdot |N|^2$$

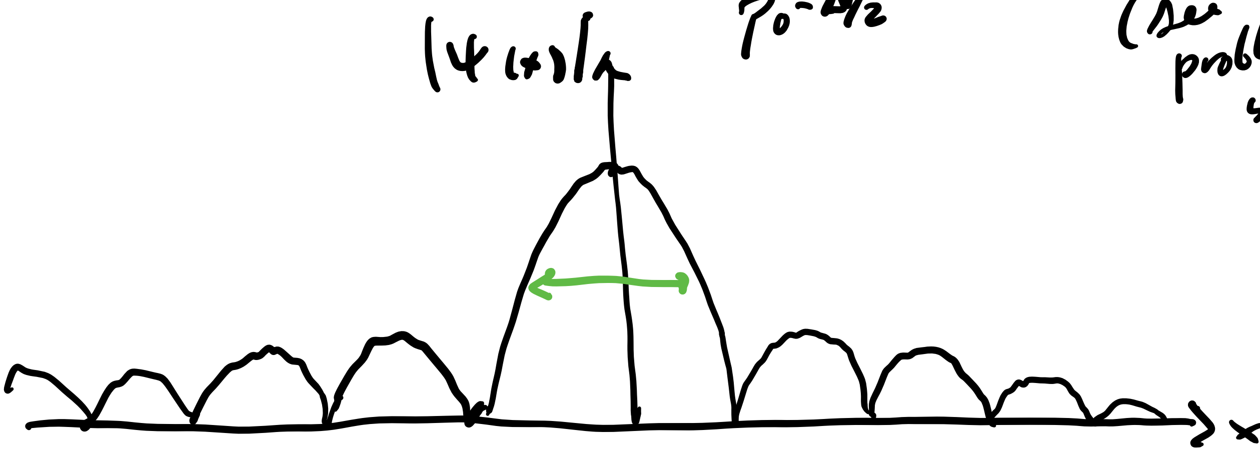
$\Rightarrow$ Normalized if pick $N = \dfrac{1}{\sqrt{\Delta p}}$. ✓

- What does wave function look like?

$$\psi(x) \doteq \langle x | p_0,\Delta p\rangle = \frac{1}{\sqrt{\Delta p}\cdot\sqrt{2\pi\hbar}} \int_{p_0-\Delta p/2}^{p_0+\Delta p/2} dp\, e^{ipx/\hbar} = \cdots$$

(see problem set)

$\Rightarrow$

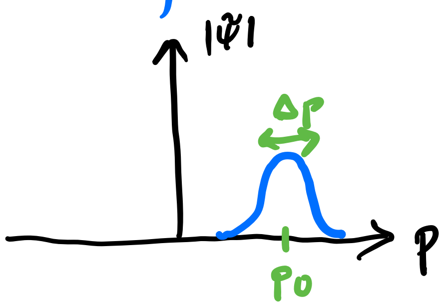


$\Delta x \sim \hbar/\Delta p$. ✓

- (Note: use Gaussians for "cleaner" wave-packets.)

- Summary:
  - Have continuum of eigenvalues but no <u>physical</u> eigenstates ⇒ only "scattering states"
  - But can make physical states with eigenvalue spread as small as you like.

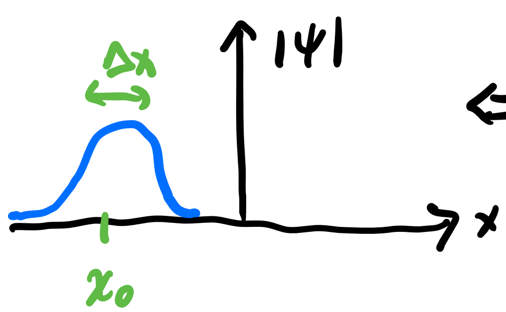
- Physical interpretation of wave packets



⇔ particle with momentum $p \sim p_0 \pm \Delta p$

⇒ velocity $\sim \frac{p_0}{m} \pm \frac{\Delta p}{m}$

↓



⇔ particle with position $x \sim x_0 \pm \Delta x$

& $\Delta x \sim \frac{\hbar}{\Delta p}$

- Expect time dependence (free particle)

$$x_{cl}(t) = x_0 + v_0 t = x_0 + \frac{p_0}{m} t$$

$$\therefore \Rightarrow \quad x(t) \sim x_0 \pm \frac{\hbar}{\Delta p} + \frac{p_0 \pm \Delta p}{m} t$$

$$\sim x_{cl}(t) \pm \underbrace{\frac{\Delta p}{m} t}_{?} \quad \text{for large } t$$

$$\Delta x(t) \overset{?}{\propto} t \qquad (?)$$

Uncertainty in x increases with time,
= "dispersion" or "spread" of $\psi(x)$

The answer (?) is wrong! Correct answer in QM (i.e., use Schrö's eqn.) is

$$\Delta x(t) \propto \sqrt{t} \qquad (!)$$

(See Townsend for calculation ...)

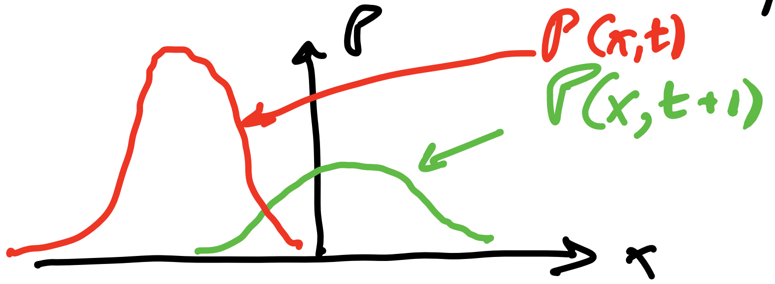
- More generally, to see time dependence, want to solve Schrö's Eqn:

$$\frac{\partial \psi(x,t)}{\partial t} = -\frac{i}{\hbar} \langle x | \hat{H} | \psi(t) \rangle$$

$$= -\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x) \cdot \psi(x,t) \right).$$

- Complicated for a general wave packet, but we really only want qualitative info, e.g. how fast does peak of wave packet move? how fast does it spread? etc.

• $|\psi(x,t)|^2 \doteq \mathcal{P}(x,t)$ = probability density for finding particle @ (x,t)



How does $\mathcal{P}$ change with time?

• Smoothly
• Total prob. $= \int \mathcal{P}\,dx = 1$ $\Big\}$ "conserved flow of probability"

$$\Longleftrightarrow \underbrace{\frac{d}{dt} P(a<x<b)}_{\text{rate of change of probability } (a<x<b)} = \underbrace{j(x=a)}_{\text{rate prob. flows in @ } x=a} - \underbrace{j(x=b)}_{\text{rate prob. flows out @ } x=b}$$

• So compute

$$\frac{\partial}{\partial t}\mathcal{P}(x,t) = \frac{\partial}{\partial t}\left(|\psi(x,t)|^2\right) = \frac{\partial \psi^*}{\partial t}\psi + \psi^*\frac{\partial \psi}{\partial t}$$

$$= +\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2} + \cancel{V\psi^*}\right)\psi - \frac{i}{\hbar}\psi^*\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \cancel{V\psi}\right)$$

$$= \frac{i\hbar}{2m}\left(\psi^*\frac{\partial^2\psi}{\partial x^2} - \psi\frac{\partial^2\psi^*}{\partial x^2}\right) = \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)\right]$$

$$\doteq -\frac{\partial}{\partial x} j(x,t)$$

So Schrö Eqn $\Rightarrow$

$$\boxed{\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0}$$

"local conservation laws"

where
$$\begin{cases} \rho \doteq |\psi|^2 & \text{prob. density} \\ j \doteq \frac{i\hbar}{2m}\left(\psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x}\right) & \doteq \text{"prob. current density"} \end{cases}$$

- Apply to $\psi(x) = Ae^{ikx}$ state

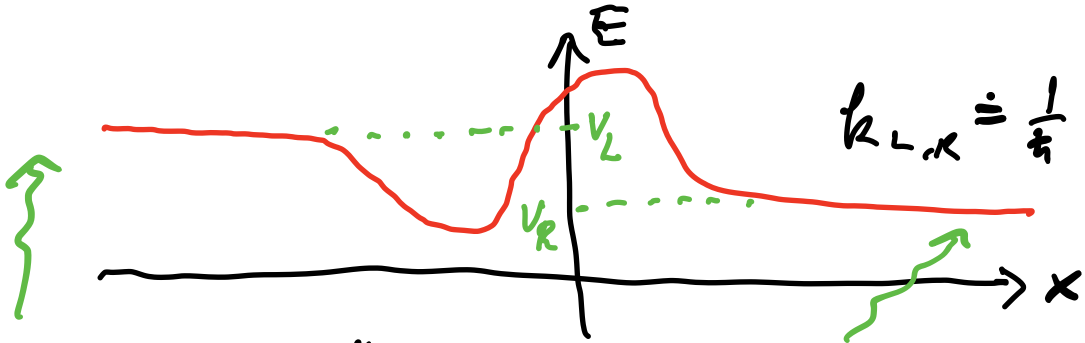
  = free particle in momentum eigenstate $p = \hbar k$

$$\Rightarrow \quad j = \frac{i\hbar}{2m}\left(Ae^{ikx} A^* \frac{d(e^{-ikx})}{dx} - A^* e^{-ikx} A \frac{d(e^{ikx})}{dx}\right)$$

$$= \frac{i\hbar}{2m}|A|^2(-ik - ik)$$

$$= |A|^2 \frac{\hbar k}{m} = |A|^2 \frac{p}{m} = |A|^2 v. \quad \checkmark$$

- Use probability current density to make physical interpretation of scattering states



$$k_{L,R} \doteq \frac{1}{\hbar}\sqrt{2m(E-V_{L,R})}$$

$$\psi_L \sim \underbrace{A e^{ik_L x}}_{\text{inc-L}} + \underbrace{B e^{-ik_L x}}_{\text{out-L}} \qquad \psi_R \sim \underbrace{C e^{ik_R x}}_{\text{out-R}} + \underbrace{D e^{-ik_R x}}_{\text{in-R}}$$

- 2 physically interesting problems:
(1) Send in particle (wave packet) from L, or
(2) " " " " " " R.

$\Rightarrow$ BC for (1): $D=0$ (i.e., no in-R)
BC for (2): $A=0$ (i.e., no in-L).

(1): Solve $\hat{H}|\varphi\rangle = E|\varphi\rangle$ ... find

$$\lim_{x\to-\infty} \varphi \sim \overset{\text{incoming}}{A} e^{ik_L x} + \overset{\text{reflected}}{B} e^{-ik_L x}$$

$$\lim_{x\to+\infty} \varphi \sim \underset{\text{transmitted}}{C} e^{ik_R x} + \underset{\text{disallowed by BC}}{D e^{-ik_R x}}$$

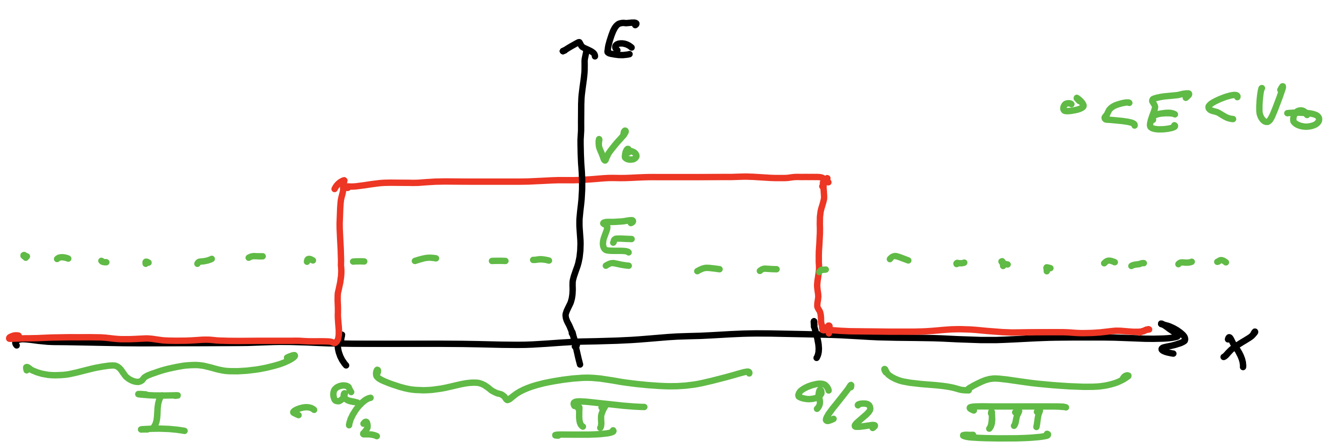
$$\Rightarrow \begin{cases} j_{in} = \dfrac{\hbar k_L}{m} |A|^2 & j_{refl} = -\dfrac{\hbar k_L}{m} |B|^2 \\ j_{trans} = \dfrac{\hbar k_R}{m} |C|^2 & \end{cases}$$

$$\therefore \boxed{\begin{aligned} R &\doteq \text{reflection probability} = \frac{|j_{refl}|}{|j_{in}|} = \frac{|B|^2}{|A|^2} \\ T &\doteq \text{transmission probability} = \frac{|j_{trans}|}{|j_{in}|} = \frac{k_R |C|^2}{k_L |A|^2} \end{aligned}}$$!!

Expect $R+T=1$. Can prove using definitions & $\partial_t \rho + \partial_x j = 0$ & $\int \rho \, dx = 1$.

(Similarly for problem (2) ...)

Example: Potential barrier



$\longrightarrow$ incoming from left $\Rightarrow$ no e^{-ikx} term in ψ_{III}

$$\psi_{I} = Ae^{ikx} + Be^{-ikx} \qquad k \doteq \frac{1}{\hbar}\sqrt{2mE}$$

$$\psi_{II} = De^{\kappa x} + Ee^{-\kappa x} \qquad \kappa \doteq \frac{1}{\hbar}\sqrt{2m(V_0 - E)}$$

$$\psi_{III} = Ce^{ikx}$$

Matching conditions @ $x = \pm a/2$:

$$\psi @ x = -\tfrac{a}{2}: \quad Ae^{-ika/2} + Be^{ika/2} = De^{-\kappa a/2} + Ee^{\kappa a/2} \quad ①$$

$$\psi' @ x = -\tfrac{a}{2}: \quad ikAe^{-ika/2} - ikBe^{ika/2} = \kappa De^{-\kappa a/2} - \kappa Ee^{\kappa a/2} \quad ②$$

$$\psi @ x = +\tfrac{a}{2}: \quad Ce^{ika/2} = De^{\kappa a/2} + Ee^{-\kappa a/2} \quad ③$$

$$\psi' @ x = +\tfrac{a}{2}: \quad ikCe^{ika/2} = \kappa De^{\kappa a/2} - \kappa Ee^{-\kappa a/2} \quad ④$$

$$③ \pm \tfrac{1}{\kappa}④ \Rightarrow \begin{cases} De^{\kappa a/2} = \frac{1}{2}\left(1 + \frac{ik}{\kappa}\right)e^{ika/2}C \\ Ee^{-\kappa a/2} = \frac{1}{2}\left(1 - \frac{ik}{\kappa}\right)e^{ika/2}C \end{cases}$$

Plug in to

$$① \Rightarrow \quad Ae^{-ika/2} + Be^{ika/2} = Ce^{ika/2}\left(\tfrac{1}{2}\right)\left[\left(1 + \tfrac{ik}{\kappa}\right)e^{-\kappa a} + \left(1 - \tfrac{ik}{\kappa}\right)e^{\kappa a}\right]$$

$$\frac{②}{ik} \Rightarrow \quad Ae^{-ika/2} - Be^{ika/2} = Ce^{ika/2}\left(\tfrac{-i\kappa}{2k}\right)\left[\left(1 + \tfrac{ik}{\kappa}\right)e^{-\kappa a} - \left(1 - \tfrac{ik}{\kappa}\right)e^{\kappa a}\right]$$

$\oplus$

$$2Ae^{-ika/2} = \tfrac{1}{2}Ce^{ika/2}\Big[\underbrace{\left(1 - \tfrac{i\kappa}{k}\right)\left(1 + \tfrac{ik}{\kappa}\right)e^{-\kappa a} + \left(1 + \tfrac{i\kappa}{k}\right)\left(1 - \tfrac{ik}{\kappa}\right)e^{\kappa a}}_{\doteq\, \xi}\Big]$$

$$\Rightarrow \frac{C}{A} = 4e^{-ika}\xi^{-1}, \quad \xi = 2\left(e^{\kappa a} + e^{-\kappa a}\right) + i\left(\frac{\kappa}{k} - \frac{k}{\kappa}\right)\left(e^{\kappa a} - e^{-\kappa a}\right)$$

$$= 4\cosh(\kappa a) + 2i\left(\frac{\kappa}{k} - \frac{k}{\kappa}\right)\sinh(\kappa a)$$

$$\therefore T = \left|\frac{C}{A}\right|^2 = \frac{16}{|\xi|^2} = \frac{16}{16\cosh^2(\kappa a) + 4\left(\frac{\kappa}{k} - \frac{k}{\kappa}\right)^2\sinh^2(\kappa a)}$$

$$\Rightarrow \boxed{T = \left[\cosh^2(\kappa a) + \frac{1}{4}\left(\frac{\kappa}{k} - \frac{k}{\kappa}\right)^2 \sinh^2(\kappa a)\right]^{-1}}$$

$$\frac{1}{4}\left(\frac{\kappa}{k} - \frac{k}{\kappa}\right)^2 = \frac{1}{4}\left(\sqrt{\frac{E}{V_0 - E}} - \sqrt{\frac{V_0 - E}{E}}\right)^2 = \frac{1}{4} \cdot \frac{1}{\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)} \doteq \varepsilon \geq 1$$

Min. ε @ $E = \frac{1}{2} V_0 \Rightarrow \varepsilon = 1$

Max. ε @ $E = 0$ or $V_0 \Rightarrow \varepsilon = \infty$

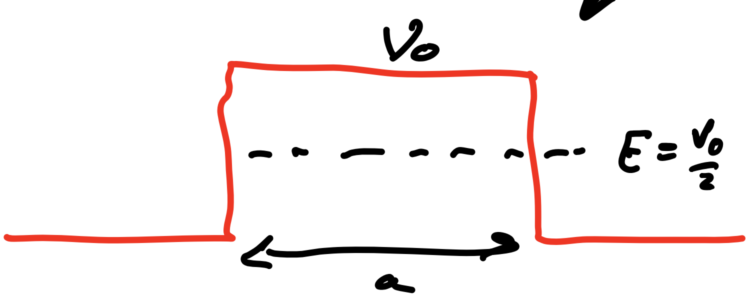
Use $\cosh^2 = 1 + \sinh^2 \Rightarrow$

$$\boxed{T = \left[1 + (1 + \varepsilon)\sinh^2(\kappa a)\right]^{-1} \quad \text{w/} \quad \varepsilon \geq 1}$$

$\Rightarrow T \leq 1$

$T = 0$ @ $\varepsilon = \infty \Rightarrow E = 0$ or V_0

T_{max} @ $\varepsilon_{min} = 1 \Rightarrow T_{max} = \left(1 + 2\sinh^2(\kappa a)\right)^{-1}$ @ $E = \frac{V_0}{2}$



$$\kappa = \frac{1}{\hbar}\sqrt{2m(V_0 - E)} = \frac{\sqrt{m V_0}}{\hbar}$$

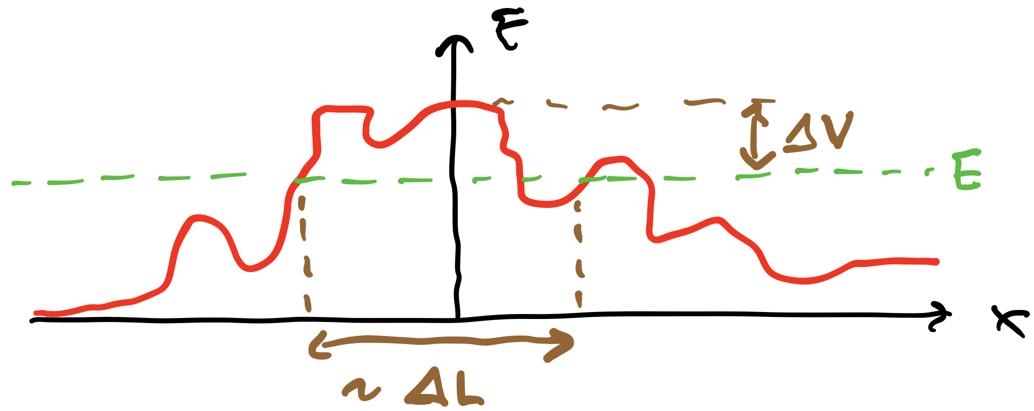
$$\therefore T_{max} = \frac{1}{1 + \frac{1}{2}\left(e^{\kappa a} - e^{-\kappa a}\right)^2} \approx 2e^{-2\kappa a}$$

for $\kappa a \gg 1$

$\therefore$ Tunnelling probability $\approx e^{-2\kappa a} = e^{-\frac{2}{\hbar} a \sqrt{m V_0}}$

Generalizes to arbitrary potential barrier as long as wide & high enough (e.g. "WKB" approx.)

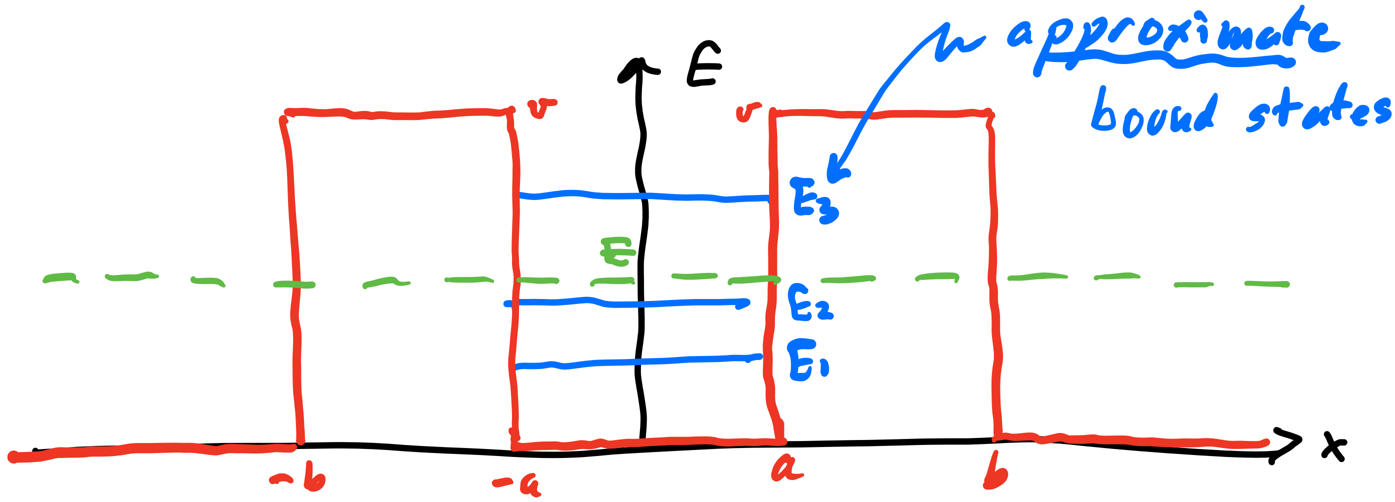
$\Rightarrow$



$$\log(\text{tunnel. prob.}) \approx -\frac{1}{\hbar}\,\Delta L\cdot\sqrt{m}\cdot\sqrt{\Delta V}$$

Extremely tiny for macroscopic $\Delta L, m, \Delta V$ ✓

Example: Resonant Tunnelling



As $E \to E_n \Rightarrow T \to 1$

no matter how high/thick pot'l barrier!

??

Resonant tunnelling example.

Resonant tunnelling from a piecewise flat potential:

$$V(x) = 0, \quad |x|>b \text{ and } |x|<a,$$
$$= v, \quad a<|x|<b,$$

with b>a>0. Define

$$k = \sqrt{2 m E} \Big/ \hbar,$$
$$\kappa = \sqrt{2 m (v - E)} \Big/ \hbar.$$

Define the matrices for matching conditions at x=±a, ±b, are

```
M1[a_] = {{e^(i k a), e^(-i k a)}, {i k e^(i k a), -i k e^(-i k a)}};
M2[a_] = {{e^(κ a), e^(-κ a)}, {κ e^(κ a), -κ e^(-κ a)}};
M1[x] // MatrixForm
M2[x] // MatrixForm
```

$$\begin{pmatrix} e^{i k x} & e^{-i k x} \\ i e^{i k x} k & -i e^{-i k x} k \end{pmatrix}$$

$$\begin{pmatrix} e^{x \kappa} & e^{-x \kappa} \\ e^{x \kappa} \kappa & -e^{-x \kappa} \kappa \end{pmatrix}$$

Then, if the wave function for |x|>b has the form

$$\psi(x) = A\, e^{i k x} + B\, e^{-i k x}, \text{ for } x < -b,$$
$$= C\, e^{i k x}, \text{ for } x > b,$$

(0 because of scattering BC.)

the matching conditions can be written as the matrix equation $\vec{a} = X\, \vec{c}$ where $\vec{a}^{\,T} = (A, B)$, $\vec{c}^{\,T} = (C, 0)$, and

```
X = Simplify[
   Inverse[M1[-b]].M2[-b].Inverse[M2[-a]].M1[-a].Inverse[M1[a]].M2[a].Inverse[M2[b]].M1[b]];
```

Then C/A = $1/X_{11}$ where

```
X11 = X[[1, 1]]
```

$$\frac{1}{16 k^2 \kappa^2} e^{-2 i a k + 2 i b k - 2 a \kappa - 2 b \kappa} \Big(-e^{4 b \kappa} (k + i \kappa)^4 - e^{4 a \kappa} (i k + \kappa)^4 + 2 e^{2 (a+b) \kappa} \left(k^2 + \kappa^2\right)^2 + e^{4 a (i k + \kappa)} \left(k^2 + \kappa^2\right)^2 - 2 e^{4 i a k + 2 a \kappa + 2 b \kappa} \left(k^2 + \kappa^2\right)^2 + e^{4 i a k + 4 b \kappa} \left(k^2 + \kappa^2\right)^2\Big)$$

so the transmission probability is given by T = $1/|X_{11}|^2$:

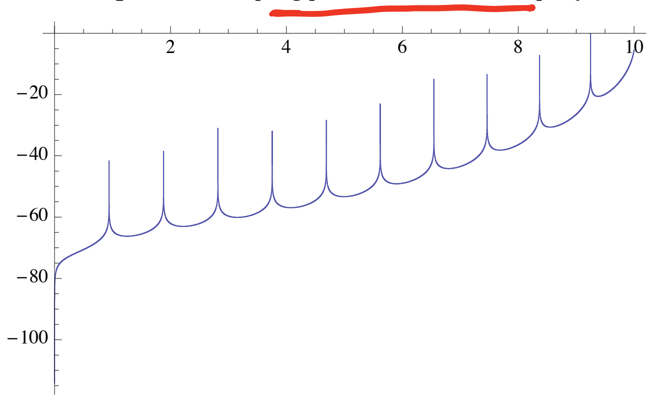
$$\frac{\kappa}{k} = \sqrt{\left(\frac{10}{n}\right)^2 - 1} = \sqrt{\frac{v}{E} - 1} \Rightarrow \frac{E}{v} = \frac{n^2}{100}$$

```
Xexp = ComplexExpand[X11];
Xconj = Xexp /. ⅈ → -ⅈ;
Xsquared = Simplify[Expand[Xexp Xconj]]
```

$$-\frac{1}{128\,k^4\,\kappa^4}\,e^{-4(a+b)\kappa}\Big(-e^{8a\kappa}k^8 - e^{8b\kappa}k^8 - 6\,e^{4(a+b)\kappa}k^8 + 4\,e^{2(3a+b)\kappa}k^8 + 4\,e^{2(a+3b)\kappa}k^8 - 4\,e^{8a\kappa}k^6\kappa^2 - 4\,e^{8b\kappa}k^6\kappa^2 +$$
$$8\,e^{4(a+b)\kappa}k^6\kappa^2 - 6\,e^{8a\kappa}k^4\kappa^4 - 6\,e^{8b\kappa}k^4\kappa^4 - 100\,e^{4(a+b)\kappa}k^4\kappa^4 - 8\,e^{2(3a+b)\kappa}k^4\kappa^4 -$$
$$8\,e^{2(a+3b)\kappa}k^4\kappa^4 - 4\,e^{8a\kappa}k^2\kappa^6 - 4\,e^{8b\kappa}k^2\kappa^6 + 8\,e^{4(a+b)\kappa}k^2\kappa^6 - e^{8a\kappa}\kappa^8 -$$
$$e^{8b\kappa}\kappa^8 - 6\,e^{4(a+b)\kappa}\kappa^8 + 4\,e^{2(3a+b)\kappa}\kappa^8 + 4\,e^{2(a+3b)\kappa}\kappa^8 + \left(e^{2a\kappa} - e^{2b\kappa}\right)^2\left(k^2+\kappa^2\right)^2$$
$$\left(-2\,e^{2(a+b)\kappa}\left(k^2+\kappa^2\right)^2 + e^{4a\kappa}\left(k^4 - 6k^2\kappa^2 + \kappa^4\right) + e^{4b\kappa}\left(k^4 - 6k^2\kappa^2 + \kappa^4\right)\right)\mathrm{Cos}[4\,a\,k] +$$
$$4\left(e^{2a\kappa} - e^{2b\kappa}\right)^3\left(e^{2a\kappa} + e^{2b\kappa}\right)k\,\kappa\left(-k^2+\kappa^2\right)\left(k^2+\kappa^2\right)^2\,\mathrm{Sin}[4\,a\,k]\Big)$$

This is a mess, but plot it for some convenient values ($a=\pi/2$, $b=\pi$, $E = n^2$, v=100, $m/(2\hbar)=1$), so that the two barriers each have thickness $\pi/2$:

```
WellTransmission = 1 / Xsquared /. {a → π / 2, b → π, k → n, κ → √(100 - n²)};
welltranplot = Plot[Log[WellTransmission], {n, 0, 10}, PlotRange → All, PlotPoints → 100 000]
```



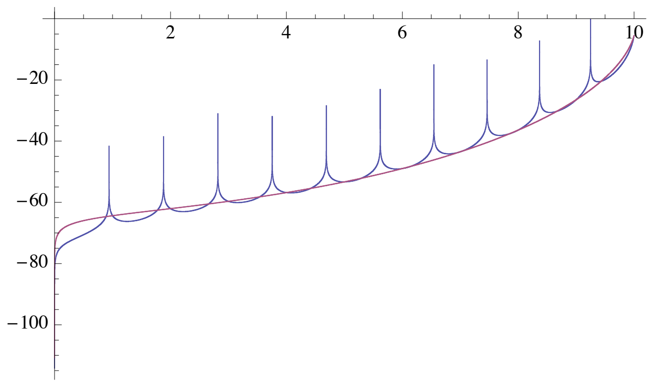
← log(T)

Note the peaks in T at n ≈ {1,2,3,4,...}. These values of n correspond to the bound state energies of the square well potential in the middle (x<|a|). These peaks in the transmission probability are called "resonant tunnelling".

For comparison, consider instead the transmission probability through a single square barrier of thickness π (i.e., without an intervening potential well). Following the same steps as above gives ...

```
B = Simplify[Inverse[M1[-b]].M2[-b].Inverse[M2[-a]].M1[-a]];
B11 = B[[1, 1]];
Bexp = ComplexExpand[B11];
Bconj  = Bexp /. ⅈ → -ⅈ;
Bsquared  = Simplify[Expand[Bexp Bconj]]
BarrierTransmission = 1 / Bsquared /. {a → 0,  b → π, k → n, κ → Sqrt[100 - n^2]};
Plot[{Log[WellTransmission], Log[BarrierTransmission]},
 {n, 0, 10}, PlotRange → All, PlotPoints → 100 000]
```

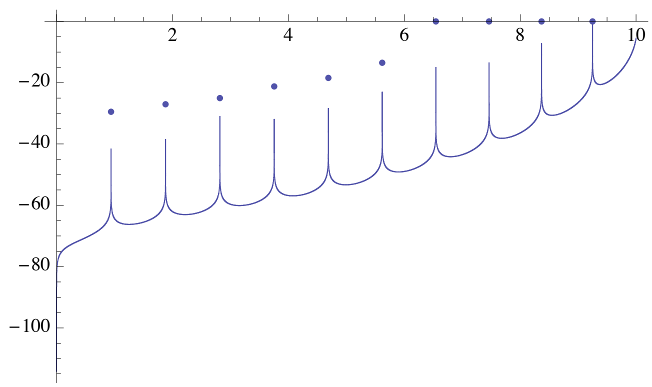
$$\frac{e^{-2(a+b)\kappa}\left(e^{4a\kappa}\left(k^2+\kappa^2\right)^2+e^{4b\kappa}\left(k^2+\kappa^2\right)^2-2e^{2(a+b)\kappa}\left(k^4-6k^2\kappa^2+\kappa^4\right)\right)}{16k^2\kappa^2}$$



... which closely follows the transmission probability for the case with an intervening potential well, except for the absence of the resonant tunnelling peaks.

[Note: In the plot the resonant tunnelling peaks only seem to rise about 10 orders of magnitude (i.e., a factor of about e^{25}) above the background, but this is just because of the numerical resolution of *Mathematica* --- in fact, they rise to values much closer to 1 (i.e., log(T) $\approx$ 0). Numerical evidence of this is just to evaluate the peak values by searching for relevant extrema of T. This gives the points in the following plot...

```
Off[FindRoot::"lstol"]
Off[Power::"infy"]
peak[1] = FindRoot[D[Denominator[WellTransmission], n] == 0, {n, .95}];
val[1] = {y → Log[Abs[WellTransmission /. peak[1]]]};
peak[2] = FindRoot[D[Denominator[WellTransmission], n] == 0, {n, 1.9}];
val[2] = {y → Log[Abs[WellTransmission /. peak[2]]]};
peak[3] = FindRoot[D[Denominator[WellTransmission], n] == 0, {n, 2.8}];
val[3] = {y → Log[Abs[WellTransmission /. peak[3]]]};
peak[4] = FindRoot[D[Denominator[WellTransmission], n] == 0, {n, 3.75}];
val[4] = {y → Log[Abs[WellTransmission /. peak[4]]]};
peak[5] = FindRoot[D[Denominator[WellTransmission], n] == 0, {n, 4.7}];
val[5] = {y → Log[Abs[WellTransmission /. peak[5]]]};
peak[6] = FindRoot[D[Denominator[WellTransmission], n] == 0, {n, 5.6}];
val[6] = {y → Log[Abs[WellTransmission /. peak[6]]]};
peak[7] = FindRoot[D[Denominator[WellTransmission], n] == 0, {n, 6.55}];
val[7] = {y → Min[Log[Abs[WellTransmission /. peak[7]]], 0]};
peak[8] = FindRoot[D[Denominator[WellTransmission], n] == 0, {n, 7.4}];
val[8] = {y → Min[Log[Abs[WellTransmission /. peak[8]]], 0]};
peak[9] = FindRoot[D[Denominator[WellTransmission], n] == 0, {n, 8.35}];
val[9] = {y → Log[Abs[WellTransmission /. peak[9]]]};
peak[10] = FindRoot[D[Denominator[WellTransmission], n] == 0, {n, 9.24}];
val[10] = {y → Log[Abs[WellTransmission /. peak[10]]]};
peaks = Table[{n /. peak[i], y /. val[i]}, {i, 1, 10}];
peakplot = ListPlot[peaks];
Show[welltranplot, peakplot]
```



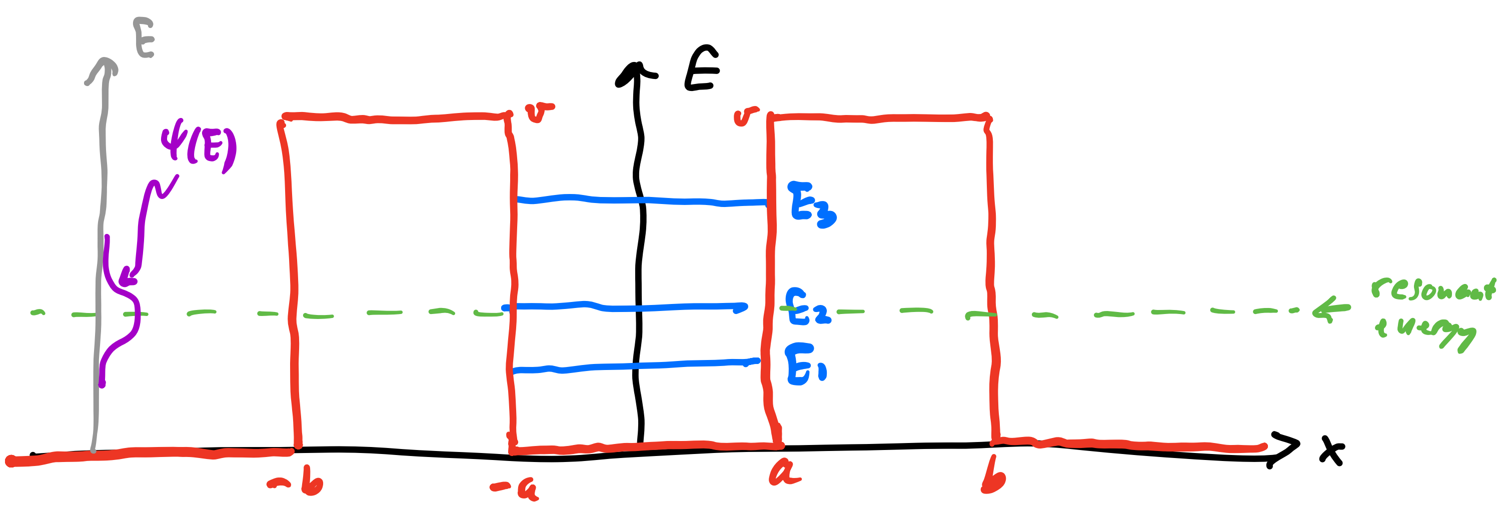
... showing another factor of e^{10} increase in T over the line plot. Also, the fact that for the last 4 peaks the value is essentially T=1 (log(T)=0), indicates that the values at the earlier peaks are probably just limited by numerical accuracy.]

This should seem like a <u>wrong</u> answer since, if true, it would be in contradiction to the classical limit.

The resolution of this paradox is that the above calculation is correct, but we are being mis-led by using unphysical scattering states instead of physical wave packet states.

We have seen that wave packets have a finite spread in energies

$$|\psi\rangle = \int dE \, \psi(E) \, |E\rangle$$



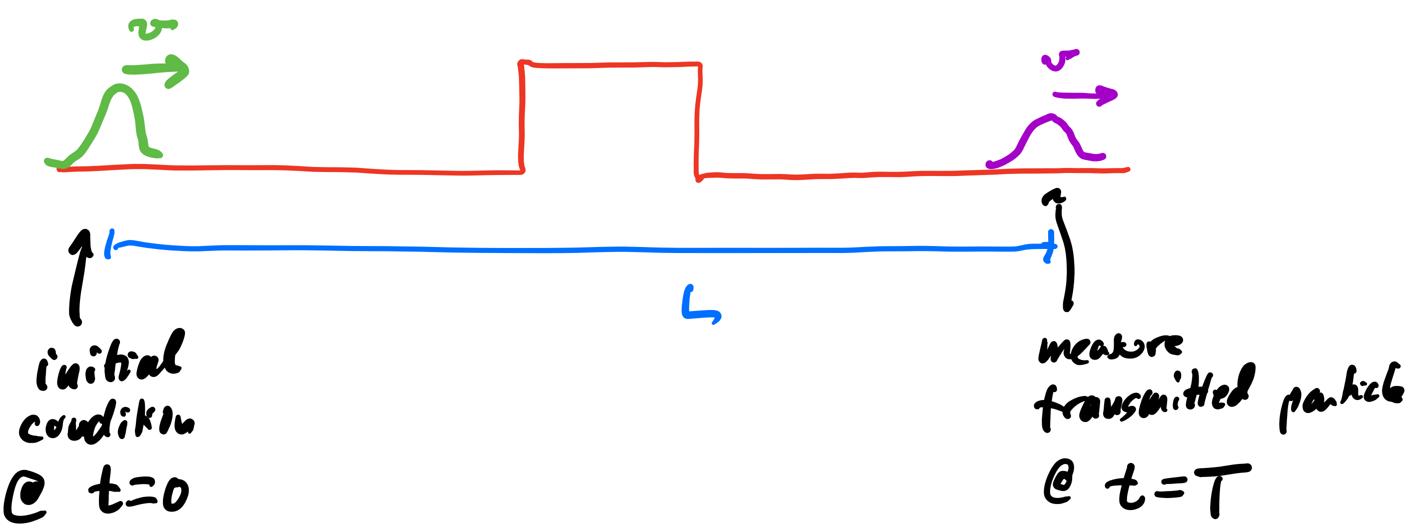
So transmission probability for <u>physical</u> state $|\psi\rangle$ is average of $T(E)$'s :

$$T(\psi) \approx \int dE \cdot T(E) \cdot |\psi(E)|^2$$

So even if exists E_n w/ $T(E_n) = 1$, if <u>width</u> of $T(E_n)$ peak is narrow, then

$T(\psi) \ll 1$. ✓

- <u>Note:</u> T & R are not the only scattering questions (experiments) one can do. Another common experiment is scattering time delay:



Time delay: $\Delta T = T - \frac{1}{v} L$.

This can also be computed using scattering states ... "scattering phase shift" ...