~~4/2/21, Week 2, Day 1/2~~ Probabilities I

(Probabilities, Half-infinite Square Well)

- We ended last class with a disturbing conclusion. Applying wave mechanics to particles seems to necessarily imply that we can no longer talk about well-defined positions & trajectories, but must rather talk about probabilities for these quantities.

- ~~Determinism~~ (in general certain deterministic outcomes still occur)

- Let's discuss particle motion a bit more

- $P_{a,b} = \int_a^b \psi^*(x,t)\psi(x,t)\,dx$

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

if $V(x)$ real + $\varphi_1(x)$ real at one point in space $\varphi_1(x)$ real for all x. $\Rightarrow$ Can choose $\varphi_1(x) = \varphi_1^*(x)$, although $\varphi_1(x)e^{i\theta}$ is also a solution with energy E_1

Suppose $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi_1(x) + V(x)\varphi_1(x) = E_1\varphi_1(x)$, $E_1 = \hbar\omega_1$

~~$V(x)$ real $\Rightarrow$ $\varphi_1(x) = \varphi_1^*(x)$~~

~~$\varphi_1(x)e^{i\theta}$ also a solution with same energy. Can choose E_1~~

2

- Then $\psi(x,t) = \varphi_1(x) e^{-i\omega_1 t}$ is a solution to t.d. schr. eqn.

$$i\hbar \frac{\partial}{\partial t}\psi = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V\psi$$

$$\Rightarrow P_{x,x+\Delta x} = \varphi_1(x) e^{-i\omega_1 t} \varphi_1(x) e^{+i\omega_1 t}{}_{\Delta x} = \varphi_1^2(x)_{\Delta x}$$

No time-dep motion

complex coefficients

- $\psi(x,t) = \alpha \varphi_1(x) e^{-i\omega_1 t} + \beta \varphi_2(x) e^{-i\omega_2 t}$, where φ_2 is energy eigenstate w/ energy E_2

is also a solution

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

$$= |\alpha|^2 \varphi_1^2(x) + |\beta|^2 \varphi_2^2(x) + \left(\alpha\beta^* e^{+i(\omega_1-\omega_2)t} + \text{c.c.}\right)\varphi_1(x)\varphi_2(x)$$

$\sim \cos[(\omega_1-\omega_2)t]$

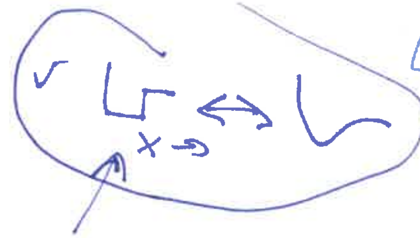
$\boxed{\text{(See next lecture for result)}}$

$\cancel{2\mathrm{Re}(\alpha\beta^*)\cos[(\omega_1-\omega_2)t+\phi]}$

$\Rightarrow$ Time-dep. motion (& more generally all time dep. for time-ind. $V(x)$) only occurs when you have superposition of energy eigenstates

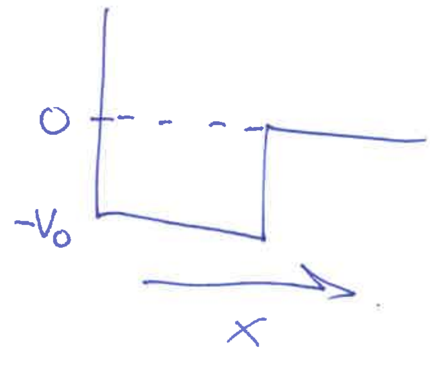
- $\boxed{\text{Show simulation}}$

We covered particle in a box.



Let's think ~~xxx~~ about more generally ~~about~~ potentials in 1D. to understand some general properties of ~~xxx~~ w.f. in different potentials.

$$V(x) = \begin{cases} \infty & x<0 \\ -V_0 & 0<x<a \\ 0 & x>a \end{cases}$$



Again let's search for periodic solutions in time

$$\psi(x,t) = \varphi_E(x) e^{-i\omega t}, \quad \text{where } E = \hbar\omega$$

$$i\hbar\frac{\partial}{\partial t}\psi = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V\psi$$

For this to be a ~~xxx~~ solution, ① $\varphi_E(x)$ is a special function... eigenfunction. ② $\hbar\omega$ is the eigenvalue $\boxed{\text{of RHS operator}}$

~~energy obtained from $i\hbar\frac{\partial}{\partial t}$ operator has to match that obtained from $\frac{-\hbar^2}{2m}\nabla^2 + V(x)$ operator~~

In other words,

(Dropping $e^{-i\omega t}$ from each side)

① $$E\,\varphi_E(x) = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\varphi_E(x) + V(x)\,\varphi_E(x)$$

Inside well $$(E+V_0)\varphi_E(x) = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\varphi_E(x)$$

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

inside well

Solutions that vanish @ $x=0$ are $\varphi_E = \sin k_v x$

That is sol'n out to $x=a$. For $x>a$, we have same thing with $V_0 \to 0$:

$$\cancel{E\,\varphi_E(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi_E(x)}$$

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

If $E>0$, then sol'n's for $x>a$ are same sines & cosines of a free particle.

If $E<0$, ($k^2<0$ &) write

$$\lambda^2 = -k^2 = \frac{-2mE}{\hbar^2}, \quad \lambda \text{ positive}$$

$$\varphi_E(x) = Ae^{-\lambda x} + Be^{\lambda x}$$

If $B \neq 0$, all weight of w.f. is @ ∞, so it's unphysical... or one could say not useful.

For $E<0$ $\Rightarrow$ $\varphi_E(x) = \begin{cases} \sin k_v x & x<a \\ Ae^{-\lambda x} & x>a \end{cases}$

What can we conclude about wavefunction properties at the boundary?

We have

Changes suddenly

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

$$= \frac{d^2}{dx^2}\varphi(x)$$

Let's integrate across boundary. Recall $\int_a^b dx \frac{df}{dx} = f\big|_b - f\big|_a$

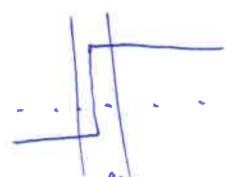
So, integrating both sides about small ϵ range across boundary

$$\int_{a-\epsilon}^{a+\epsilon} dx\, \varphi''(x) = \int_{a-\epsilon}^{a+\epsilon} dx\, \frac{2m}{\hbar^2}(V(x)-E)\,\varphi(x) \rightarrow 0$$

since $V(x)$ & φ finite

$$\| $$

$$\varphi'\big|_{a+\epsilon} - \varphi'\big|_{a-\epsilon}$$



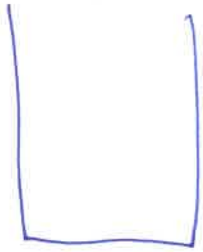
area vanishes as $\epsilon \to 0$

$\Rightarrow$ φ' does not change across boundary if $V(x)$ finite. ~~is smooth, no kink~~

Do that operation again & we find φ does not change across boundary either.

$\Rightarrow$ $\varphi_E(x)$ is continuous (no jumps) & smooth (no kinks) for finite potentials.

For infinite potentials, we lose smoothness e.g. infinite well



$\varphi_1(x) =$ 

But we still maintain continuity.
(Real world potentials are finite, so we can say w.f.s are smooth & continuous)

But we can approach infinite case & if we lost continuity, we would have a problem.

$\frac{\partial}{\partial x}$ is momentum operator & we would be saying that we had a region of $\to\infty$ momentum. Would be a problem

---

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

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

$\Updownarrow$

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

If Bound ($k^2<0$) ($\lambda^2>0$)

Bound solutions, $E<0$

$$\varphi_E(x) = \begin{cases} \sin k_v x, & x<a \\ A\, e^{-\lambda x}, & x>a \end{cases}$$

(continuity of $\varphi_E(x)$) $\longrightarrow$ $\sin k_v a = A e^{-\lambda a}$

(No sudden jump in φ)

$$\varphi_E'(x) = \begin{cases} k_v \cos k_v x, & x<a \\ -\lambda A e^{-\lambda x}, & x>a \end{cases}$$

(smoothness of $\varphi_E(x)$) $\longrightarrow$ $k_v \cos k_v a = -\lambda A e^{-\lambda a}$

(No sudden change of slope of φ)

Solve graphically

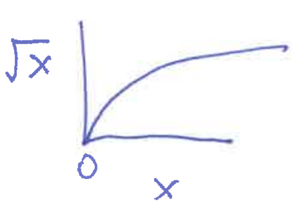
$$k_v a \cot k_v a = -\lambda a$$

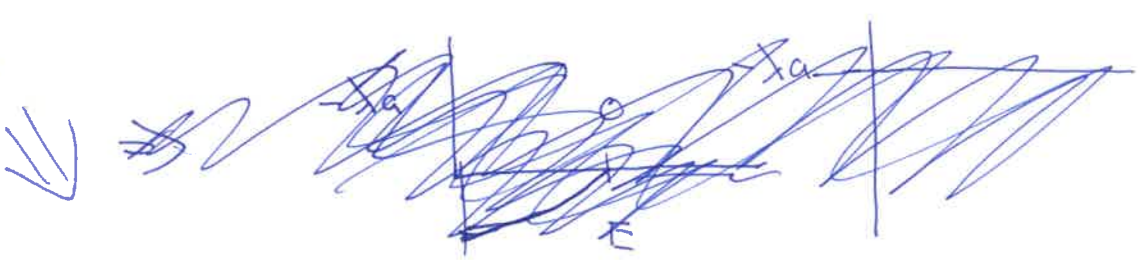
Multiplied both sides by a to make them unitless.

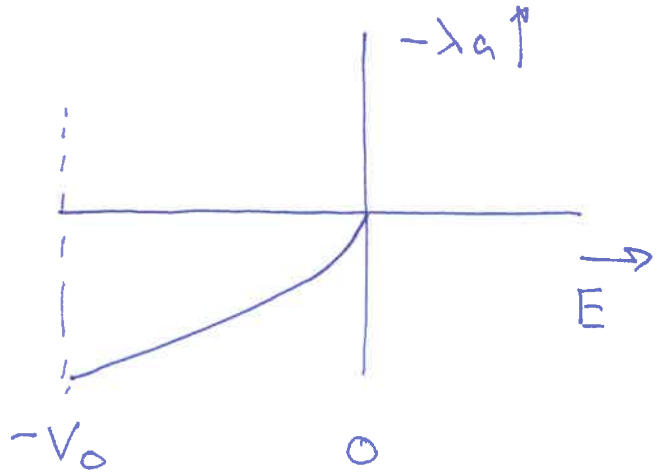
$\rightarrow$ Plot both sides vs E & find intersections

RHS

$$\lambda^2 = \frac{-2mE}{\hbar^2} \rightarrow -\lambda a = -a\sqrt{\frac{-2mE}{\hbar^2}}$$





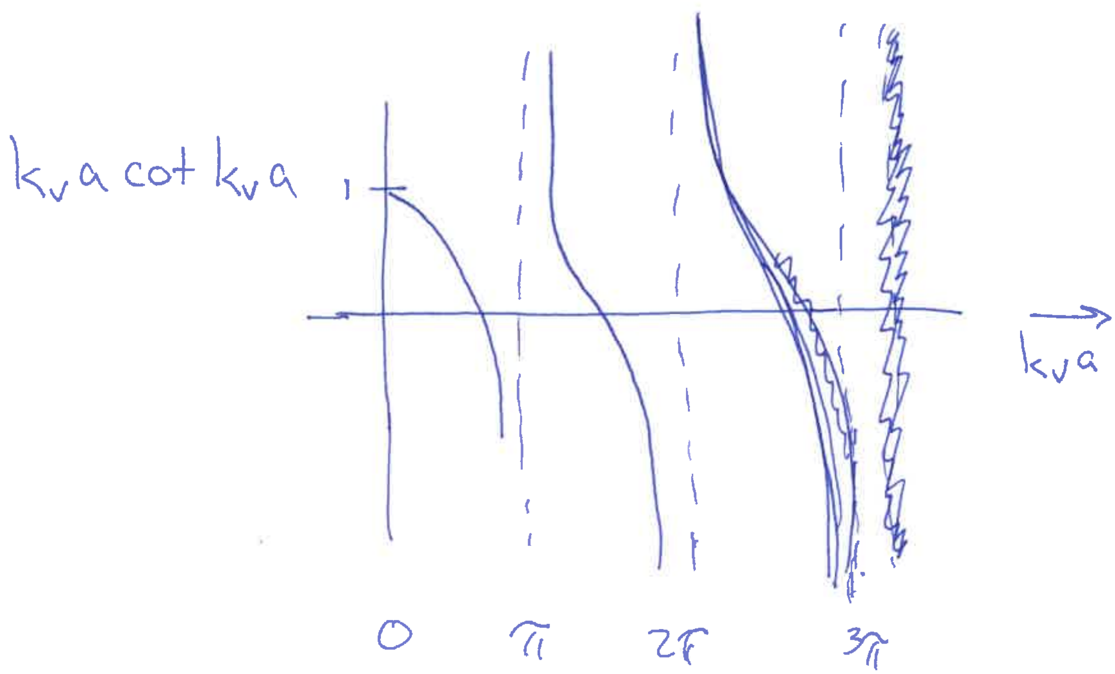


LHS

$$k_v^2 = \frac{2m(E+V_0)}{\hbar^2} \Rightarrow 0 < k_v^2 < \frac{2mV_0}{\hbar^2}$$

$$k_v a \cot k_v a \Big|_{k_v \to 0} = 1 \quad , \quad \text{since} \quad x\frac{\cos x}{\sin x} \to 1 \text{ as } x \to 0$$

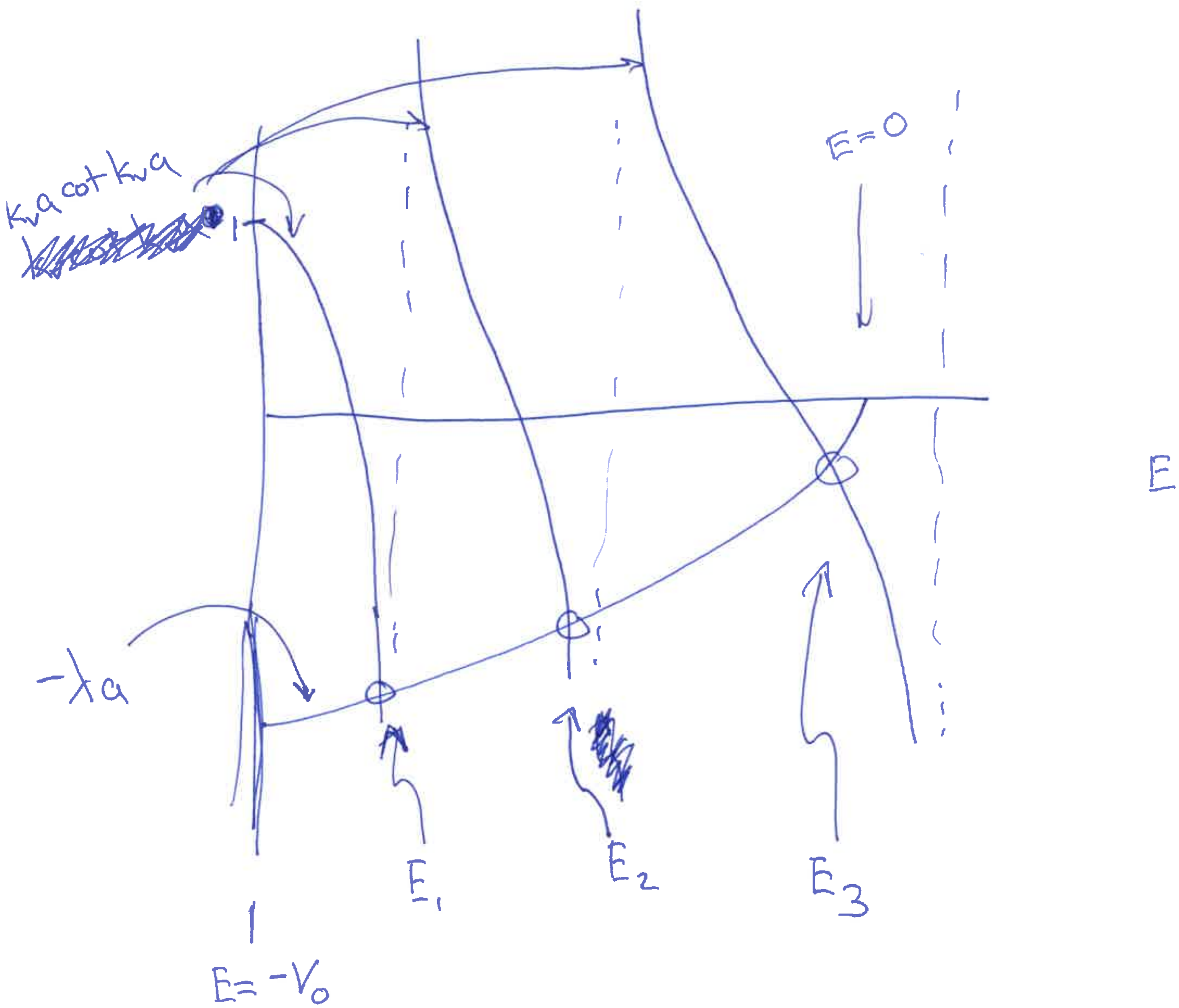
& $\cot k_v a \to \pm\infty$ at $k_v a = \pi, 2\pi, 3\pi$



Now plot vs. E. Notice that $k_v \propto \sqrt{E+V_0}$

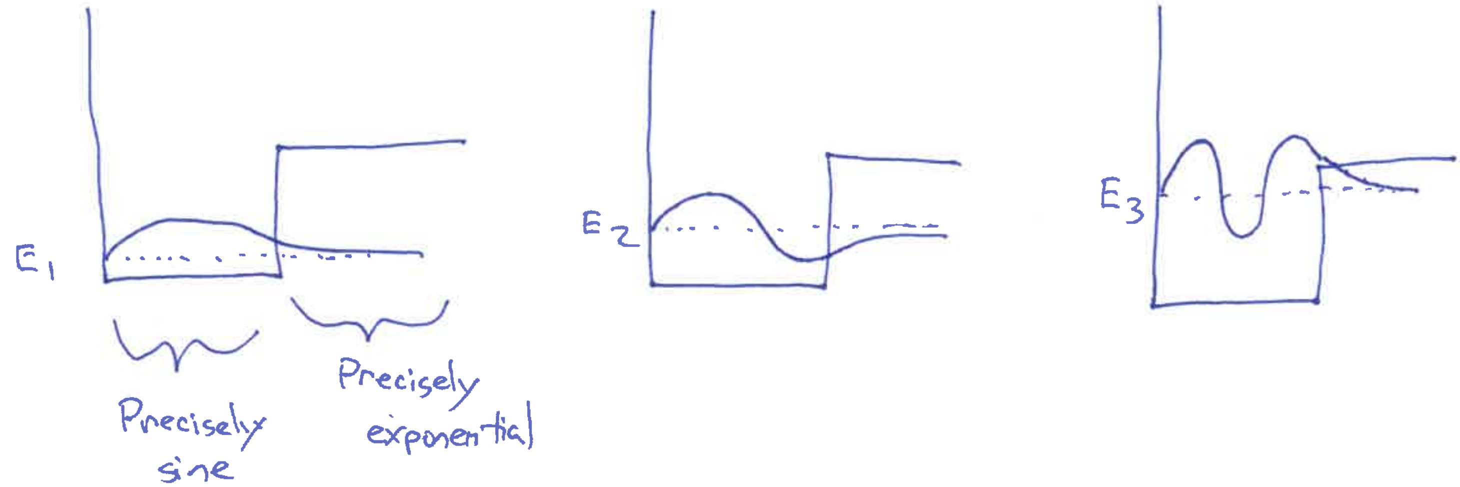
$\Rightarrow$ So as $E \uparrow$, we need to take increasingly larger steps in E to get same change in k_v

$\Rightarrow$ Infinities get further apart

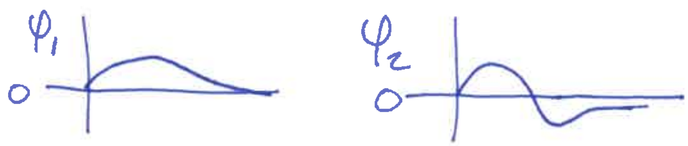


(zero K.E. relative to bottom of well)

At these 3 solutions, we satisfy smoothness & continuity at boundary.



- Don't be confused by axis shifts in above plots



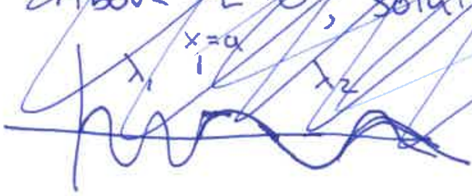
- Note that $E_1 > -V_0$ ⇒ always some K.E.

- The precise number of bound solutions depends on unitless parameter $k_v a = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}\, a$

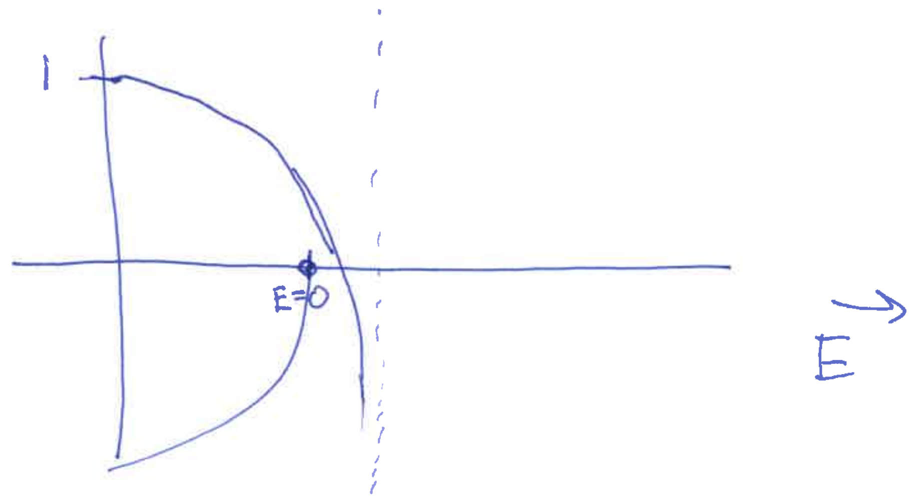
Increasing V_0 changes shape & scaling of plot, but more importantly allows larger E interval

Increasing a packs in more ∞'s per E interval

- ~~Above E=0, solutions are sines & cosines with any k allowed.~~

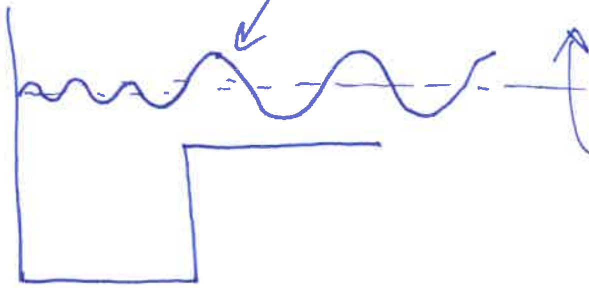


Could have any number of bound solutions, including zero:



Unbound solutions are sines + cosines, w/ different wavelengths

longer amplitude + longer wavelength



momentum smaller outside box

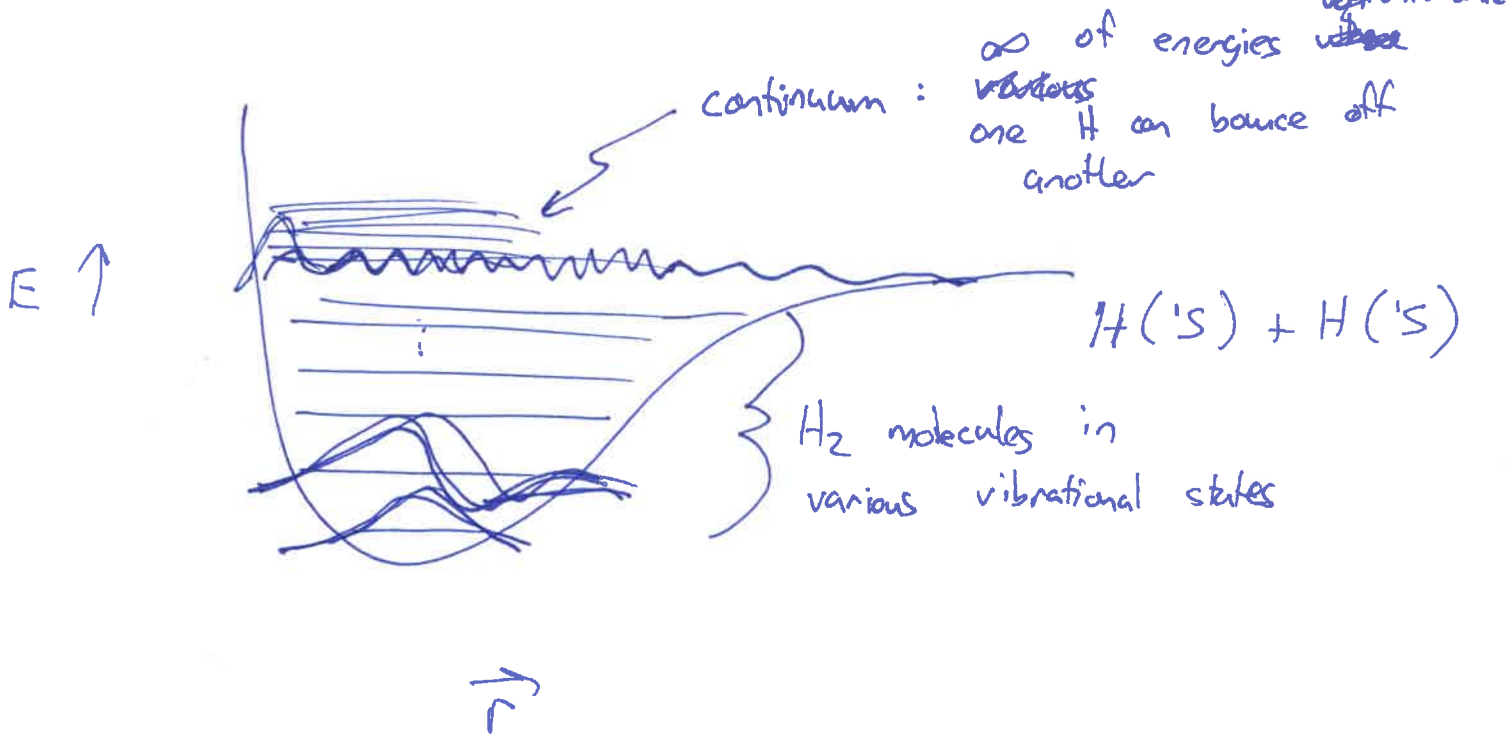
Spends less time per unit length in box, since moving faster there (E same everywhere, + more of E is kinetic in box)

So, we have $E_1, E_2 \ldots E_n$ (n finite) for $E<0$ & Any $E>0$ allowed

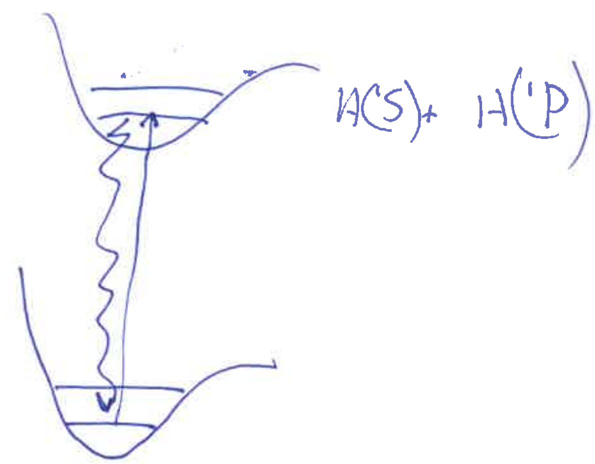
That behavior is typical of potentials which are const as $x \to \infty$.

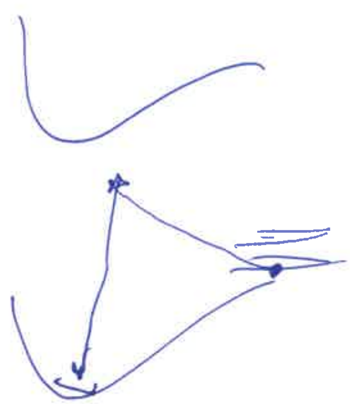
"Discrete" & "Continuous" spectrum

For instance diatomic molecule



Photoassociation





If on other had $V \to \infty$ at $x = \pm\infty$ (e.g. HM)

only solutions are bound solutions