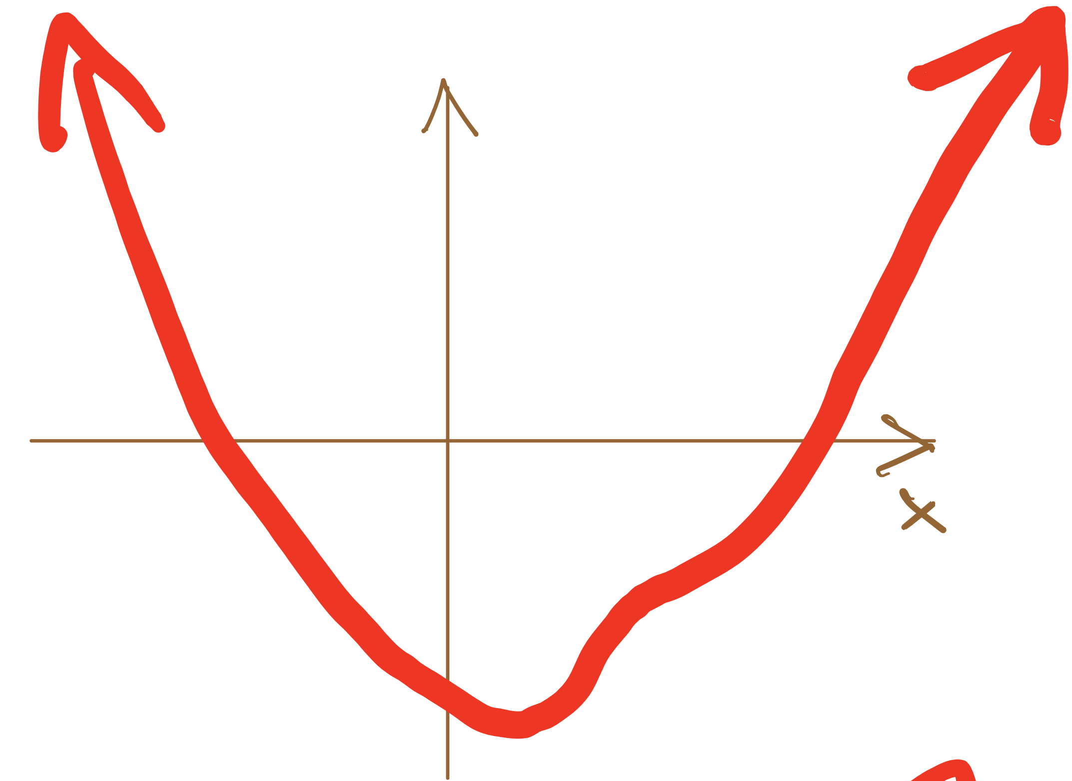
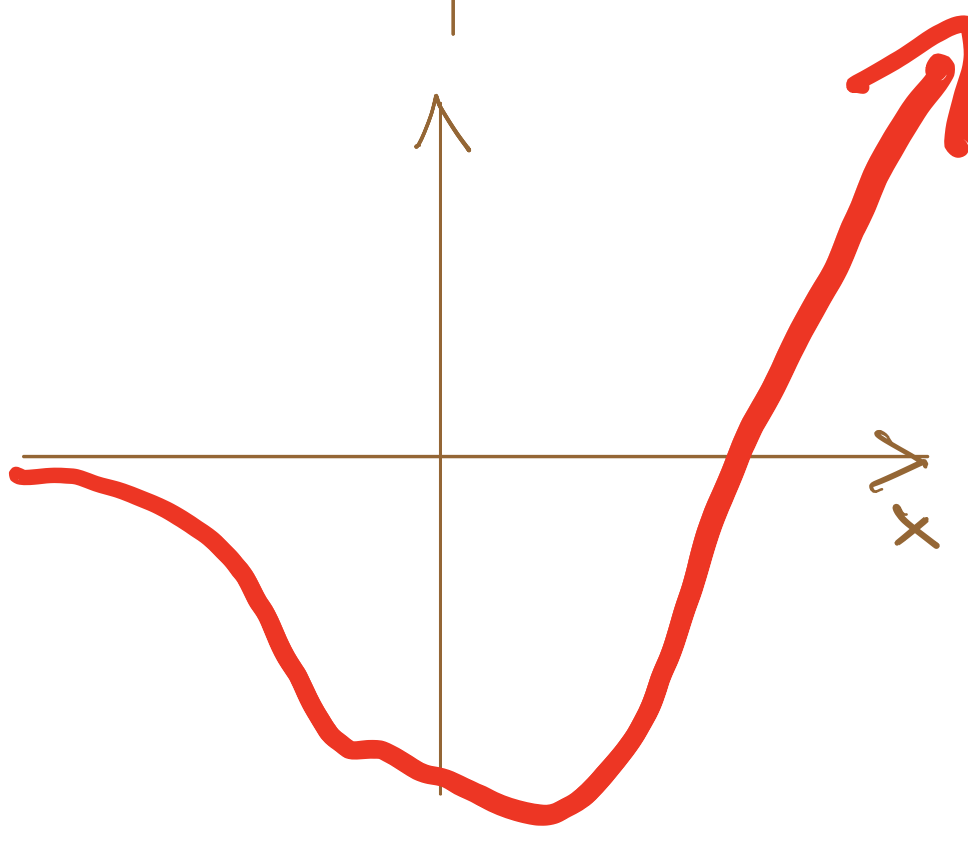
Relationship between V and the nature of solutions of the Schrödinger equation

- bound states have DISCRETE ENERGY LEVELS
- unbound states have CONTINUOUS SPECTRA


x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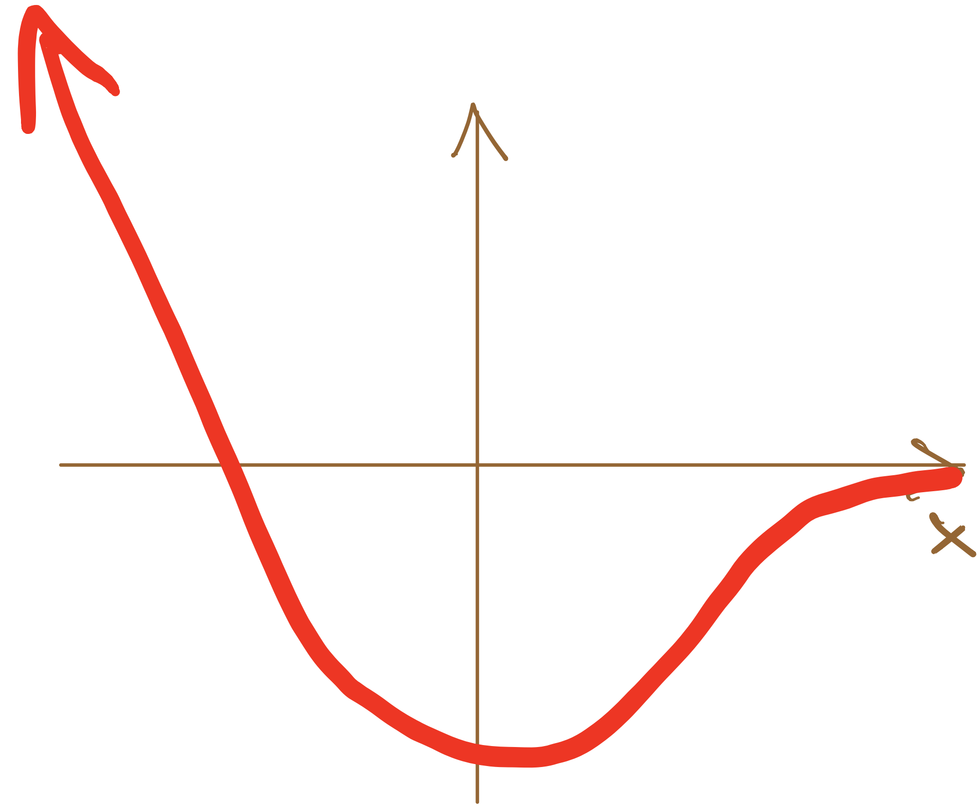
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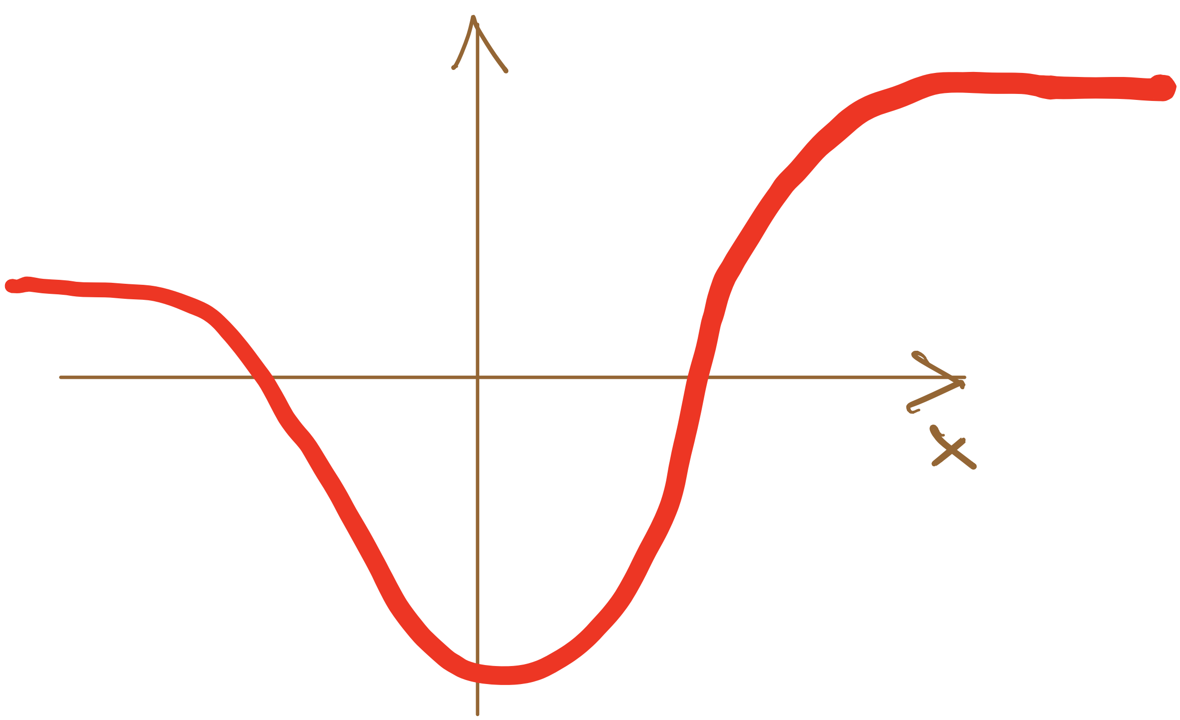
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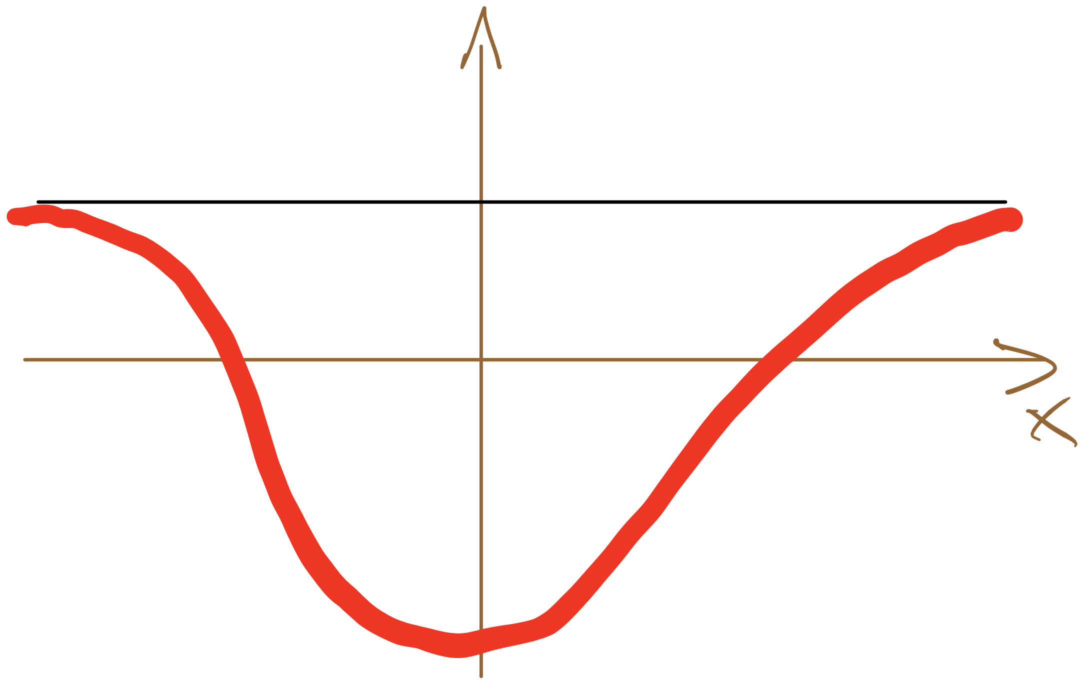
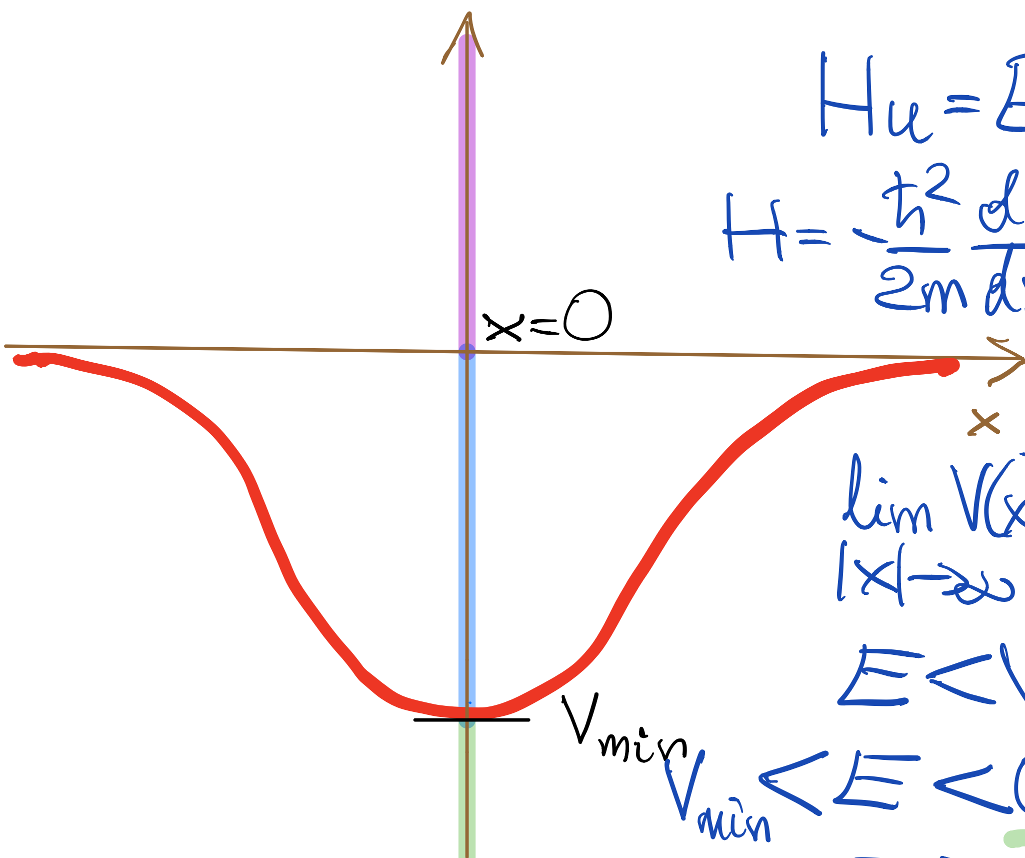



$$Hu = Eu$$

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

$$\lim_{|x|\to\infty} V(x) = 0$$

$$E < V_{min}$$

$$V_{min} < E < 0$$

$$E > 0$$

$$\kappa(x) = \frac{1}{u(x)} \frac{d^2u}{dx^2}$$

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

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

$$\kappa(x) = \frac{1}{u}\frac{d^2u}{dx^2} = \frac{2m}{\hbar^2}\left[V(x) - E\right]$$

$\kappa(x) > 0$

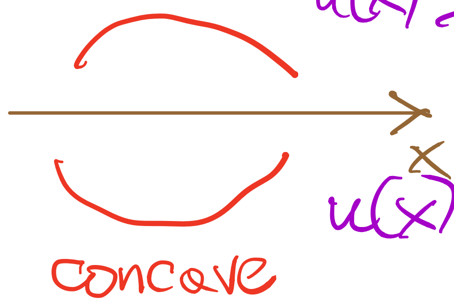

$u(x) > 0, \frac{d^2u}{dx^2} > 0$

$u(x) < 0, \frac{d^2u}{dx^2} < 0$

Convex

$\varkappa(x) < 0$

$u(x) > 0, \ \frac{d^2u}{dx^2} < 0$




$u(x) < 0, \ \frac{d^2u}{dx^2} > 0$

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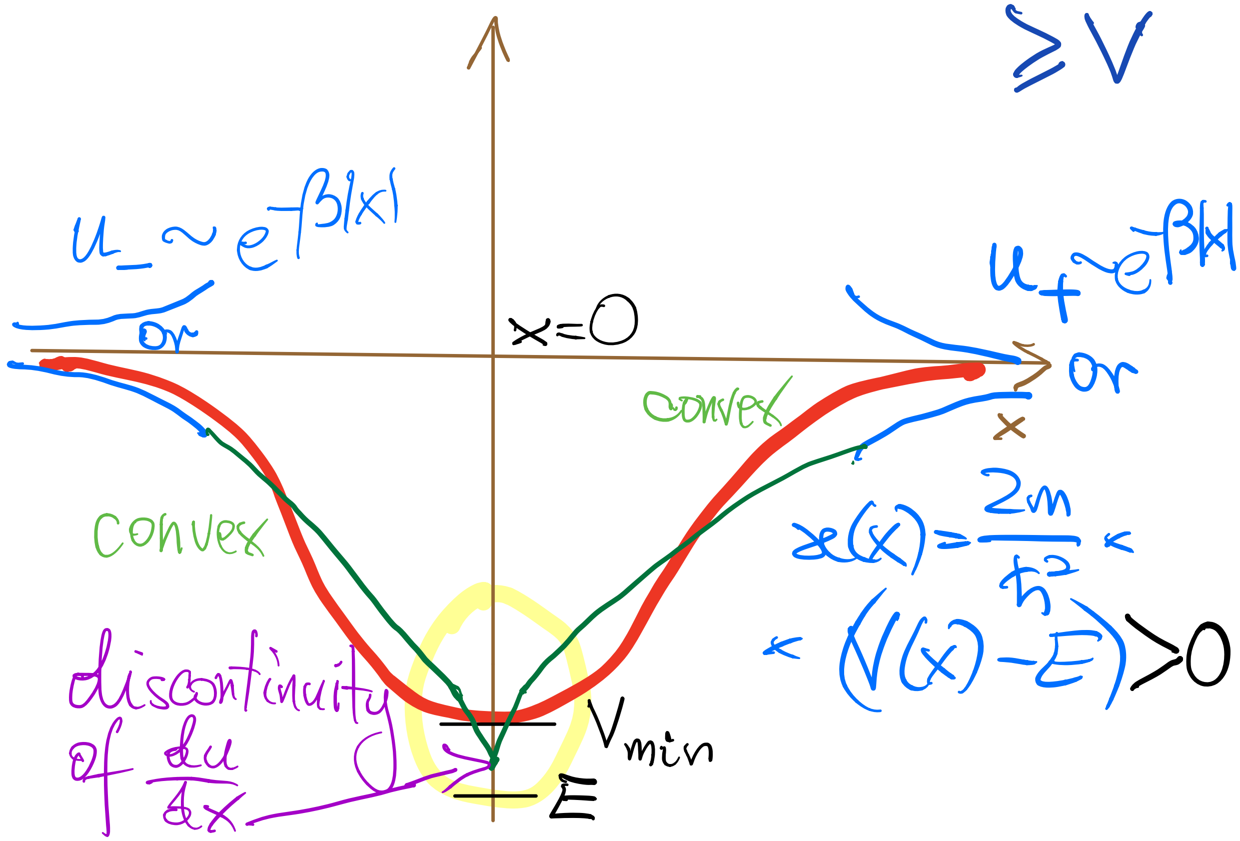
- $E < V_{min}$

In CM,
$E = T + V \geq V$




$\varkappa(x) = \frac{2m}{\hbar^2} (V(x) - E) > 0$

$$|x| \to \infty ; \quad -\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} = Eu, \quad E<0$$

$$u(x) = Ae^{-\beta x} + Be^{\beta x}$$

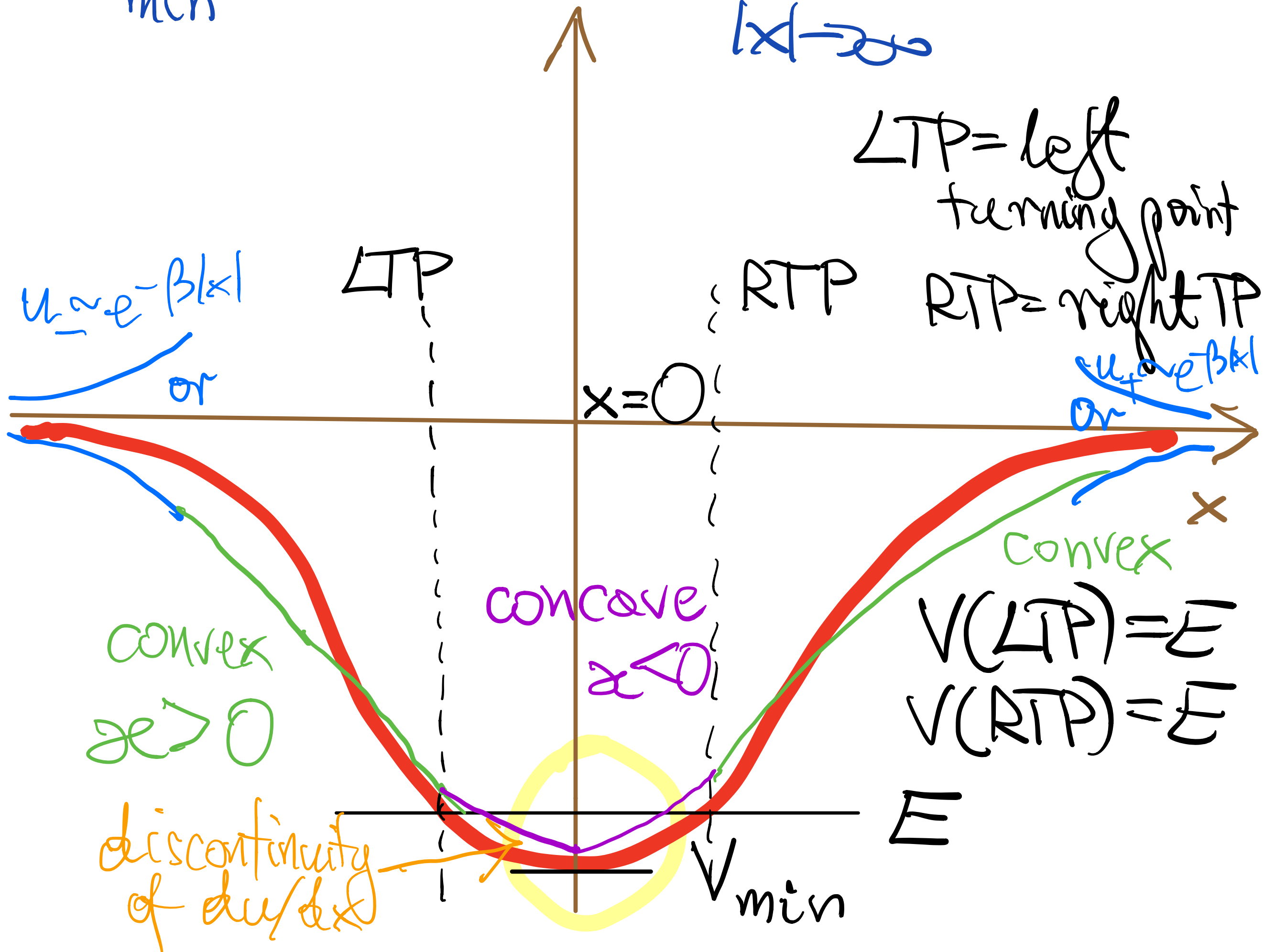
$$\beta = \sqrt{\frac{-2mE}{\hbar^2}}$$

$$\left.\begin{array}{l} x \gg 0, \ B = 0 \\ x \ll 0, \ A = 0 \end{array}\right\} \sim e^{-\beta|x|}$$

NO SOLUTIONS EXIST WITH $E < V_{min}$

(similarly to CM)

- $V_{min} < E < 0 = \lim_{|x|\to\infty} V(x)$




For $x < LTP$ and $x > RTP$

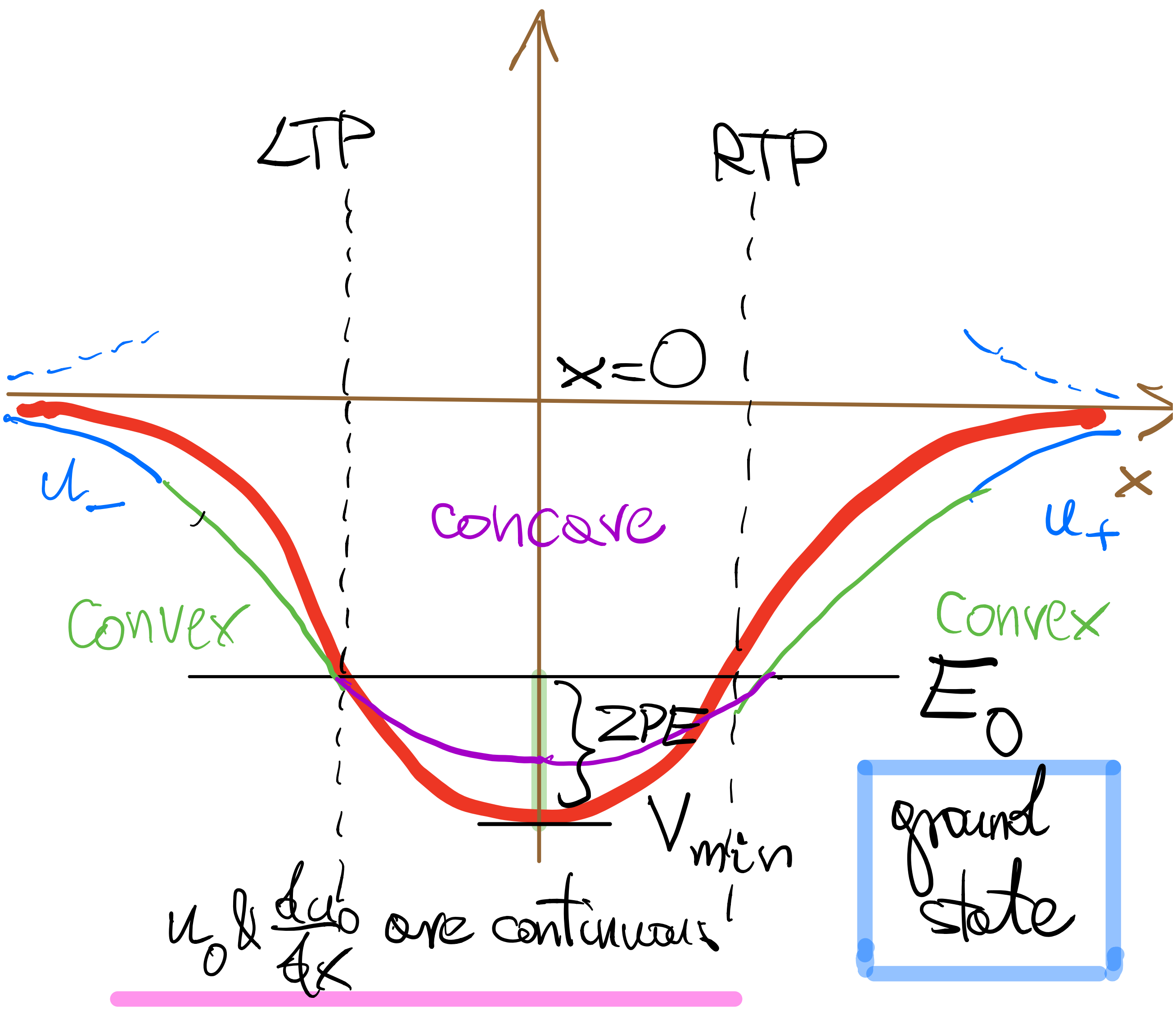
$$\varkappa(x) = \frac{2m}{\hbar^2}[V(x) - E] > 0$$

convex

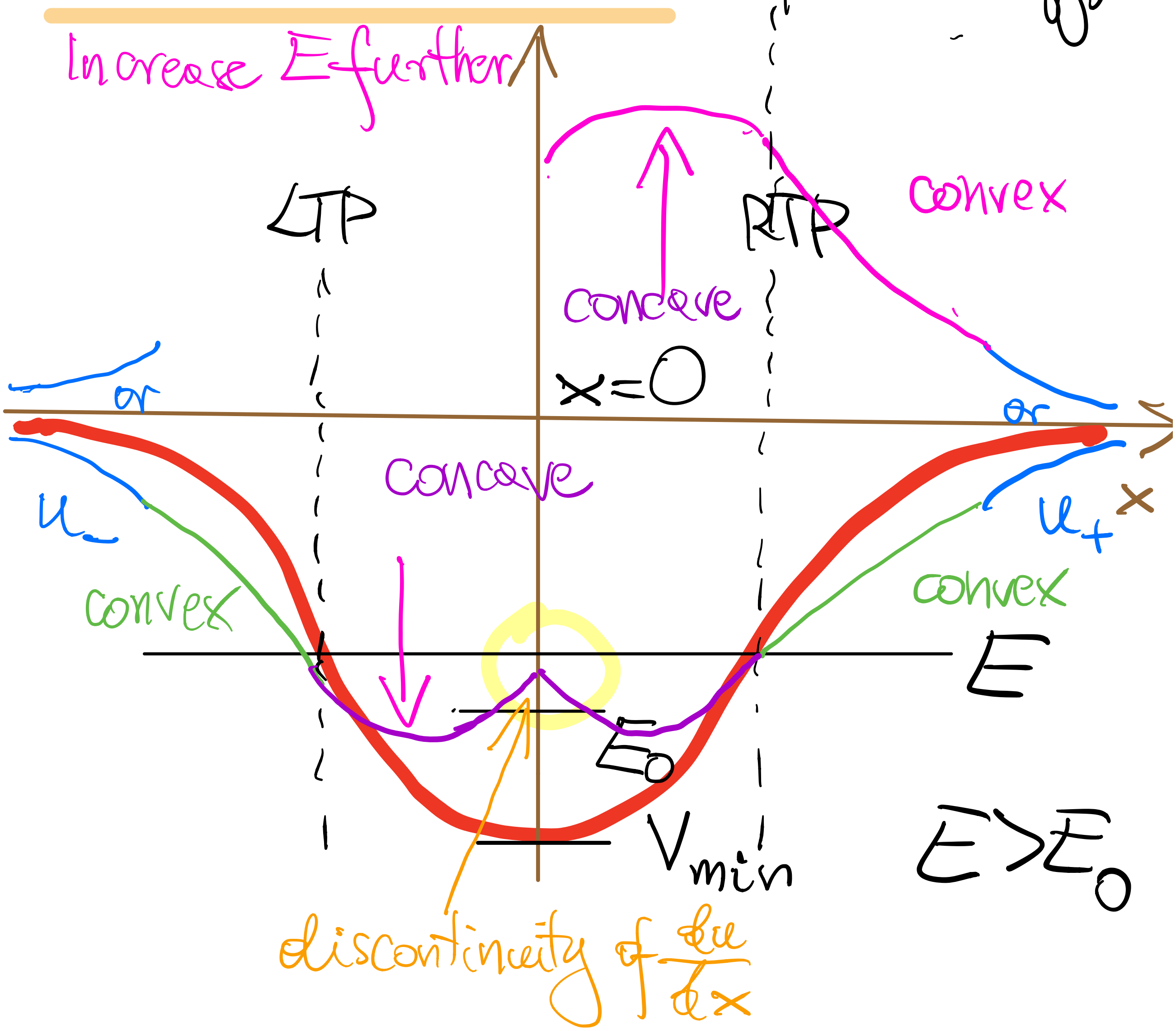
$x \in (LTP, RTP)$

$\varkappa(x) < 0$ concave

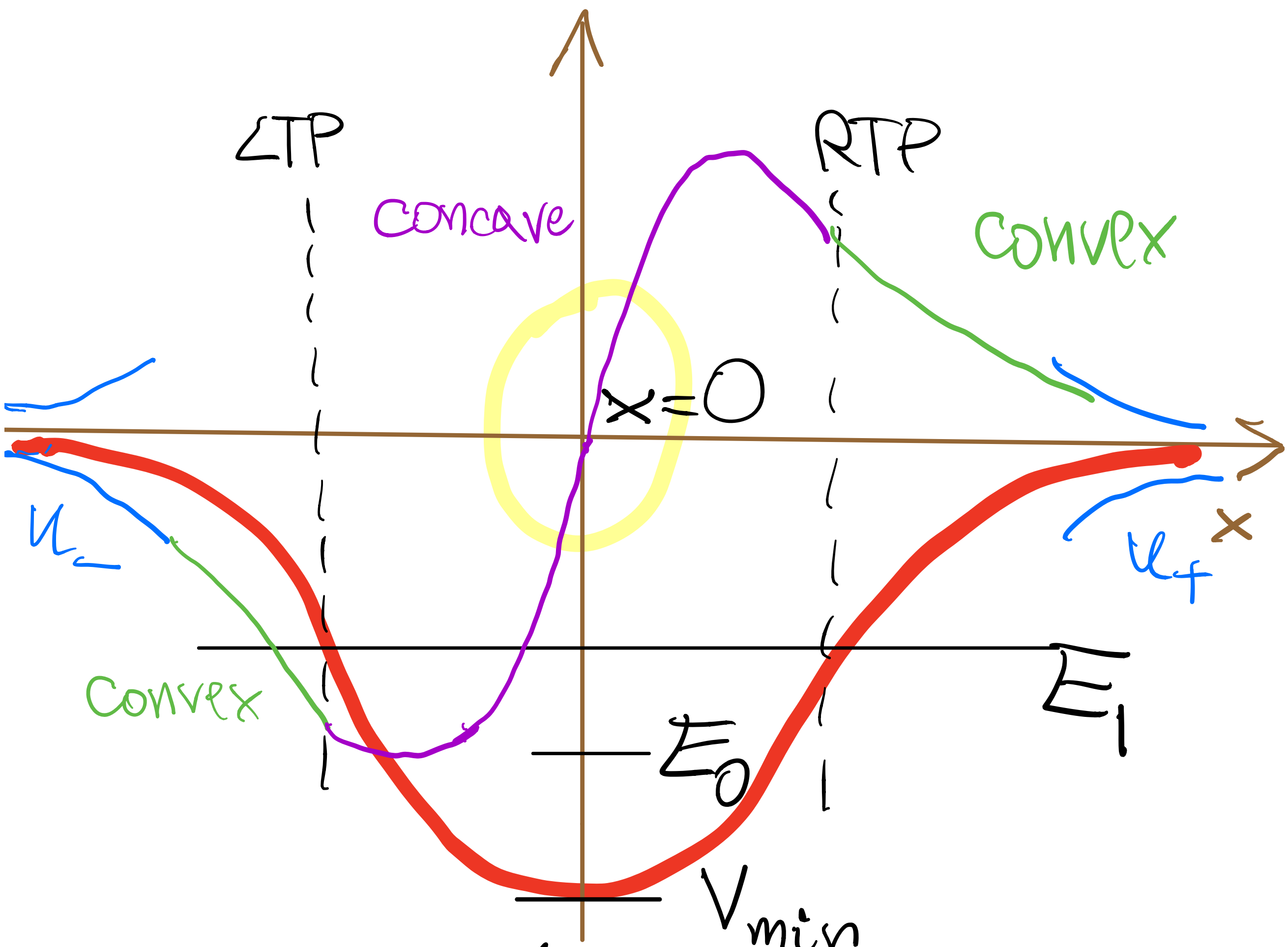
Let us increase $E$ to widen the (LTP, RTP) region.



$Hu_0 = E_0 u_0$, $u_0$ has no nodes, most of $u_0$ is localized between turning points, $E_0 > V_{min}$ (zero-point energy) ZPE



Increase $E$ even more

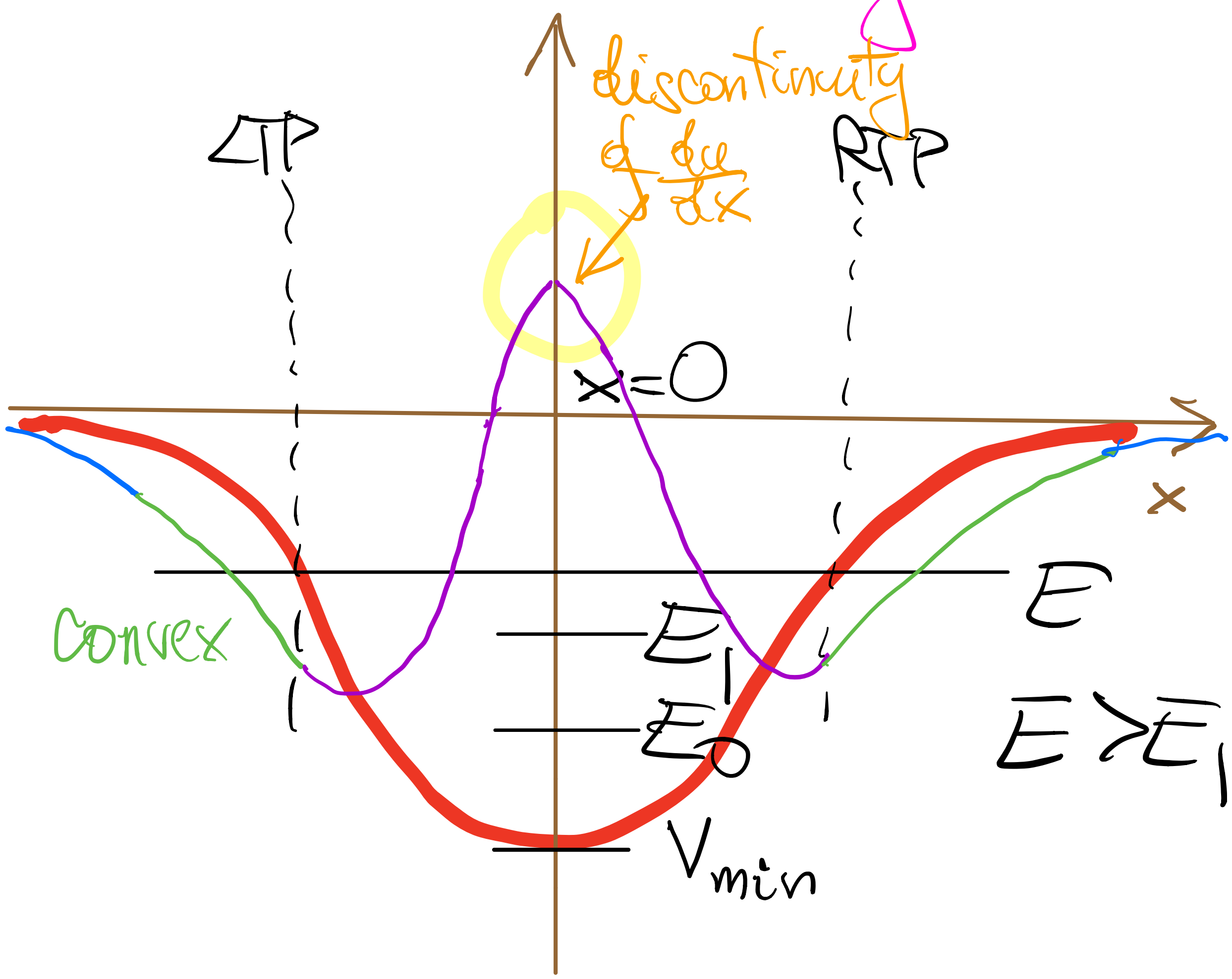


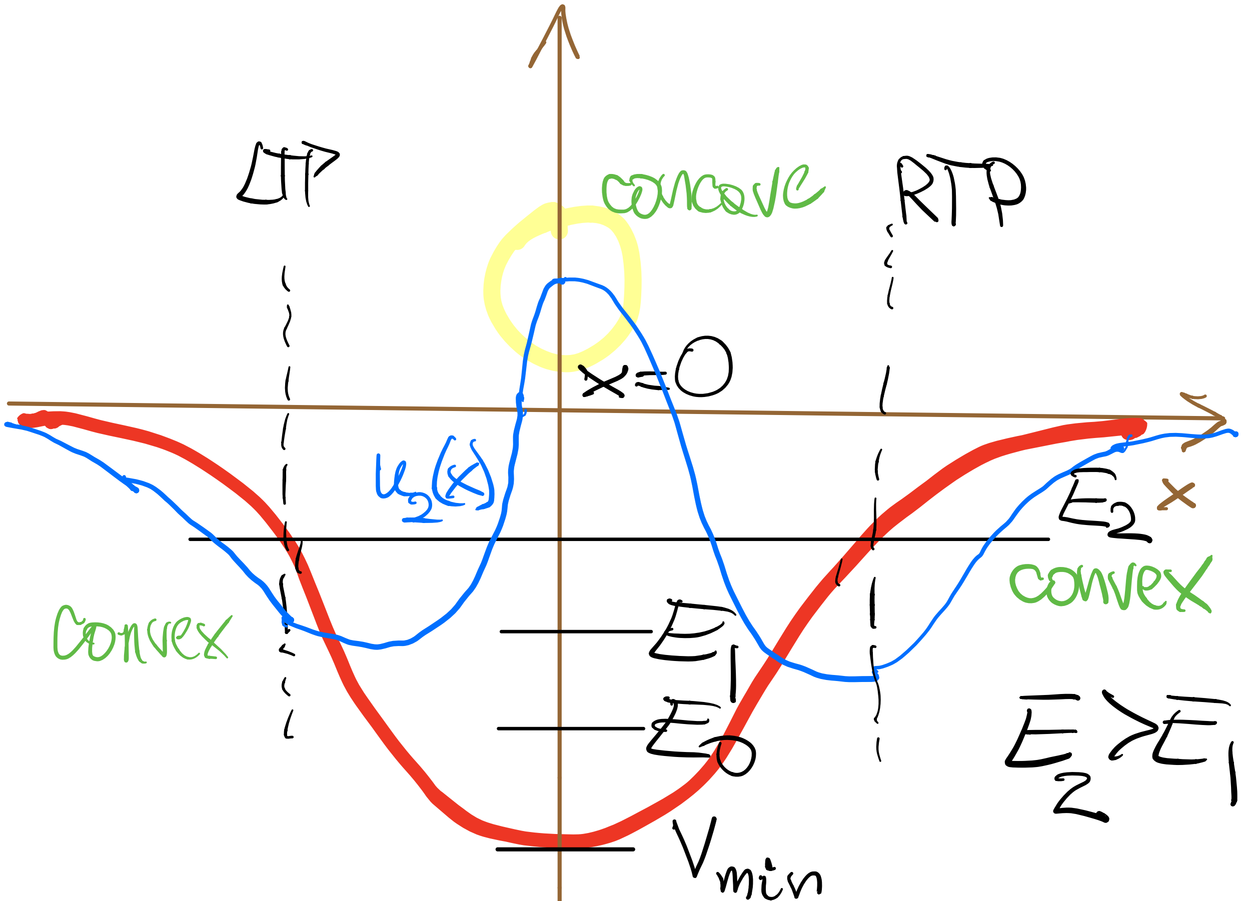

$u_1, \frac{du_1}{dx}$ are continuous

$0 > E_1 > E_0 > V_{min}$

$u_1$ has one node

Continue increasing $E$






$u_2$, $\frac{du_2}{dx}$ are continuous

$$V_{min} < E_0 < E_1 < E_2 < \dots < 0$$

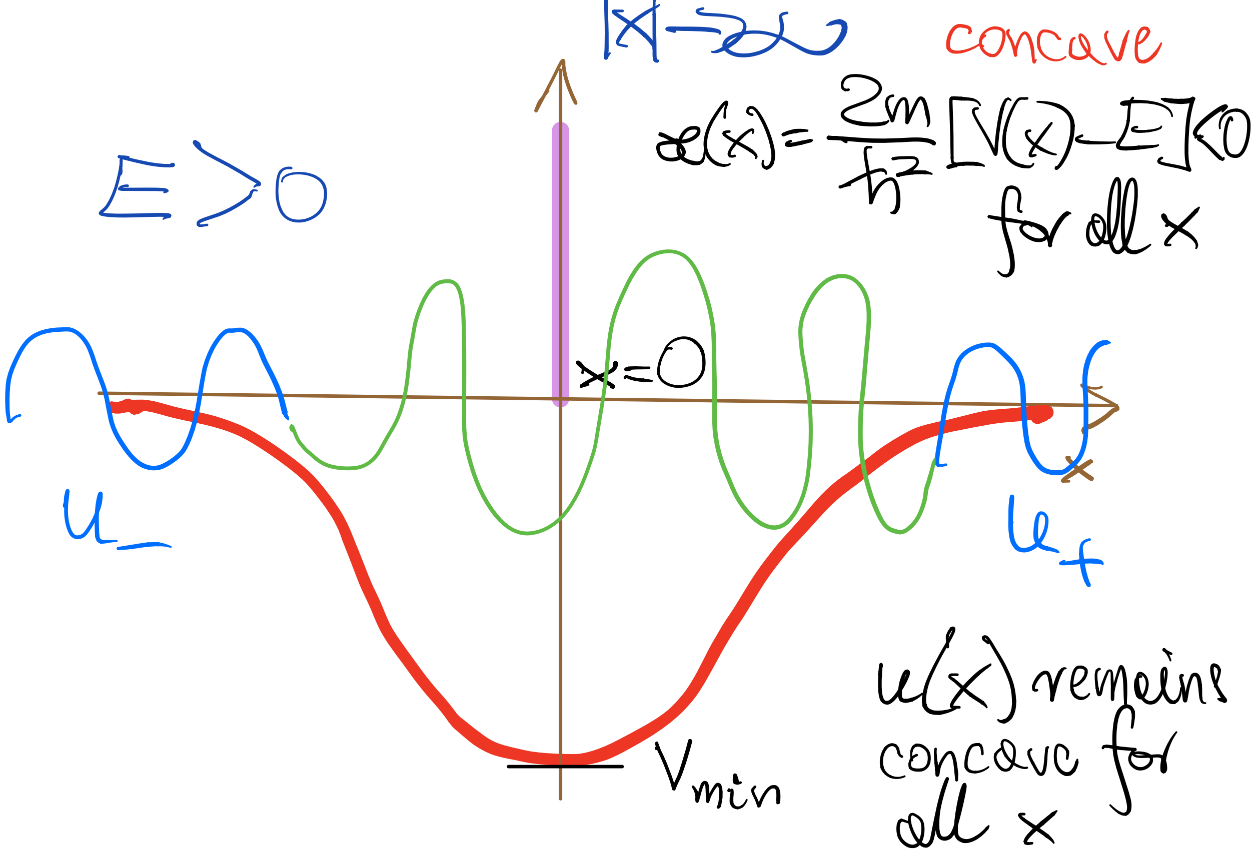
$$Hu_n = E_n u_n \checkmark$$

$u_n(x)$ has $n$ nodes

Each $u_n(x)$ is localized between turning points

# BOUND STATES

- $E > 0 = \lim_{|x| \to \infty} V(x)$



Asymptotically $\boxed{E > 0}$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} = Eu$$

$$u_\pm(x) = A_\pm \sin\alpha x + B_\pm \cos\alpha x$$

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}}$$

$$= \sqrt{A_\pm^2 + B_\pm^2}\left(\frac{A_\pm}{\sqrt{A_\pm^2+B_\pm^2}}\sin\alpha x + \frac{B_\pm}{\sqrt{A_\pm^2+B_\pm^2}}\cos\alpha x\right)$$

$$\frac{A_\pm}{\sqrt{A_\pm^2+B_\pm^2}} = \cos\gamma_\pm \qquad \frac{B_\pm}{\sqrt{A_\pm^2+B_\pm^2}} = \sin\gamma_\pm$$

$$u_\pm(x) = C_\pm \sin(ax + \varphi_\pm)$$

phase shift controlled by

$$C_\pm = \sqrt{A_\pm^2 + B_\pm^2}$$

$$\tan\varphi_\pm = \frac{\sin\varphi_\pm}{\cos\varphi_\pm} = \frac{B_\pm}{A_\pm}$$

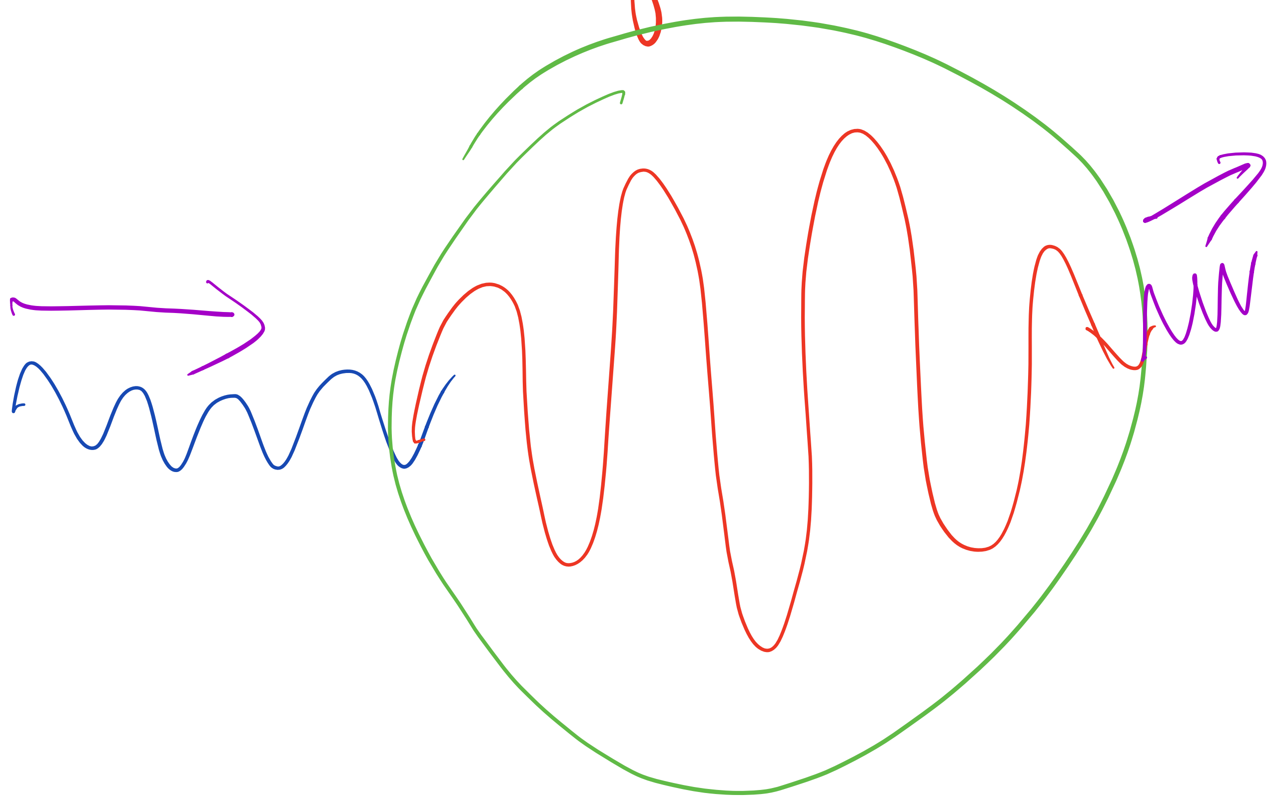
For $E > 0$, we can find smooth solutions for ANY value of $E$.

$$Hu = Eu$$

set $E$, solve for $u$

continuous spectrum

functions u corresponding to
continuous spectra
describe SCATTERING
STATES; they are
no longer localized



# GENERAL CASE

- If $V \to \infty$ as $|x_j| \to \infty$, $j=1,\dots,3N$, there is an infinite set of discrete energy levels,

bound stat

$$V_{min} < E_0 < E_1 < E_2 < \dots$$

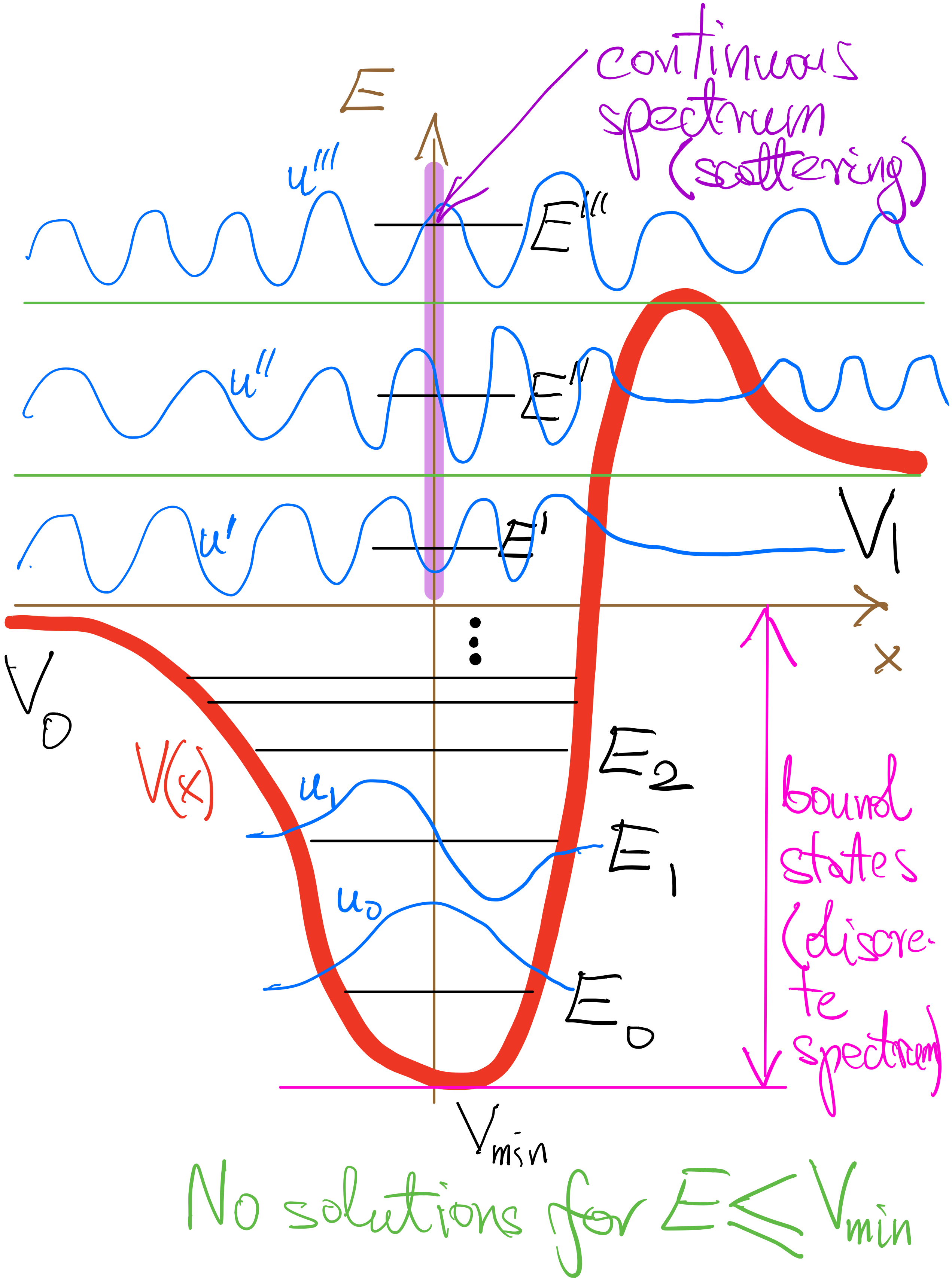
$u_n$ has $n$ nodes
(no scattering states)

- If $V$ is bounded as some (or all) $|x_j| \to \infty$, there is an infinite or finite number of

discrete energy levels.
Let us designate the asymptotes of $V$ as

$$V_0(\infty) < V_1(\infty) < V_2(\infty) < \ldots.$$

In this case, we obtain discrete energy levels for $V_{min} < E < V_0(\infty)$ and continuous spectrum for $E > V_0(\infty)$.

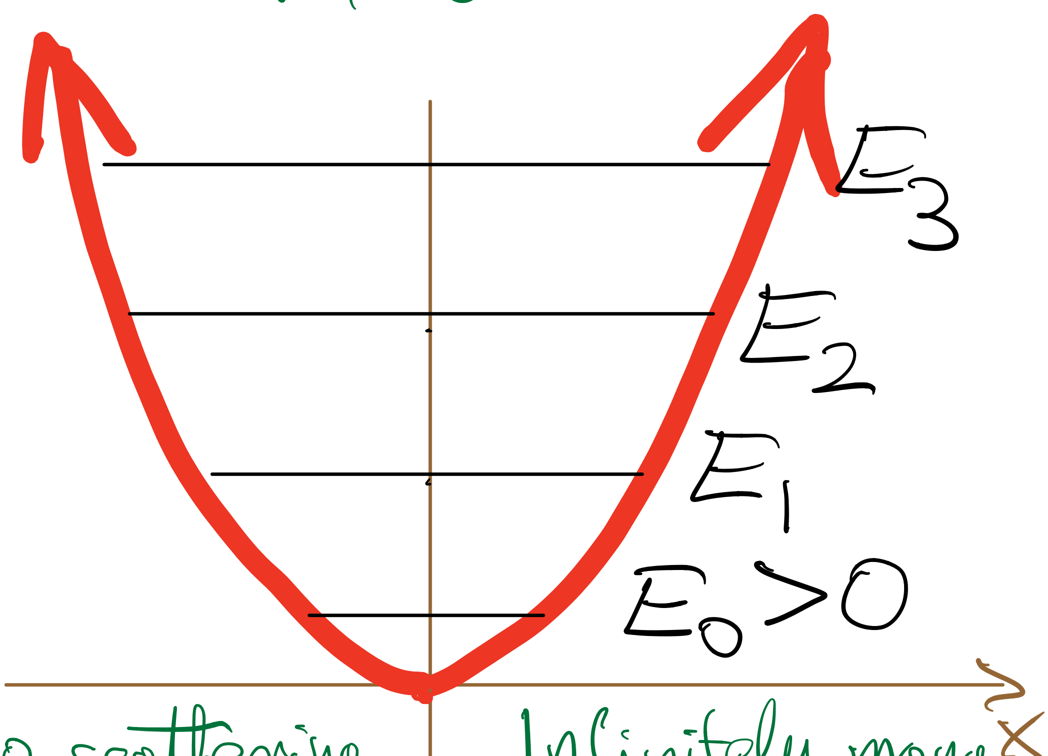

E
continuous spectrum (scattering)
u'''
E'''
u''
E''
u'
E'
V1
x
V0
V(x)
E2
u1
E1
u0
E0
bound states (discrete spectrum)
Vmin
No solutions for E ≤ Vmin

Examples:

1. $V(x) = \frac{1}{2}kx^2$

(harmonic oscillator)

$\lim_{|x|\to\infty} V(x) = \infty$, $V_{min} = 0$



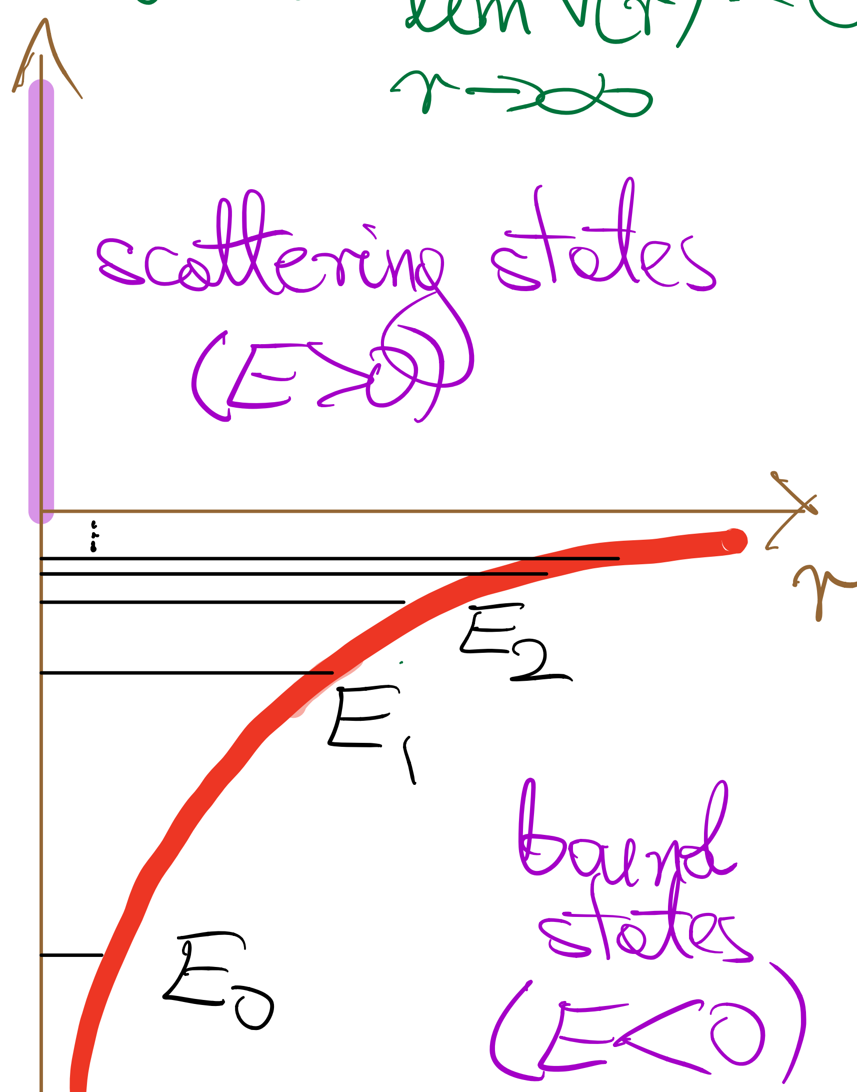

No scattering states, bound states only

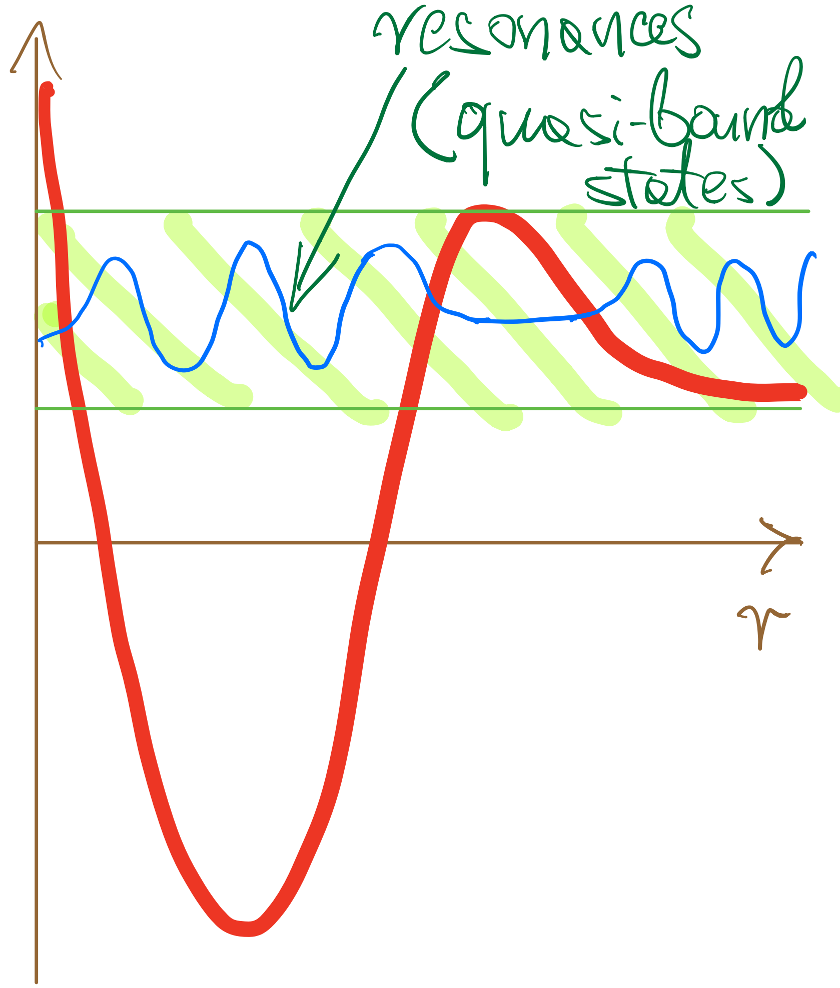
Infinitely many discrete levels, $0 < E_0 < E_1 < \ldots$

2. $V(r) = -\dfrac{Ze^2}{r}$

(hydrogenic atom)

$\lim_{r\to\infty} V(r) = 0$




resonances
(quasi-bound
states)
r