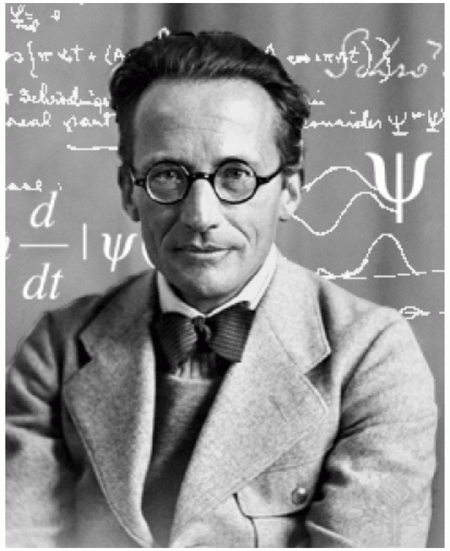
Schrödinger Equation in Position Space



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

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + V(\hat{x})$$

$$\langle x|\hat{p}_x|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle \Longrightarrow \langle x|\hat{p}_x^2|\psi\rangle = \frac{\hbar^2}{i^2}\frac{\partial^2}{\partial x^2}\langle x|\psi\rangle$$

$$\langle x|\frac{\hat{p}_x^2}{2m}|\psi\rangle = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\langle x|\psi\rangle$$

$$\langle x|V(\hat{x})|\psi\rangle = \langle x|V(x)|\psi\rangle = V(x)\langle x|\psi\rangle$$

$$\langle x|V(\hat{x}) = \langle x|\left(V(0)+V'(0)\hat{x}+\frac{1}{2!}V''(0)\hat{x}^2+\dots\right) = \langle x|\left(V(0)+V'(0)x+\frac{1}{2!}V''(0)x^2+\dots\right) = \langle x|V(x)$$

$$\langle x|\hat{x} = \langle x|x$$

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

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

$$\langle x|\psi(t)\rangle = \psi(x,t)$$

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

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

Time-dependent Schrödinger equation in position space

Consider $\hat{H}$ eigenstate: $|\Psi\rangle = |E\rangle$

$$|\Psi(t)\rangle = e^{-\frac{i\hat{H}t}{\hbar}}|E\rangle = e^{-\frac{iEt}{\hbar}}|E\rangle$$

$$\Psi_E(x,t) = \langle x|\Psi(t)\rangle = e^{-\frac{iEt}{\hbar}}\langle x|E\rangle$$

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

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\langle x|E\rangle \cancel{e^{-\frac{iEt}{\hbar}}} = \cancel{i\hbar}\cdot\left(\frac{-\cancel{i}E}{\cancel{\hbar}}\right)\cancel{e^{-\frac{iEt}{\hbar}}}\langle x|E\rangle$$

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\underbrace{\langle x|E\rangle}_{\Psi(x} = E\underbrace{\langle x|E\rangle}_{\Psi(x)}$$

$$\langle x|\hat{H}|E\rangle = E\langle x|E\rangle$$

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x) = E\Psi(x)$$

Time — dependent Schrödinger Eq. in position space

For any time-dependent wave function $\psi(x,t)=\langle x|\psi(t)\rangle$

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

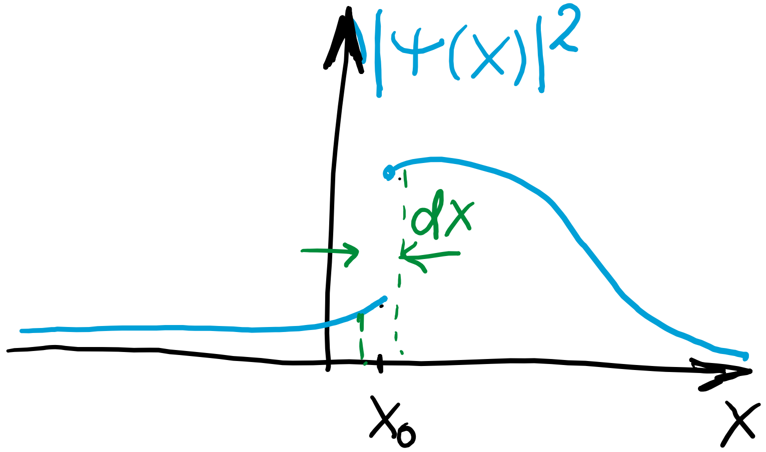
Time- independent Schrödinger Eq. in position space

For eigenstate of $\hat{H}$: $\psi_E(x,t)=e^{\frac{-iEt}{\hbar}}\langle x|\psi\rangle=e^{\frac{-iEt}{\hbar}}\psi(x)$

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

Properties of Solutions of time-independent Schrödinger Eq.

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



1) $P(x) = |\psi(x_0)|^2 \cdot dx$ ← Prob. to find in dx-vicinity of X_0

If $\psi(x)$ is discontinuous at X_0 $\Rightarrow$ $P(X_0)$ is not defined

$\psi(x)$ is continuous

VERY IMPORTANT

$\Rightarrow$ 2-nd derivative of discontinuous function in Schrödinger Eq.!

---

2) $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi \Rightarrow \frac{d^2\psi}{dx^2}=\frac{2m}{\hbar^2}\left[V(x)-E\right]\psi$$

$$\int_{x_0-\varepsilon}^{x_0+\varepsilon} \frac{d^2\psi}{dx^2}\,dx = \int_{x_0-\varepsilon}^{x_0+\varepsilon} \frac{2m}{\hbar^2}\left[V(x)-E\right]\psi\,dx$$

$$\lim_{\varepsilon\to 0} \left(\frac{d\psi}{dx}\right)_{x_0+\varepsilon} - \left(\frac{d\psi}{dx}\right)_{x_0-\varepsilon} = \frac{2m}{\hbar^2}\int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x)\psi\,dx - \underbrace{\frac{2mE}{\hbar^2}\int_{x_0-\varepsilon}^{x_0+\varepsilon}\psi\,dx}_{0}$$

$$\left(\frac{d\psi}{dx}\right)_{x_0^+} - \left(\frac{d\psi}{dx}\right)_{x_0^-} = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon} V(x)\psi\,dx$$

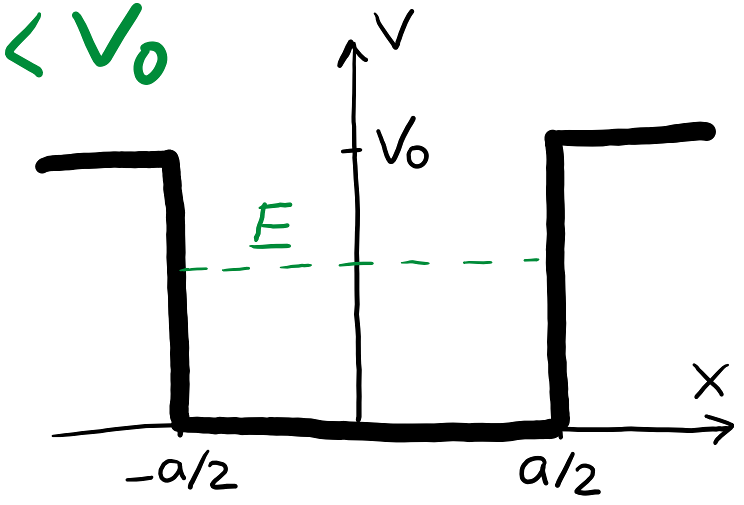
VERY IMPORTANT

If $V(x)$ is finite at x_0 $\Rightarrow$ $\left(\frac{d\psi}{dx}\right)_{x_0^+} = \left(\frac{d\psi}{dx}\right)_{x_0^-}$ $\Leftrightarrow$ $\frac{d\psi}{dx}$ is continuous at x_0

Example

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

$0 < E < V_0$



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

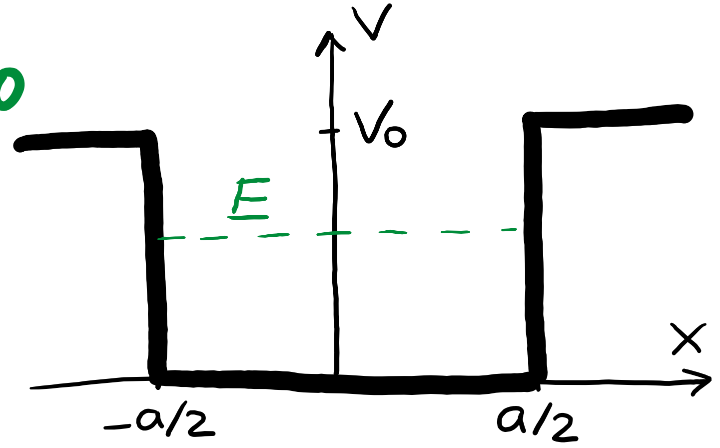
1) $-a/2 < x < a/2$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \Rightarrow \frac{d^2\psi}{dx^2} = -\underbrace{\frac{2mE}{\hbar^2}}_{K^2}\psi \Rightarrow \frac{d^2\psi}{dx^2} = -K^2\psi$$

$$\psi(x) = A\sin Kx + B\cos Kx \quad \text{or} \quad \psi(x) = A' e^{iKx} + B' e^{-iKx}$$

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

$0<E<V_0$



2) $x<-a/2$ or $x>a/2$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V_0\psi=E\psi \Rightarrow \frac{d^2\psi}{dx^2}=\underbrace{\frac{2m}{\hbar^2}(V_0-E)}_{\Rightarrow q^2}\psi \Rightarrow \frac{d^2\psi}{dx^2}=q^2\psi$$

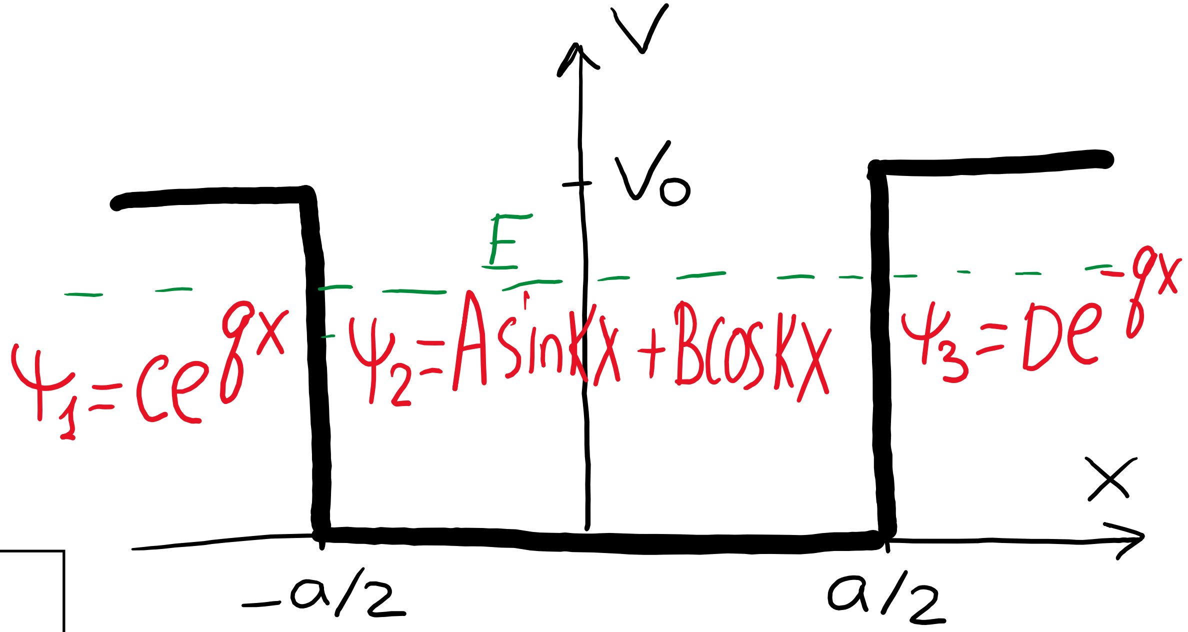
$$\psi(x)=Ce^{qx}+De^{-qx}$$

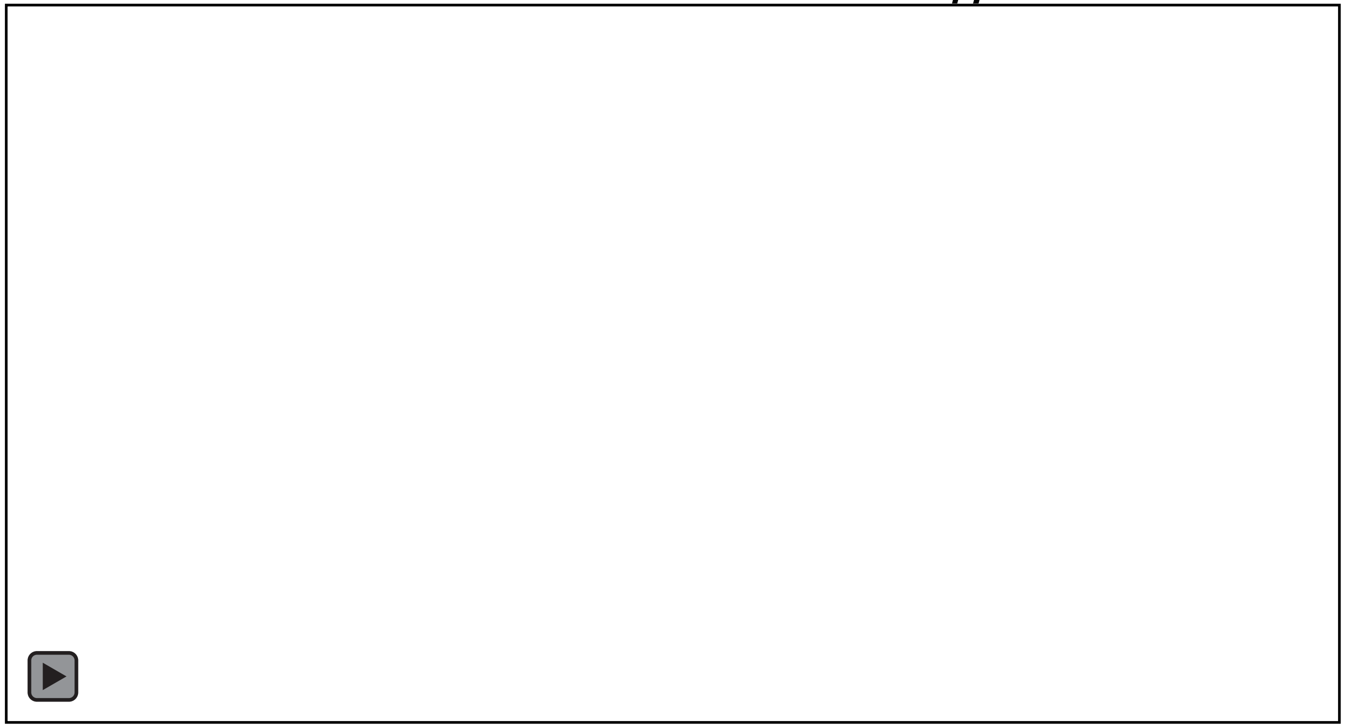
FOR $x<-a/2$: $D=0 \Rightarrow \psi(x)=Ce^{qx}$

FOR $x>a/2$: $C=0 \Rightarrow \psi(x)=De^{-qx}$

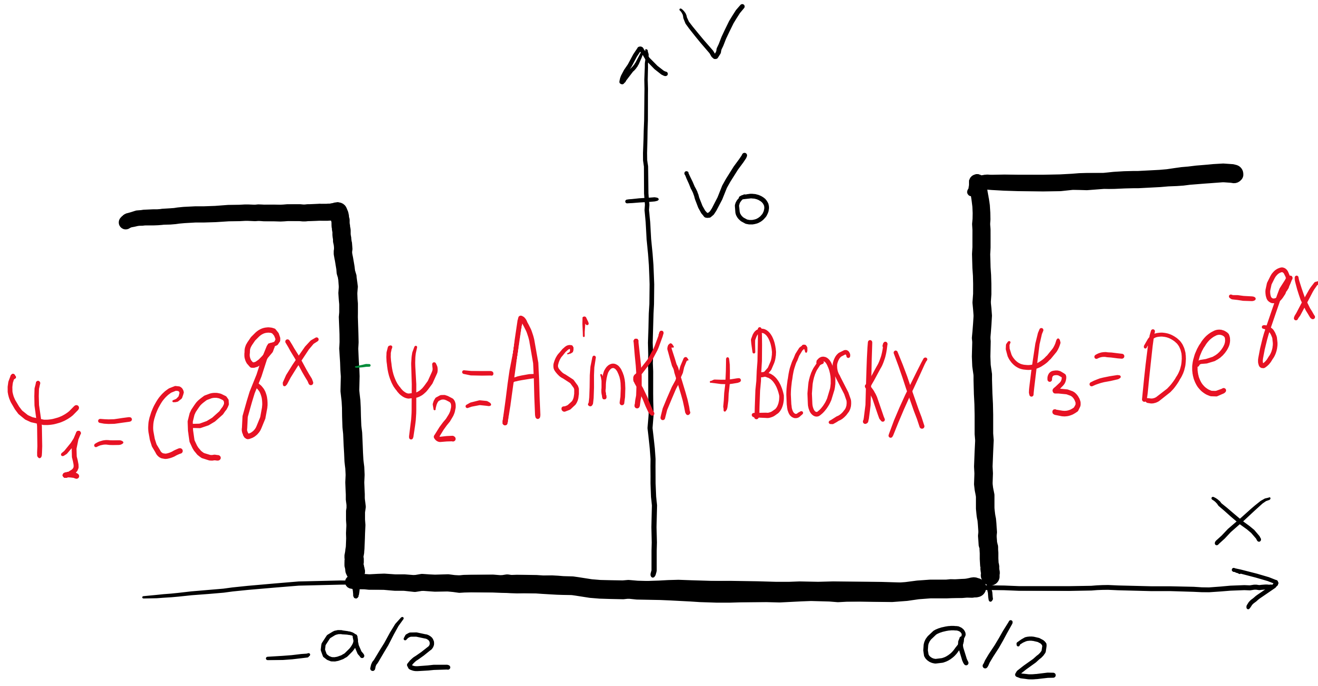
$$P(x>a/2) = \int_{a/2}^{\infty} |\psi(x)|^2 \, dx =$$

$$= |D|^2 \int_{a/2}^{\infty} e^{-2qx} \, dx = |D|^2 \left. \frac{e^{-2qx}}{-2q} \right|_{a/2}^{\infty} = |D|^2 \frac{e^{-qa}}{2q} > 0$$





Match at Boundaries



1) $x = -a/2$

a) Continuity:

$$\psi_1\left(-\frac{a}{2}\right) = \psi_2\left(-\frac{a}{2}\right)$$

$$Ce^{-\frac{qa}{2}} = A\sin\left(-\frac{ka}{2}\right) + B\cos\left(-\frac{ka}{2}\right)$$

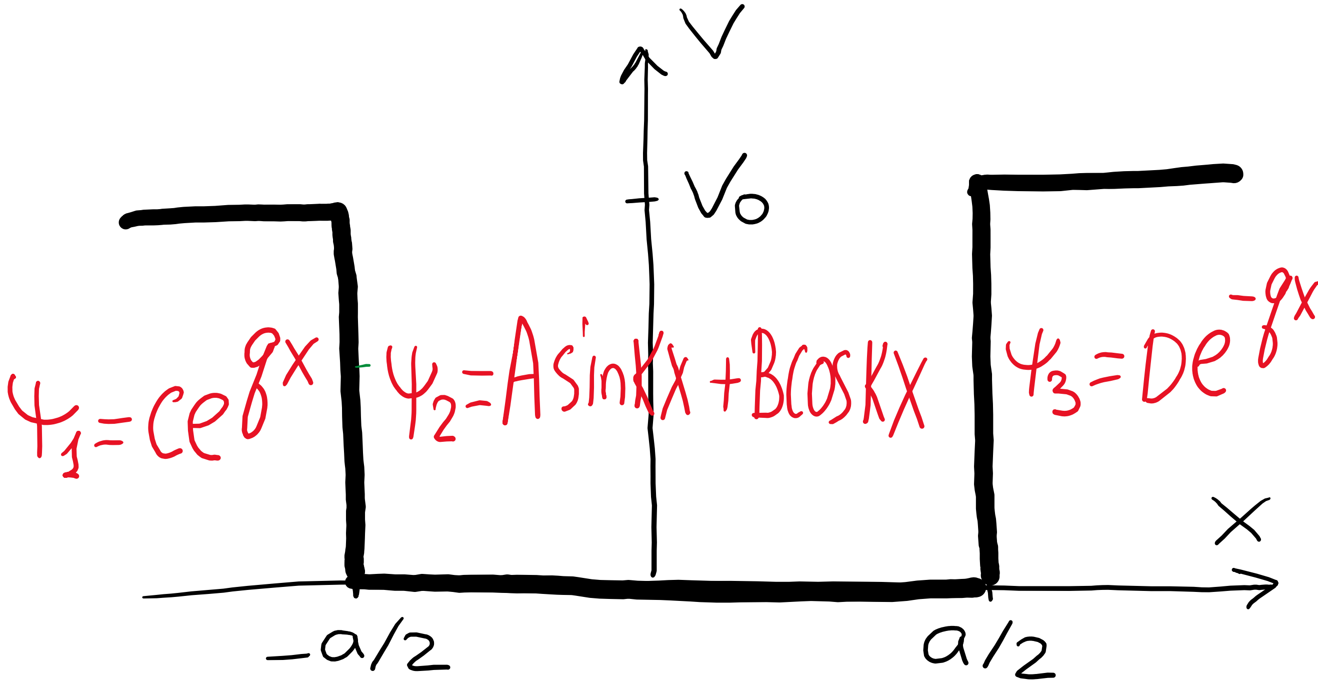
b) $V(-a/2)$ is finite $\Rightarrow$ smoothness $\Rightarrow$ $\left.\frac{d\psi_1}{dx}\right|_{-a/2} = \left.\frac{d\psi_2}{dx}\right|_{-a/2}$

$$Cqe^{-\frac{qa}{2}} = Ak\cos\left(-\frac{ka}{2}\right) - Bk\sin\left(-\frac{ka}{2}\right)$$

2) $x = a/2$

a) Continuity:

$$\psi_2\left(\frac{a}{2}\right) = \psi_3\left(\frac{a}{2}\right)$$



$$A\sin\left(\frac{ka}{2}\right) + B\cos\left(\frac{ka}{2}\right) = De^{-\frac{qa}{2}}$$

b) $V(a/2)$ is finite $\Rightarrow$ smoothness $\Rightarrow$ $\left.\frac{d\psi_2}{dx}\right|_{a/2} = \left.\frac{d\psi_3}{dx}\right|_{a/2}$

$$Ak\cos\left(\frac{ka}{2}\right) - Bk\sin\left(\frac{ka}{2}\right) = -Dqe^{-\frac{qa}{2}}$$

$$Ce^{-\frac{qa}{2}} = -A\sin\left(\frac{ka}{2}\right) + B\cos\left(\frac{ka}{2}\right)$$

$$Cqe^{-\frac{qa}{2}} = Ak\cos\left(\frac{ka}{2}\right) + Bk\sin\left(\frac{ka}{2}\right)$$

$$A\sin\left(\frac{ka}{2}\right) + B\cos\left(\frac{ka}{2}\right) = De^{-\frac{qa}{2}}$$

$$Ak\cos\left(\frac{ka}{2}\right) - Bk\sin\left(\frac{ka}{2}\right) = -Dqe^{-\frac{qa}{2}}$$

+ Normalization

We can eliminate
A, B, C, D

and get 1 equation
with k, q, a.

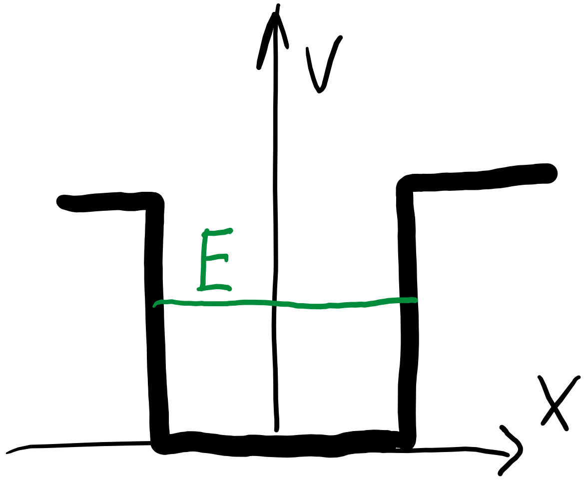
$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad q = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

We arrive to algebraic equation for E

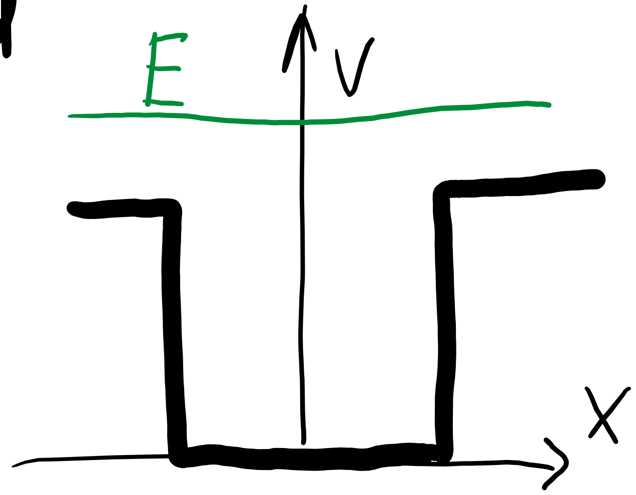
It will have discrete solutions! $(E_1, E_2, \ldots)$

If the particle is (classically) constrained

it's energy eigenvalues are discrete (quantized)



If the particle is not constrained



It has continuous energy spectrum (i.e. E can take any value within certain interval)