Finite square well

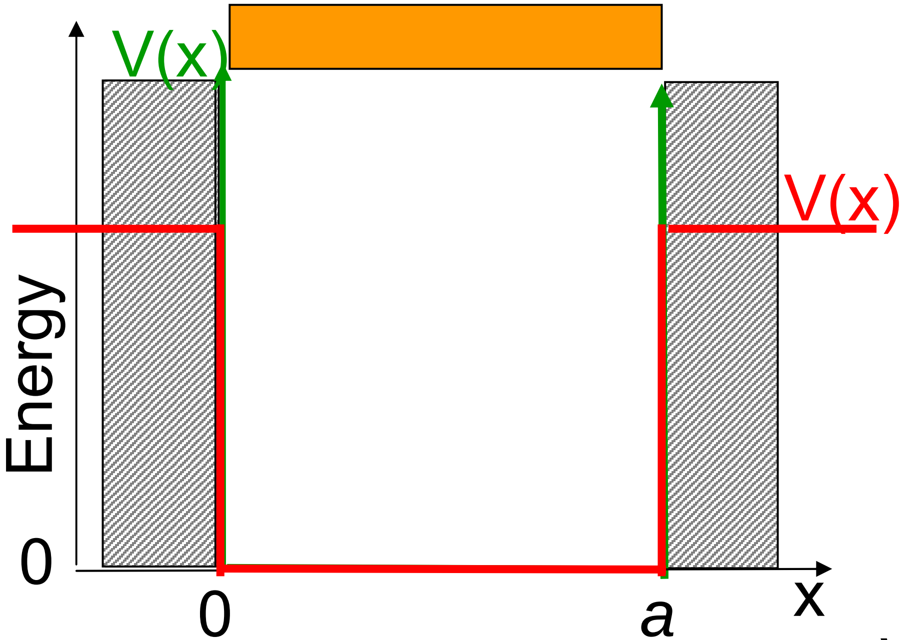
Announcements:

- Homework due on Wednesday
- Normal problem solving sessions 3-5 on Monday and Tuesday.
- 2nd exam is a week from tomorrow (April 7) in MUEN 0046 from 7:30 – 9:00 pm.
- Average score on HW9 was 42.4.
- Homework which comes out Wednesday will mostly be review and will be extra credit.

Today: Details and implications of the finite square well

Tomorrow: Quantum tunneling

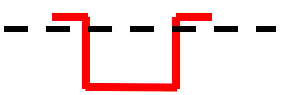
Motivation for a *finite* square well



Infinite square well approximation assumes that electrons never get out of the well so $V(0)=V(a)=\infty$ and $\psi(0)=\psi(a)=0$.

A more accurate potential function V(x) gives a chance of the electron being outside

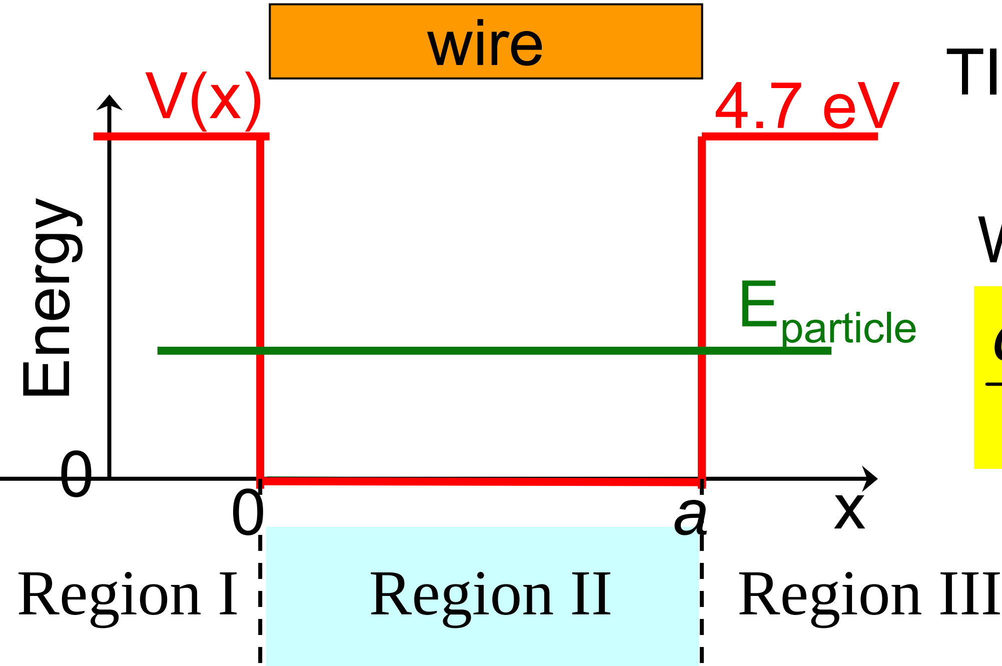
What if the particle energy is higher?



What about two wires very close together?

These scenarios require the more accurate potential

Analyzing the finite square well



TISE: $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$

We rewrite the TISE as

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

Consider three regions

In Region II: total energy E > potential energy V so $V - E < 0$

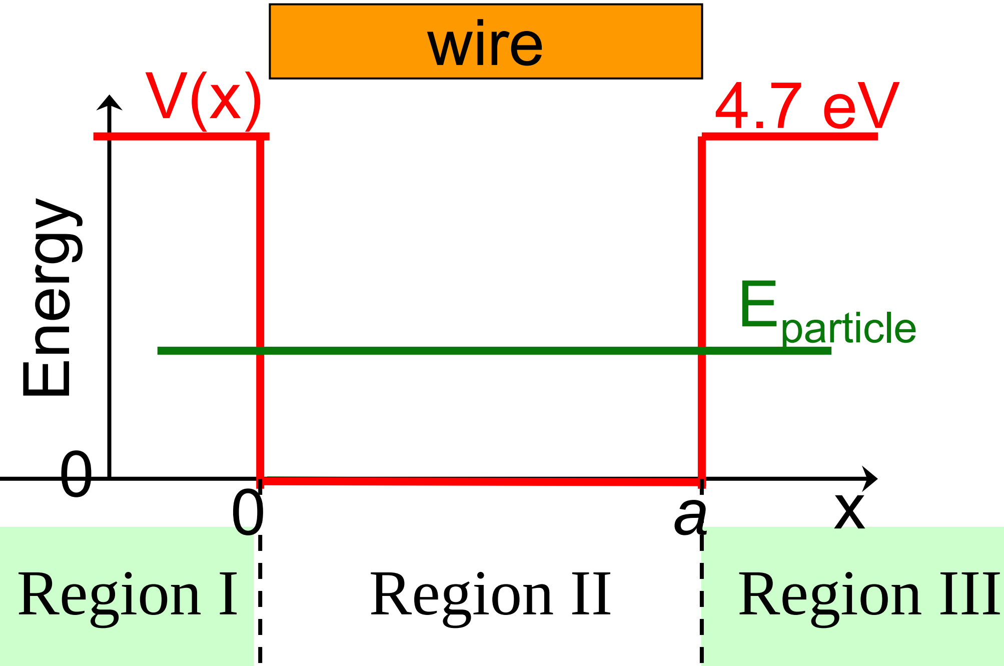
Replace $\frac{2m}{\hbar^2}\left[V(x)-E\right]$ with $-k^2$ to get $\frac{d^2\psi(x)}{dx^2}=-k^2\psi(x)$ (k is real)

Same as infinite square well so sin(kx) and cos(kx) or e^{ikx} and e^{-ikx}

Region II: $\psi_{\mathrm{II}}(x)=A\cos(kx)+B\sin(kx)$

Clicker question 2

the finite square well to DA



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

<u>In Region I & III:</u> E < V
so V − E > 0

Replace $\frac{2m}{\hbar^2}\left[V(x) - E\right]$ with α^2 to get $\frac{d^2\psi(x)}{dx^2} = \alpha^2\,\psi(x)$

(α is real)

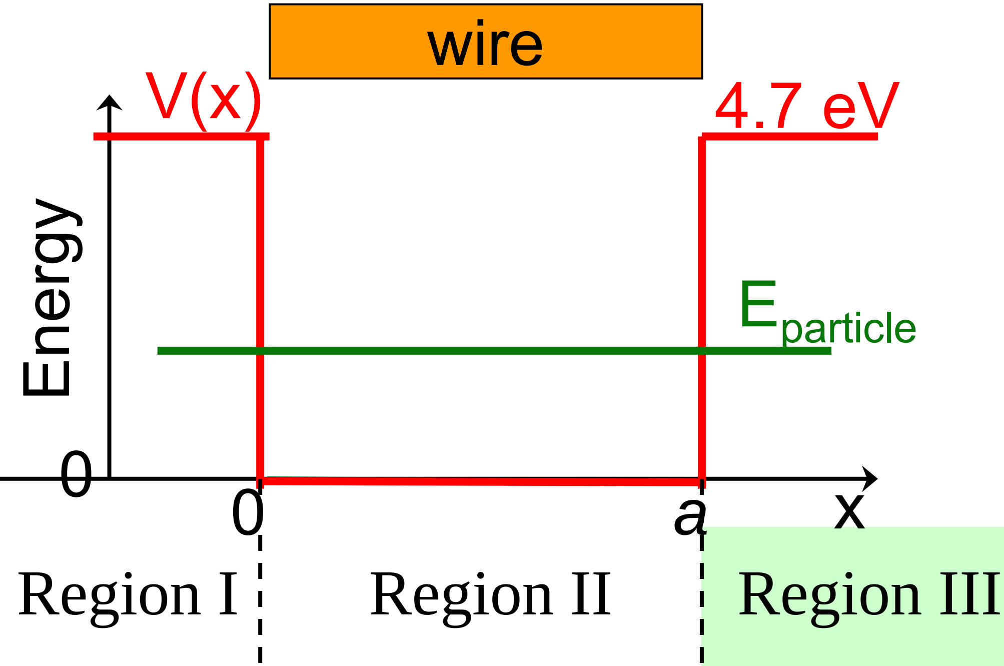
Which functional forms of ψ(x) work?

A. $\cos\alpha x$
B. $\sin\alpha x$
C. $e^{\alpha x}$
D. $e^{i\alpha x}$
E. More than one

A,B,D give a minus sign so $\frac{d^2\psi(x)}{dx^2} = -\alpha^2\,\psi(x)$
This is not what we want.

Both $e^{\alpha x}$ and $e^{-\alpha x}$ give us what we want $\frac{d^2\psi(x)}{dx^2} = \alpha^2\,\psi(x)$

Analyzing the finite square well



Rewritten TISE:

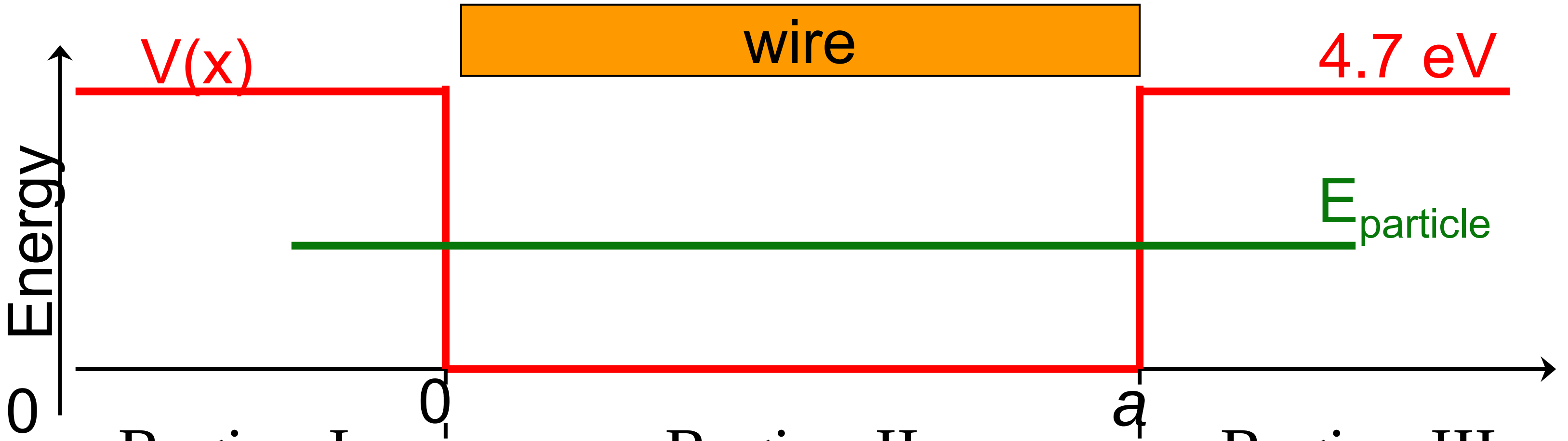
$$\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2}\left[V(x) - E\right]\psi(x)$$

In Region I & III solutions are of the form $e^{\alpha x}$ and $e^{-\alpha x}$.

Assume $\alpha > 0$. Then for Region III, $e^{\alpha x}$ gives exponential growth and $e^{-\alpha x}$ gives exponential decay

Region III: $\psi_{\text{III}}(x) = Ce^{\alpha x} + De^{-\alpha x}$

Clicker question 3 — the finite square well / Set frequency to DA



Region I	Region II	Region III
$\psi_{\mathrm{I}}(x) = Ee^{\alpha x} + Fe^{-\alpha x}$	$\psi_{\mathrm{II}}(x) = A\cos(kx) + B\sin(kx)$	$\psi_{\mathrm{III}}(x) = Ce^{\alpha x} + De^{-\alpha x}$

What will the wave function in Region III look like? What can we say about the constants *C* and *D* (assuming α>0)?

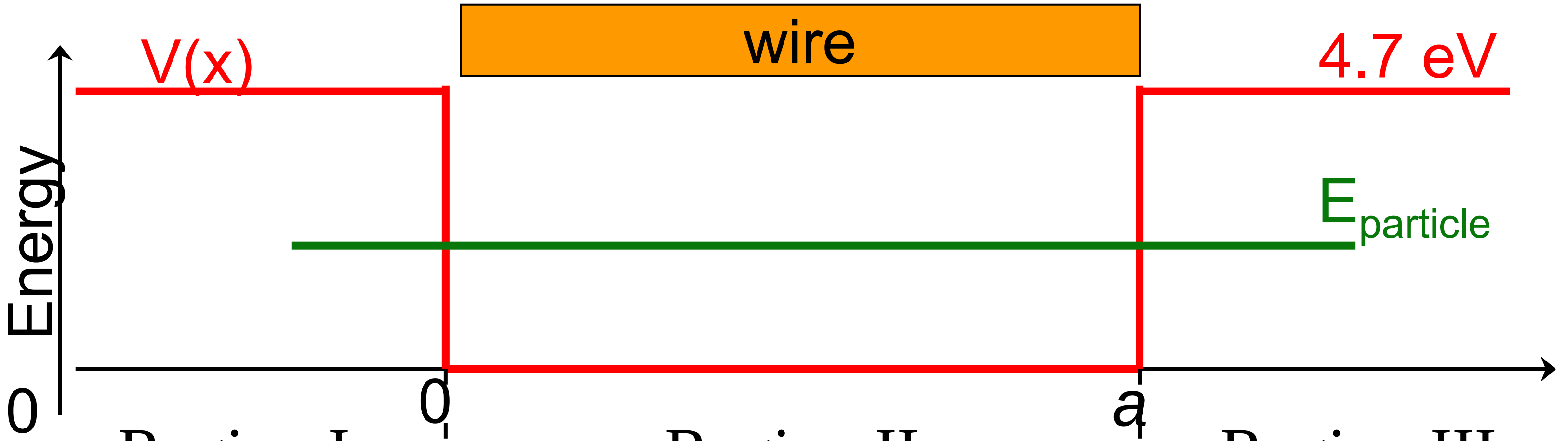
A. C = 0
B. D = 0
C. C = D
D. C = D = 0
E. C & D can be anything; need more information

If *C* ≠ 0 then $Ce^{\alpha x} \rightarrow \infty$ as $x \rightarrow \infty$

Makes it impossible to normalize

For *D* ≠ 0 $De^{-\alpha x} \rightarrow 0$ as $x \rightarrow \infty$ so it is OK.

Clicker question 4 — the finite square well to DA



Region I	Region II	Region III
$\psi_{\mathrm{I}}(x) = Ee^{\alpha x} + Fe^{-\alpha x}$	$\psi_{\mathrm{II}}(x) = A\cos(kx) + B\sin(kx)$	$\psi_{\mathrm{III}}(x) = Ce^{\alpha x} + De^{-\alpha x}$

What will the wave function in Region I look like? What can we say about the constants *E* and *F* (assuming α>0)?

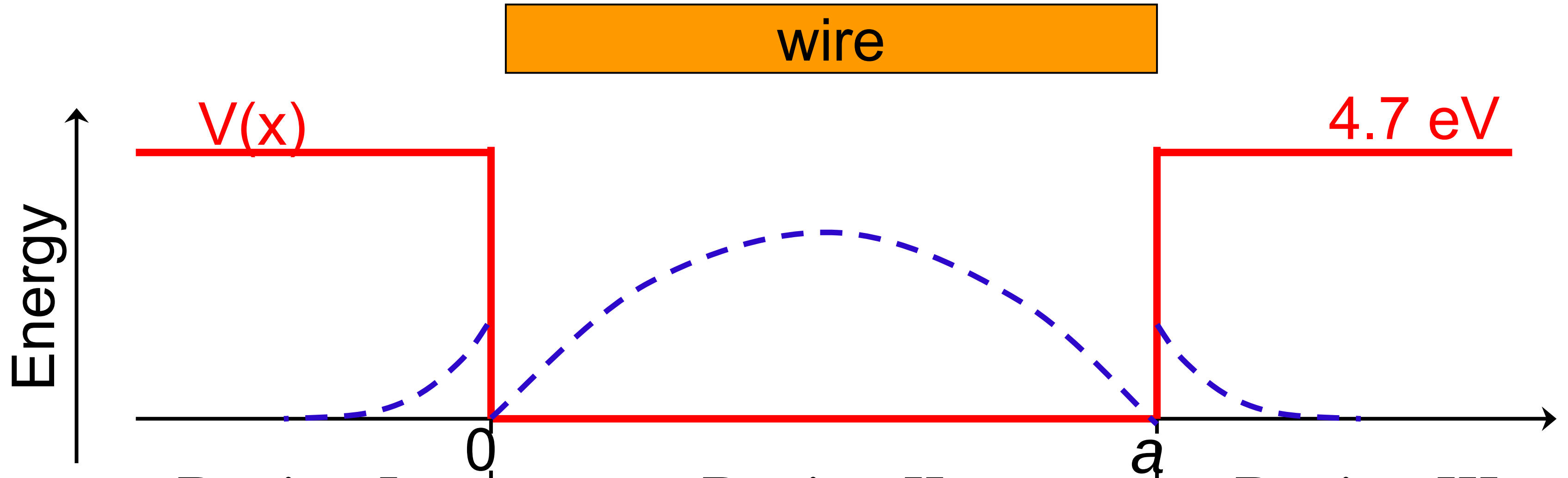
A. E = 0
B. F = 0
C. E = F
D. E = F = 0
E. E & F can be anything; need more information

If *F* ≠ 0 then $Fe^{-\alpha x} \rightarrow \infty$ as $x \rightarrow -\infty$

Makes it impossible to normalize

For *E* ≠ 0 $Ee^{\alpha x} \rightarrow 0$ as $x \rightarrow -\infty$ so it is OK.

Matching boundary conditions



Region I: $\psi_{\mathrm{I}}(x) = Ee^{\alpha x}$

Region II: $\psi_{\mathrm{II}}(x) = A\cos(kx) + B\sin(kx)$

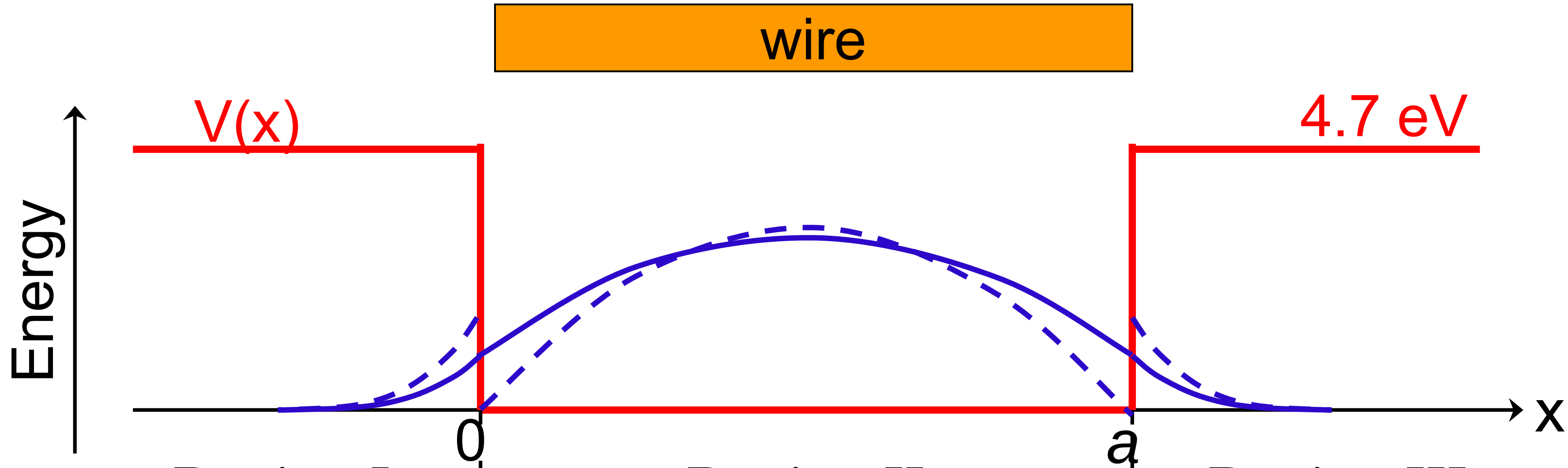
Region III: $\psi_{\mathrm{III}}(x) = De^{-\alpha x}$

Matching boundary conditions at x=0 and x=a requires:

ψ(x) is continuous so $\psi_{\mathrm{I}}(0) = \psi_{\mathrm{II}}(0)$ and $\psi_{\mathrm{II}}(a) = \psi_{\mathrm{III}}(a)$

$\frac{d\psi(x)}{dx}$ is continuous so $\frac{d\psi_{\mathrm{I}}(0)}{dx} = \frac{d\psi_{\mathrm{II}}(0)}{dx}$ and $\frac{d\psi_{\mathrm{II}}(a)}{dx} = \frac{d\psi_{\mathrm{III}}(a)}{dx}$

Matching boundary conditions



Region I

$$\psi_{\mathrm{I}}(x) = Ee^{\alpha x}$$

Region II

$$\psi_{\mathrm{II}}(x) = A\cos(kx) + B\sin(kx)$$

Region III

$$\psi_{\mathrm{III}}(x) = De^{-\alpha x}$$

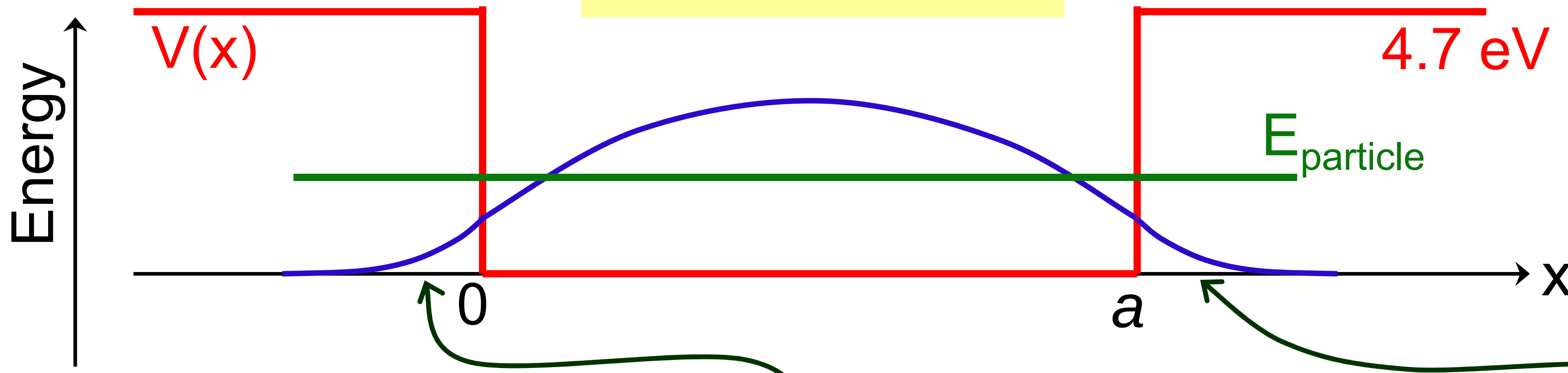
$$\frac{d^2\psi_{\mathrm{I}}(x)}{dx^2} = \alpha^2\psi_{\mathrm{I}}(x) \qquad \frac{d^2\psi_{\mathrm{II}}(x)}{dx^2} = -k^2\psi_{\mathrm{II}}(x) \qquad \frac{d^2\psi_{\mathrm{III}}(x)}{dx^2} = \alpha^2\psi_{\mathrm{III}}(x)$$

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

We won't actually work out the math; we'll just look at results.

Evaluating results

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



Potential well is not infinite so particle is not strictly contained

Particle location extends into *classically forbidden region*

In the classically forbidden regions, the particle has total energy **less than** the potential energy!

Comparison of infinite and finite potential wells

Electron in finite square well
(*a*=2 nm and V=1.0 eV)

Infinite potential well
(*a* = 2 nm and V = ∞)