Infinite (and finite) square well potentials

Announcements:

Homework set #8 is posted this afternoon and due on Wednesday. Note I received an email from a student that problem 5c had a typo and should say exp(-iEt/hbar). I corrected the homework set this morning.

Second Midterm is Thursday, Nov. 7 – 7:30 – 9:00 pm in this room.

Some wave function rules

$\psi(x)$ and $d\psi(x)/dx$ must be continuous

These requirements are used to match boundary conditions.

$|\psi(x)|^2$ must be properly normalized $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$

This is necessary to be able to interpret $|\psi(x)|^2$ as the probability density

$\psi(x) \rightarrow 0 \quad \text{as} \quad x \rightarrow \pm\infty$

This is required to be able to normalize $\psi(x)$

Infinite square well (particle in a box) solution

After applying boundary conditions we found $\psi(x) = B\sin(kx)$

and $k = \frac{n\pi}{a}$ which gives us an energy of $E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$

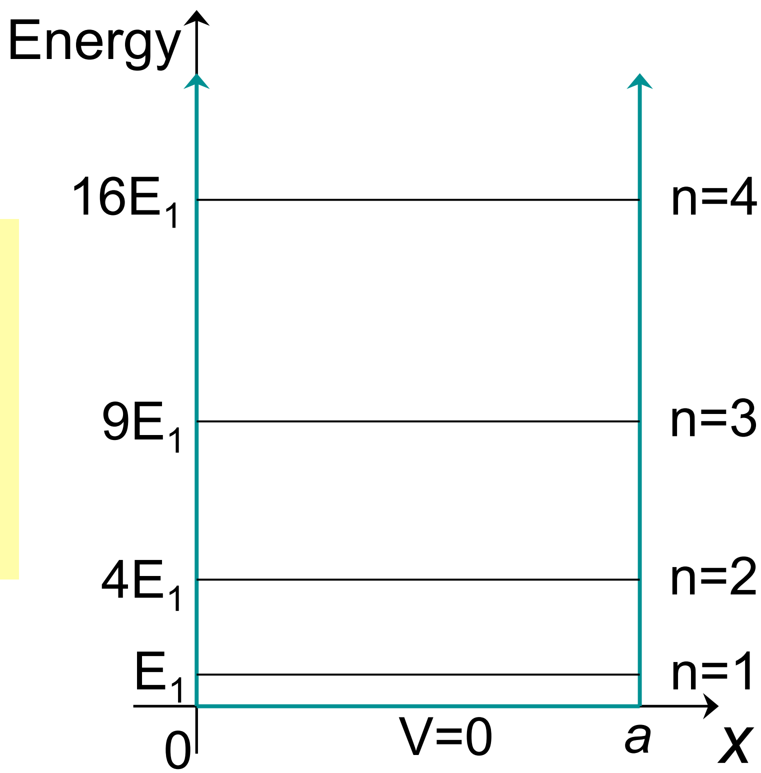
Things to notice:

Energies are quantized.

Minimum energy E_1 is **not** zero.

Consistent with uncertainty principle. *x* is between 0 and *a* so Δ*x*~a/2. Since Δ*x*Δ*p*≥ħ/2, must be uncertainty in *p*. But if *E*=0 then *p*=0 so Δ*p*=0, violating the uncertainty principle.

When *a* is large, energy levels get closer so energy becomes more like continuum (like classical result).



Finishing the infinite square well

We need to normalize ψ(x). That is, make sure that $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$

For the region x<0 and x>a the probability |ψ(x)|^2 is zero so we just need to ensure that $\int_0^a |\psi(x)|^2 dx = 1$

Putting in $\psi(x) = B\sin(kx)$ and doing the integral we find $B = \sqrt{2/a}$

Therefore $\psi(x) = \sqrt{2/a}\,\sin(kx)$

But we also know $k = n\pi / a$

So we can write the solution as $\psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$

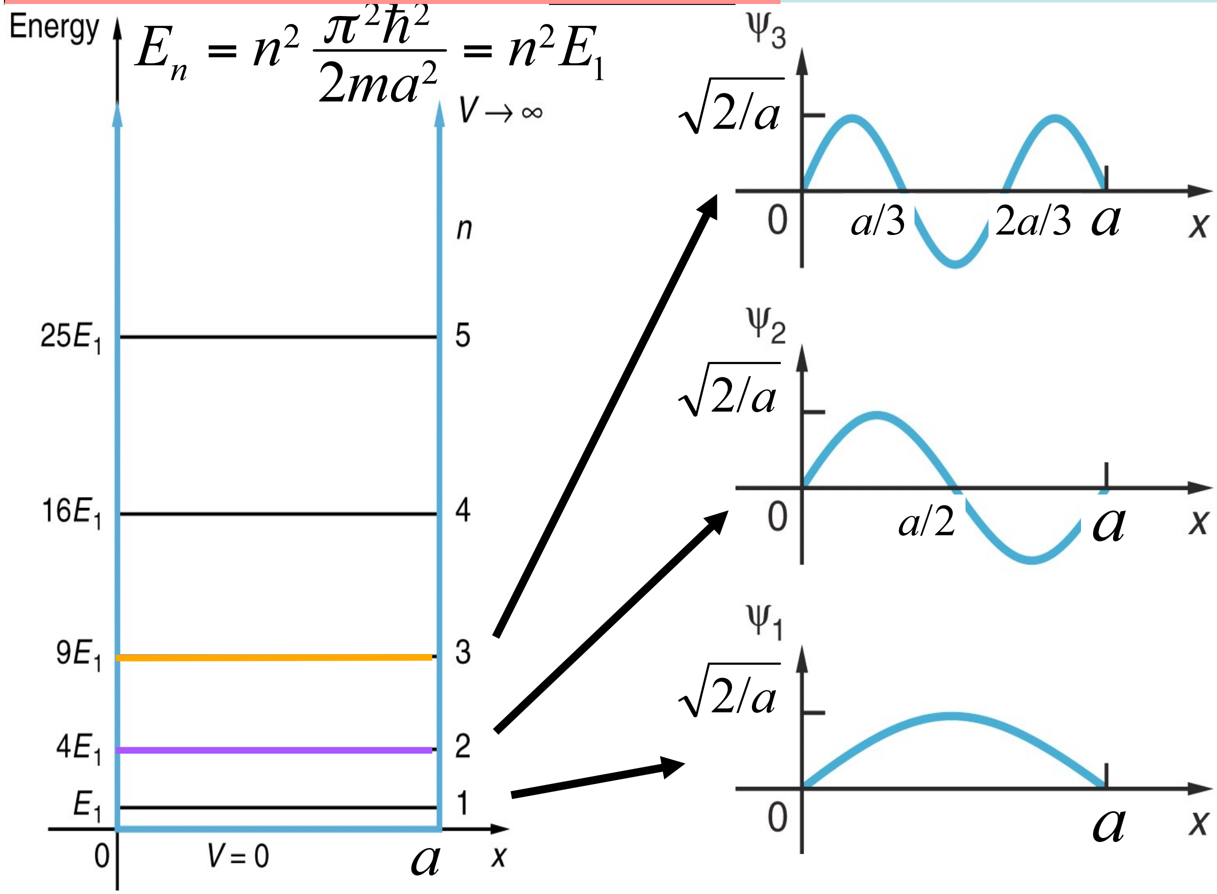
Adding in the time dependence: $\Psi(x,t) = \psi(x)\phi(t) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)e^{-iEt/\hbar}$

Is it still normalized? $\phi^*(t)\,\phi(t)$ is not a function of *x* so can pull out of the integral and find $\phi^*(t)\phi(t) = e^{iEt/\hbar}e^{-iEt/\hbar} = 1$

So the time dependent piece is already normalized.

Clicker question 1

Set frequency to DA



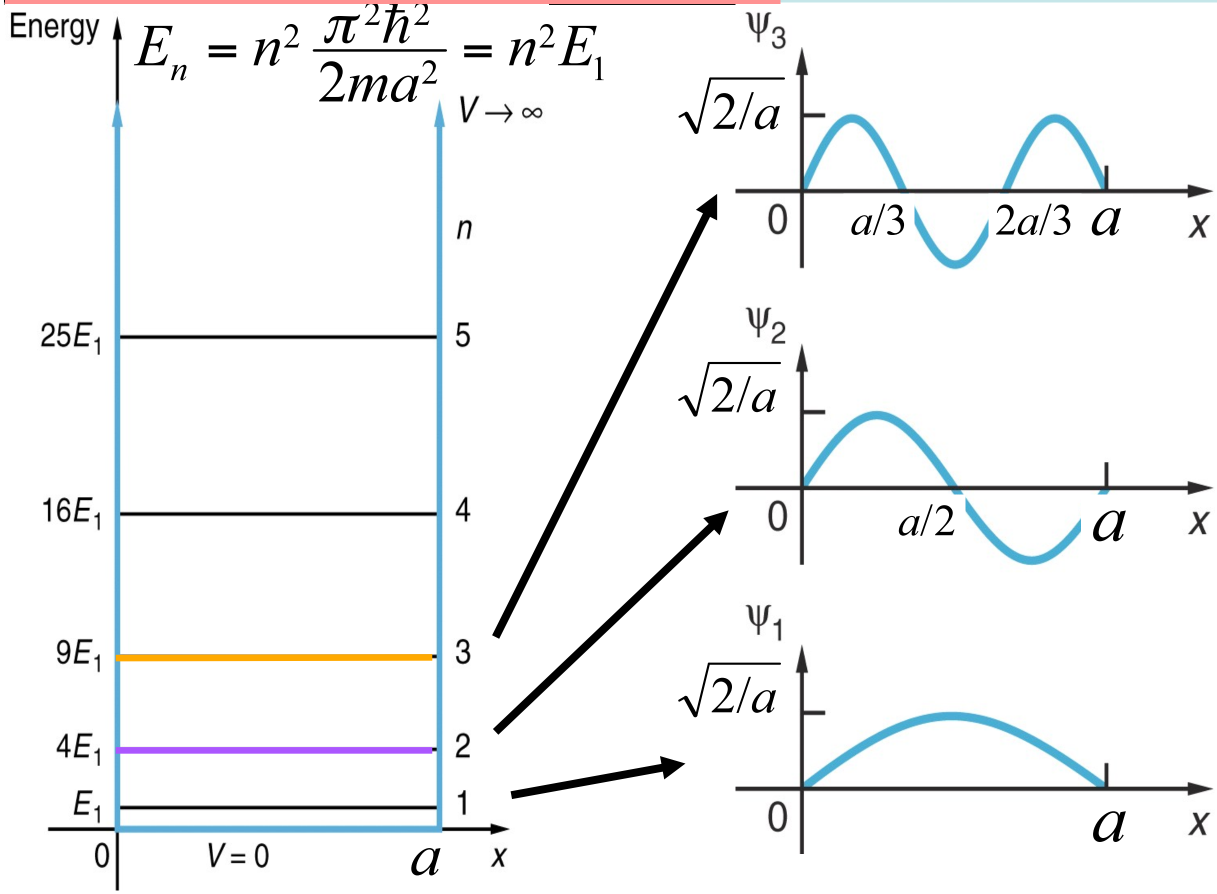
Am I more likely to find the particle close to $a/2$ in the n=2 or n=3 state?

A. n=2 state

B. n=3 state

C. No difference

Clicker question 1 | Set frequency to DA



Am I more likely to find the particle close to *a*/2 in the n=2 or n=3 state?

A. n=2 state

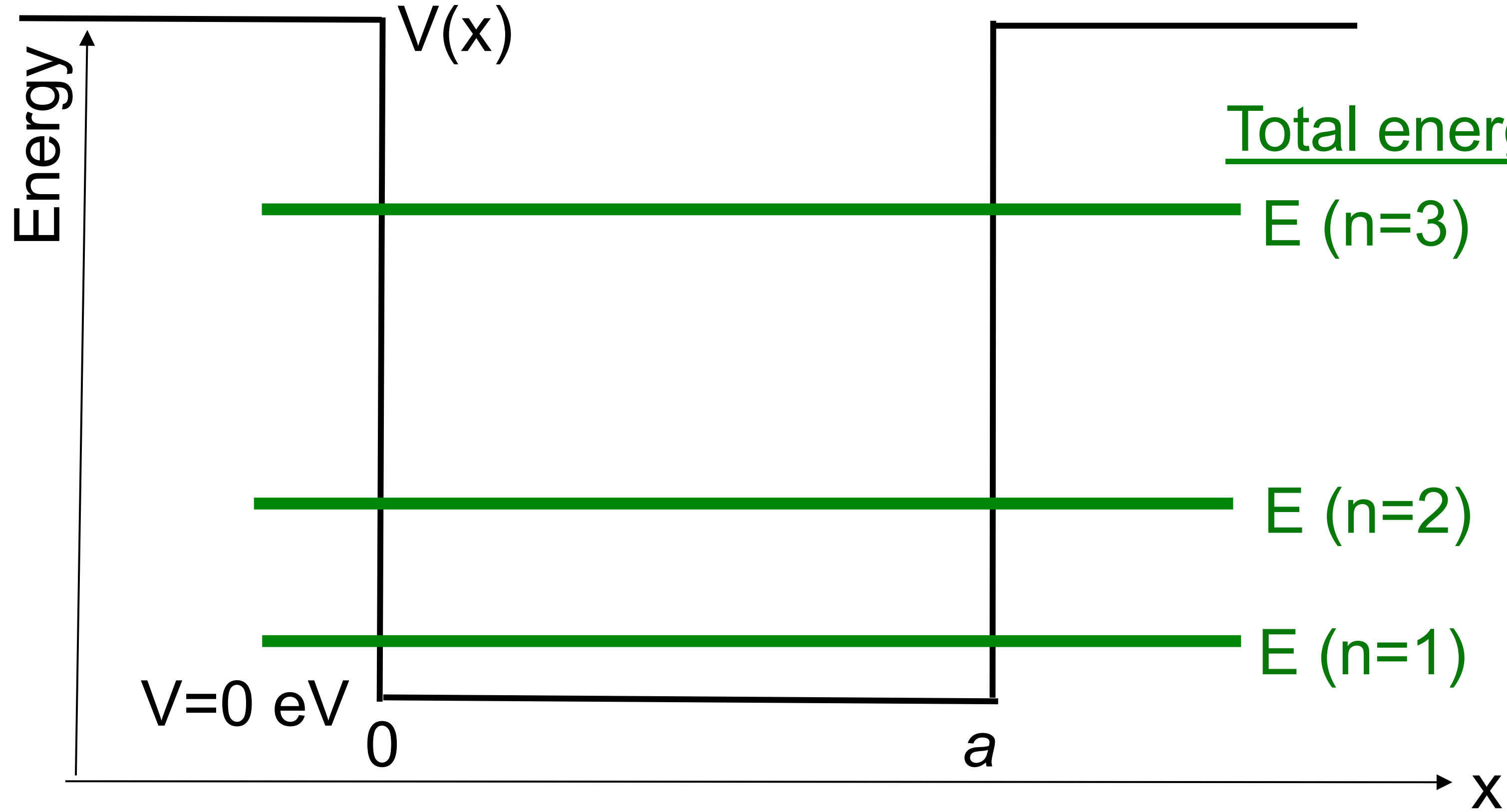
B. n=3 state

C. No difference

For n=2 state: $|\psi_2(a/2)|^2 = 0$

For n=3 state: $|\psi_3(a/2)|^2 = 2/a$

Be careful to understand everything we plot…



Sometimes plot three things on the same graph!

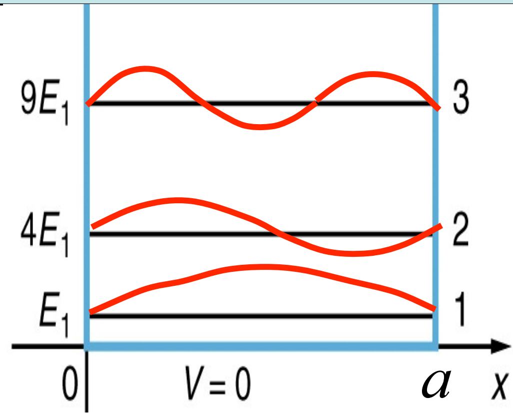
Potential Energy V(x)

Total Energy E

Wave Function ψ(x)

http://phet.colorado.edu/simulations/sims.php?sim=Quantum_Bound_States

Comparing classical and quantum results



$$\Psi(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)e^{-iE_n t/\hbar} \qquad E_n = n^2\frac{\pi^2\hbar^2}{2ma^2} = n^2 E_1$$

Note: time dependence depends on energy

Classical physics	Quantum physics
Particle can have any energy	Particle can only have particular energies (quantized)
Lowest kinetic energy is 0 (particle is at rest)	Lowest energy state in box has kinetic energy (zero point motion)

How small would a box need to be for E_1 to be 4.7 eV?

$$a = \frac{n\pi\hbar}{\sqrt{2mE_n}} = \frac{\pi(6.58\times10^{-16}\text{ eVs})(3\times10^{8}\text{ m/s})}{\sqrt{2(0.511\times10^{6}\text{ eV})(4.7\text{ eV})}} = 2.8\times10^{-10}\text{ m}$$

About the size of an atom so our model wouldn't work anyway

Reading Quiz 1 | Set frequency to DA

Please answer this question on your own.
No discussion until after.

Q. *Classically forbidden regions* are where…

A. a particle's total energy is less than its kinetic energy
B. a particle's total energy is greater than its kinetic energy
C. a particle's total energy is less than its potential energy
D. a particle's total energy is greater than its potential energy
E. None of the above.

Reading Quiz 1 | Set frequency to DA

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A. a particle's total energy is less than its kinetic energy
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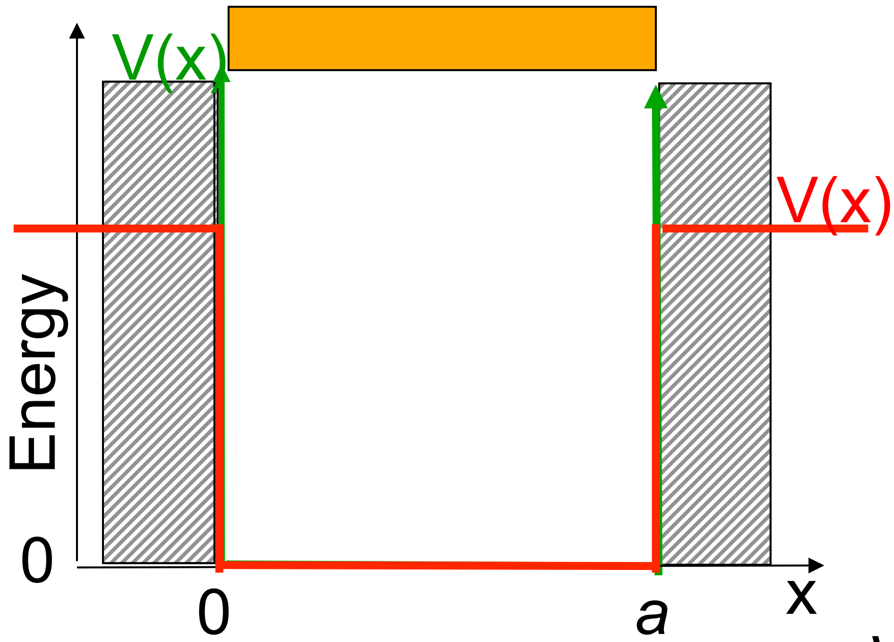
C. a particle's total energy is less than its potential energy
D. a particle's total energy is greater than its potential energy
E. None of the above.

This would imply that the kinetic energy is negative which is forbidden (at least classically).

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 $\psi(0)=\psi(a)=0$.

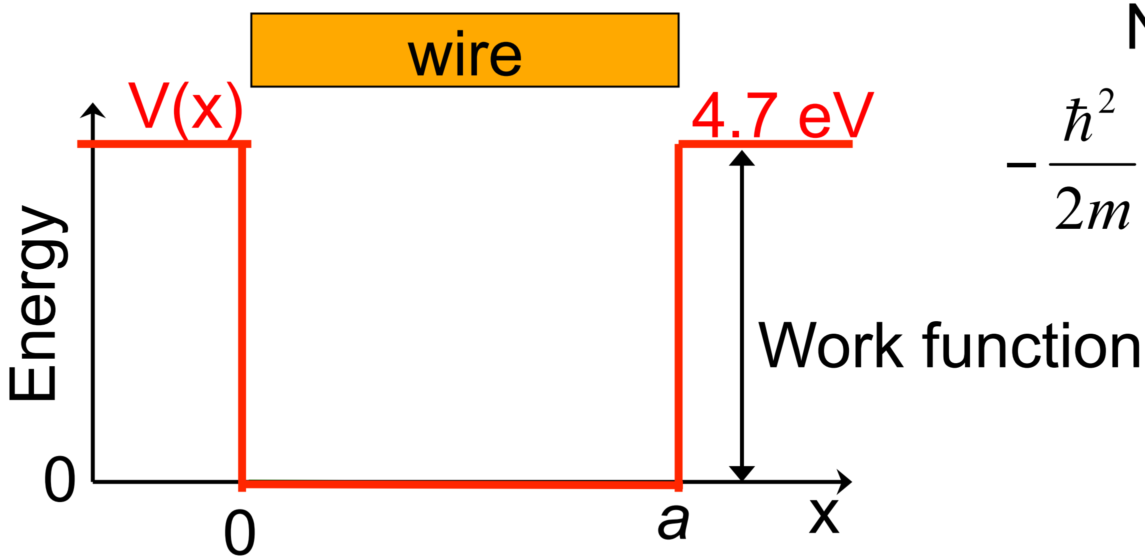
A more accurate potential function V(x) gives a chance of the electron being outside

What if the particle energy is higher?

What about two wires very close together?

These scenarios require the more accurate potential

Need to solve the *finite* square well



Need to solve TISE:

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

$x < 0$: $V(x) = 4.7$ eV

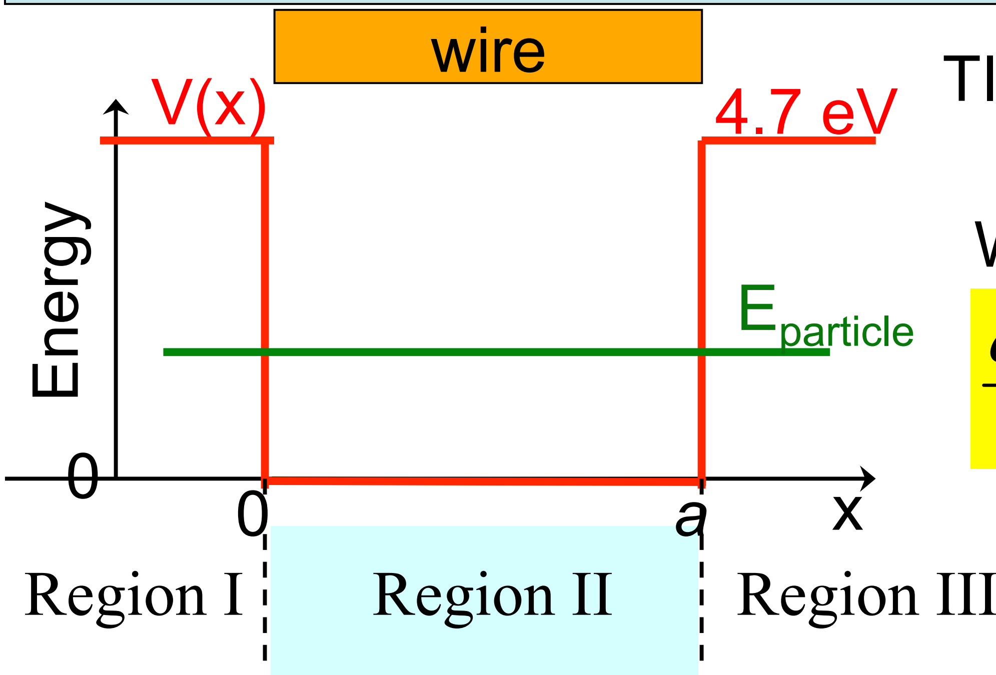
$x > a$: $V(x) = 4.7$ eV

$0 < x < a$: $V(x) = 0$

This will be used to understand *quantum tunneling* which provides the basis for understanding

- Radioactive decay
- Scanning Tunneling Microscope which is used to study surfaces
- Binding of molecules

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 $V - E < 0$

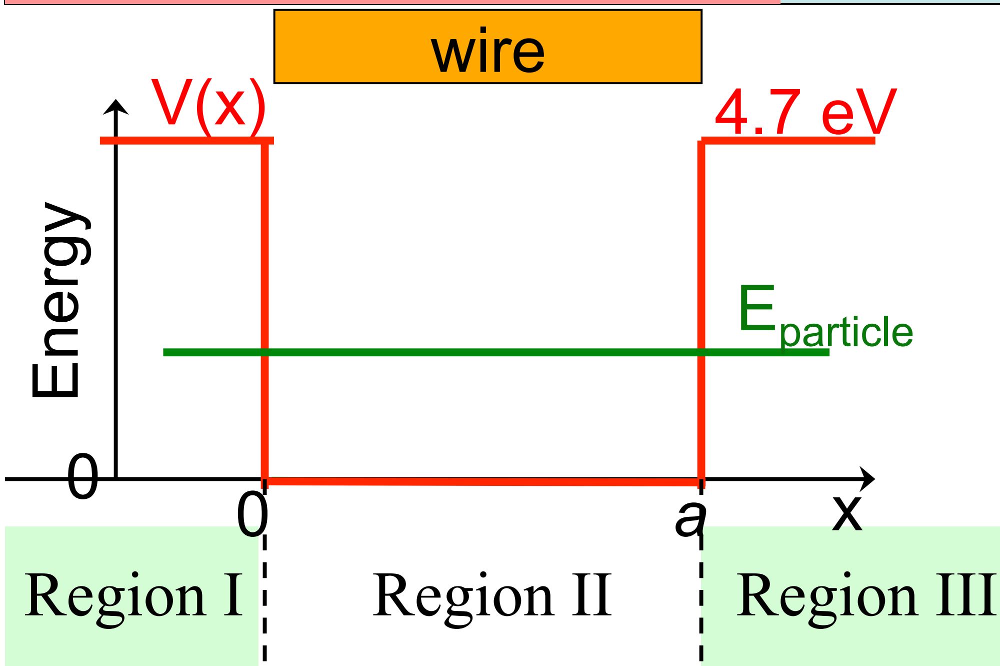
Replace $\frac{2m}{\hbar^2}\left[V(x) - E\right]$ with $-k^2$ to get $\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x)$ (k is real)

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

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

Clicker question 2

…the finite square well to DA



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

In Region I & III: 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?

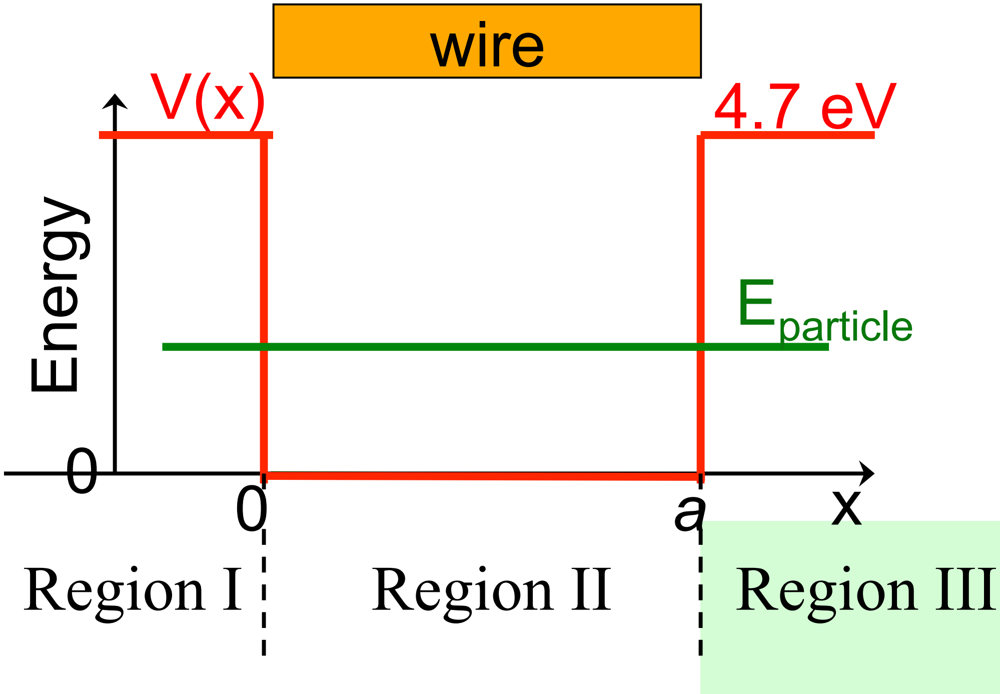
A. $\cos\alpha x$
B. $\sin\alpha x$
C. $e^{\alpha x}$
D. $e^{i\alpha x}$
E. More than one

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:

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

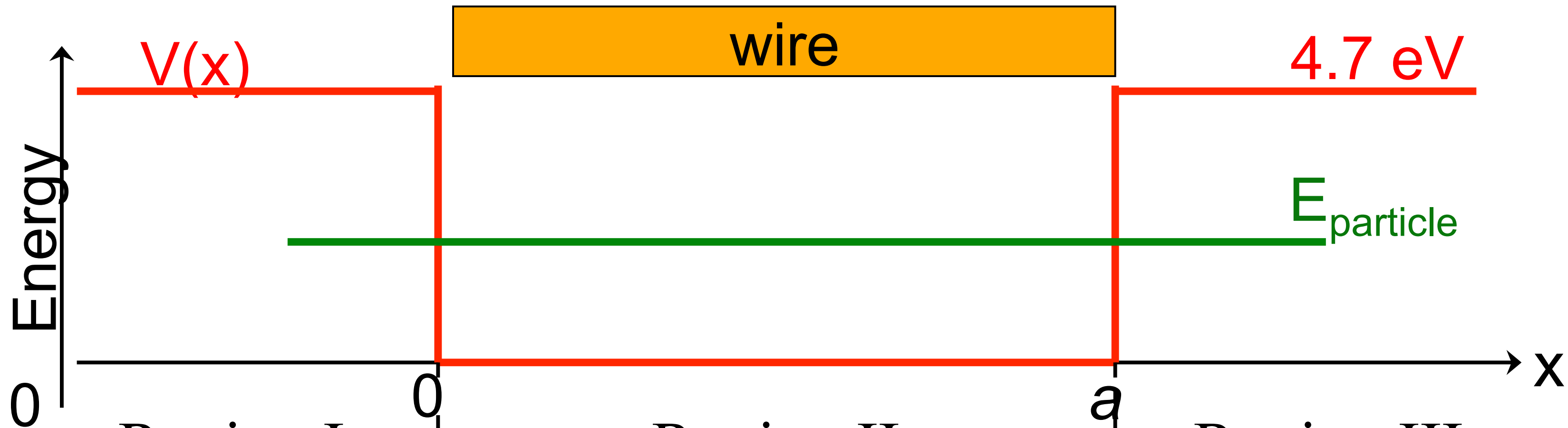
<u>In Region I & III</u> solutions are of the form $e^{\alpha x}$ and $e^{-\alpha x}$.

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

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

Clicker question 3

the finite square well to DA

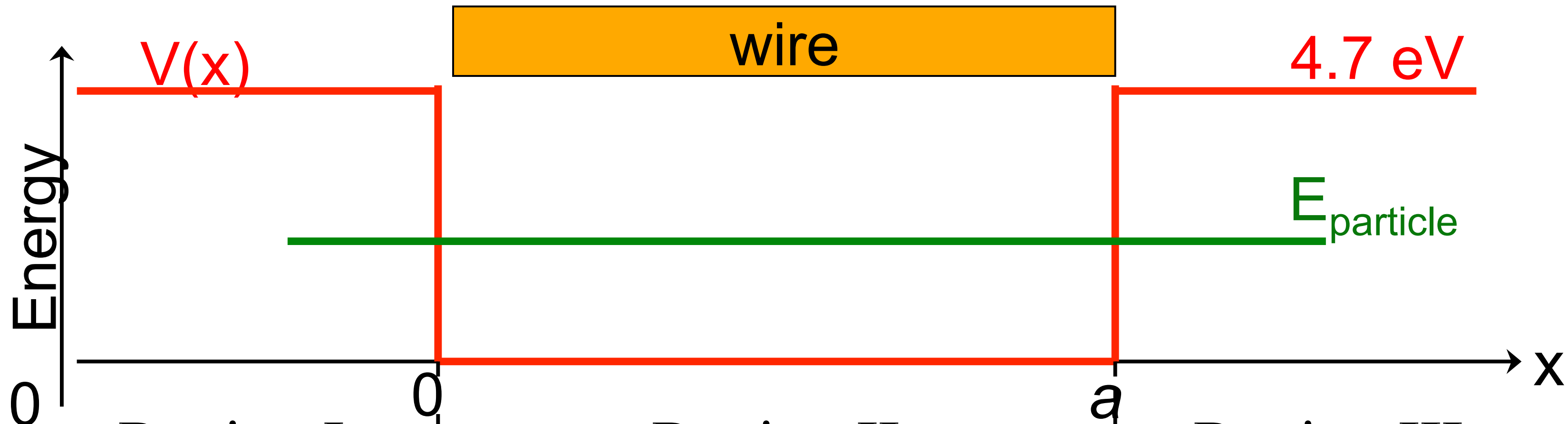


Region I	Region II	Region III
$\psi_{\mathrm{I}}(x) = Ee^{\alpha x} + Fe^{-\alpha x}$	$\psi_{\mathrm{II}}(x) = A\cos(kx) + B\sin(kx)$	$\psi_{\mathrm{III}}(x) = Ce^{\alpha x} + De^{-\alpha x}$

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

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

Clicker question 3 — the finite square well to DA



Region I: $\psi_I(x) = Ee^{\alpha x} + Fe^{-\alpha x}$

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

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

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

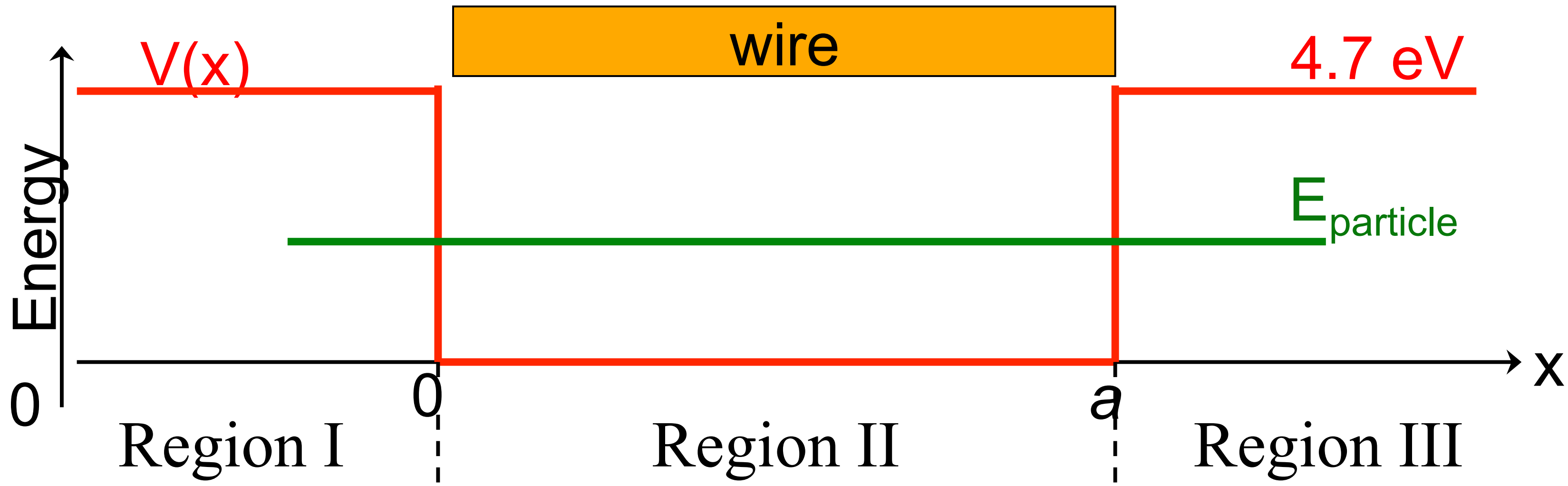
A. C = 0
B. D = 0
C. C = D
D. C = D = 0
E. C & D can be anything; need more information

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

Makes it impossible to normalize

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

Clicker question 4 the finite square well to DA

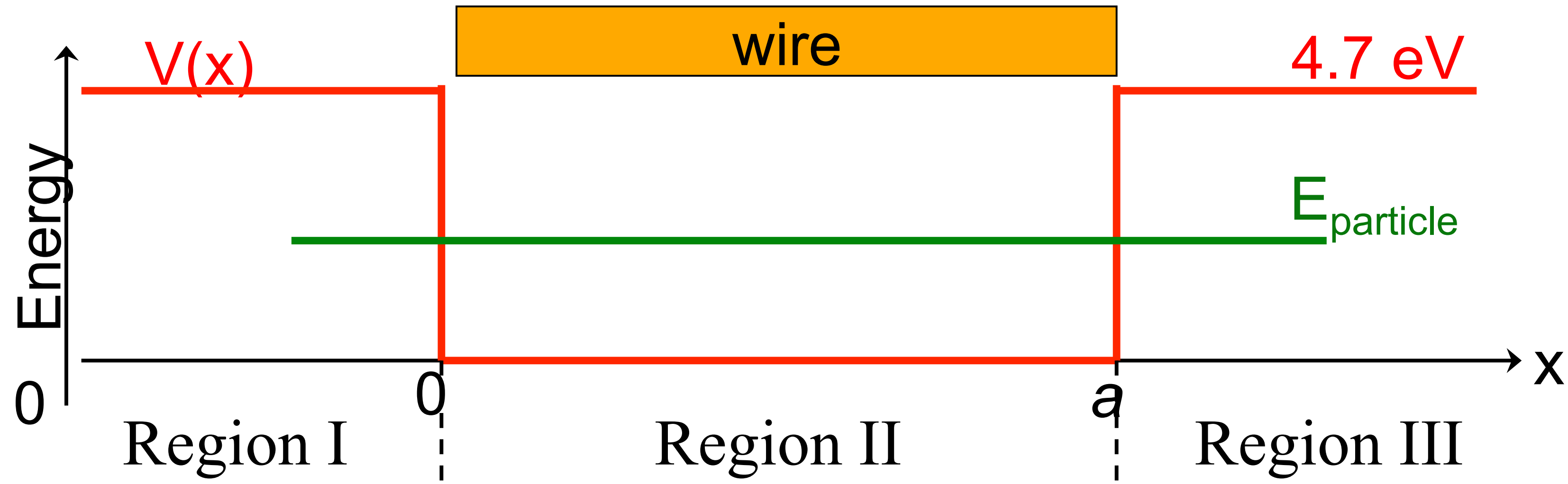


$\psi_{\text{I}}(x) = Ee^{\alpha x} + Fe^{-\alpha x}$ $\psi_{\text{II}}(x) = A\cos(kx) + B\sin(kx)$ $\psi_{\text{III}}(x) = Ce^{\alpha x} + De^{-\alpha x}$

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

Clicker question 4 — the finite square well to DA



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

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

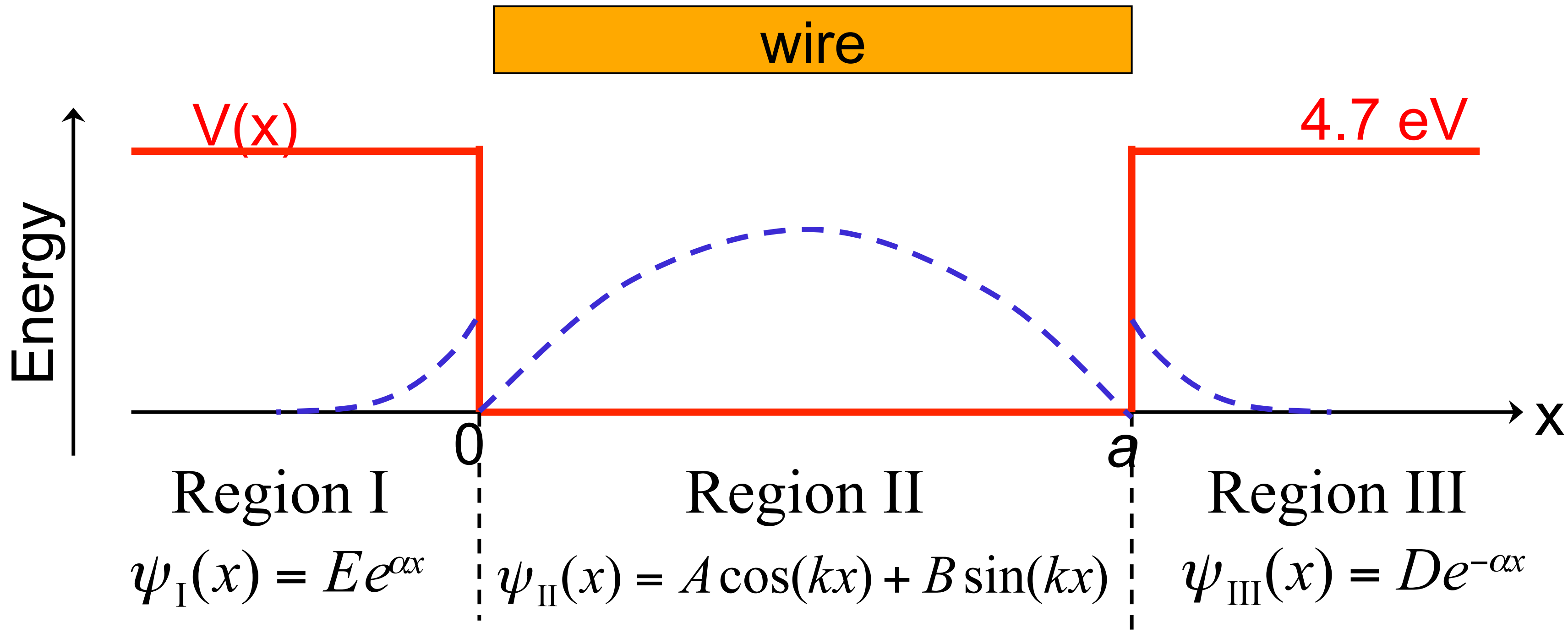
A. E = 0
B. F = 0
C. E = F
D. E = F = 0
E. E & F can be anything; need more information

If $F \neq 0$ then $Fe^{-\alpha x} \to \infty$ as $x \to -\infty$

Makes it impossible to normalize

For $E \neq 0$ $Ee^{\alpha x} \to 0$ as $x \to -\infty$ so it is OK.

Matching boundary conditions

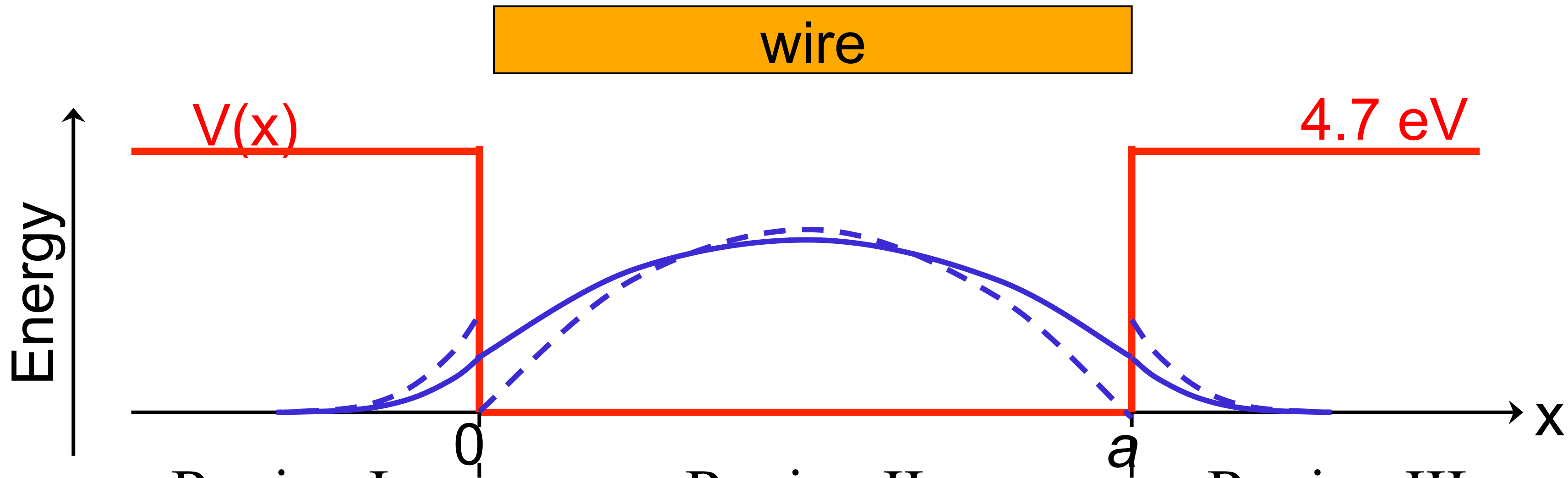


Matching boundary conditions at x=0 and x=a requires:

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



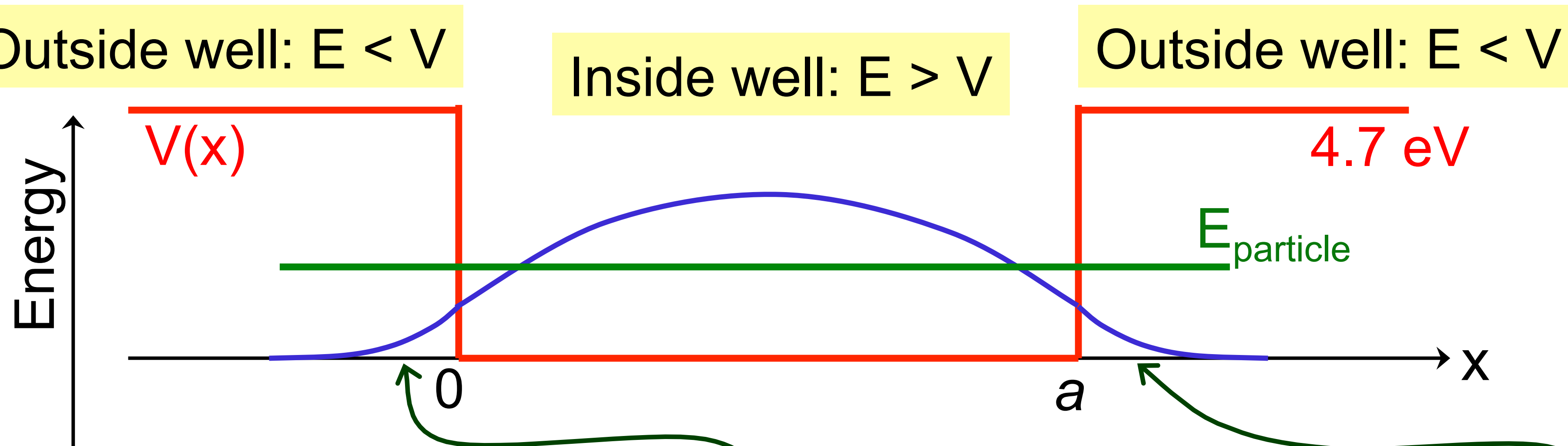
Region I	Region II	Region III
$\psi_{\mathrm{I}}(x) = Ee^{\alpha x}$	$\psi_{\mathrm{II}}(x) = A\cos(kx) + B\sin(kx)$	$\psi_{\mathrm{III}}(x) = De^{-\alpha x}$
$\frac{d^2\psi_{\mathrm{I}}(x)}{dx^2} = \alpha^2\psi_{\mathrm{I}}(x)$	$\frac{d^2\psi_{\mathrm{II}}(x)}{dx^2} = -k^2\psi_{\mathrm{II}}(x)$	$\frac{d^2\psi_{\mathrm{III}}(x)}{dx^2} = \alpha^2\psi_{\mathrm{III}}(x)$

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

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 = ∞)