Infinite (and finite) square well potentials

Announcements:

- There will be a homework set put up this afternoon and due Wednesday after break.
- No class on Friday.
- HW1-8 and Exam 1 grades are now in CULearn. Please check to make sure they are correct.

In case you are curious, the average scores (of those turned in) are below:

	EX1	HW1	HW2	HW3	HW4	HW5	HW6	HW7	HW8
Avg:	75.0	44.2	43.7	42.2	35.6	32.7	39.2	39.2	37.7

EX1 is out of 100, HW4 is out of 40 and the rest are out of 50

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

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

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 $E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$

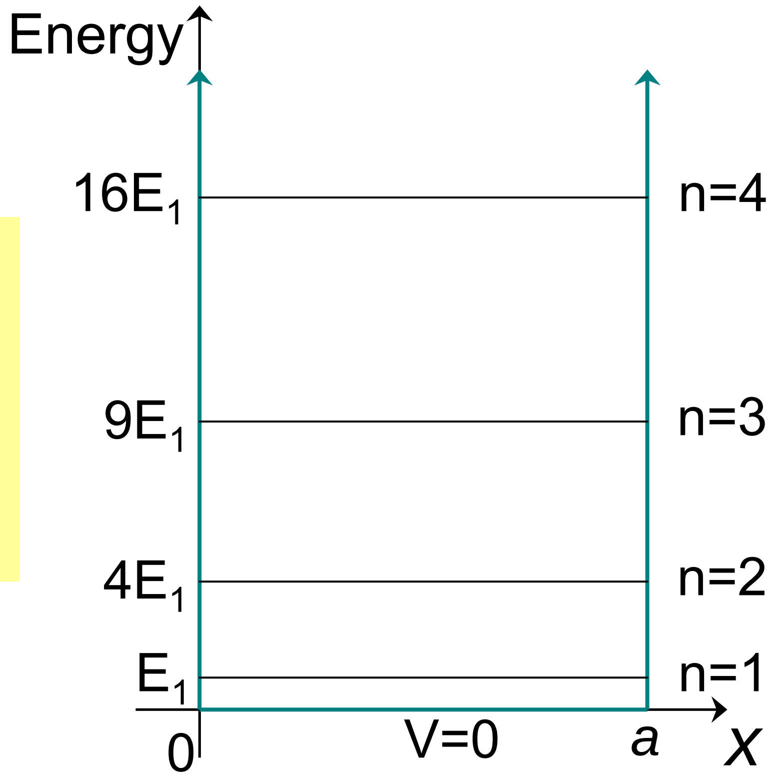
<u>Things to notice:</u>

Energies are quantized.

Minimum energy E_1 is **<u>not</u>** zero.

Consistent with uncertainty principle. *x* is between 0 and *a* so $\Delta x \sim a/2$. Since $\Delta x \Delta p \geq \hbar/2$, must be uncertainty in *p*. But if *E*=0 then *p*=0 so Δp=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 $|\psi(x)|^2$ 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 $\psi(x) = \sqrt{2/a}\,\sin(kx)$

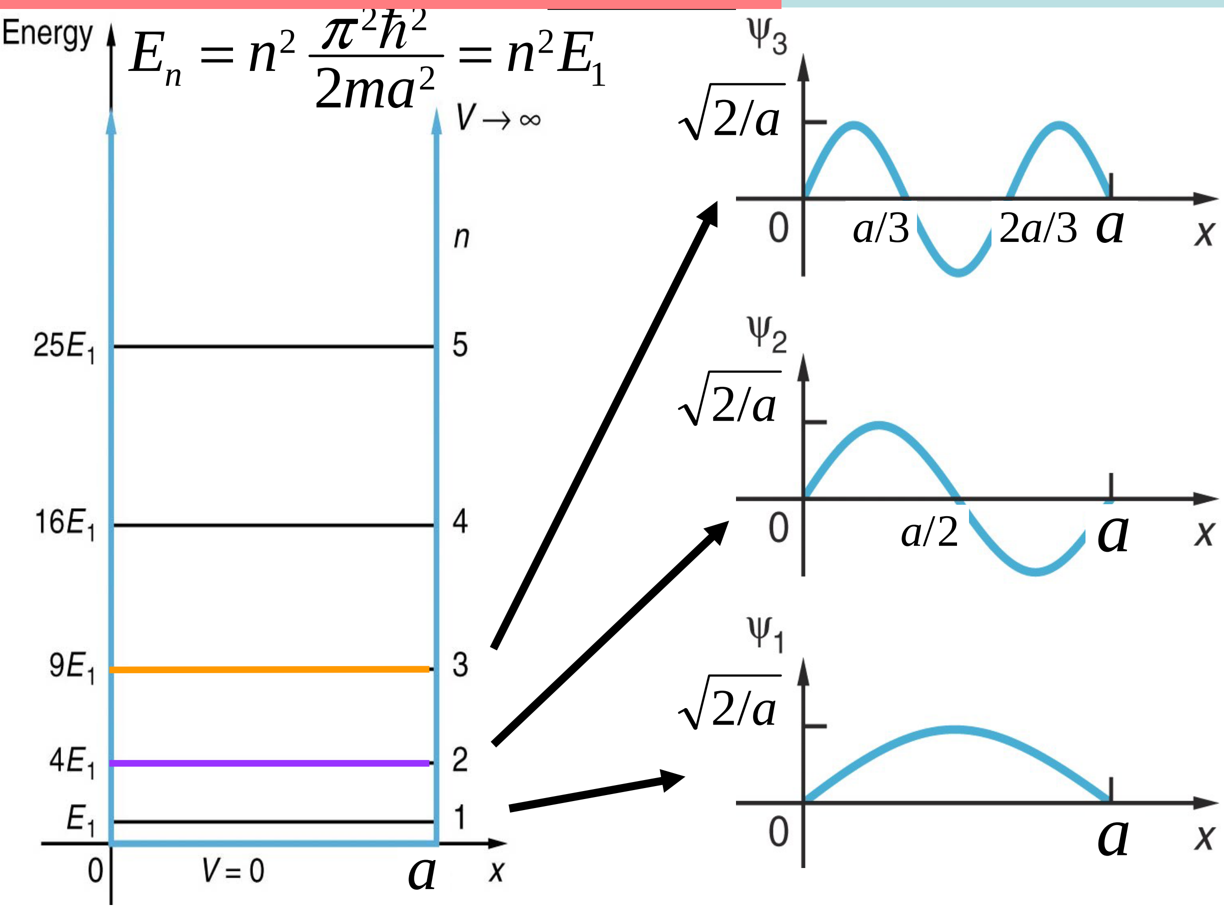
But we also know $k = n\pi / a$

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.



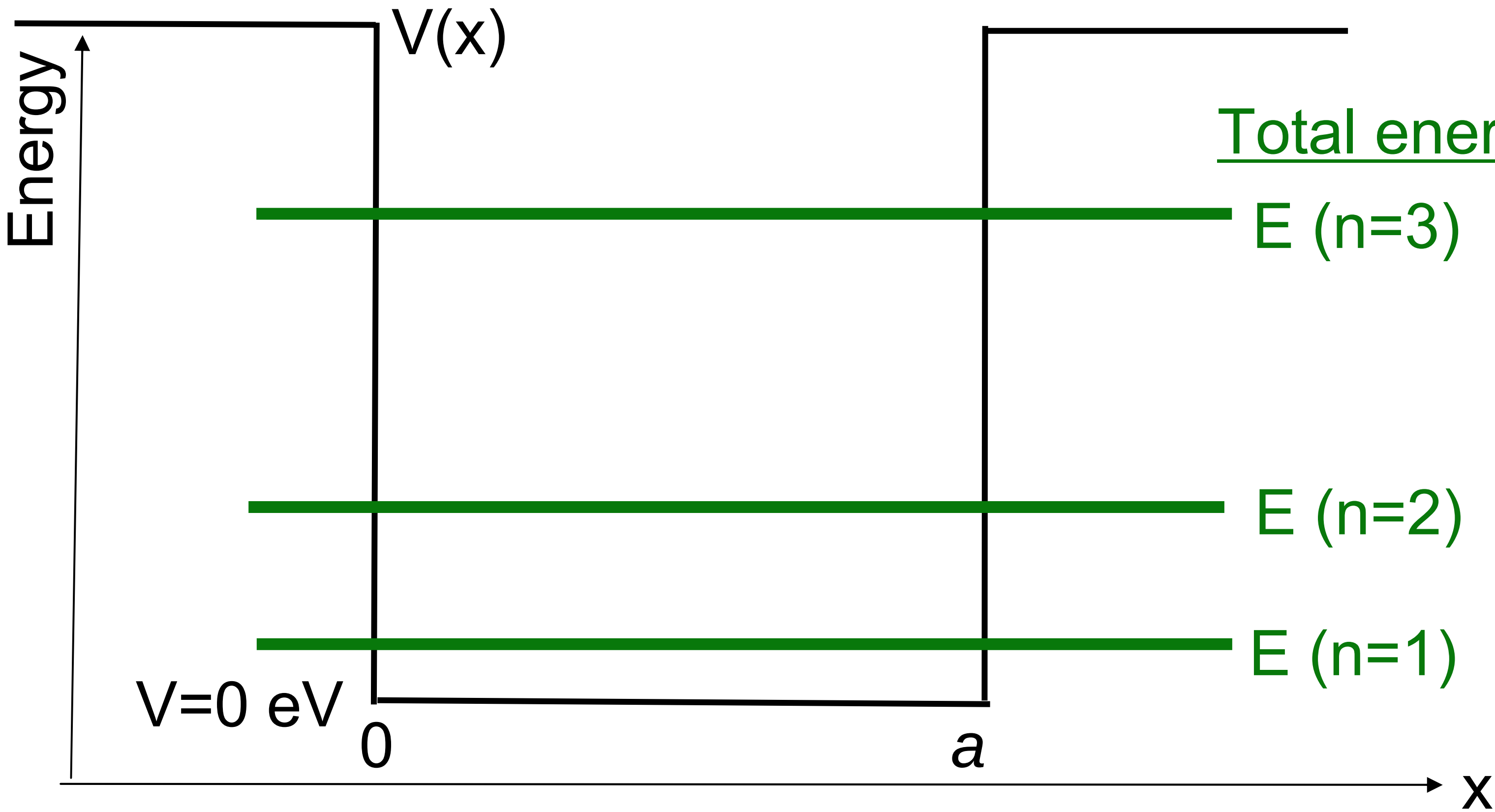
Am I more likely to find the particle close to *a*/2 in the n=2 or n=3 state?

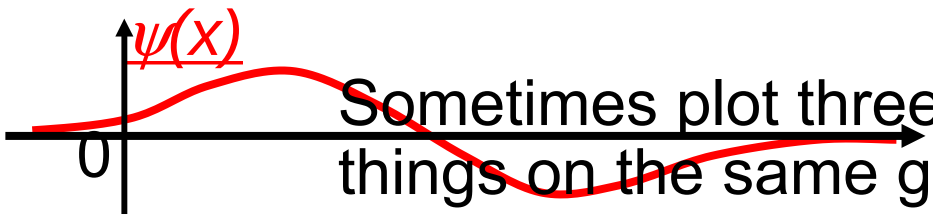
A. n=2 state
B. n=3 state
C. No difference

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!

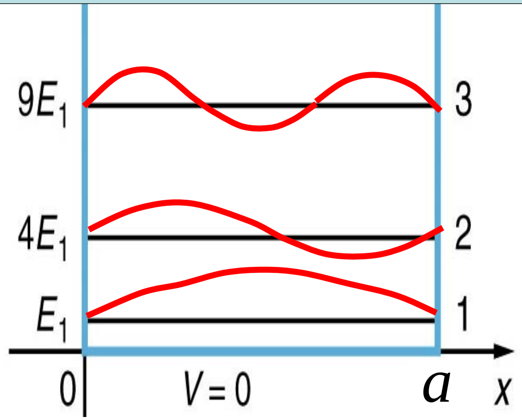
Potential Energy V(x)

Total Energy E

Wave Function $\psi(x)$

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

Comparing classical and quantum results



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

$$E_n = n^2 \frac{\pi^2\hbar^2}{2ma^2} = n^2 E_1$$

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

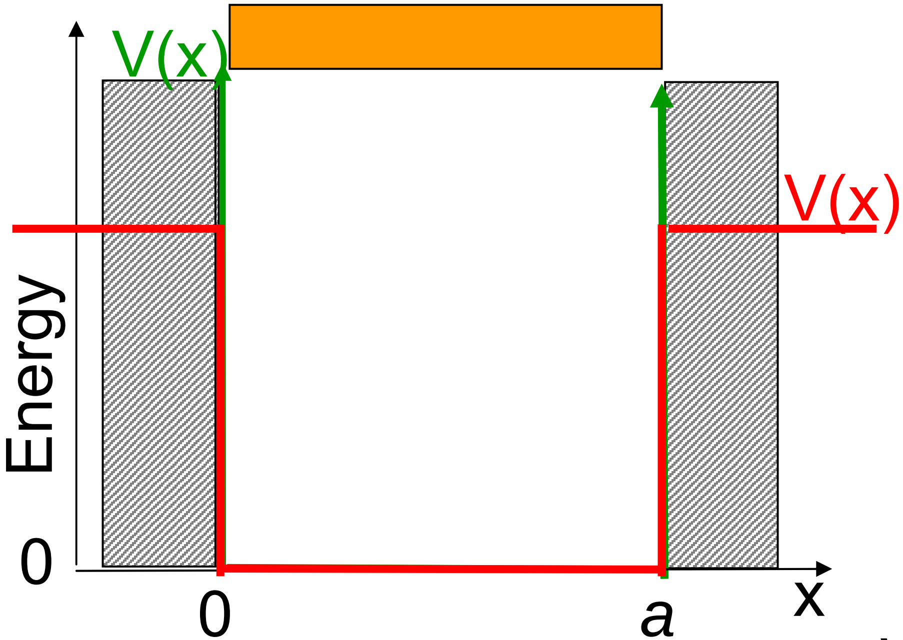
Please answer this question on your own.
No discussion until after.

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.

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

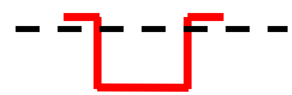
Motivation for a *finite* square well



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

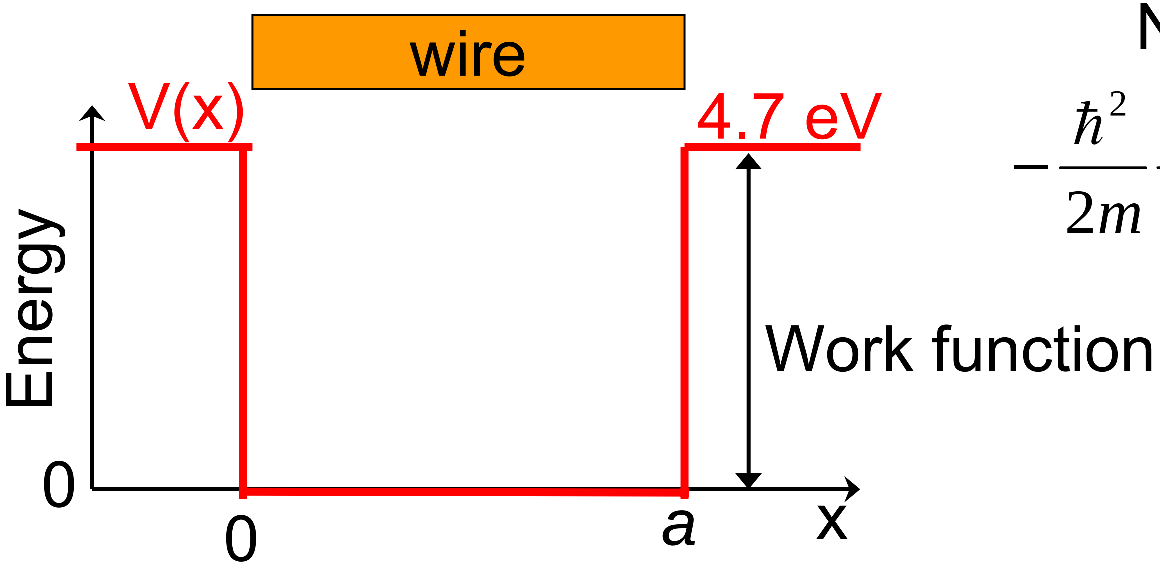
What if the particle energy is higher?



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

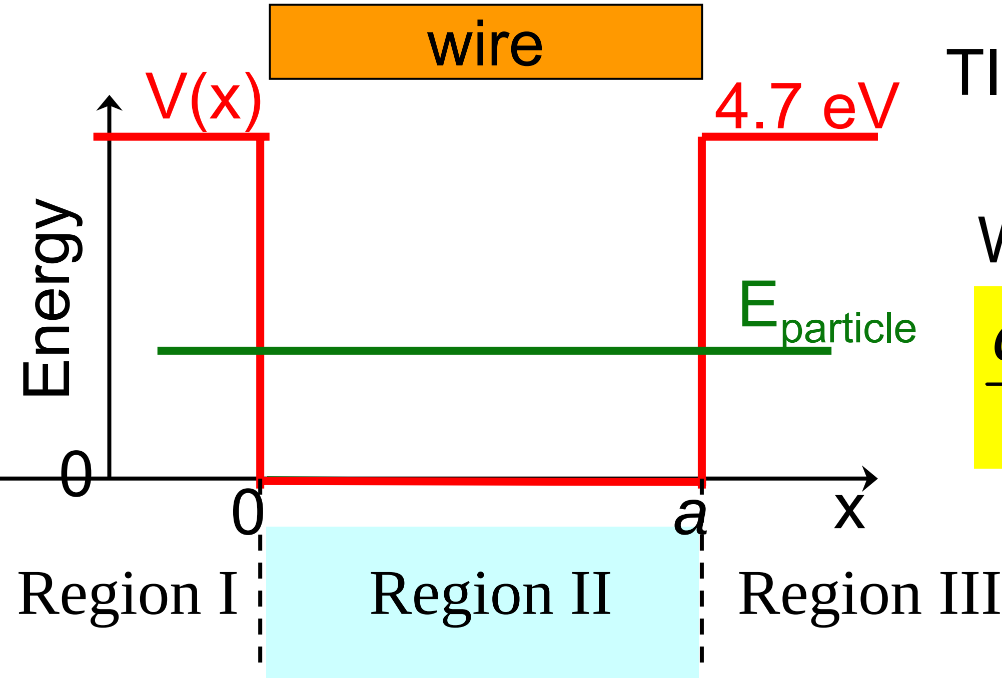
This will be used to understand *quantum tunneling* which provides the basis for understanding

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

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

<u>Consider three regions</u>

<u>In Region II:</u> 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: $\psi_{II}(x) = A\cos(kx) + B\sin(kx)$