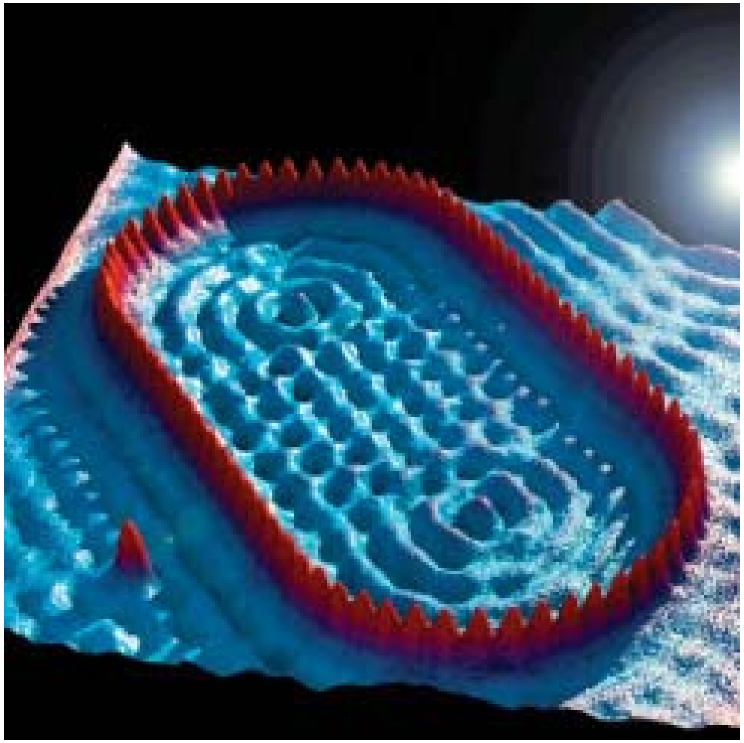
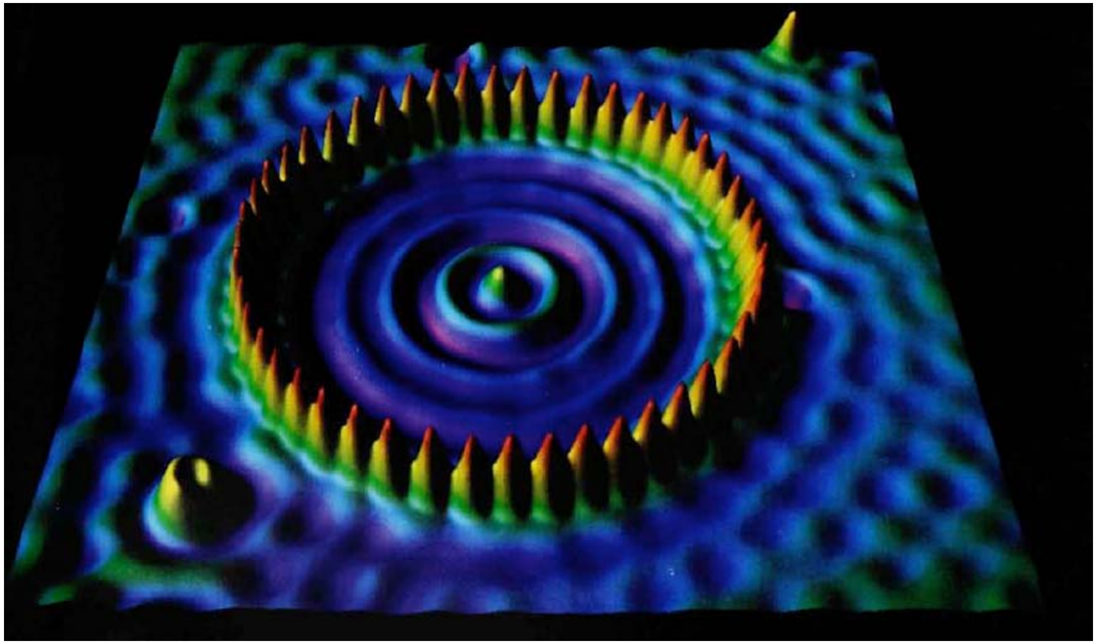
Infinite square well (particle in a box)

Announcements:

- Homework set 9 is due Wednesday.
- There will be no class on Friday, March 20.





Today we will be investigating the infinite square well (particle in a box).

Free particle

The general (spatial part) solution for a free particle is:

$$\psi(x) = A\cos(kx) + B\sin(kx)$$

Using some identities you will be proving in the homework, this can also be written as $\psi(x) = Ce^{ikx} + De^{-ikx}$

To get the full wave function we multiply by the time dependence:

$$\Psi(x,t) = \psi(x)e^{-i\omega t} = Ce^{i(kx-\omega t)} + De^{-i(kx+\omega t)}$$

This is the sum of two traveling waves, each with momentum ħk and energy ħω.

The *C* wave is moving right and the *D* wave is moving left.

Lets pick the right going wave and check it one more time.

Check free particle solution in TDSE

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

For a free particle, *V(x,t)=0*. The solution for a particle moving to the right is $\Psi(x,t) = Ce^{i(kx-\omega t)}$

If we plug this into the TDSE, what do we get?

$$\frac{\partial^2\Psi(x,t)}{\partial x^2} = C(ik)(ik)e^{i(kx-\omega t)} = -Ck^2e^{i(kx-\omega t)} = -k^2\Psi(x,t)$$

$$\frac{\partial\Psi(x,t)}{\partial t} = -Ci\omega e^{i(kx-\omega t)} = -i\omega\Psi(x,t)$$

Putting it all together gives: $$\frac{\hbar^2k^2}{2m}\Psi(x,t) = \hbar\omega\Psi(x,t)$$

Kinetic energy = Total energy

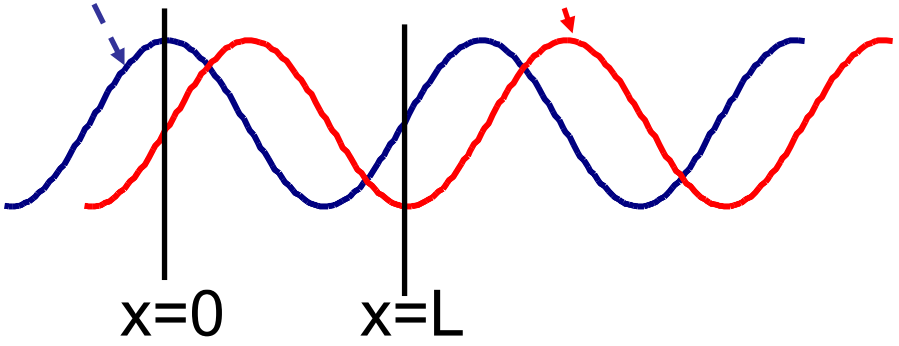
It all works!

Clicker question 1 — Set frequency to DA

Left moving free particle wave function is: $\Psi(x,t) = Ce^{i(kx-\omega t)}$

Can also write as $\Psi(x,t) = C\cos(kx-\omega t) + iC\sin(kx-\omega t)$

The probability of finding the particle at x=0 is __________ to the probability of finding the particle at x=L.



A. Always larger
B. Always smaller
C. Always equal
D. Oscillates between smaller & larger
E. Depends on other quantities like *k*

Get probability from $|\Psi(x,t)|^2$.

$$\Psi^*\Psi = \left(C\cos(kx-\omega t) - iC\sin(kx-\omega t)\right)\left(C\cos(kx-\omega t) + iC\sin(kx-\omega t)\right)$$
$$= C^2[\cos^2(kx-\omega t) + \sin^2(kx-\omega t)] = C^2$$

or $\Psi^*\Psi = Ce^{-i(kx-\omega t)}Ce^{i(kx-\omega t)} = C^2$

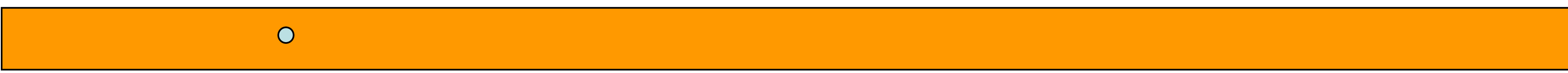
Probability is constant (same everywhere and everywhen)

Electrons in wire

We just solved the free particle in 1D problem.

Remember, free particle means there is no force acting on it.

An electron in a very long (technically infinite) copper wire with no voltage on it would have the <u>same</u> wave function.



<u>Next: Wave function of electron in a *short* (length *a*) copper wire.</u>

Use TISE:

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

We will first figure out V(x), then find the solution, and finally analyze what the solution means physically.

Clicker question 2

Set frequency to DA

What can we say about V(x) for an electron inside a copper wire which extends from x=0 to x=a?

Hint: consider what we learned from the photoelectric effect.

A. V(x) is smaller in the region 0<x<a

B. V(x) is constant over all values of x

C. V(x) is constant in the region x<0 and x>a

D. More than one of the above

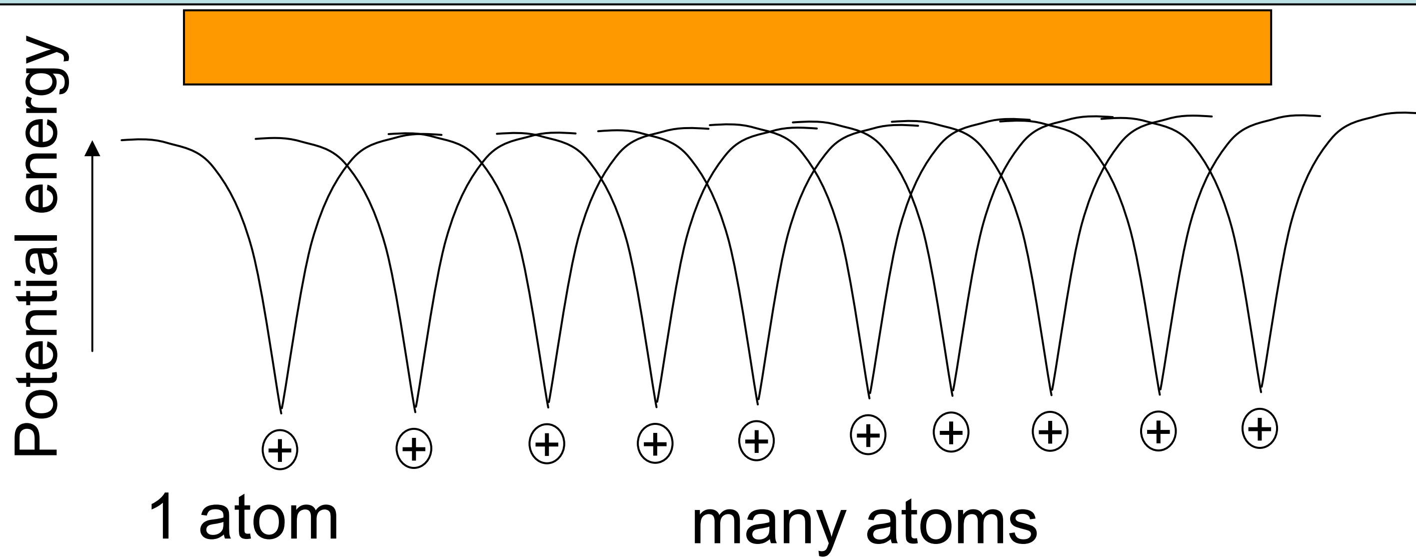
E. None of the above

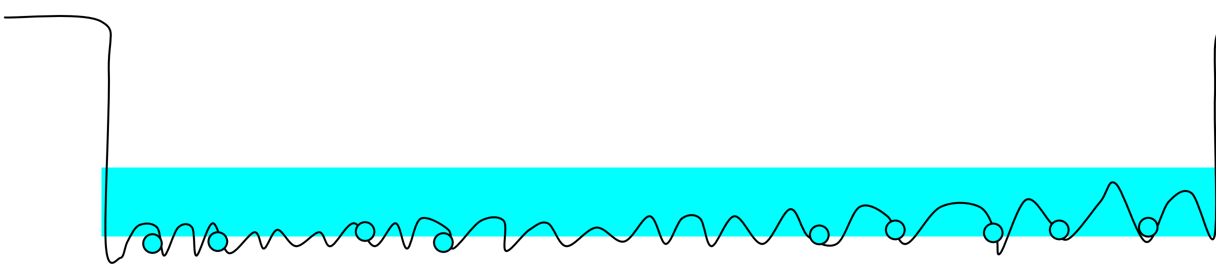
Photoelectric effect showed us that it takes energy to remove an electron from a metal

So electron “wants” to be in the metal (smaller PE)

Outside the wire (x<0 or x>a) it’s a free particle: V(x) is constant

Potential energy in a metal





electrons move around to points of lowest potential

The electrons fill in and are uniformly distributed.

The potential energy ends up being constant

Potential energy in a metal

The regular array of positive charges creates the “potential well”

The electrons fill in the well up to a certain level

The top most electrons in the well are the easiest to remove

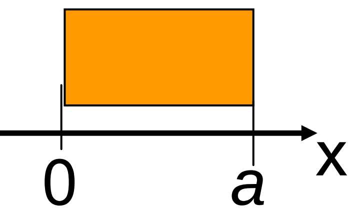
What energy is required to remove the top most electron?

The work function of the metal (4.7 eV for copper).

Clicker question 3

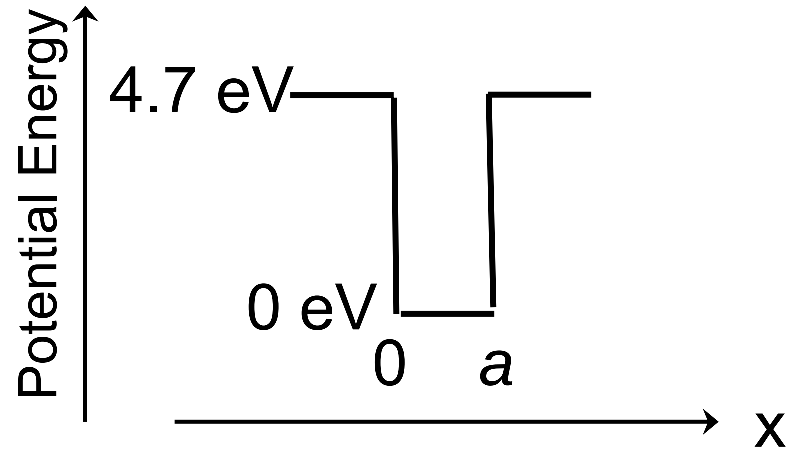
Set frequency to DA

Physical picture



Potential energy V(x)

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



The thermal energy of an electron is approximately $k_B T$ which is equal to ~0.025 eV at room temperature.

How likely is it that the electron is outside the well?

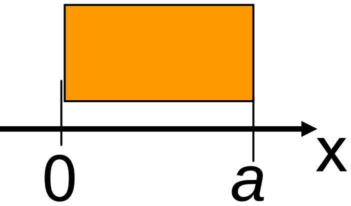
A. impossible
B. very unlikely
C. somewhat unlikely
D. likely
E. impossible to tell

Likelihood is about $e^{-4.7/0.025} = 10^{-82}$ which is a very small probability indeed!

Note, we could have made the bottom of the well -4.7 eV and the top 0 eV. Get the same results but a little more complicated.

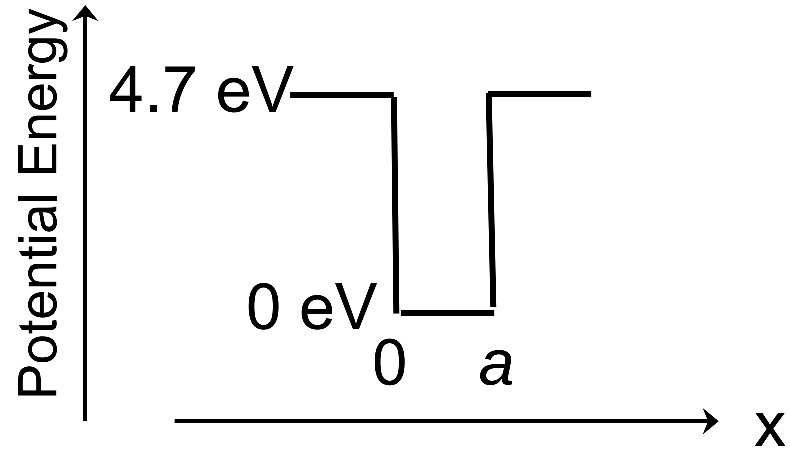
Set frequency to DA

Physical picture



Potential energy V(x)

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



For this scenario, what can we say about ψ(x)?

A. $\psi(x)$ is the same for all x

B. $\psi(x)$ is ~0 for $0<x<a$ and not 0 for $x<0$ and $x>a$

C. $\psi(x)$ is ~0 for $x<0$ and $x>a$ and not 0 for $0<x<a$

D. $\psi(x)$ is not ~0 anywhere

This is similar to the guitar string boundary condition

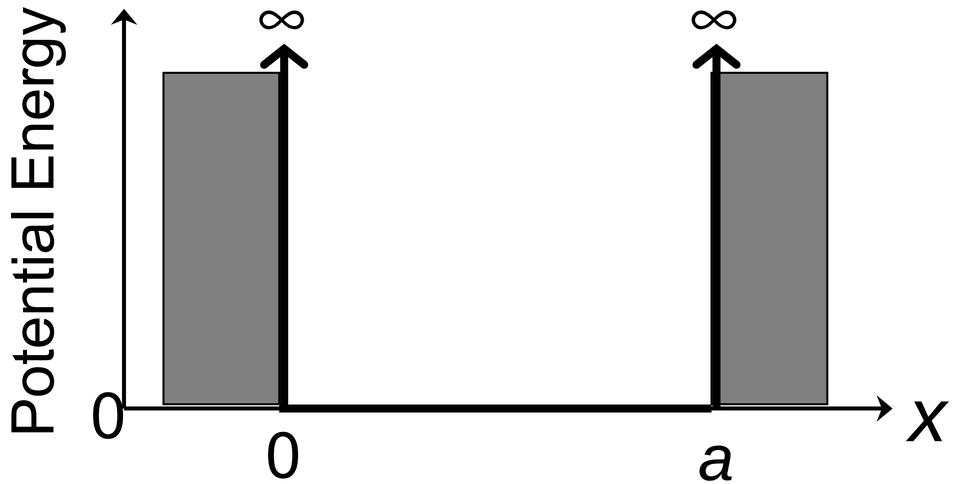
The infinite square well (particle in a box)

So the approximate potential energy function is

$x < 0$: $V(x) \approx \infty$

$x > a$: $V(x) \approx \infty$

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



This is called the *infinite square well* (referring to the potential energy graph) or *particle in a box* (since the particle is trapped inside a 1D box of length *a*.

We are interested in the region $0 < x < a$ where $V(x) = 0$ so

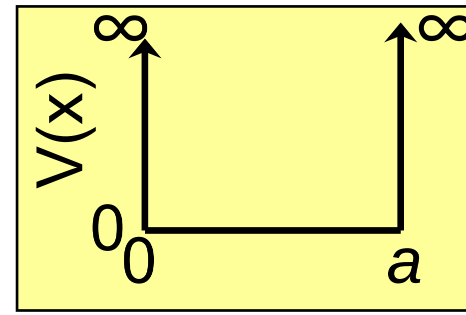
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad \text{becomes} \quad -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

This is the same equation as the free particle. But now we will also need to apply the boundary conditions $\psi(0) = 0$ and $\psi(a) = 0$.

Infinite square well solution

From the free particle we know the functional form of the solution to $-\dfrac{\hbar^2}{2m}\dfrac{d^2\psi(x)}{dx^2} = E\psi(x)$

is $\psi(x) = A\cos(kx) + B\sin(kx)$



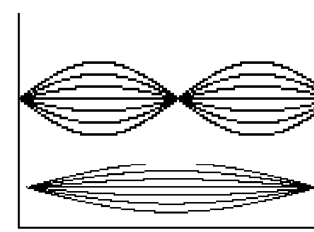
Now we apply the boundary conditions

Putting in $x = 0$ gives $\psi(0) = A$ so $A = 0$

Putting in $x = a$ gives $\psi(a) = B\sin(ka)$

To get $\sin(ka) = 0$ requires $ka = n\pi$

Get the condition $k = \dfrac{n\pi}{a}$; same as the guitar string.



We also know $k = \dfrac{2\pi}{\lambda}$ so that $\lambda = \dfrac{2a}{n}$

Clicker question 5 — Set frequency to DA

For an infinite square well, what are the possible values for *E*?

A. $E_n = \dfrac{\pi^2\hbar^2}{nma^2}$

B. $E_n = \dfrac{nhc}{2a}$

C. $E_n = \dfrac{n^2\pi^2\hbar^2}{2ma^2}$

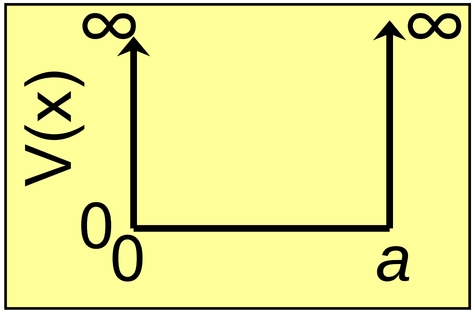
D. $E_n = \dfrac{n\pi^2\hbar^2}{ma^2}$

E. Any value (*E* is not quantized)

$$k = \frac{2\pi}{\lambda}$$

$$k = \frac{n\pi}{a}$$

$$\lambda = \frac{2a}{n}$$



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

$$\psi(x) = B\sin(kx)$$

Putting $\psi(x) = B\sin(kx)$ into the TISE $-\dfrac{\hbar^2}{2m}\dfrac{d^2\psi(x)}{dx^2} = E\psi(x)$

gives $\dfrac{\hbar^2 k^2}{2m}\psi(x) = E\psi(x)$ so $E = \dfrac{\hbar^2 k^2}{2m}$ (just kinetic energy)

Putting in the *k* quantization condition gives $E = \dfrac{n^2\pi^2\hbar^2}{2ma^2}$