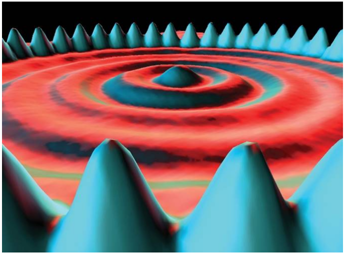
Chapter 7 - Quantum Mechanics



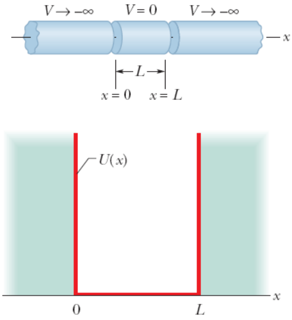
“Not all chemicals are bad. Without chemicals such as hydrogen and oxygen, for example, there would be no way to make water, a vital ingredient in beer.”

-Dave Barry

David J. Starling
Penn State Hazleton
PHYS 214

Infinite Square Well

Let's consider an electron confined to a small region.



Infinite Square Well

Infinite Square Well
Finite Square Well
Electron Traps

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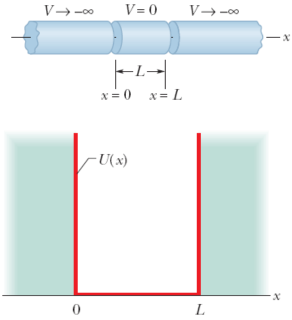

In this case, $\psi(x) = 0$ for $x < 0$ and $x > L$.

Infinite Square Well

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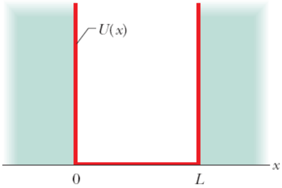
Electron Traps

Inside the well, $U = 0$, *and so the electron is a "free particle."*



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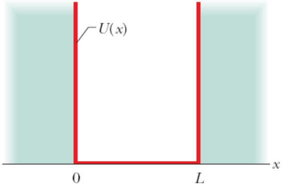

Free particles behave sinusoidally:

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

with $k = 2\pi/\lambda$.

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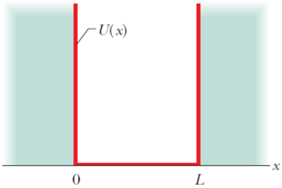
Electron Traps

How do we find k? We impose **boundary conditions.**



Infinite Square Well

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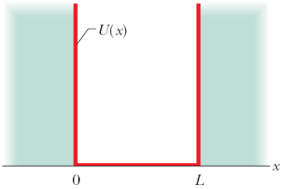

- The wavefunction must be 0 outside the well.
- The wavefunction must be continuous.
- Therefore, $\psi(0) = 0$ and $\psi(L) = 0$.

Infinite Square Well

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Electron Traps

First condition:

$$\psi(0) = A\sin(0) + B\cos(0) = B = 0$$

Infinite Square Well

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Second condition:

$$\begin{aligned} \psi(L) &= A\sin(kL) = 0 \\ \sin(kL) &= 0 \\ kL &= n\pi, \text{ for } n = 1, 2, 3, \ldots \\ k &= \frac{n\pi}{L} \end{aligned}$$

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Final result:

$$\psi(x) = A\sin\left(\frac{n\pi}{L}x\right) \text{ for } n = 1, 2, 3, \ldots$$

Infinite Square Well

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The integer n is called the **principle quantum number** *of the wavefunction.*

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Infinite Square Well

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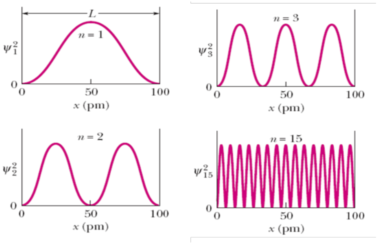
We square the wavefunction to get the probability density:



Infinite Square Well

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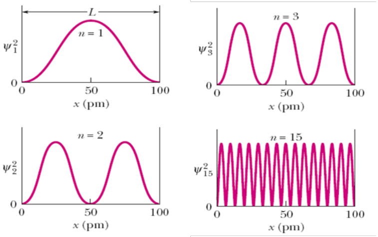
Electron Traps

The probability of finding the electron between the range x_1 and x_2 is

$$P = \int_{x_1}^{x_2} |\psi_n(x)|^2 dx$$



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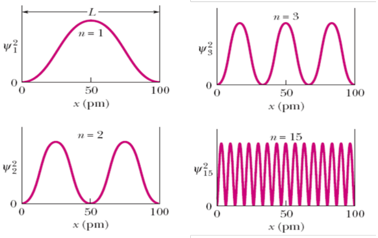

The total probability is of course 1 (100%).

$$P = 1 = \int_{-\infty}^{\infty} |\psi_n(x)|^2 dx$$

Infinite Square Well

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Electron Traps

To find the normalization constant A, we use the probability integral:

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$$1 = \int_0^L \left| A \sin\left(\frac{n\pi}{L} x\right) \right|^2 dx$$

Infinite Square Well

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Finite Square Well
Electron Traps

To find the normalization constant A, we use the probability integral:

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\end{aligned}$$

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$$
\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)
$$

Infinite Square Well

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Finite Square Well
Electron Traps

To find the total energy of the electron for each quantum number, recall that

$$E = K + U = \frac{1}{2}mv^2 + 0 = \frac{p^2}{2m}$$

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Finally, we note that $\lambda = 2\pi/k = 2L/n$, giving

$$E_n = \left(\frac{h^2}{8mL^2}\right)n^2, \text{ for } n = 1, 2, 3, \ldots$$

Infinite Square Well

When the electron (or any other particle) is confined, its energies are **quantized** *and there exist discrete states!*

$$E_n = \left(\frac{h^2}{8mL^2}\right) n^2, \text{ for } n = 1, 2, 3, ...$$

$$\psi_n(x) = A \sin\left(\frac{n\pi}{L}x\right) \text{ for } n = 1, 2, 3, ...$$

Infinite Square Well

For the infinite square well, the energies get farther apart with higher n.

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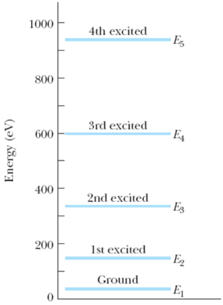
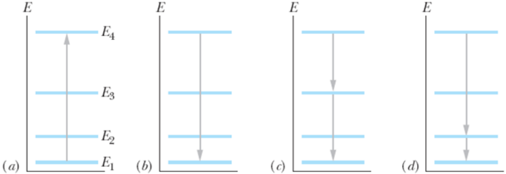


Infinite Square Well

A photon can be absorbed by the electron only if its energy hf is equal to the energy difference between the electron state and a higher state.



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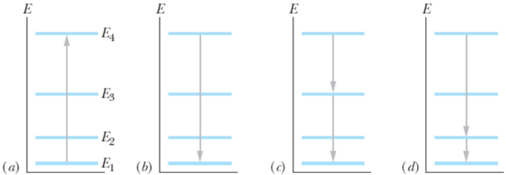


$$E_\gamma = hf = E_{high} - E_{low}$$

When the electron decays, it can do so in a number of ways.

Infinite Square Well

Infinite Square Well
Finite Square Well
Electron Traps

Lecture Question 7.1

Which one of the following transitions between two energy states in the infinite square well requires the largest energy to excite the electron?

(a) $n = 1$ to $n = 2$

(b) $n = 1$ to $n = 4$

(c) $n = 1$ to $n = 14$

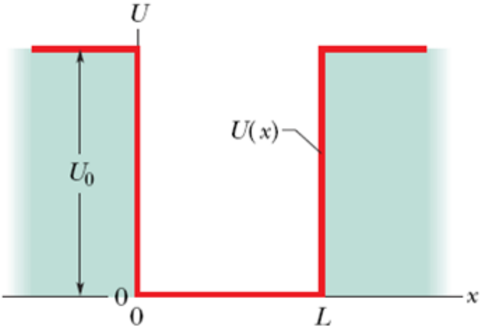
(d) $n = 99$ to $n = 100$

(e) $n = 100$ to $n = 101$

Finite Square Well

Infinite Square Well
Finite Square Well
Electron Traps

The finite square well has walls of finite potential energy U_0.



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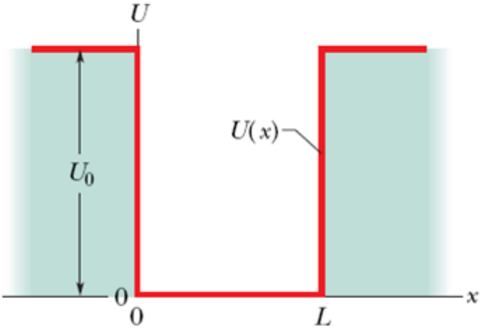

If the particle has energy $E < U_0$, then the particle is trapped within the well like before.

Finite Square Well

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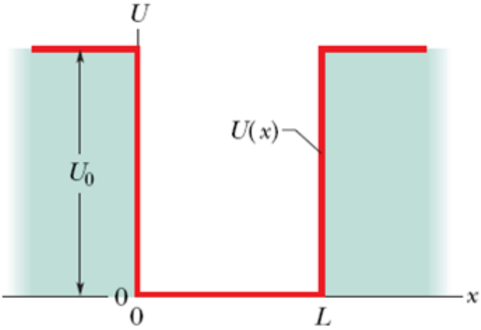

If the particle has energy $E < U_0$, then the particle is trapped within the well like before.

However—the particle can tunnel into the nearby walls.

Finite Square Well

Infinite Square Well
Finite Square Well
Electron Traps

To find the wave function and energy levels, we must again resort to Schrödinger's equation.

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - U)\psi = 0$$

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- Outside the well, we have exponentially decaying solutions.

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$$\psi(x) = \begin{cases} Ae^{ax} & x < 0 \\ B\cos(kx) + C\sin(kx) & 0 < x < L \\ De^{-cx} & x > L \end{cases}$$

Finite Square Well

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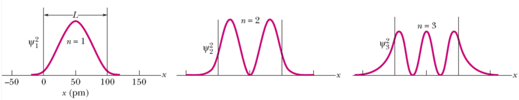
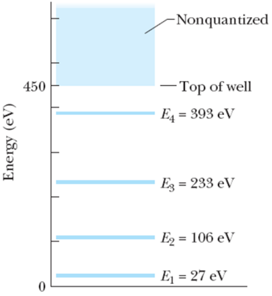
The constants A, B, C, D, a and c need to be determined using normalization, continuity, smoothness and even-ness of the solution.

Finite Square Well

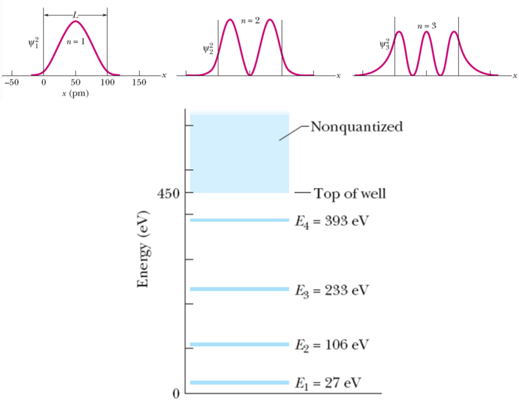
The resulting wavefunctions and energies look similar to the infinite square well.





Finite Square Well

The resulting wavefunctions and energies look similar to the infinite square well.

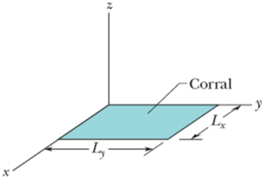


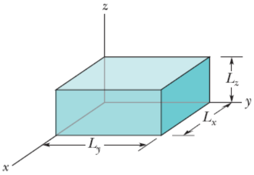
Notice the continuous spectrum of energies above the top.

Electron Traps

Infinite Square Well
Finite Square Well
Electron Traps

Any structure that confines an electron is known as an electron trap.





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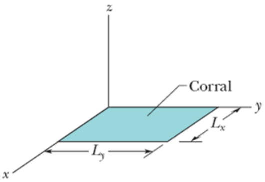
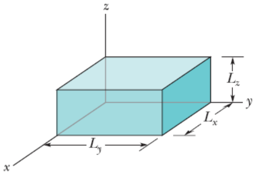


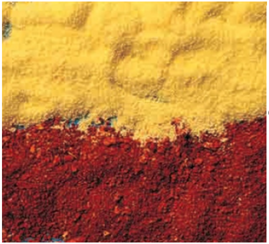


These devices have various uses.

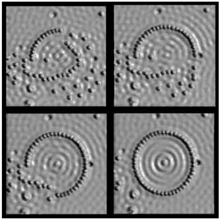
Electron Traps

Infinite Square Well
Finite Square Well
Electron Traps

We can construct granules that have particular colors, or control atoms one at a time.



(a) (c)



(b) (d)

Electron Traps

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Finite Square Well

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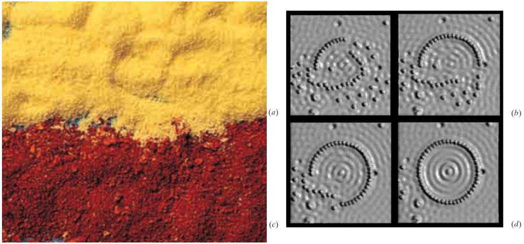
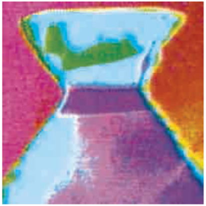


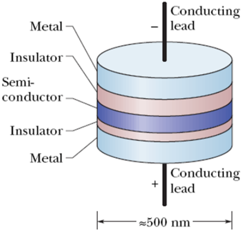
Cadmium selenide of small (top) and large (bottom) granule sizes, and a quantum corral using iron atoms.

Electron Traps

Infinite Square Well
Finite Square Well
Electron Traps

A quantum dot is a useful type of tunable electron trap using semiconductors.





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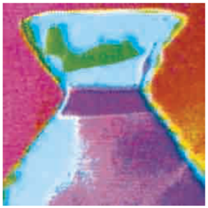

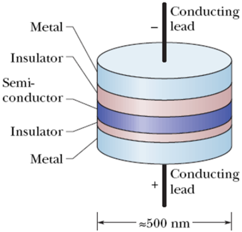

Electrons can be added or subtracted using voltages at the leads.

Infinite Square Well

Infinite Square Well
Finite Square Well
Electron Traps

Lecture Question 7.2

If an electron in a potential trap had zero energy, the electron would be stationary and its momentum would be zero. In such a case, what would be the uncertainty in the *position* of the electron, according to the Heisenberg uncertainty principle?

(a) zero

(b) negative and small

(c) positive and small

(d) negative and infinite

(e) positive and infinite