Quantum Wells

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Lecture 24

Traveling Waves vs Standing Waves

- On a stretched string we can set up both traveling waves and standing waves.
  - A traveling wave, on a long string, can have any frequency.
  - A standing wave, set up on a string with a finite length, can have only discrete frequencies.
- In other words, confining the wave to a finite region of space leads to quantization of the motion — to the existence of discrete states for the wave, each state with a sharply defined frequency.

- This observation applies to waves of all kinds, including matter waves. For matter waves, however, it is more convenient to deal with the energy E of the associated particle than with the frequency f of the wave.
- Consider the matter wave associated with an electron moving in the positive x direction and subject to no net force — a so-called free particle. The energy of such an electron can have any reasonable value, just as a wave traveling along a stretched string of infinite length can have any reasonable frequency.

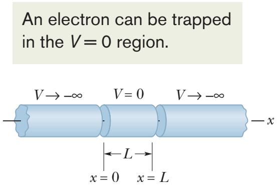
- Consider next the matter wave associated with an atomic electron, perhaps the valence (least tightly bound) electron. The electron — held within the atom by the attractive Coulomb force between it and the positively charged nucleus — is a bound particle. It can exist only in a set of discrete states, each having a discrete energy E. This sounds much like the discrete states and quantized frequencies that apply to a stretched string of finite length.
- For matter waves, then, as for all other kinds of waves, we may state a confinement principle: Confinement of a wave leads to quantization — that is, to the existence of discrete states with discrete energies.

Outline

- An Electron in an Infinite Potential Well
- An Electron in a Finite Potential Well
- Two- and Three-Dimensional Electron Traps

One-Dimensional Infinite Potential Well

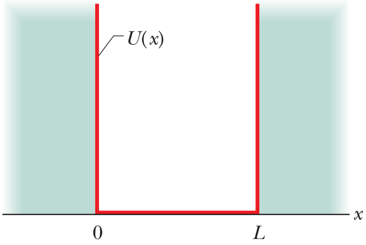
- Consider a nonrelativistic electron confined to a one-dimensional electron trap (or a limited region of space).



- The trap consists of two semi-infinitely long cylinders, each of which has an electric potential approaching $-\infty$; between them is a hollow cylinder of length L, which has an electric potential of zero.
- We put a single electron into this central cylinder to trap it.

- When the electron is in the central cylinder, its potential energy $U = -eV$ is zero.
- If the electron could not get out of this region, its potential energy would be positively infinite outside.
- It is a potential "well" because an electron placed in the central cylinder cannot escape from it.

An electron can be trapped in the $U = 0$ region.



Standing Waves in a 1D Trap

- We examine by analogy with standing waves on a string of finite length, stretched along an x axis and confined between rigid supports.
- Because the supports are rigid, the two ends of the string are nodes, or points at which the string is always at rest.
- The states, or discrete standing wave patterns in which the string can oscillate, are those for which the length L of the string is equal to an integer number of half-wavelengths; that is, the string can occupy only states for which

$$L = \frac{n\lambda}{2}, \text{ for } n = 1, 2, 3, \ldots .$$

- Each value of the integer n identifies a state of the oscillating string.
- For a given n, the transverse displacement of the string at any position x along the string is given by

$$y_n(x) = A \sin\left(\frac{n\pi}{L} x\right),$$

where A is the amplitude of the standing wave.
- For the electron in the trap, we promote the transverse displacement to wave function $\psi_n(x)$.

Probability of Detection

- Classically, we expect to detect the electron anywhere in the infinite well with a constant probability density.
- Quantum mechanically, we find the probability density

$$p_n(x) = |\psi_n(x)|^2 = |A|^2 \sin^2\left(\frac{n\pi}{L}x\right)$$

  for a given n.
- The constant A (up to a phase) can be determined by the **normalization** condition

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = \int_0^L |\psi_n(x)|^2 dx = 1,$$

  so $A = \sqrt{2/L}$.

Energies of the Trapped Electron

- The de Broglie wavelength λ of the electron is defined as

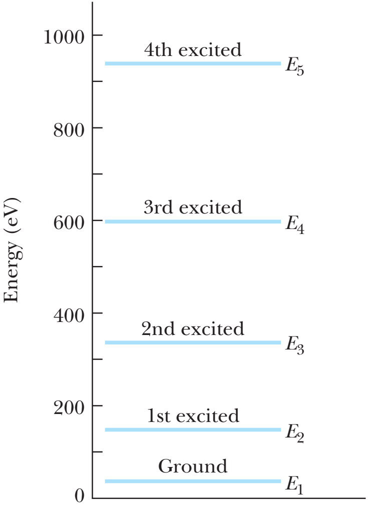
$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mK}},$$

  where $K = p^2/(2m)$ is the kinetic energy of the nonrelativistic electron.
- For an electron moving within the central cylinder, where $U = 0$, the total (mechanical) energy E is equal to the kinetic energy K.

- Therefore, the total energy for an electron moving in the central cylinder is

$$E_n = \left(\frac{h^2}{8mL^2}\right) n^2$$

for $n = 1, 2, 3, \ldots$.
- The positive integer n here is the **quantum number** of the electron's quantum state in the trap.

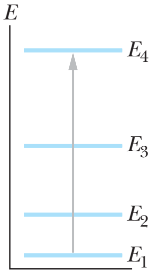


- The quantum state with the lowest possible energy level E_1 with quantum number $n = 1$ is called the **ground state** of the electron.
- Why is $n = 0$ not allowed? Choosing $n = 0$ would indeed yield a lower energy of zero. However, as we will see below, the corresponding probability density is $|\psi|^2 = 0$, which we can interpret only to mean that there is no electron in the well; so $n = 0$ is not a possible quantum number.
- It is an important conclusion of quantum physics that confined systems must always have a certain minimum energy called the **zero-point energy**.

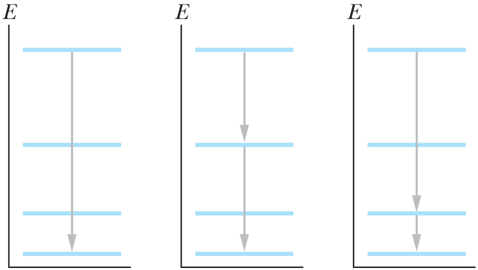
- Electrons can be excited or de-excited by the absorption or emission of a photon with energy

$$\hbar\omega = \frac{hc}{\lambda} = \Delta E = E_{\mathrm{high}} - E_{\mathrm{low}}.$$

The electron is excited to a higher energy level.



It can de-excite to a lower level in several ways (set by chance).



Wave Functions of the Trapped Electron

- If we solve Schroedinger's equation, as in the previous lecture, for an electron trapped in the 1D infinite well of width L, we could write the solutions as

$$\psi_n(x) = \exp\left(i\frac{n\pi}{L}x\right) \text{ or } \psi_n(x) = \exp\left(-i\frac{n\pi}{L}x\right).$$

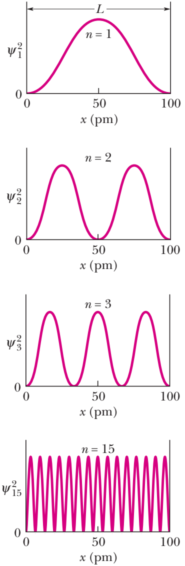
- However, the traveling waves do not satisfy the boundary conditions

$$\psi_n(0) = \psi_n(L) = 0.$$

- The appropriated solutions can only be certain linear combinations of the traveling wave functions, given by

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

for $0 \leq x \leq L$. The constant A is to be determined.
- Note that the wave functions $\psi_n(x)$ have the same form as the displacement functions $y_n(x)$ for a standing wave on a string stretched between rigid supports.

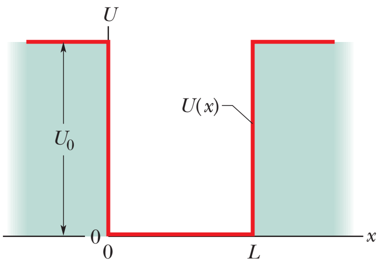


- For sufficiently large n, the probability of detection becomes more and more uniform across the well. This result is an instance of a general principle called the **correspondence principle**: At large enough quantum numbers, the predictions of quantum physics merge smoothly with those of classical physics.

An Electron in a Finite Well

- We can picture an electron trapped in a one-dimensional well between infinite-potential walls as being a standing matter wave. The solutions must be zero at the infinite walls.
- For finite walls, however, the analogy between waves on a stretched string and matter waves fails. Matter wave nodes no longer exist at $x = 0$ and at $x = L$; wave function can penetrate the walls into *classically forbidden* regions.

- To find the wave functions describing the quantum states of an electron in a finite well, we must resort to the time-independent Schroedinger's equation

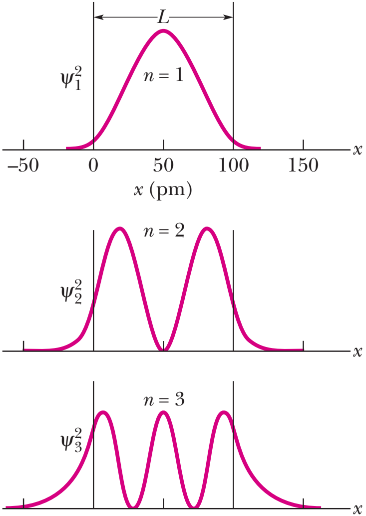


$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\psi(x) = E\psi(x)$$

- Rather than solving this equation for the finite well, much alike what we did in the case of a potential barrier, we proceed with a qualitative discussions.

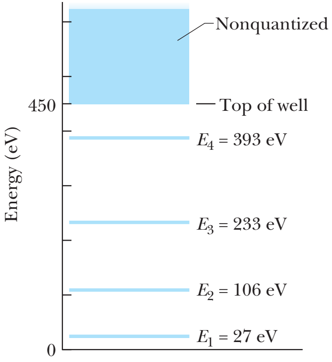
Wave Functions of the Trapped Electron

- As in the tunneling problem, the matter wave "leaks" into the walls of a finite potential energy well; the leakage is greater for greater value of quantum number n.
- As a result, the wavelength λ for any given quantum state is greater when the electron is trapped in a finite well than when it is trapped in an infinite well of the same length L.



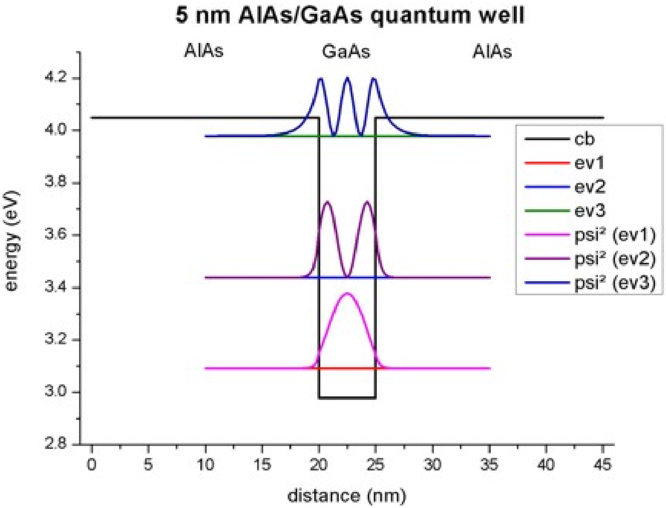
Energies of the Trapped Electron

- Thus, the corresponding energy $E = (h/\lambda)^2/(2m)$ for an electron in any given state is less in the finite well than in the infinite well.
- An electrons with an energy greater than the well depth has too much energy to be trapped in the finite well.



- Thus, there is a continuum of energies beyond the top of the well; a high-energy electron is not confined, and its energy is not quantized.

Semiconductor Quantum Wells



Schroedinger's Equation in High Dimensions

- Assuming $U = 0$. We can generalize Schroedinger's equation to 2D (and similarly to 3D) as

$$E\Psi(x,y) = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]\Psi(x,y).$$

- We are interested in a family of wave functions $\Psi(x,y) = X(x)Y(y)$, whose Schroedinger's equation is equivalent to

$$E = -\frac{\hbar^2}{2m}\frac{1}{X(x)}\frac{\partial^2 X(x)}{\partial x^2} - \frac{\hbar^2}{2m}\frac{1}{Y(y)}\frac{\partial^2 Y(y)}{\partial y^2}.$$

- This has the form $E = F(x) + G(y)$, which can only be satisfied when $F(x) = E_1$ and $G(y) = E - E_1$, i.e., each function must separately be a constant.
- As a consequence, separation of variables breaks the multivariate partial differential equation into a set of independent ordinary differential equations (ODEs).
- We can solve the ODEs for $X(x)$ and $Y(y)$. The wave function for the original equation is simply their product $X(x)Y(y)$.

- Separation of variables was first used by L'Hospital in 1750. It is especially useful in solving equations arising in mathematical physics, such as Laplace's equation, Helmholtz's equation, and Schroedinger's equation.
- Success requires choice of an appropriate coordinate system and may not be attainable at all depending on the equation. In particular, it works when

$$U(x, y) = U_x(x) + U_y(y),$$

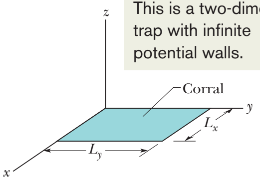
or, in a central potential in spherical coordinates,

$$U(r, \theta, \phi) = V(r).$$

2D & 3D Infinite Potential Wells

- Consider a 2D infinite potential well of widths L_x and L_y (e.g., for an electron on a surface).

This is a two-dimensional trap with infinite potential walls.



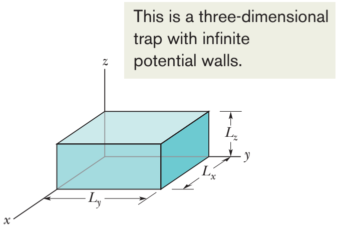
- The normalized wave functions are

$$\psi_n(x, y) = \frac{2}{\sqrt{L_x L_y}} \sin\left(\frac{n_x \pi}{L_x} x\right) \sin\left(\frac{n_y \pi}{L_y} y\right),$$

with two quantum numbers n_x and n_y, and the corresponding energies are

$$E_{n_x, n_y} = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2}\right).$$

- An electrons can also be trapped in a 3D infinite potential well with a volume $V = L_x L_y L_z$. Now a trapped electron has three quantum numbers n_x, n_y, and n_z.



- The normalized wave functions and their energies are

$$\psi_n(x, y, z) = \sqrt{\frac{8}{V}} \sin\left(\frac{n_x \pi}{L_x} x\right) \sin\left(\frac{n_y \pi}{L_y} y\right) \sin\left(\frac{n_z \pi}{L_z} z\right),$$

$$E_{n_x, n_y} = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right).$$

Summary

- For an electron in an infinite potential well, understand
  - the energies of the trapped electron,
  - how photon absorption or emission can change the electron's energy,
  - the wave functions of the trapped electron, and
  - the probability of detecting the electron anywhere in the infinite well.
- Understand the electron energies and wave functions in a finite potential well.
- Understand the energies and wave functions in an infinite well in higher dimensions.

- Understand that the confinement of waves (string waves, matter waves—any type of wave) leads to quantization—that is, discrete states with certain energies. States with intermediate energies are not allowed.

- A free electron has an *extended* wave function:

$$\psi \sim e^{ikx}.$$

- An example of the *localized* wave function is the ground-state wave function of the hydrogen atom,

$$\psi \sim e^{-r/a_B}.$$

Reading

Halliday, Resnick & Krane:

- Chapter 47: Electrons in Potential Wells.