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.

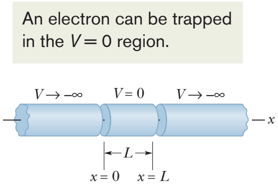
- Consider next the matter wave associated with an atomic electron, perhaps the valence (least tightly bound) electron. The electron — held within the atom by the attractive Coulomb force between it and the positively charged nucleus — is a bound particle. It can exist only in a set of discrete states, 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

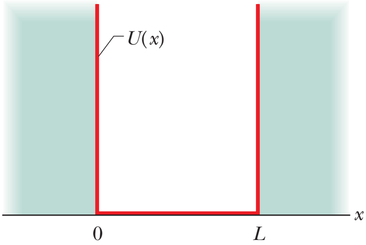
- Consider a nonrelativistic electron confined to a one-dimensional electron trap (or a limited region of space).



- The trap consists of two semi-infinitely long cylinders, each of which has an electric potential approaching $-\infty$, i.e., $U = -|q|V \to +\infty$ with $V \to -\infty$; 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 $(0 \leq x \leq L)$ 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

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

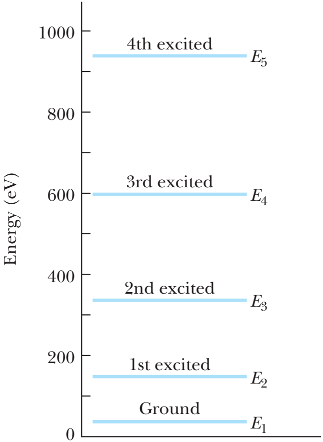
  where $K = p^2/(2m)$ is the kinetic energy of the nonrelativistic electron.
- For an electron moving within the central cylinder, where $U = 0$, the total (mechanical) energy E is equal to the kinetic energy K.

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

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

for $n = 1, 2, 3, \ldots$.
Narrower well (smaller L) $\Rightarrow E_n \nearrow$.

- The positive integer n here is the **quantum number** of the electron's quantum state in the trap.

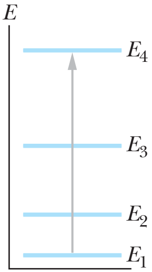


- The quantum state with the lowest possible energy level E_1 with quantum number $n = 1$ is called the **ground state** of the electron.
- Why is $n = 0$ not allowed? Choosing $n = 0$ would indeed yield a lower energy of zero. However, as we will see below, the corresponding probability density is $|\psi|^2 = 0$, 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 non-zero minimum energy called the **zero-point energy**.

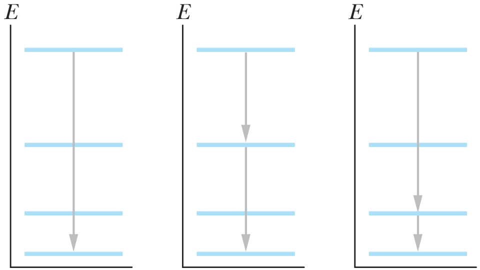
- Electrons can be excited or de-excited by the absorption or emission of a photon with energy

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

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 time-independent 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 above traveling waves do not satisfy the boundary conditions

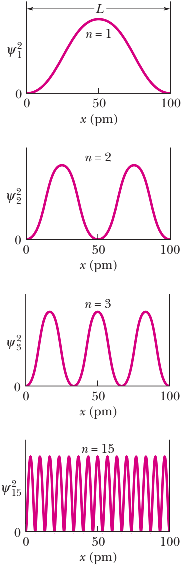
$$\psi_n(0) = \psi_n(L) = 0.$$

- The appropriate 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 $0 \le x \le L$. 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.

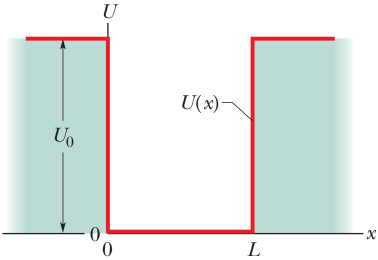


- For sufficiently large n, the probability of detection becomes more and more uniform across the well in the coarse-grained scale. This result is an instance of a general principle called the **correspondence principle**: At large enough quantum numbers, the predictions of quantum physics merge smoothly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

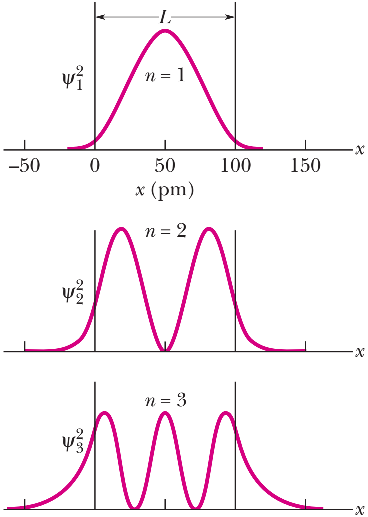


$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+U(x)\psi(x)=E\psi(x).$$

- 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 discussion.

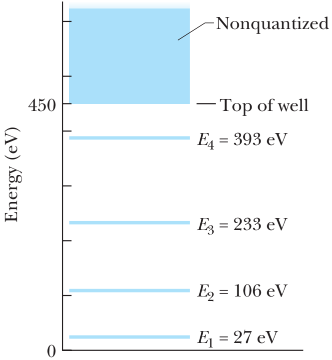
Wave Functions of the Trapped Electron ($E < U_0$)

- 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.



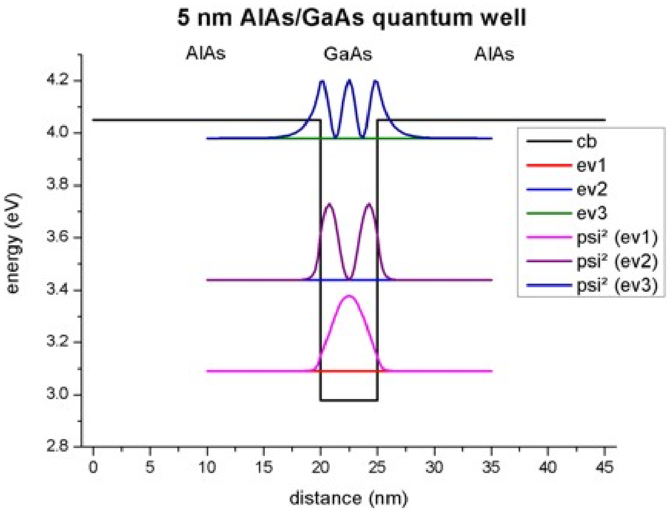
Energies of the Trapped Electron

- Thus, the corresponding energy $E \approx (h/\lambda)^2/(2m)$ 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 $(E > U_0)$ 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 $X(x)Y(y)$. [In which case $\Psi(x, y)$ can be written in the form of $\Psi(x, y) = X(x)Y(y)$, and in which case cannot be?]

- 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

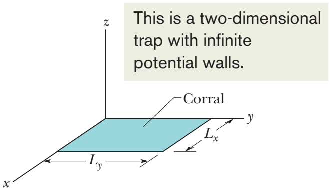
$$U(x, y) = U_x(x) + U_y(y),$$

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).
- The normalized wave functions are



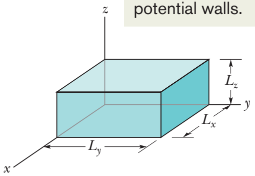
$$\psi_n(x, y) = \frac{2}{\sqrt{L_x L_y}} \sin\left(\frac{n_x \pi}{L_x} x\right) \sin\left(\frac{n_y \pi}{L_y} y\right),$$

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.

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



- The normalized wave functions and their energies are

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

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

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 discrete energies are allowed. 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.