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Modern physics

4. Barriers and wells

Outline

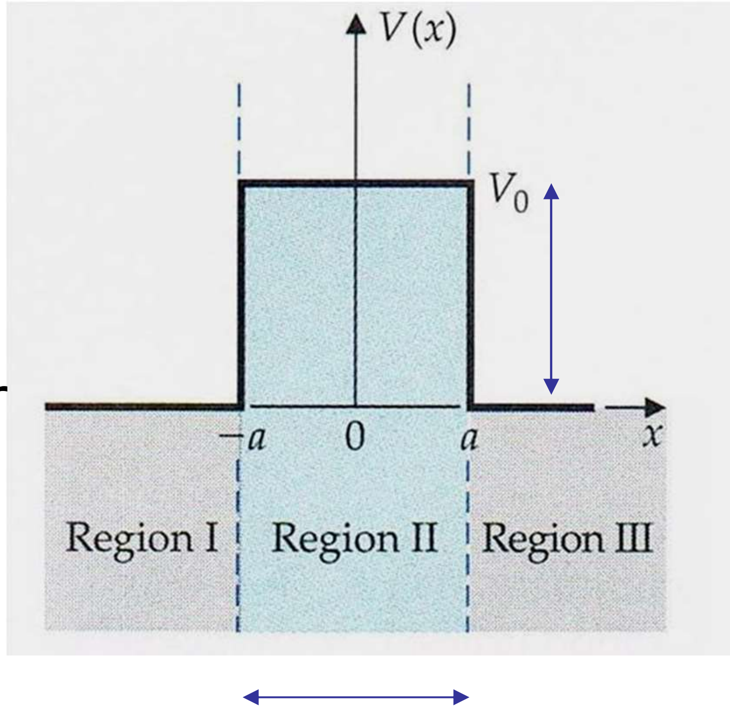
4.1. Particle motion in the presence of a potential barrier
4.2. Wave functions in the presence of a potential barrier
4.3. Tunneling through the potential barrier
4.4. Applications and examples of tunneling: alpha decay, nuclear fusion, scanning tunneling microscope STM
4.5. Bound states
4.6. Quantum corrals

4.1. Particle motion in the presence of a potential barrier

A one-dimensional potential barrier is formed by a potential-energy function of the form

$$V(x)=\begin{cases} 0 \text{ for } x<-a \text{ (region I)} \\ V_0 \text{ for } -a<x<a \text{ (region II)} \\ 0 \text{ for } x>+a \text{ (region III)} \end{cases}$$

barrier height V_0



barrier width $2a$

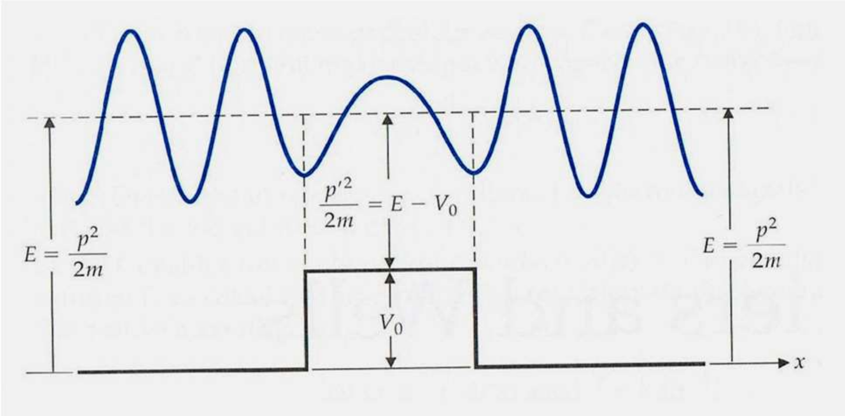
When particle of fixed momentum and energy approaches this potential barrier it can be scattered. The result obtained in classical physics (transmission or reflection) depends on the relationship between the particle energy and barrier height. It is quite different in quantum mechanics

4.1. Particle motion in the presence of a potential barrier

Classically:

if $E>V_0$, then the particle will pass the barrier

if $E<V_0$, then the particle hits a wall and is reflected back



$$p = \sqrt{2mE} \;\Rightarrow\; p = \sqrt{2m(E - V_0)} \;\Rightarrow\; p = \sqrt{2mE}$$

the momentum p changes when the particle is at the top of the barrier but returns to its original value when x=a

4.1. Particle motion in the presence of a potential barrier

In quantum mechanics :

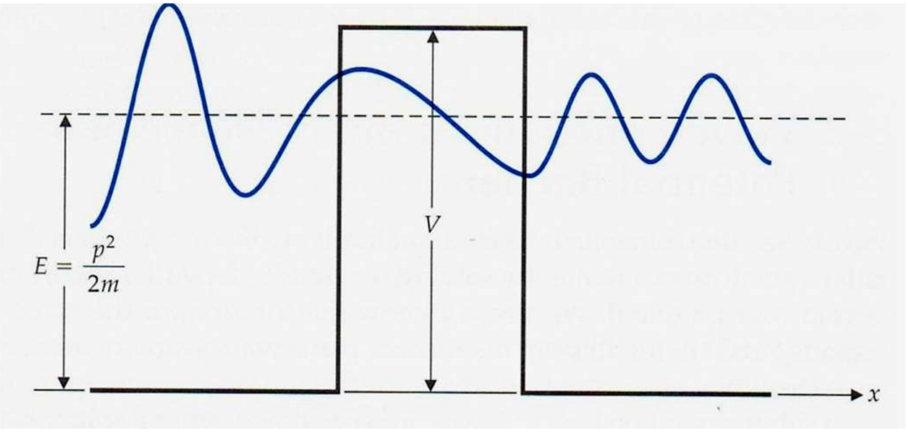
if $E>V_0$, then the particle will pass the barrier or will be reflected from it

if $E<V_0$, then there is a non-zero probability that the particle will be transmitted through the barrier (**barrier tunneling**)

de Broglie wavelength, λ

$$\lambda = \frac{2\pi\hbar}{p} = \frac{2\pi\hbar}{\sqrt{2mE}}$$

is real and the same for x>a and x<-a



For –a<x<a, λ is imaginary

$$\lambda = \frac{2\pi\hbar}{\sqrt{2m(E-V_0)}}$$

classically we have evanescent waves, the exponential decay with x, that is why the amplitude of the wave function for x>a is attenuated

4.2. Wave functions in the presence of a potential barrier

- Wave functions will be obtained as solutions of the time-independent Schrödinger equation

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

- In region I and III, when V(x)=0, the solutions are in the form of well-known plane waves moving either to the right or to the left

4.2. Wave functions in the presence of a potential barrier

- Region I

$$u(x) = \underbrace{\exp(ikx)}_{\text{incident wave}} + \underbrace{R\ \exp(-ikx)}_{\text{reflected wave}} \qquad k^2 = \frac{2mE}{\hbar^2}$$

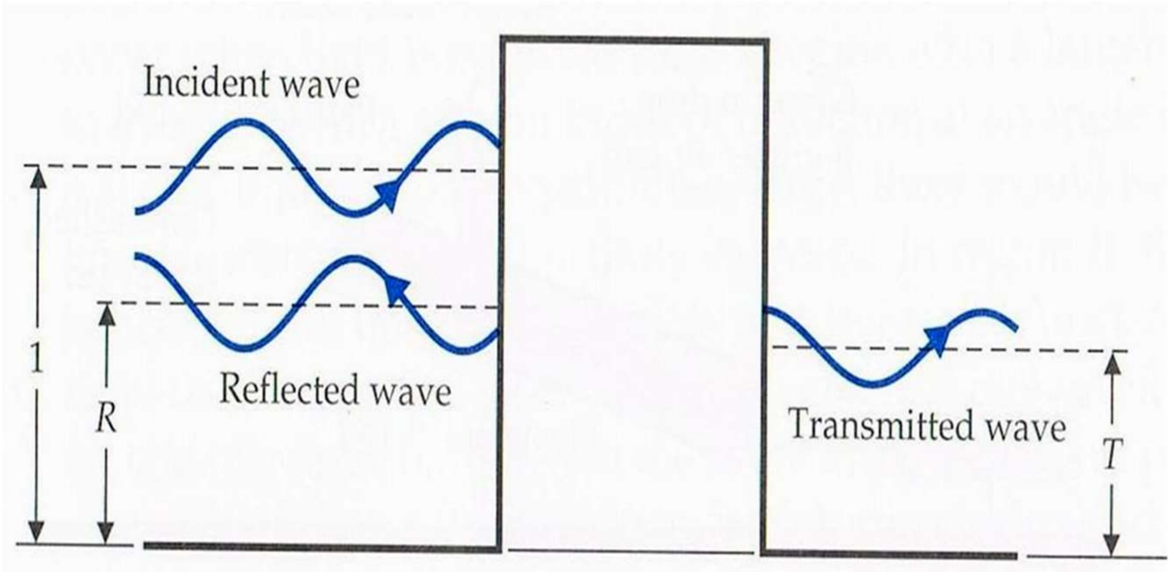
- Region II

$$u(x) = A\exp(iqx) + B\ \exp(-iqx) \qquad q^2 = \frac{2m}{\hbar^2}(E - V_0)$$

coefficients A and B will be found after specifying the physical conditions

- Region III

$$u(x) = \underbrace{T\exp(ikx)}_{\text{transmitted wave, only}}$$



4.2. Wave functions in the presence of a potential barrier

- **Continuity conditions**

As the probability density has to be continuous and the realizable potential is never infinite we insist that:

the wave function and its first derivative be continuous everywhere

When we apply these physical conditions at boundaries $x=-a$ and $x=a$ *(to be done at home)* we finally obtain

$$R=\frac{i(q^2-k^2)\sin(2qa)}{2kq\cos(2qa)-i(k^2+q^2)\sin(2qa)}\exp(-2ika)$$

R is a measure of reflectance

$$T=\frac{2qk}{2kq\cos(2qa)-i(k^2+q^2)\sin(2qa)}\exp(-2ika)$$

T is a measure of transmittance

Properties of solutions for E>V_0

We remember that: $k^2 = \frac{2mE}{\hbar^2}$ $q^2 = \frac{2m}{\hbar^2}\left(E - V_0\right)$

1. From these two relations we see that when E>V_0, q is real and when $V_0 \neq 0$, q ≠k thus R is not zero

At energies for which, classically, the particle would not be reflected, in quantum mechanical there is still a possibility that it will be reflected

$$R = \frac{i(q^2 - k^2)\sin(2qa)}{2kq\cos(2qa) - i(k^2 + q^2)\sin(2qa)}\exp(-2ika)$$

2. When E>>V_0, then q≈k, and $R \cong \frac{V_0}{E}$ In this limit $T \to 1$

3. Always $|T|^2 + |R|^2 = 1$ and $|R|^2 \leq 1$

4.3. Tunneling through the potential barrier

Solutions for E<V_0

Classically, a particle will bounce back from such a barrier in perfect reflection. In quantum mechanics the particle has a chance to tunnel through the barrier, especially if the barrier is thin.

In such a case:

$$q^2 = \frac{2m}{\hbar^2}(E - V_0) < 0$$

q is imaginary and the solutions for T show an exponential decay

$$|T|^2 = \frac{16k^2\kappa^2}{(k^2+\kappa^2)^2}\exp(-4\kappa a)$$

$$\kappa^2 = \frac{2m}{\hbar^2}(V_0 - E)$$

a is the barrier thickness

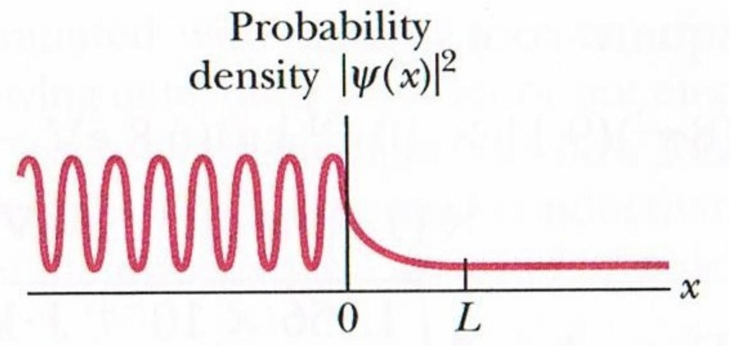
4.3. Tunneling through the potential barrier

The transmission coefficient $|T|^2$ gives the probability with which the particle is transmitted through the barrier, i.e. the probability of tunneling.

Example: If $|T|^2$=0.020, then of every 1000 particles (electrons) approaching a barrier, 20 (on average) will tunnel through it and 980 will be reflected.

$$\boxed{|T|^2 \cong \exp(-4\kappa a)}$$

$$\kappa^2 = \frac{2m}{\hbar^2}(V_0 - E)$$



Because of the exponential form the transmission coefficient is very sensitive to the three variables on which it depends: particle mass m, barrier thickness a, and energy difference V_0-*E*

4.4. Applications and examples of tunneling: alpha decay, nuclear fusion, scanning tunneling microscope STM

Barrier tunneling has many applications (especially in electronics), i.e., **tunnel diode** in which a flow of electrons produced by tunneling can be rapidly turned on and off by controlling the barrier height.

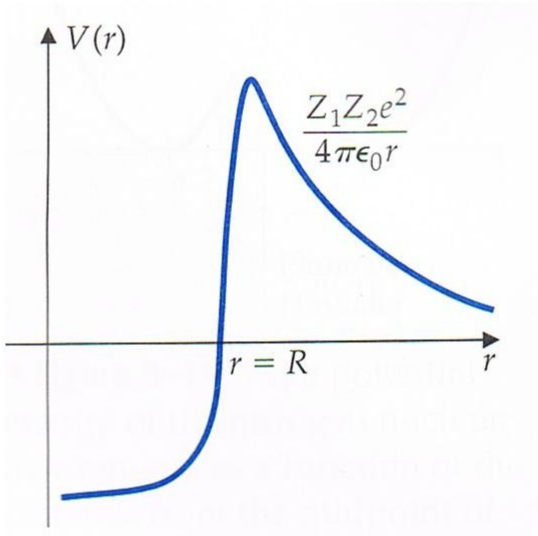
- In 1973 Nobel Prize in physics was shared by Leo Esaki (for tunneling in semiconductors), Ivar Giaever (for tunneling in superconductors) and Brian Josephson (for the Josephson junction, rapid quantum switching device based on tunneling)
- In 1986 Gerd Binning and Heinrich Rohrer for development of scanning tunneling microscope STM
- The earliest (late 1920s) application of tunneling was to nuclear physics: alpha decay (George Gamow, Ronald Gurney, Edward U. Condon) and nuclear fusion.

Alpha decay

An unstable parent nucleus converts into a daughter nucleus with the emission of an alpha particle α– a helium nucleus, ${}^{4}_{2}\mathrm{He}$

A-atomic weight

$$\underbrace{{}^{A}Z}_{\text{parent nucleus}} \rightarrow \underbrace{{}^{A-4}Z}_{\text{daughter nucleus}} + \alpha$$



Example:

$$^{241}Am \rightarrow {}^{237}Np + \alpha$$

Alpha decay can be perfectly explained by the tunneling phenomenon in which α particle tunnels through the Coulomb barrier formed by the combination of the Coulomb and nuclear potential energies.

Alpha decay

The success of the application of tunneling to the explanation of alpha decay manifested itself in the first determination of the radius R of nucleus

$$R \cong 1.5 A^{1/3}\, fm$$

This early result revealed that the volume of the nucleus:

$$V = \frac{4\pi}{3} R^3$$

was proportional to its atomic weight *A*, so that the nuclear density was almost constant.

The result also demonstrated just how small the nucleus was.

Nuclear fusion

Nuclear fusion has a potentially important technological application to the production of **clean nuclear power**.

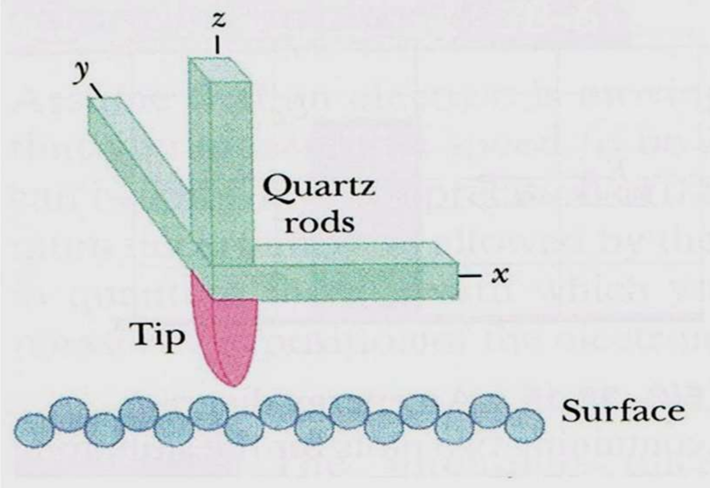
An important reaction involves the fusion of two deuterons to make a triton and a neutron, with the release of a great deal of energy.

$$\underbrace{{}^{2}H + {}^{2}H}_{\text{deuteron}} \rightarrow \underbrace{{}^{3}H}_{\text{triton}} + \underbrace{n}_{\text{neutron}} + \underbrace{6.4\times10^{-13}\,J}_{\text{energy released}}$$

Coulomb repulsion between two deuterons inhibits this process. This process can take place only because of **tunneling** through the Coulomb barrier. However, it is necessary to reach a temperature on the order of 10^4K to have a practical reaction rate.

Scanning tunneling microscope STM

Three quartz rods are used to scan a sharply pointed conducting tip across the surface.



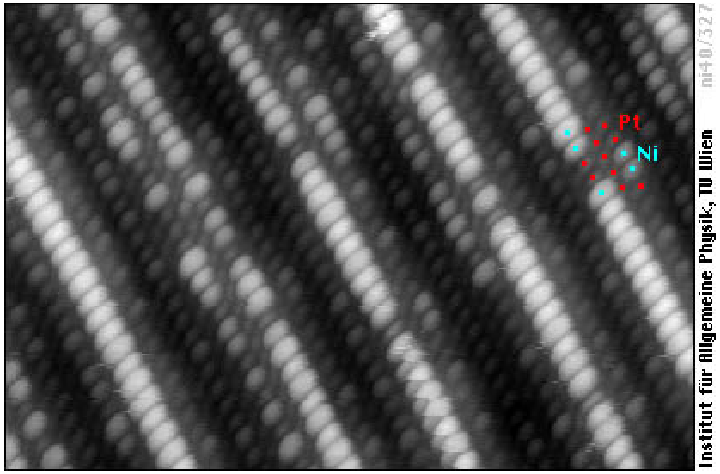
Principle of operation

A weak positive potential is placed on an extremely fine tungsten tip. When the distance between the tip and the metallic surface is small, a tunneling effect takes place. The number of electrons that flow from the surface to the tip per unit time (electric current) is very sensitive to the distance between the tip and the surface.

Quartz rods form a piezoelectric support, their elastic properties depend on the applied electric fields. The magnitude of the tunneling current is detected and maintained to keep a constant separation between tip and the surface. The tip moves up and down to match the contours of the surface and a record of its movement forms a map of the surface, an image.

Scanning tunneling microscope STM

The resolution of image depends on the size of the tip. By heating it and applying a strong electric field, one can effectively pull off the tungsten atoms from the tip layer by layer, till one is left with a tip that consists of a single atom, of size 0.1 nm.

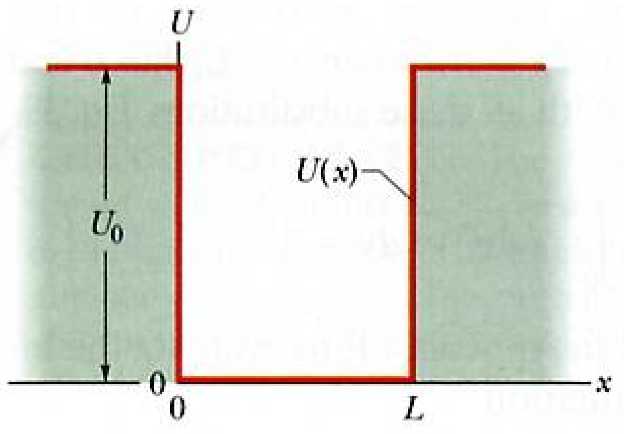


Another important application of STM is in **nanotechnology**. The tip can lift single atoms out of the metallic surface, one at a time and form a new structure at the nano-scale. It is of great value in construction of ultrasmall circuits and the creation of new, artificial molecules.

4.5. Bound states

A potential energy well of **infinite depth** is an idealization. A **finite well** in which the potential energy of electron outside the well has a finite positive value U_o (wall depth) is realizable.

finite well



To find the wave functions describing the quantum states of an electron in the finite potential well, the Schrödinger equation has to be solved. The continuity conditions at the well boundaries (x=0 and x=L) have to be imposed.

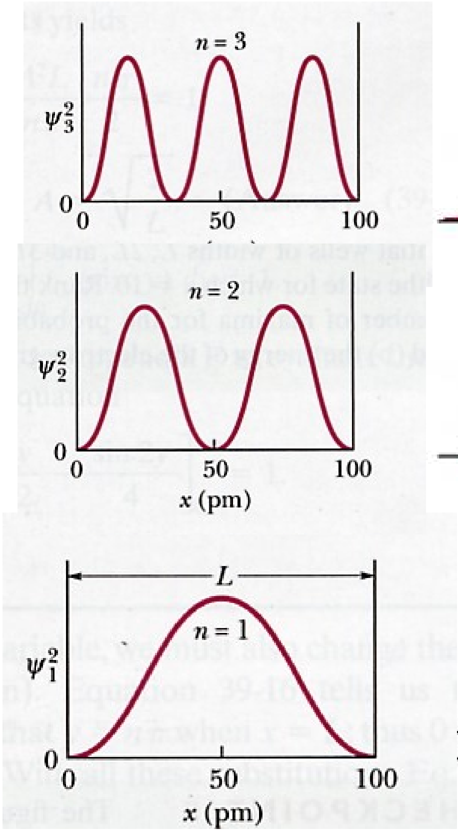
4.5. Bound states

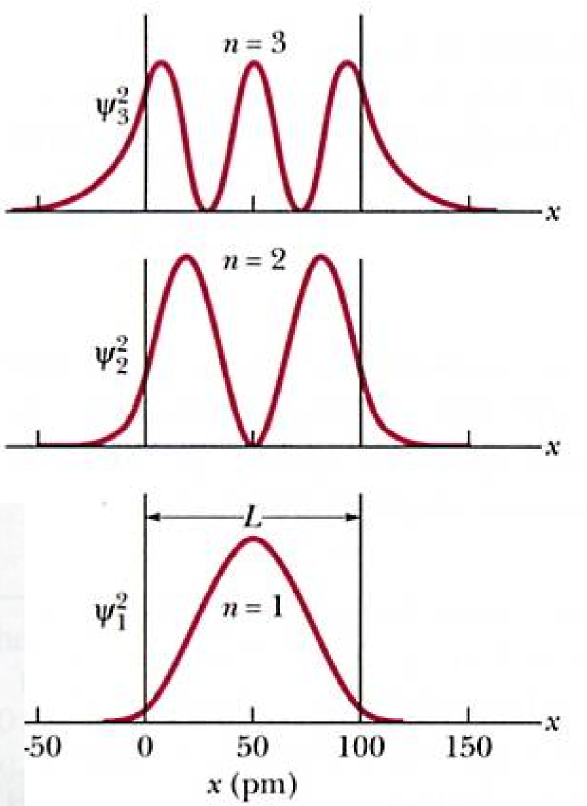
Probability density for an electron confined to the potential well

infinite well | finite well

Basic difference between the infinite and finite well is that for a finite well, the electron matter wave penetrates the walls of the well (leaks into the walls). Newtonian mechanics does not allow electron to exist there.

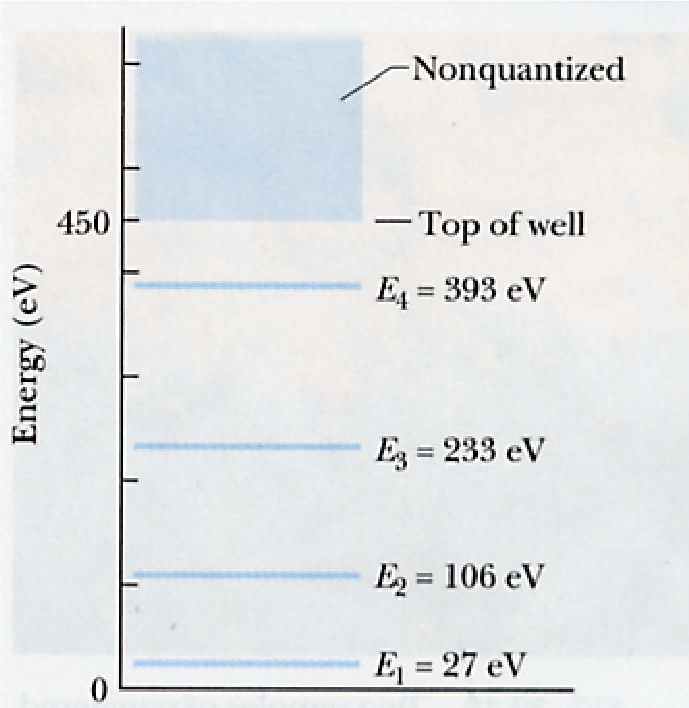
Because a matter wave ***does* leak** into the walls the wavelength λ for any given quantum state is greater when the electron is trapped in a finite wave than when it is trapped in an infinite wave





4.5. Bound states

The energy level diagram for finite well



From:
$$\lambda = \frac{\hbar}{\sqrt{2mE}}$$

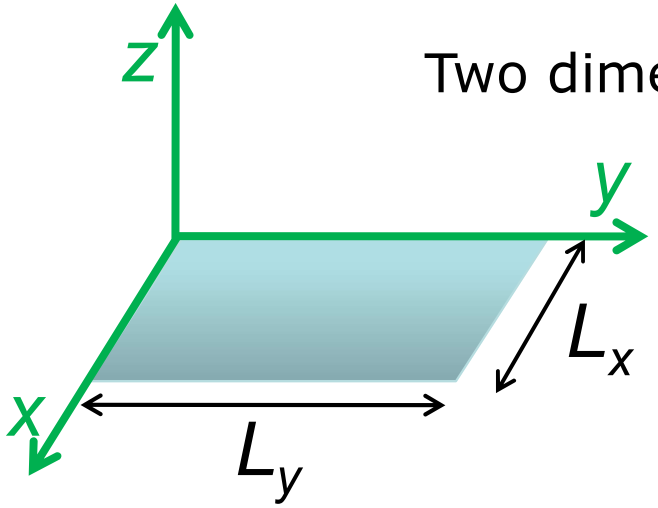
we see that the energy *E* for an electron in any given state is less in the finite well than in the infinite well

The electron with an energy greater than U_0 (450 eV in this example) has too much energy to be trapped. Thus it is **not confined** and its energy is **not quantized**.

For a given well (e.g. U_0=450 eV and L=100 pm) only a limited number of states can exist (in this case n=1,2,3,4). We say that up to a certain energy electron will be **bound (trapped).**

4.6. Quantum corrals

Rectangular corral
Two dimensional 2D infinitive potential well



An electron can be trapped in the rectangular area with widths L_x and L_y as in 2D infinitive potential well.
The rectangular corral might be on the surface of a body that somehow prevents the electron from moving parallel to the *z* axis and thus from leaving the surface.

Solution of Schrödinger's equation for the rectangular corral, shows that, for the electron to be trapped, its matter wave must fit into each of the two widths separately, just as the matter wave of a trapped electron must fit into a 1D infinitive potential well. This means the wave is separately quantized in L_x and L_y.

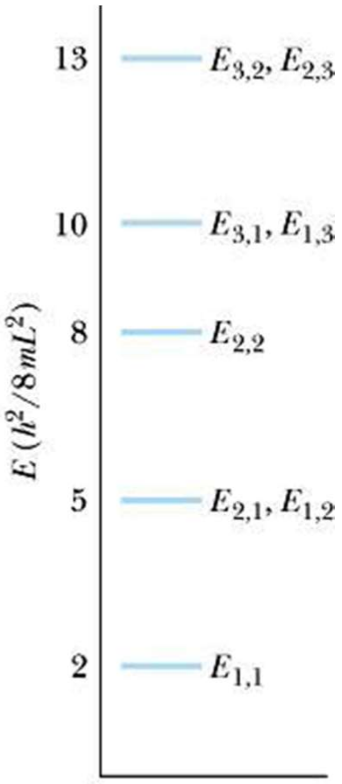
4.6. Quantum corrals

$L_x = L_y$

The energy of the electron depends on both quantum numbers and is the sum of the energy of the electron along x axis and y axis.

$$E_{nx,ny} = \left(\frac{h^2}{8mL_x^2}\right) n_x^2 + \left(\frac{h^2}{8mL_y^2}\right) n_y^2$$

n_x, n_y – quantum numbers, positive integers only



Different states with the same energy are called **degenerate**

Example of degenerate states:

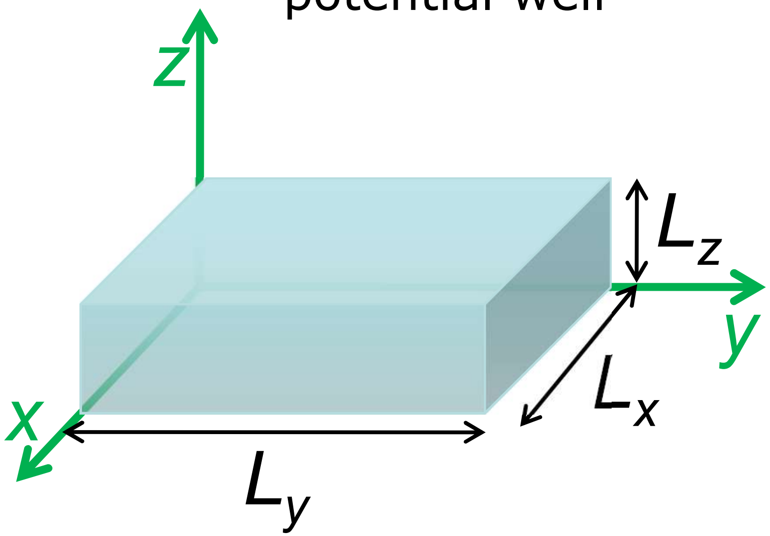
for $L_x=L_y$ the states characterized by quantum numbers $n_x=2$; $n_y=1$ and $n_x=1$; $n_y=2$ have the same energy $E_{21}=E_{12}$

The energy level diagram for an electron trapped in a square corral $L_x=L_y$

Degenerate states cannot occur in a one-dimensional well.

4.6. Quantum corrals

Rectangular box
Three dimensional infinitive potential well



An electron can be trapped in 3 D infinitive potential well – a rectangular box with widths L_x, L_y, L_z.
Then from the Schrödinger's equation we get the energy of electron as:

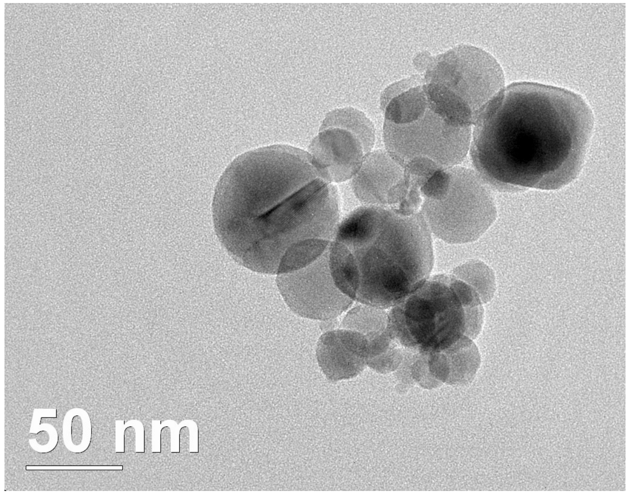
$$E_{nx,ny,nz} = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)$$

In the three dimensional world (real world) there are three quantum numbers to characterize the energetic state of an electron. In the simple model of the infinite potential well (rectangular box) they are denoted as: n_x, n_y, n_z. The real 3D potential of an atom is more complicated but still we get three quantum numbers.

Examples of electron traps

Nanocrystallites

Powders whose granules are small – in the nanometer range – change colour as compared with powder of larger size.



Each such granule – each **nanocrystallite** – acts as a potential well for the electron trapped within it.

For the infinite quantum well we have shown that the energy *E* of the electron is

$$E = \frac{h^2}{8mL^2} n^2$$

When the width *L* of the well is decreased, the energy levels increase. The electron in the well will absorb light with higher energy i.e. shorter wavelength. The same is true for nanocrystallites.

Examples of electron traps

Nanocrystallites

A given nanocrystallite can absorb photons with an energy above a certain threshold energy E_t (=hf_t). Thus, the wavelength below a corresponding threshold wavelength

$$\lambda_f = \frac{c}{f_t} = \frac{ch}{E_t}$$

will be absorbed while that of wavelength longer than λ_f will be scattered by the nanocrystallite.

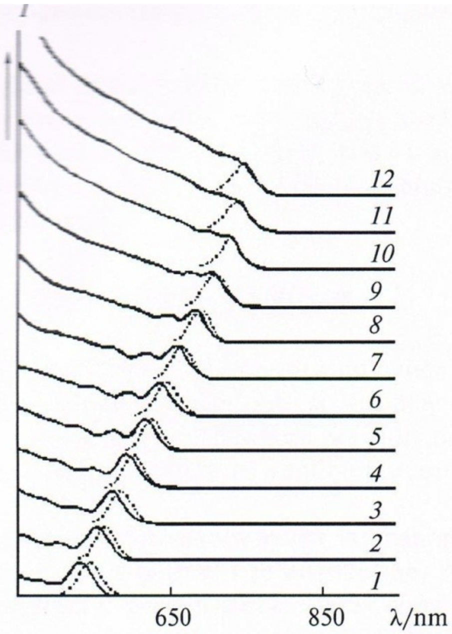
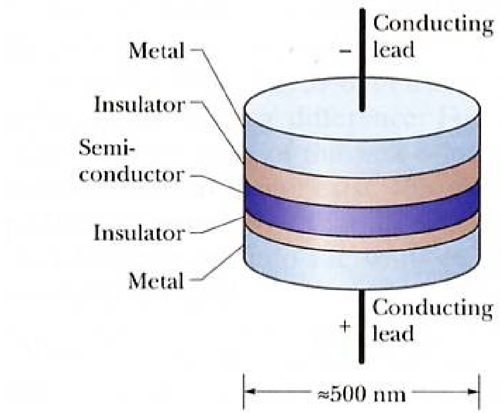


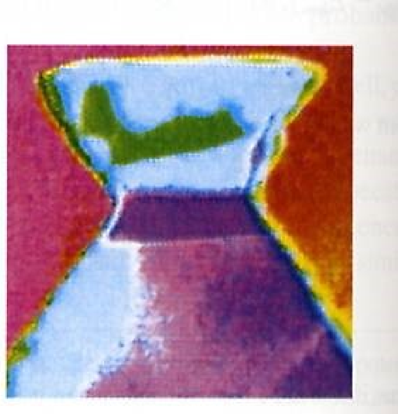
Fig. 2. Shift of absorption bands (solid curves) and photoluminescence bands (dashed lines) with an increase in the size of CdTe nanoparticles[14]: d = 3.2 (*1*), 3.3 (*2*), 3.5 (*3*), 3.6 (*4*), 3.8 (*5*), 4.2 (*6*), 4.6 (*7*), 5.3 (*8*), 6.2 (*9*), 7.7 (*10*), 8.4 (*11*), and 9.1 nm (*12*).

Therefore, when the size of a nanocrytallite is reduced, its colour changes (from red to yellow, for instance).

Examples of electron traps

Quantum dots –artificial atoms





Central semiconducting layer (purple) is deposited between two insulating layers forming a potential energy well in which electrons are trapped. The lower insulating layer is thin enough to permit electrons to tunnel through it if an appropriate potential difference is applied between two metal leads. In this way the number of electrons confined to the well can be controlled.

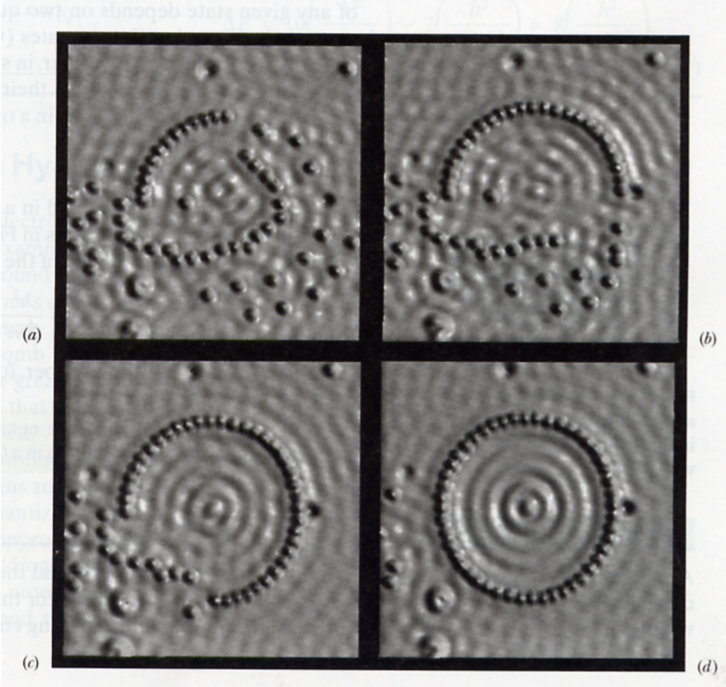
Quantum dots can be constructed in two-dimensional arrays, and have promising applications in computing systems of great speed and storage capacity.

Examples of electron traps

With the use of STM, the scientists at IBM's Almaden Research Center, moved Fe atoms across a carefully prepared Cu surface at low temperature 4K. Atoms forming a circle were named a **quantum corral.**

This structure and especially the ripples inside it are the straightforward demonstration of the existence of matter waves. The ripples are due to electron waves.

Quantum corral



A quantum coral during four stages of construction. Note the appearance of ripples caused by electrons trapped in the corral when it is almost complete.

Conclusions

- The wavelike aspect of matter produces some surprising results. These effects are evident for potential energies with a steplike structures: wells, walls, and barriers.
- The calculation of wave functions for barriers and wells involves solution of Schrödinger equation with the application of continuity conditions at boundaries between different values of the potential energy
- The results obtained are different from those for classical waves. One such feature of a special interest is the penetration of potential-energy barriers. The probability of tunneling might be small but this phenomenon is of great importance
- Examples of tunneling are: in the alpha decay, fusion of deuterons, STM, tunnel diodes and other electronic devices
- Electrons can be trapped in finite potential wells: nanocrystallites, quantum dots and corrals