Lecture 4

Semiconductor physics II

Introduction to Quantum Mechanics

What is Quantum Mechanics

- **Classical theoretical physics**

  -- Newton's laws of motion.

  -- The motion of large objects, such as planets and satellites.

- **Quantum mechanics** （量子物理）

  -- **the behaviors of electrons** （fermions费米子）

  -- the behaviors of high-frequency electromagnetic waves (bosons波色子)

- **Wave mechanics:** The formulation of quantum mechanics to describe behavior and characteristics of these electrons.

  -- Schrodinger wave equation

Principles of Quantum Mechanics

↓

Schrodinger wave equation

↓

The electron behavior in a crystal

↓

The operation and characteristics of semiconductor devices

Principles of Quantum Mechanics

- The principle of energy quanta
  （能量量子化）
- The wave-particle duality principle
  （波粒二象性）
- The uncertainty principle
  （不确定原理）

Principle of energy quanta

Experiment of **photoelectric effect**

-To demonstrate the invalidation of the classical theoretical physics

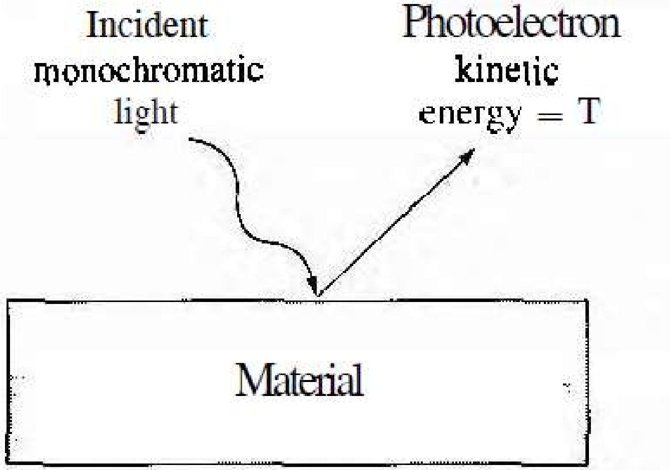


Fig The photoelectric effect

If monochromatic （单色） light is incident on a clean surface of a material, then **under certain conditions**, electrons (photoelectrons) are emitted from the surface.

--- condition in classical theoretical physics: **intensity of the light independent of frequency**.

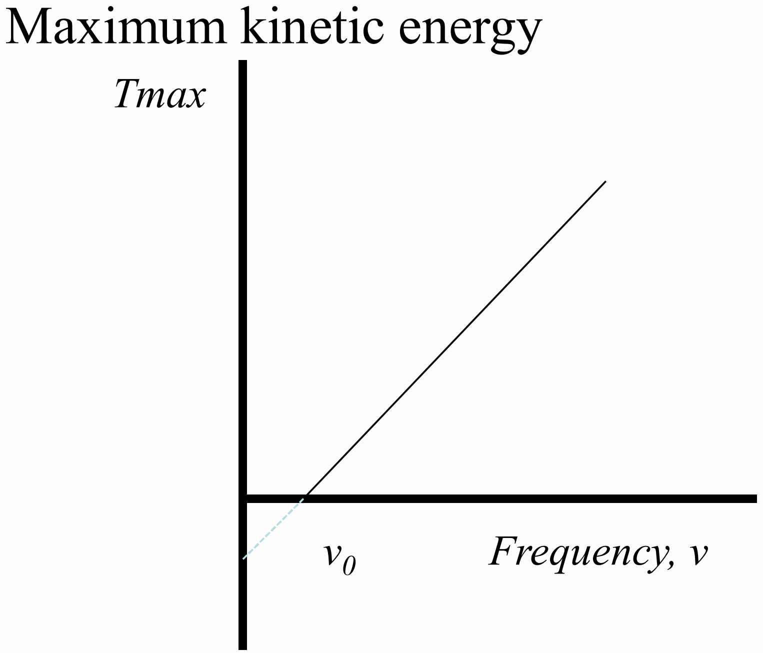


Fig The maximum kinetic energy （动能）of the photoelectron as a function of incident frequency.

Quanta（量子）

－thermal radiation （热辐射） emitted from a heated surface in discrete packets of energy

－Postulated by Planck in 1900

The energy of these quanta

$$E = hv$$

h is a constant known as Planck's constant ($h = 6.625 \times 10^{-34}$ J-s).

v is frequency of the radiation.

If the incident intensity varies at a constant frequency, the rate of photoelectron emission （光电发射效率） changes, but the maximum kinetic energy remains the same.

Photon (光子)– the particle-like packet of energy

In 1905. Einstein interpreted the photoelectric results：
a light wave is also contained in discrete packets or bundles, whose energy is also given by $E = hv$.

A photon with sufficient energy, then, can knock an electron from the surface of the material.

The **work function** （功函数） of the material:

The minimum energy required to remove an electron from the surface, which is hv_0.

The maximum kinetic energy of the photoelectron

$$T_{\max} = \frac{1}{2}mv^2 = hv - hv_0 \quad (v \geq v_0)$$

where hv is the incident photon energy.

hv_0 is the minimum energy, or work function.

Example:

To calculate the photon energy corresponding to a particular wavelength. Consider an x-ray with a wavelength of 0.708 × 10^{-8}cm. Calculate its photon energy.

Solution:

$$E = h\nu = \frac{hc}{\lambda} = \frac{(6.625\times10^{-34})(3\times10^{10})}{0.708\times10^{-8}}$$

$$= 2.81\times10^{-15}\,J$$

c: velocity of light

The reciprocal relation（互反关系） between photon energy and wavelength :

A large energy corresponds to a short wavelength.

Wave-Particle Duality

- The existence of a wave-particle duality principle.

De Broglie hypothesis: since waves exhibit particle-like behavior, then particles should be expected to show wave-like properties. (**subatomic particles（亚原子粒子）: electrons, protons（质子）, and neutrons（中子）**)

- The **momentum** （动量） of a photon is:

$$p = \frac{h}{\lambda}$$

the wavelength of the light wave

The **wavelength** of a particle is:

$$\lambda = \frac{h}{p}$$

de Broglie wavelength of the matter wave

Example:

To calculate the de Broglie wavelength of a particle.

Consider an electron traveling at a velocity of $10^7\,\text{cm/sec} = 10^5\,\text{m/s}$

Solution:

The momentum is given by

$$p = mv = (9.11\times10^{-31})(10^5)$$
$$= 9.11\times10^{-26}$$

Then the de Broglie wavelength is

$$\lambda = \frac{h}{p} = \frac{6.625\times10^{-34}}{9.11\times10^{-26}} = 7.27\times10^{-9}\,m$$

The Uncertainty Principle

- The **Heisenberg uncertainty principle**

  --- given in 1927.

  --- we cannot describe with absolute accuracy the behavior of subatomic particles, including **position** and **momentum** and also **energy** and **time**.

- It is impossible to simultaneously describe with absolute accuracy the position and momentum of a particle.

$$\Delta p \Delta x \geq \hbar$$

the uncertainty in the momentum

the uncertainty in the position

a modified Planck's constant

$$\hbar = \frac{h}{2\pi} = 1.054 \times 10^{-34} \text{ J-s}$$

It is impossible to simultaneously describe with absolute accuracy the energy of a particle and the instant of time the particle has this energy.

$$\Delta E \Delta t \geq \hbar$$

the uncertainty in energy

the uncertainty in time

◆ The simultaneous measurements of position and momentum and of energy and time are in error to a certain extent.

◆ We will develop a **probability density function** （概率密度函数） that will allow us to determine the probability that an electron has a particular energy.

◆ The uncertainty principle is only **significant for subatomic particles**.

Schrodinger's Wave Equation

- Provided by Schrodinger, in 1926.
- Called **wave mechanics**, which incorporated **the principles of quanta** introduced by Planck, and **the wave-particle duality principle** introduced by de Broglie.
- The motion of electrons in a crystal can be described by wave

The one-dimensional, **nonrelativistic** （非相对论）Schrodinger's wave equation

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

the mass of
the particle

the potential function
assumed to be independent of time

the wave function

Using the technique of **separation of variables** **（分离变量法）**

$$\Psi(x,t) = \psi(x)\phi(t)$$

a function of the position   a function of time

Substituting this form of the solution into Schrodinger's wave equation:

$$\frac{-\hbar^2}{2m}\phi(t)\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x)\phi(t) = j\hbar\psi(x)\frac{\partial\phi(t)}{\partial t}$$

Dividing it by the total wave function

$$\frac{-\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = j\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t}$$

(nonrelativistic)=>
a function of position = a function of time = constant

☐ The time-dependent portion

a separation constant $\eta = j\hbar \dfrac{1}{\phi(t)} \dfrac{\partial \phi(t)}{\partial t}$

The solution $\phi(t) = e^{-j(\eta/h)t}$ **---a sinusoidal wave**

η / h is the **radian frequency（角频率）**

We have $E = h\nu$ or $E = h\omega / 2\pi$

Then $\omega = \dfrac{\eta}{h} = E / \hbar$

The separation constant is equal to the total energy *E* of the particle

The time-independent portion

$$\frac{-\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)=E$$

$$\Downarrow$$

$$\boxed{\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2m}{\hbar^2}(E-V(x))\psi(x)=0}$$

This time-independent Schrodinger's wave equation can also be justified on the basis of the classical wave equation.

- The time-independent classical wave equation, in terms of voltage, $\frac{\partial^2 V(x)}{\partial x^2}+(\frac{\omega^2}{v_p^2})V(x)=0$ let $\psi(x)=V(x)$

From the wave-particle duality principle

$$\frac{\omega^2}{v_p^2}=(\frac{2\pi}{\lambda})^2=\frac{2m}{\hbar^2}(\frac{p^2}{2m})=\frac{2m}{\hbar^2}(E-V)$$

$$\frac{p^2}{2m}=T=E-V$$

Physical Meaning of the Wave Function

--- to use the wave function to describe the behavior of an electron in a crystal

the wave function $\Psi(x,t) = \psi(x)\phi(t) = \psi(x)e^{-j(E/\hbar)t}$

$\left|\Psi(x,t)\right|^2 dx$ a **probability density function**, or the probability of finding the particle between Δx *and* $\Delta x + dx$ *at a given time*

$\Psi(x,t)\Psi^*(x,t) = \psi(x)\psi^*(x) = \left|\psi(x)\right|^2$ **independent of time**

---in agreement with the Heisenberg uncertainty principle

Comparisons:

In classical mechanics, the position of a particle can be determined precisely. In quantum mechanics, the position of a particle is found in terms of a probability independent of time.

Boundary Conditions

- Since $|\Psi(x,t)|^2$ represents the probability density function

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

- The wave function and its first derivative must have the following properties if the total energy *E* and the potential *V(x)* are finite everywhere.

Condition 1. *Ψ(x)* must be finite, single valued and continuous.

If *Ψ(x)* were infinite, the probability of finding the particle at some point would be certain. – violate the uncertainty principle.

Condition 2. $\partial\psi(x)/\partial x$ **must be finite, single-valued, and continuous**.

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$$

The second derivative is finite, so the first derivative is continuous.

Application of Schrodinger’s Wave Equation

☐ Electron in Free Space

- ✓ Consider the motion of an electron in free space.
- ✓ There is no force acting on the particle, then the potential function *V*(*x*) will be constant. Assume *V(x)=0.*
- ✓ Then the time-independent wave equation:

$$\boxed{\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2mE}{\hbar^2}\psi(x)=0}$$

Its solution $$\psi(x)=A\exp[\frac{jx\sqrt{2mE}}{\hbar}]+B\exp\left[\frac{-jx\sqrt{2mE}}{\hbar}\right]$$

a traveling wave
in the +*x* direction

a traveling wave
in the -*x* direction

✓ Recall that the time-dependent portion $\psi(t) = e^{-j(\eta/h)t}$

Then the total solution for the wave function

$$\Psi(x,t) = \text{Aexp}\left[\frac{j}{\hbar}(x\sqrt{2mE} - Et)\right] + \text{Bexp}\left[\frac{-j}{\hbar}(x\sqrt{2mE} + Et)\right]$$

☐ Assume, there is the +x traveling wave, which is

$$\Psi(x,t) = \text{Aexp}[j(kx - \omega t)]$$ **----Travelling wave （行波）**

The wave number $k = \dfrac{2\pi}{\lambda}$

the wavelength $\lambda = \dfrac{h}{\sqrt{2mE}}$

The probability density function is a constant AA^*.

A free particle with a well-defined momentum can be found anywhere with equal probability.
$\Rightarrow$ a precise momentum implies an undefined position.
$\Rightarrow$ in agreement with the Heisenberg uncertainty principle

□The Infinite Potential Well (无限深势阱)

The problem of a particle in the infinite potential well is a classic example of a **bound particle**.

The particle is assumed to exist in region II.

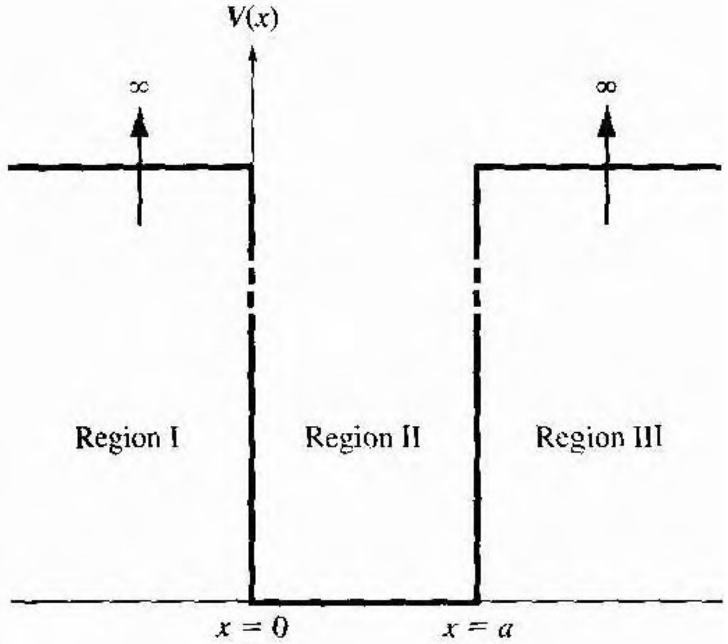


Fig Potential function of the infinite potential well.

The time-independent Schrodinger's wave equation

$$\boxed{\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2m}{\hbar^2}(E-V(x))\psi(x)=0}$$

Assume *V=0* in region II

$$\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2mE}{\hbar^2}\psi(x)=0$$

Its solution

$$\psi(x)=A_1\cos Kx+A_2\ \sin Kx$$

$$\boxed{K=\sqrt{\frac{2mE}{\hbar^2}}}$$

The wave function must be zero in both regions I and region III since the probability of finding the particle in regions I and region III is zero.

=> One boundary condition is that the wave function must be continuous

$$\psi(x=0)=\psi(x=a)=0$$

=> $A_1 = 0$ and $\boxed{K=\dfrac{n\pi}{a}}$

Since $\int_{-\infty}^{\infty}\psi(x)\psi^*(x)dx=1$

$$\int_0^a A_2^2\sin^2 Kxdx=1 \Longrightarrow A_2=\sqrt{\frac{2}{a}}$$

Finally, the time-independent wave solution is

$$\psi(x)=\sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})\quad \text{when}\quad n=1,2,3...$$

----standing wave
（驻波）

The electron in the infinite potential well is a standing wave solution

Comparison:

- **The free electron is represented by a traveling wave.**
- **The bound particle is represented by a standing wave.**

Equating the two expressions for *K*. we obtain

$$k_n^2 = \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2}$$

The total energy can then be written as $\boxed{E = E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}}$

For the particle in the infinite potential well, the wave function is

$$\boxed{\psi(x) = \sqrt{\frac{2}{a}} \sin Kx \qquad K = \frac{n\pi}{a}}$$

- **the energy of the particle is quantized.**
- **contrary to results from classical physics**, which would allow the particle to have continuous energy values.

Example

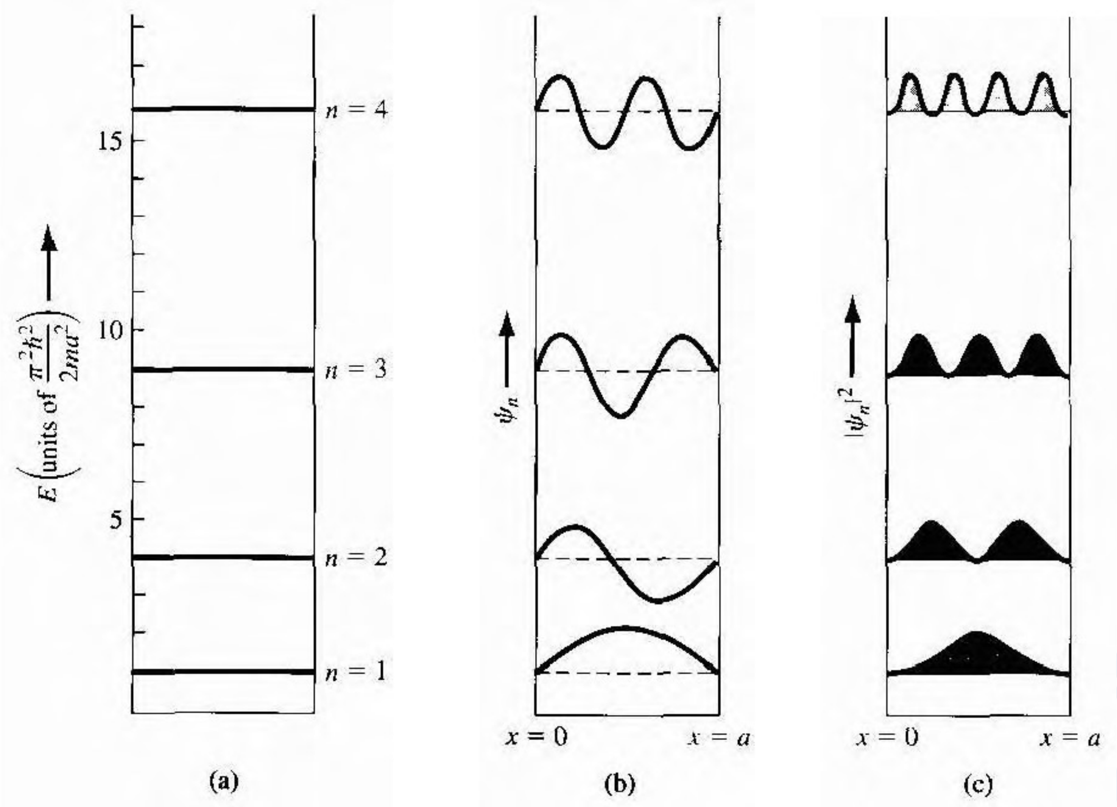
Consider an electron in an infinite potential well of width 5 A. To calculate the first three energy levels of an electron in an infinite potential well.

Solution:

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} = \frac{n^2(1.054\times10^{-34})^2\pi^2)}{(2(9.11\times10^{-31})(5\times10^{-10})^2} = n^2(2.41\times10^{-19})J$$

$$E_n = \frac{n^2(2.41\times10^{-19})}{1.6\times10^{-19}} = n^2(1.51)\ eV$$

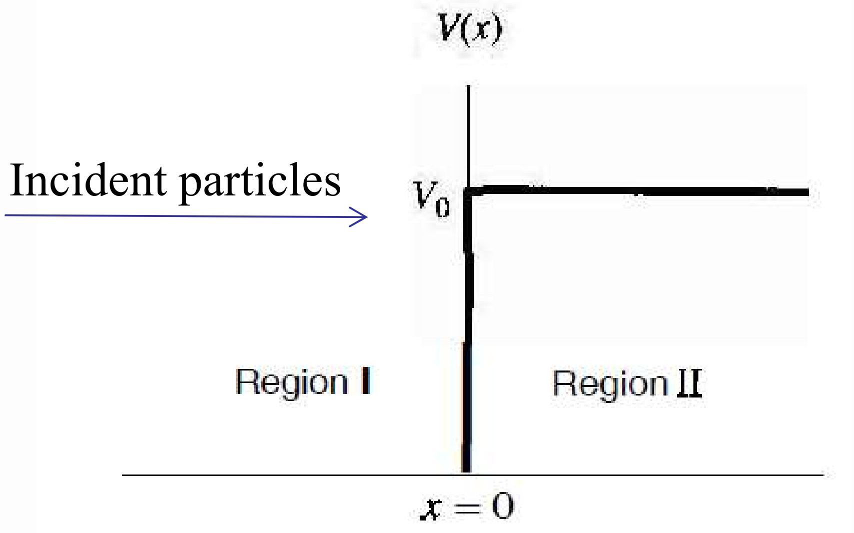
$$E_1 = 1.51\ eV \quad E_2 = 6.04\ eV \quad E_3 = 13.59\ eV$$



As the energy increases, the probability of finding the particle at any given value of x becomes more uniform.

Fig Particle in an infinite potential well:
(a) Four lowest discrete energy levels.
(b) Corresponding wave functions.
(c) Corresponding probability functions

□The Step Potential Function (阶跃势函数)



- A flux of particles is incident on the potential barrier.
- The total energy of the particle is less than the barrier height, or $E < V_0$.
- The wave equation

$$\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2m}{\hbar^2}(E-V(x))\psi(x)=0$$

In region I, $V = 0$

$$\boxed{\frac{\partial^2\psi_1(x)}{\partial x^2}+\frac{2m}{\hbar^2}\psi_1(x)=0}$$

$$\psi_1(x)=A_1e^{jK_1x}+B_1e^{-jK_1x}\quad(x\le 0)\quad K_1=\sqrt{\frac{2mE}{\hbar^2}}$$

the **incident** and **reflected** particles are represented by **traveling waves**

$A_1 A_1^*$ is the probability density function of the incident particles

$v_i A_1 A_1^*$ the flux of incident particles; $v_r B_1 B_1^*$ the flux of reflected particles

v_i is the velocity of the incident wave, and v_r is the velocity of reflected wave.

In region II, the potential is $V = V_0$ Since $E < V_0$,

$$\boxed{\frac{\partial^2\psi_2(x)}{\partial x^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi_2(x) = 0}$$

$$\psi_2(x) = A_2 e^{-K_2 x} + B_2 e^{+K_2 x} \quad (x \geq 0) \quad K_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

- One boundary condition: **the wave function must remain finite**

$$\Rightarrow B_2 = 0 \quad \Rightarrow \quad \psi_2(x) = A_2 e^{-K_2 x} \quad (x \geq 0)$$

- The second boundary condition: **The wave function** at $x = 0$ **must be continuous** => $\psi_1(0) = \psi_2(0)$ => $A_1 + B_1 = A_2$

- The third boundary condition: **the first derivative of the wave function must also be continuous**

$$\Rightarrow \quad \left.\frac{\partial\psi_1(x)}{\partial x}\right|_{x=0} = \left.\frac{\partial\psi_2(x)}{\partial x}\right|_{x=0}$$

$$\Rightarrow \quad B_1 = \frac{-(K_2^2 + 2jK_1K_2 - K_1^2)A_1}{(K_2^2 + K_1^2)} \quad A_2 = \frac{2K_1(K_1 - jK_2)A_1}{(K_2^2 + K_1^2)}$$

The reflected probability density function

$$B_1 \bullet B_1^* = \frac{(K_2^2 - K_1^2 + 2jK_1K_2)(K_2^2 - K_1^2 - 2jK_1K_2)A_1 \bullet A_1^*}{(K_2^2 + K_1^2)^2}$$

Reflection coefficient

$$R = \frac{v_r \bullet B_1 \bullet B_1^*}{v_1 \bullet A_1 \bullet A_1^*}$$

the ratio of the reflected flux to the incident flux

In region I, *V* = *0* so that *E* = *T* (the kinetic energy of the particle)

$$T = \frac{1}{2}mv^2 \quad \Rightarrow \quad K_1 = \sqrt{\frac{2m}{\hbar^2}\left(\frac{1}{2}mv^2\right)} = \sqrt{m^2\frac{v^2}{\hbar^2}} = \frac{mv}{\hbar}$$

=> The incident velocity and the reflected velocity

$$v_i = \frac{\hbar}{m} \bullet K_1 = v_r = \frac{\hbar}{m} \bullet K_1$$

The reflection coefficient is $R = \dfrac{v_r \bullet B_1 \bullet B_1^*}{v_1 \bullet A_1 \bullet A_1^*} = \dfrac{B_1 \bullet B_1^*}{A_1 \bullet A_1^*} = 1$

- In Region I, the result of $R=1$ implies that all of the particles incident on the potential barrier for $E < V$, are eventually reflected. --- consistent with classical physics

- In region II, $\psi_2(x) = A_2 e^{-K_2 x}$

For the case of $E < V_0$, the coefficient A_2 is not zero.
$\Rightarrow$There is a finite probability that the incident particle will penetrate the potential barrier and exist in region II.

--- difference between classical and quantum mechanics

Although there is a finite probability that the particle may penetrate the barrier, since the reflection coefficient in region I is unity, the particle in region II must eventually turn around and move back into region I.

Example:

Consider an incident electron that is traveling at a velocity of 1×10^5 m/s in region I. To calculate the penetration depth of a particle impinging on a potential barrier $V_0 = 2E$.

Solution

With $V(x)=0$, the total energy is also equal to the kinetic energy

$$E = T = \frac{1}{2}mv^2 = 4.56\times10^{-21} J = 2.85\times10^{-2}\ \text{eV}$$

The wave function: $\psi_2(x) = A_2 e^{-K_2 x}$ $\quad K_2 = \sqrt{2m(V_0 - E)/\hbar^2}$

We want to determine the distance $x = d$ at which the wave function magnitude has decayed to **e^{-1}** of its value at $x = 0$.

$$1 = d\sqrt{\frac{2m(2E-E)}{\hbar^2}} = d\sqrt{\frac{2mE}{\hbar^2}}$$

The distance $\quad d = \sqrt{\frac{\hbar^2}{2mE}} = \frac{1.054\times10^{-34}}{\sqrt{2(9.11\times10^{-31})(4.65\times10^{-21})}} = 11.6\times10^{-10} m$

□The Potential Barrier

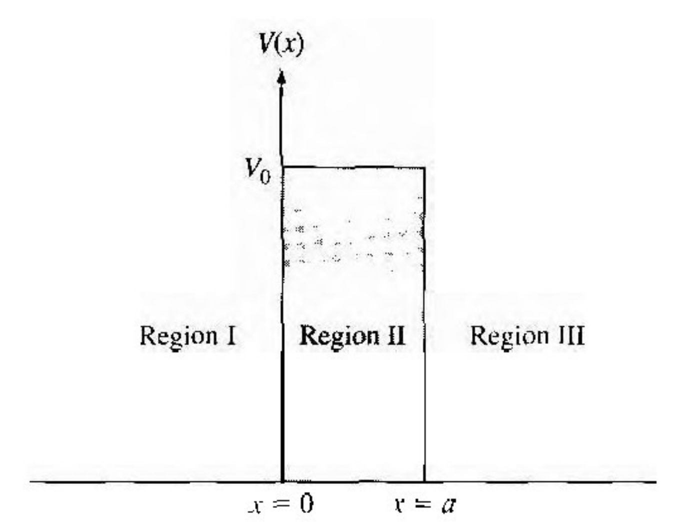


Fig The potential barrier function

- ● A flux of incident particles originating on the negative x axis travel in the $+x$ direction.
- ● The total energy of an incident particle is $E < V_0$

The solutions of the wave equation in regions I, II, and III are

$$\psi_1(x) = A_1 e^{jK_1 x} + B_1 e^{-jK_1 x}$$

$$K_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi_2(x) = A_2 e^{jK_2 x} + B_2 e^{-jK_2 x}$$

$$K_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$$\psi_3(x) = A_3 e^{jK_1 x} + B_3 e^{-jK_1 x}$$

- The coefficient B_3 presents a negative traveling wave in region III. However, once a particle gets into region III, there are no potential changes to cause a reflection. => $B_3 = 0$

- We have four boundary relations for the boundaries at $x = 0$ and $x = a$ corresponding to the wave function and its first derivative being continuous.

  $\Rightarrow$ We can solve for the four coefficients B_1 , A_2, B_2 ,and A_3 in terms of A_1

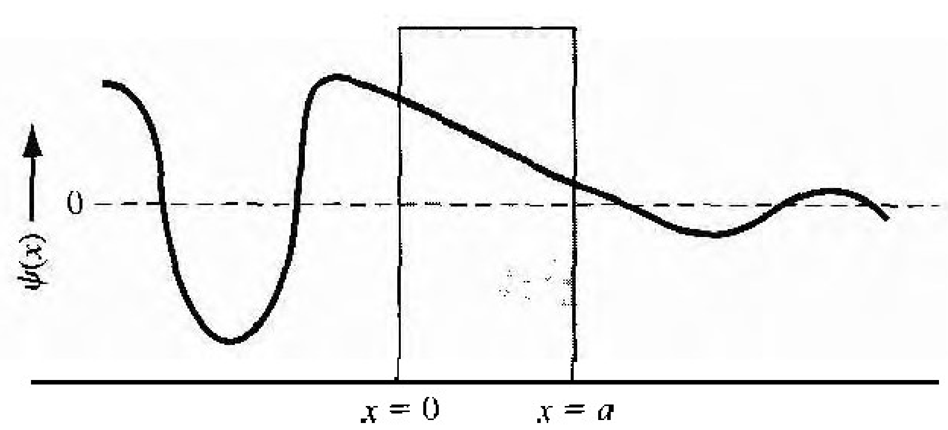


Fig The wave functions through the potential barrier.

The **transmission coefficient**, in this case defined as the ratio of the transmitted flux in region III to the incident flux in region I

$$T = \frac{v_t \bullet A_3 \bullet A_3^*}{v_i \bullet A_1 \bullet A_1^*} = \frac{A_3 \bullet A_3^*}{A_1 \bullet A_1^*}$$

v_t: velocity of transmitted particle; v_i: velocity of incident particle.

For the special case when $E << V_0$, we find that

$$\boxed{T \approx 16\left(\frac{E}{V_0}\right)\left(1 - \frac{E}{V_0}\right)\exp(-2K_2 a)}$$

There is a finite probability that a particle impinging a potential barrier will penetrate the barrier and will appear in region III.

--- **tunneling phenomenon（隧穿效应）**contradicts classical mechanics

The application of this quantum mechanical tunneling phenomenon: semiconductor device characteristics, such as in the **tunnel diode**

Example:

Consider an electron with energy of 2eV impinging on a potential barrier with V_0 = 20 eV and a width of 3 A.

To calculate the probability of an electron tunneling through a potential barrier.

Solution:

The tunneling probability

$$K_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = \sqrt{\frac{2(9.11\times10^{-31})(20-2)(1.6\times10^{-19})}{(1.054\times10^{-34})^2}}$$

The transmission coefficient

$$T \approx 16(\frac{E}{V_0})(1-\frac{E}{V_0})\exp(-2K_2 a)$$

$$=16(0.1)(1-0.1)\exp[-2(2.17\times10^{10})(3\times10^{-10})] = 3.17\times10^{-6}$$

The tunneling probability may appear to be a small value, but it is not zero. If a large number of particles impinge on a potential barrier, a significant number can penetrate the barrier.

Extensions of the Wave Theory to Atoms

The One-Electron Atom

Bohr theory: In the atom, the nucleus is a heavy, positively charged proton （质子） surrounded by electrons which are light, negatively charged particles.

The potential function due to the coulomb attraction between the proton and electron and is

$$V(r) = \frac{-e^2}{4\pi\varepsilon_0 r}$$

spherically symmetric →a three dimensional problem in spherical coordinates.

e is the magnitude of the electronic charge

ε_0 is the permittivity of free space

The time-independent Schrodinger's wave equation in three dimensional spherical coordinates is

$$\nabla^2\psi(r,\theta,\phi)+\frac{2m_0}{\hbar^2}(E-V(r))\psi(r,\theta,\phi)=0$$

m_0 is the rest mass of the electron.

Laplace operator in spherical coordinates can be written as

$$\begin{aligned}&\frac{1}{r^2}\bullet\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin^2\theta}\bullet\frac{\partial^2\psi}{\partial\phi^2}+\frac{1}{r^2\sin^2\theta}\bullet\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)\\&+\frac{2m_0}{\hbar^2}(E-V(r))\psi=0\end{aligned}$$

By the separation-of-variables technique

$$\psi(r,\theta,\phi)=R(r)\bullet\Theta(\theta)\bullet\Phi(\phi)$$

$$\frac{\sin^2\theta}{R}\bullet\frac{\partial}{\partial r}(r^2\frac{\partial R}{\partial r})+\frac{1}{\Phi}\bullet\frac{\partial^2\Phi}{\partial\phi^2}+\frac{\sin\theta}{\Theta}\bullet\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\Theta}{\partial\theta})$$

$$+r^2\sin^2\theta\frac{2m_0}{\hbar^2}(E-V)=0$$

Since the second term is a function of φ only

$$\frac{1}{\Phi}\bullet\frac{\partial^2\Phi}{\partial\phi^2}=-m^2$$

m is a separation of variables constant

$$\Phi=e^{jm\phi}\qquad m=0,\pm1,\pm2,\pm3,\ldots$$

We can define two additional separation-of-variables constants l and n for variable θ and r,

$n, l,$ and m are known as **quantum numbers**

$$\boxed{\begin{aligned}&n=1,2,3,\ldots\\&l=n-1,n-2,n-3,\ldots,0\\&|m|=l,l-1,\ldots,0\end{aligned}}$$

Each set of quantum number corresponds to a quantum state which the electron may occupy.

The electron energy is written in the form

$$\boxed{E_n = \frac{-m_0 e^4}{(4\pi\varepsilon_0)^2 2\hbar^2 n^2}}$$

n is the principal quantum number.

- The negative energy indicates that the electron is bound to the nucleus.
- The energy of the bound electron is quantized.
- If the energy were to become positive, then the electron would no longer be a bound particle and the total energy would no longer be quantized.

The solution of the wave equation may be designated by ψ_{nlm}

For the lowest energy state, $n = 1$, $l = 0$, and $m = 0$, the wave function is

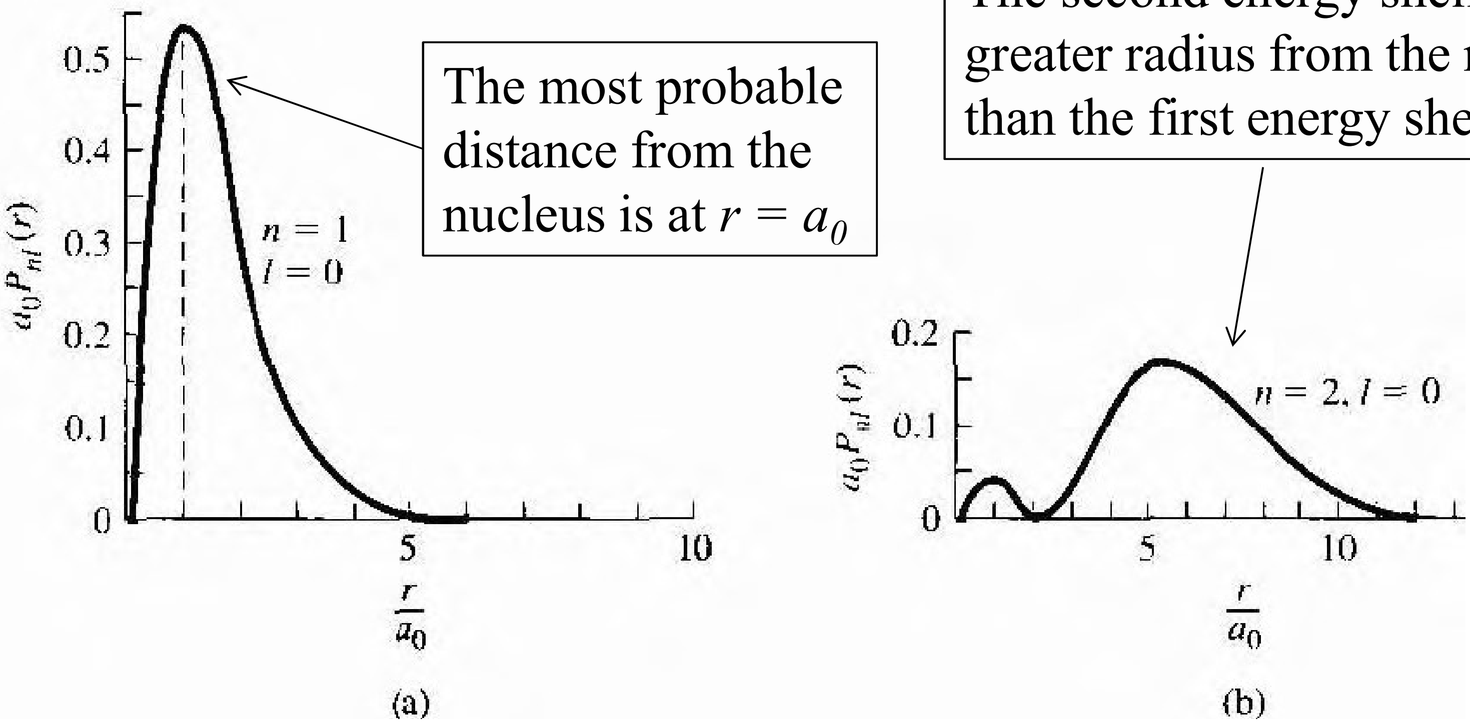
$$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

This function is spherically symmetric, and the parameter a_o is **Bohr radius（波尔半径）**.

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_0 e^2} = 0.529\,\mathring{\mathrm{A}}$$

The radial probability density function （径向概率密度函数）
—the probability of finding the electron at a particular distance from the nucleus,
—proportional to the product $\psi_{100}\psi^*_{100}$

Electron cloud or **energy shell**



The most probable distance from the nucleus is at $r = a_0$

The second energy shell is at a greater radius from the nucleus than the first energy shell.

Fig The radial probability density function for the one-electron atom in the (a) lowest energy state (n=1,l=0,m=0) (b) next-higher energy state (n=2,l=0,m=0)

For the case of $n = 2$ and $l = 1$. there are three possible states corresponding to the three allowed values of the quantum number m （m=1,-1,0）. The wave functions are no longer spherically symmetric.

□The Periodic Table

Schrodinger's wave equation + Two concepts

- **Electron spin (电子自旋)**

---The electron has an intrinsic angular momentum, or spin, which is quantized and may take on one of two possible values $S=+1/2$ and $S=-1/2$.

Four basic quantum numbers: n, l, m, s.

- **Pauli exclusion principle**

--- In any given system (an atom, molecule, or crystal), no two electrons may occupy the same quantum state.

--- In an atom, no two electrons may have the same set of quantum numbers.

Table Initial portion of periodic table

Element	Notation	n	l	m	s
Hydrogen (1)	$1s^1$	1	0	0	$+\frac{1}{2}\ or -\frac{1}{2}$
Helium (2)	$1s^2$	1	0	0	$+\frac{1}{2}\ and -\frac{1}{2}$
Lithium (3)	$1s^2 2s^1$	2	0	0	$+\frac{1}{2}\ or -\frac{1}{2}$
Beryllium (4)	$1s^2 2s^2$	2	0	0	$+\frac{1}{2}\ and -\frac{1}{2}$
Boron (5)	$1s^2 2s^2 2p^1$	2	1		$m = 0, -1, +1$ $s = +\frac{1}{2}, -\frac{1}{2}$
Carbon (6)	$1s^2 2s^2 2p^2$	2	1		
Nitrogen (7)	$1s^2 2s^2 2p^3$	2	1		
Oxygen (8)	$1s^2 2s^2 2p^4$	2	1		
Fluorine (9)	$1s^2 2s^2 2p^5$	2	1		
Neon (10)	$1s^2 2s^2 2p^6$	2	1		

1s represents the first energy shell, n=1, l=0, m=0, s=+1/2,-1/2, two electrons.

2s2p represents the second energy shell,

$n=2, \quad l=0, \quad m=0, \qquad s=+1/2,-1/2,$

$n=2, \quad l=1, \quad m=0,+1,-1, \quad s=+1/2,-1/2,$

can accommodate eight electrons.

The energy shell is determined by the main quantum number n, and can accommodate $\sum_{l=0}^{n-1} 2(2l+1) = 2n^2$ **electrons.**

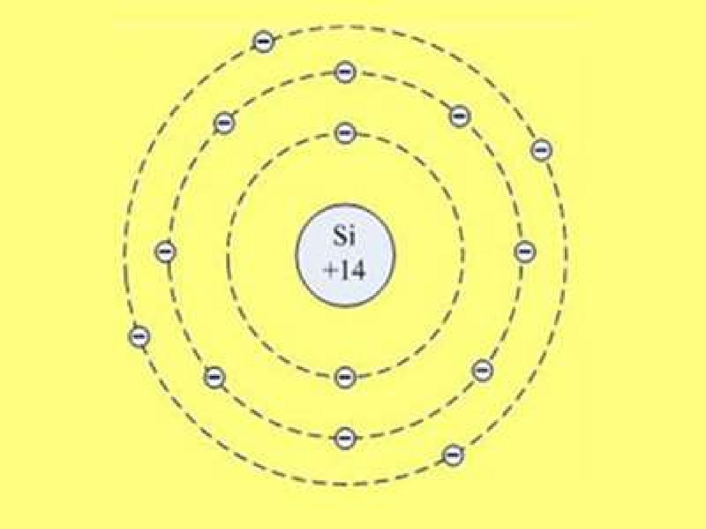


Fig 2D structure of Si atom

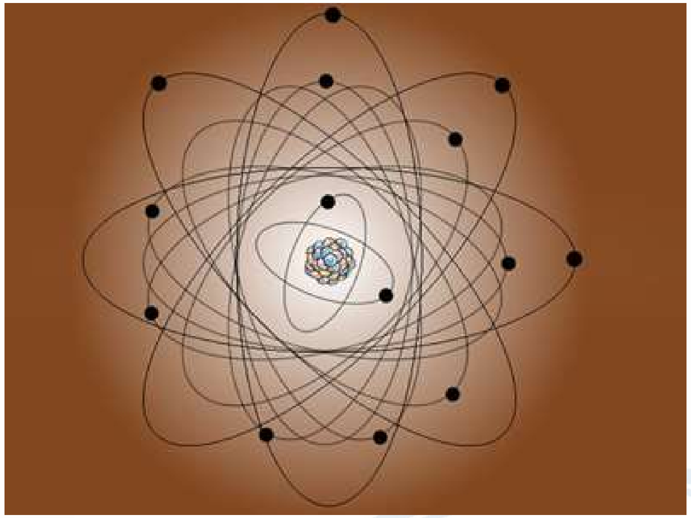


Fig 3D structure of Si atom

✓The inner shells are full and the **chemical activity** of an element is **determined primarily by the valence**, or outermost, electrons.

✓If all of the energy shells are full, the element doest not react with other elements and is an **inert element** （**惰性元素**）.

✓Semiconductor elements are in Group III, V, and VI.

Homework3

A one-dimensional infinite potential well with a width of 12 A contains an electron.

(a) Calculate the first two energy levels that the electron may occupy.

(b) If an electron drops from the second energy level to the first, what is the wavelength of a photon that might be emitted?

Summary

- ✓ The basic concepts of quantum mechanics can be used to describe the behavior of electrons under various potential functions.
- ✓ The wave-particle duality principle： Particles can have wave-like behavior and waves can have particle-like behavior.
- ✓ Schrodinger's wave equation forms the basis for describing and predicting the behavior of electrons.
- ✓ applying Schrodinger‘s wave equation to a bound particle： energy of the bound particle is quantized.
- ✓ applying Schrodinger‘s wave equation to an electron incident on a potential barrier： there is a finite probability of tunneling.
- ✓ applying Schrodinger‘s wave equation to the one-electron： the periodic table.