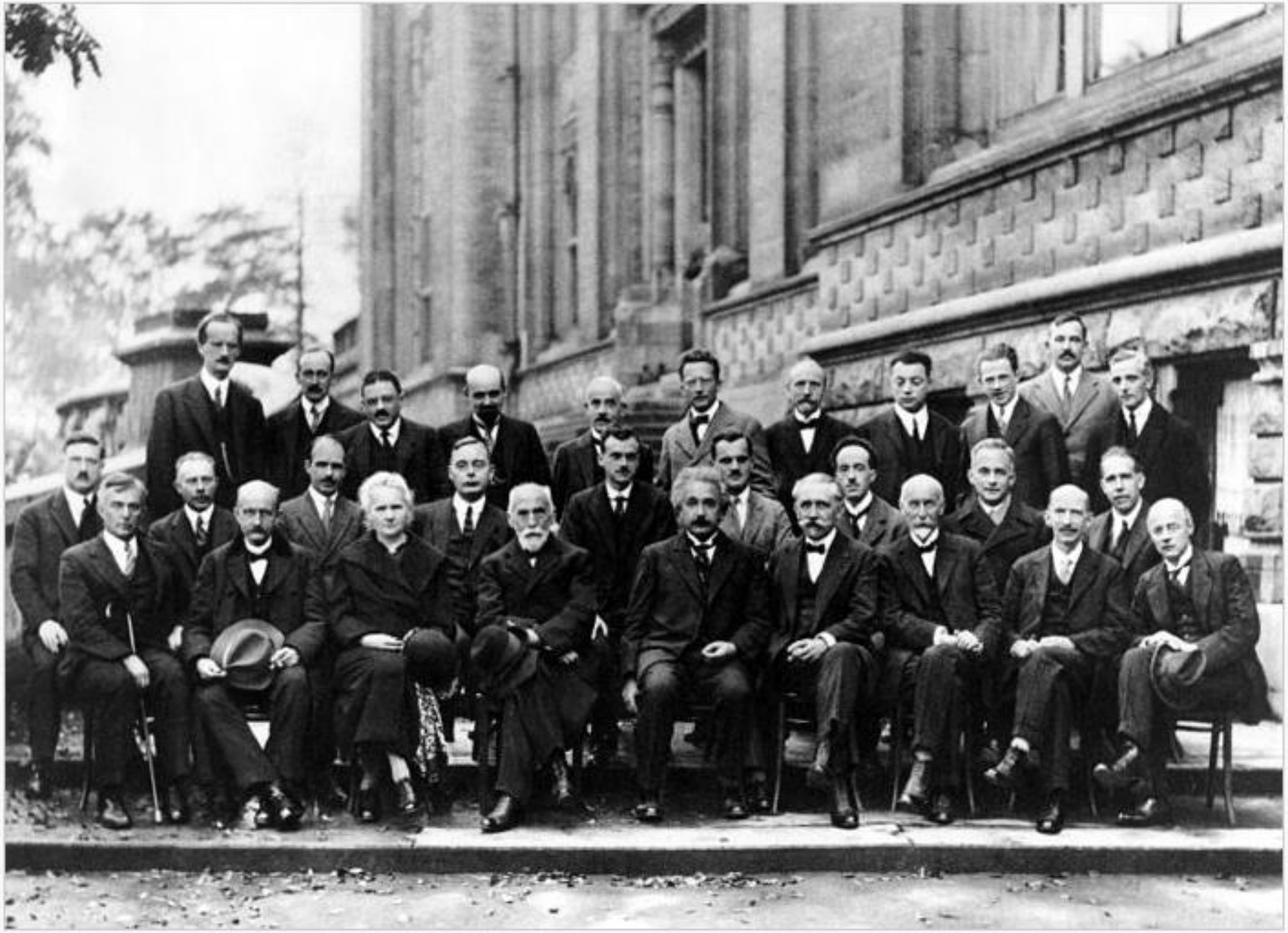
Semiconductor Materials and Devices
(반도체 재료 및 소자)

Chapter 2. Introduction to Quantum Mechanics

Young Min Song
Assistant Professor
School of Electrical Engineering and Computer Science
Gwangju Institute of Science and Technology
http://www.gist-foel.net
ymsong@gist.ac.kr, ymsong81@gmail.com
A207, ☎2655

The 5th Solvay Conference



A. Piccard, E. Henriot, P. Ehrenfest, E. Herzen, Th. de Donder, E. Schrödinger, J.E. Verschaffelt, W. Pauli, W. Heisenberg, R.H. Fowler, L. Brillouin;

P. Debye, M. Knudsen, W.L. Bragg, H.A. Kramers, P.A.M. Dirac, A.H. Compton, L. de Broglie, M. Born, N. Bohr;

I. Langmuir, M. Planck, M. Skłodowska-Curie, H.A. Lorentz, A. Einstein, P. Langevin, Ch.-E. Guye, C.T.R. Wilson, O.W. Richardson

Fifth conference participants, 1927. Institut International de Physique Solvay in Leopold Park.

'Brief' History of Quantum Mechanics

1900, Plank constant, black body radiation, Plank

1905, Photoelectric effect, Einstein

1913, Bohr's atom model, Bohr

1923, Matter wave, wave-particle duality, de Broglie

1924, Pauli's exclusion principle, Pauli

1926, Schrodinger's equation, wave mechanics, Schrodinger

1927, Uncertainty principle, Heisenberg

1927, Copenhagen interpretation, 5^{th} Solvay Conference

1935, EPR paradox, Schrodinger's cat

Energy Quanta

"Light can behave like a stream of particles of zero rest-mass. The only way to explain a vast number of experiments is to view light as a stream of discrete entities or energy packets called photons, each carrying a quantum of energy hν , and momentum h/λ."

Photoelectric Effect

The KE of the emitted electron is independent of I → Only the number of electrons ejected depends on the light intensity.

The KE of the emitted electron depends on the frequency of light."

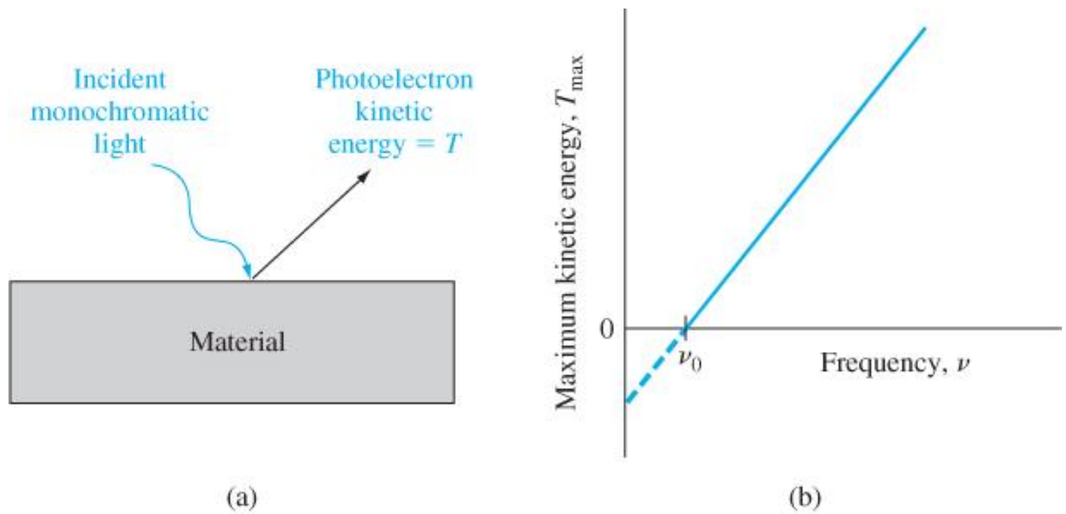
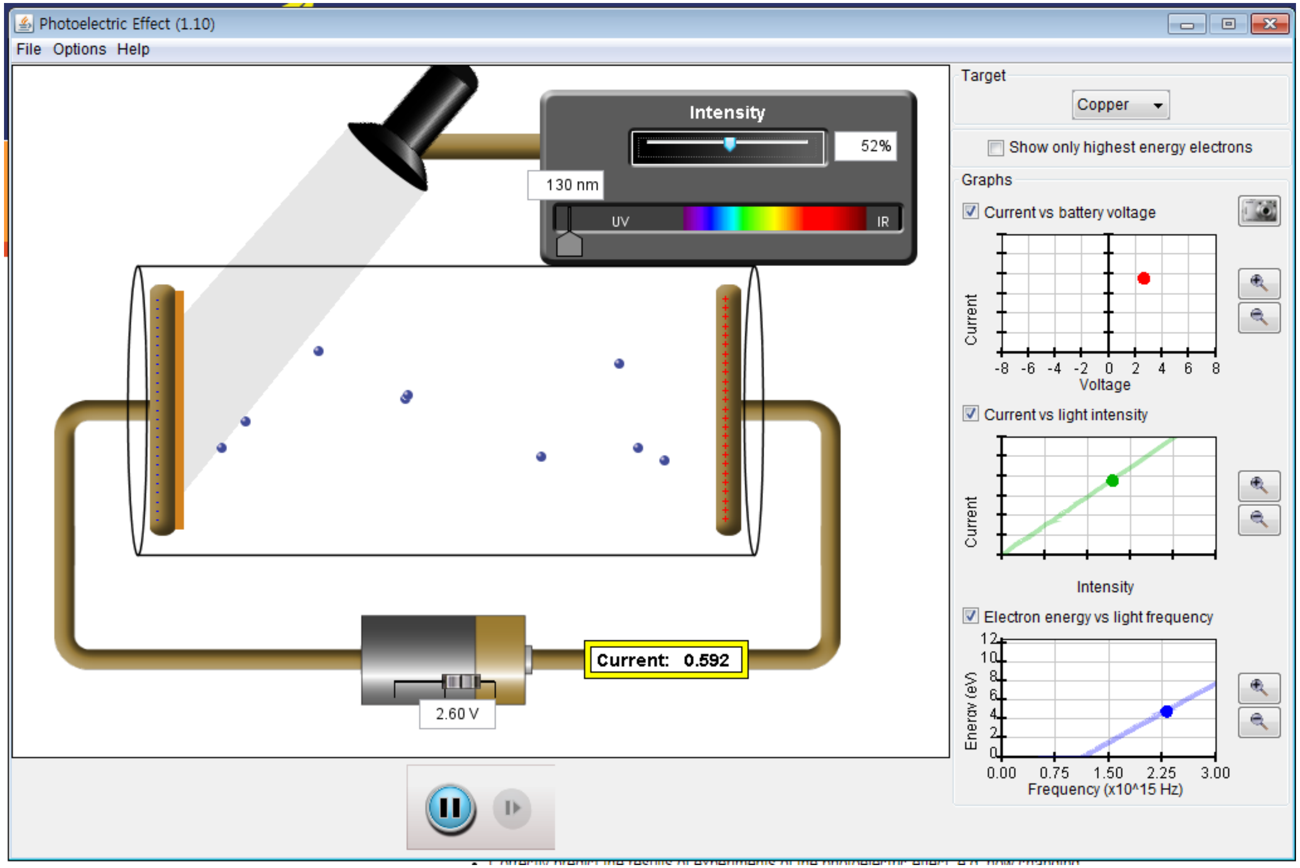


Figure 2.1 | (a) The photoelectric effect and (b) the maximum kinetic energy of the photoelectron as a function of incident frequency.

$$T_{\max} = \frac{1}{2} m\upsilon^2 = h\nu - \underbrace{h\nu_0}_{\text{work function}}$$

Photoelectric Effect experiments

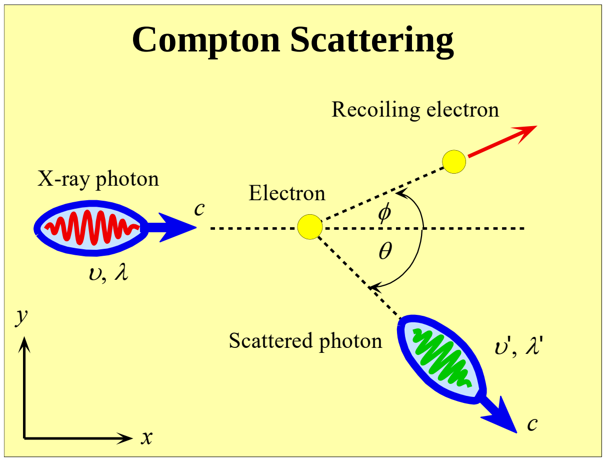
→ HW) experimental results with three variables (light intensity, wavelength, and materials) and discussion



http://phet.colorado.edu/en/simulation/photoelectric

Wave-Particle Duality : Matter Wave

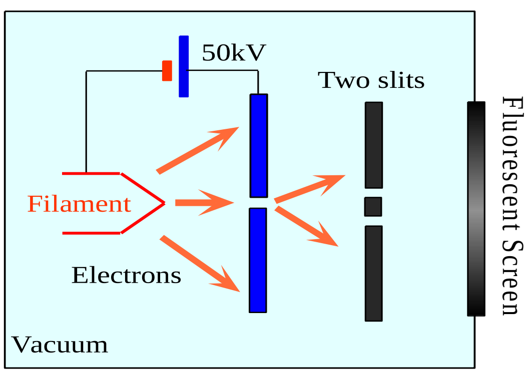
"Just as a photon has a light wave associated with it that governs its motion, so a material particle (e.g., an electron) has an associated matter wave (or pilot wave) that governs its motion." ----- A Grand Symmetry of Nature



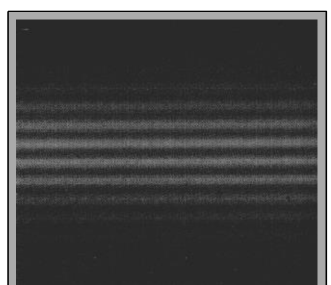
$$KE_m = h\nu - h\nu'$$

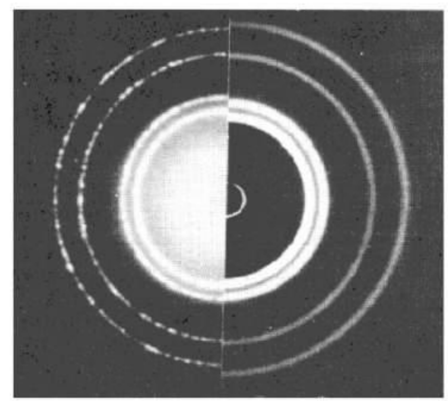
"It has been found that an electron traveling with a momentum p behaves like a wave of wavelength λ given by :

$$\lambda = \frac{h}{p}$$: *de Broglie* wavelength



Electron diffraction fringes on the screen





(d) Composite photograph showing diffraction patterns produced with an aluminum foil by X-rays and electrons of similar wavelength. Left: X-rays of λ = 0.071 nm. Right: Electrons of energy 600 eV.

The electromagnetic frequency spectrum

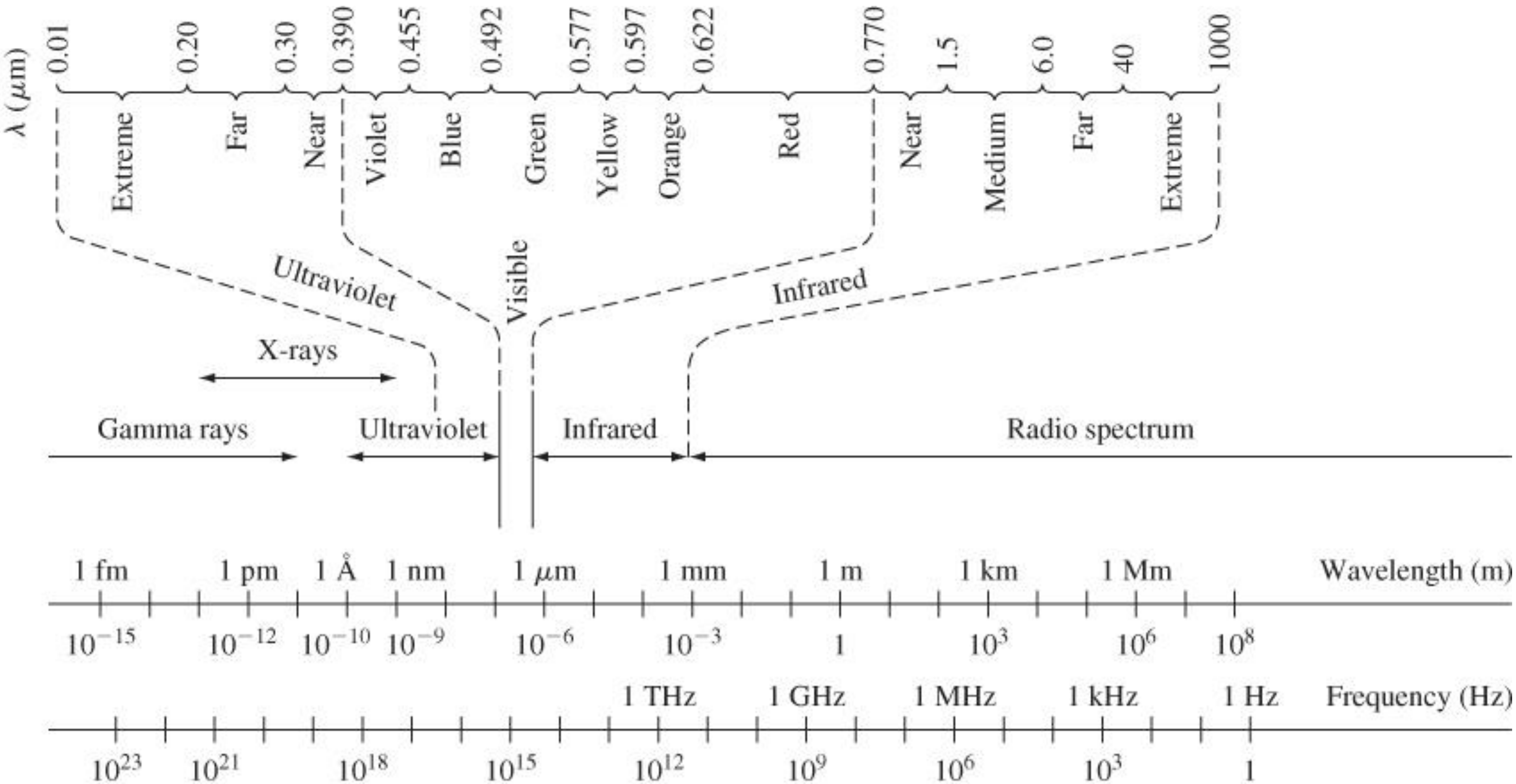


Figure 2.4 | The electromagnetic frequency spectrum.

An electron traveling at 10^5 m/s :

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

$$\lambda = \frac{h}{p} = \frac{6.625 \times 10^{-34}}{9.11 \times 10^{-26}} = 7.27 \times 10^{-9} \text{ m} \qquad \lambda = 72.7 \text{ Å}$$

A general equation that describes the wave-like behavior of a particle as a function of appropriate potential energy and boundary conditions :

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

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

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

$$E=j\hbar\cdot\frac{1}{\phi(t)}\cdot\frac{\partial\phi(t)}{\partial t}$$

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

$$\phi(t)=e^{-j(E/\hbar)t}$$

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

Physical Meaning of the Wave Function :

$$|\Psi(x,t)|^2=\Psi(x,t)\cdot\Psi^*(x,t) \qquad \Psi(x,t)=\psi(x)\phi(t)=\psi(x)e^{-j(E/\hbar)t}$$

$$\Psi(x,t)\Psi^*(x,t)=\left[\psi(x)e^{-j(E/\hbar)t}\right]\left[\psi^*(x)e^{+j(E/\hbar)t}\right]=\psi(x)\psi^*(x)$$

$$|\Psi(x,t)|^2=\psi(x)\psi^*(x)=|\psi(x)|^2$$

: The probability of finding the electron per unit volume at x, y, z, at time t.

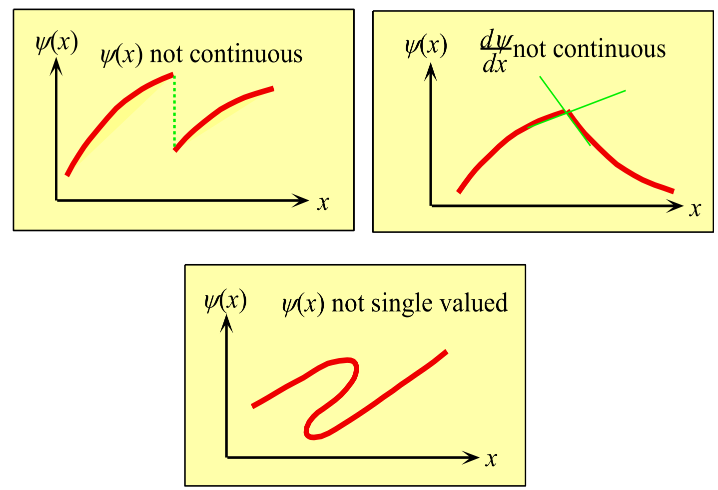
Boundary Conditions

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

To be the total energy *E* and the potential *V(x)* finite,

- ✓ $\psi(x)$: finite, single-valued, and continuous
- ✓ $d\psi(x)/dx$: finite, single-valued, and continuous

Unacceptable forms of $\psi(x)$



Unacceptable forms of $\psi(x)$

Potential function and wave function

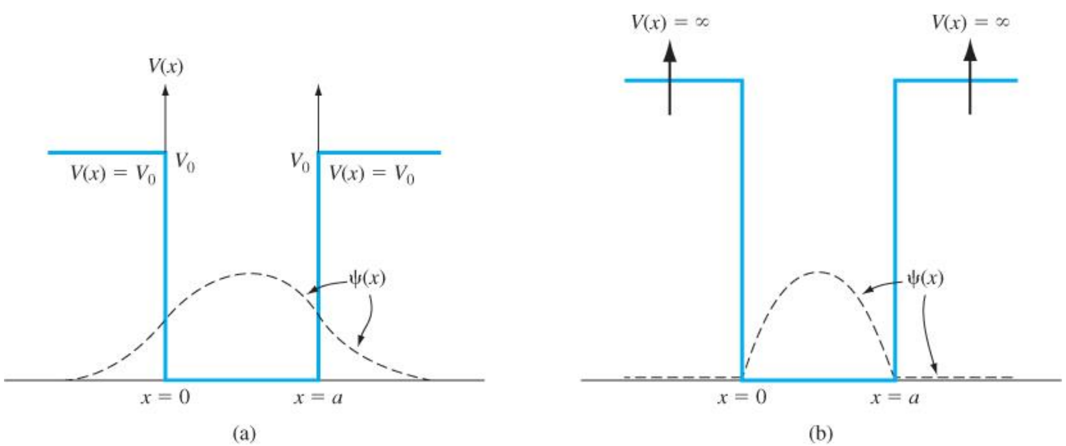


Figure 2.5 | Potential functions and corresponding wave function solutions for the case (a) when the potential function is finite everywhere and (b) when the potential function is infinite in some regions.

Electrons in Free Space

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0 \Longrightarrow \psi(x) = A\exp\left[\frac{jx\sqrt{2mE}}{\hbar}\right] + B\exp\left[\frac{-jx\sqrt{2mE}}{\hbar}\right]$$

$$\Psi(x,t) = A\exp\left[\frac{j}{\hbar}(x\sqrt{2mE} - Et)\right] + B\exp\left[\frac{-j}{\hbar}(x\sqrt{2mE} + Et)\right] \Longleftarrow \psi(t) = e^{-j(E/\hbar)t}$$

Assume that only a particle traveling in the +x direction,

$$\Psi(x,t) = A\exp[j(kx - \omega t)] \qquad k^2 = \frac{2m}{\hbar^2}E \qquad k = \frac{2\pi}{\lambda} \Longrightarrow \lambda = \frac{h}{\sqrt{2mE}} \qquad \lambda = \frac{h}{p}$$

$\Psi(x,t)\Psi^*(x,t) = AA^*$: constant over the entire space

※ The uncertainty Δx in its position is infinite.

※ Since the electron has a well-defined wavenumber k, its momentum p is also well-defined by virtue of $p = \hbar k$. Therefore, the uncertainty Δp in its momentum is zero.

Electrons in the Infinite Potential Well

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

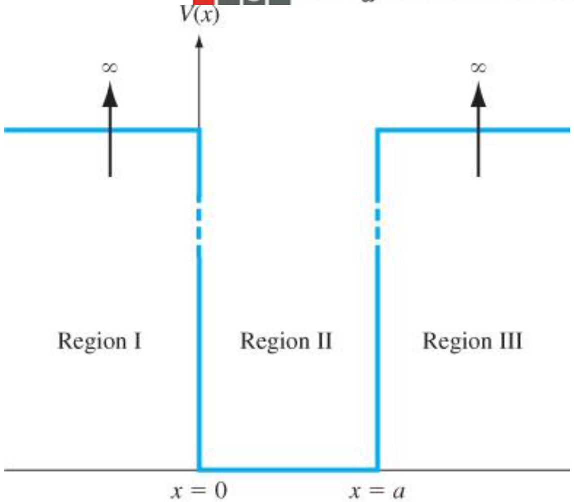


Figure 2.6 | Potential function of the infinite potential well.

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

$\Longrightarrow$ $\psi(x) = A_1 \cos Kx + A_2 \sin Kx \quad K = \sqrt{\frac{2mE}{\hbar^2}}$

Boundary condition : $\psi(x=0) = \psi(x=a) = 0$

$$\psi(x=a) = 0 = A_2 \sin Ka \Longrightarrow K = \frac{n\pi}{a}$$

$$\int_{-\infty}^{\infty} \psi(x)\psi^*(x)\,dx = 1 \Longrightarrow \int_0^a A_2^2 \sin^2 Kx\,dx = 1 \Longrightarrow A_2 = \sqrt{\frac{2}{a}}$$

$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ where $n = 1, 2, 3, \ldots$ (Standing waves)

$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2} \Longrightarrow \boxed{E = E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}}$ where $n = 1, 2, 3, \ldots$

The energy of electron is quantized, the energy can only have particular discrete values.

Electrons in the Infinite Potential Well

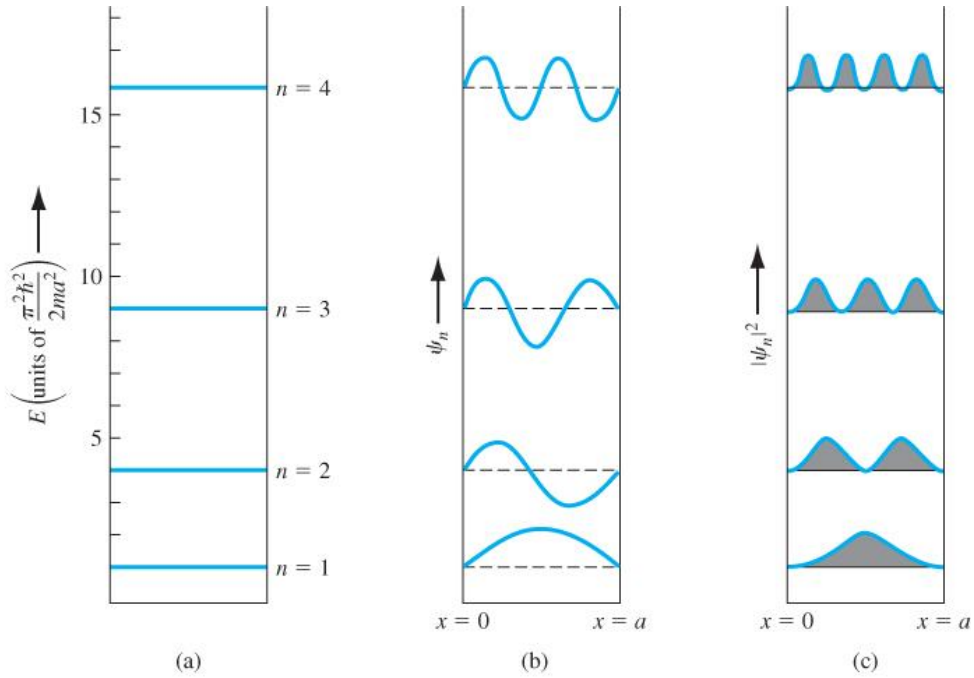


Figure 2.7 | Particle in an infinite potential well: (a) four lowest discrete energy levels, (b) corresponding wave functions, and (c) corresponding probability functions. *(From Pierret [10].)*

Consider an electron in an infinite potential well of width 5Å

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

$$E_n = \frac{n^2(2.41 \times 10^{-19})}{1.6 \times 10^{-19}} = n^2(1.51) \text{ eV}$$

$$E_1 = 1.51 \text{ eV}, \quad E_2 = 6.04 \text{ eV}, \quad E_3 = 13.59 \text{ eV}$$

The Potential Barrier

$$\psi_1(x) = A_1 e^{jK_1 x} + B_1 e^{-jK_1 x} \qquad K_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi_2(x) = A_2 e^{K_2 x} + B_2 e^{-K_2 x}$$

$$\psi_3(x) = A_3 e^{jK_1 x} + B_3 e^{-jK_1 x} \qquad K_2 = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

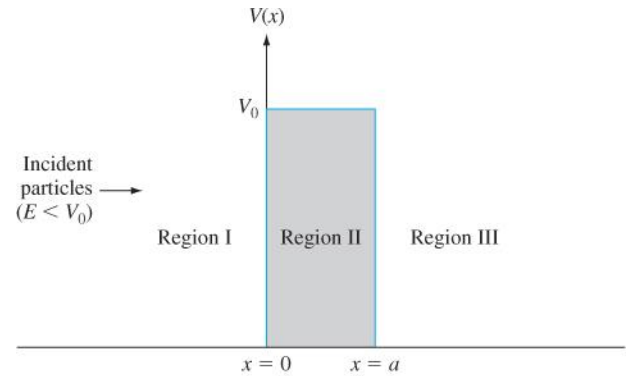


Figure 2.9 | The potential barrier function.

B_3 is zero, and B_1, A_2, B_2, and A_3 can be defined in terms of A_1 by solving four boundary conditions.

$$T = \frac{v_t \cdot A_3 \cdot A_3^*}{v_i \cdot A_1 \cdot A_i^*} = \frac{A_3 \cdot A_3^*}{A_1 \cdot A_1^*} \qquad T \approx 16\left(\frac{E}{V_0}\right)\left(1 - \frac{E}{V_0}\right)\exp\left(-2K_2 a\right)$$

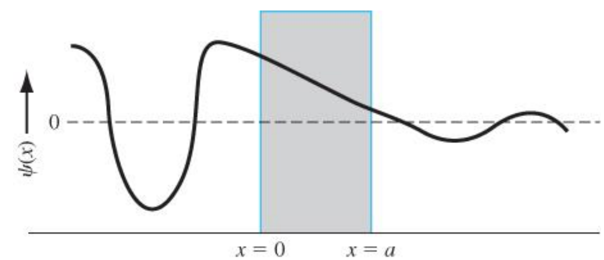


Figure 2.10 | The wave functions through the potential barrier.

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

$$K_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = \sqrt{\frac{2(9.11 \times 10^{-31})(20 - 2)(1.6 \times 10^{-19})}{(1.054 \times 10^{-34})^2}} \qquad K_2 = 2.17 \times 10^{10} \text{ m}^{-1}$$

$$T = 16(0.1)(1 - 0.1)\exp\left[-2(2.17 \times 10^{10})(3 \times 10^{-10})\right] \qquad T = 3.17 \times 10^{-6}$$

Hydrogen Atom : solving Schrodinger's equation

$$V(r) = \frac{-e^2}{4\pi\epsilon_0 r}$$

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

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

$$\frac{\sin^2\theta}{R}\cdot\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{1}{\Phi}\cdot\frac{\partial^2\Phi}{\partial\phi^2} + \frac{\sin\theta}{\Theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\cdot\frac{\partial\Theta}{\partial\theta}\right) + r^2\sin^2\theta\cdot\frac{2m_0}{\hbar^2}(E - V) = 0$$

Separation-of-variable Constants

$$\frac{1}{\Phi}\cdot\frac{\partial^2\Phi}{\partial\phi^2} = -m^2 \longrightarrow \Phi = e^{jm\phi}$$

$$m = 0, \pm1, \pm2, \pm3, \ldots$$

$$E_n = \frac{-m_0 e^4}{(4\pi\epsilon_0)^2 2\hbar^2 n^2}$$

$$n = 1, 2, 3, \ldots$$
$$l = n-1, n-2, n-3, \ldots, 0$$
$$|m| = l, l-1, \ldots, 0$$

The three quantum numbers comes out from the mathematical solution of Schrodinger's wave equation of hydrogen atom.

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

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_0 e^2} = 0.529\ \text{Å}$$

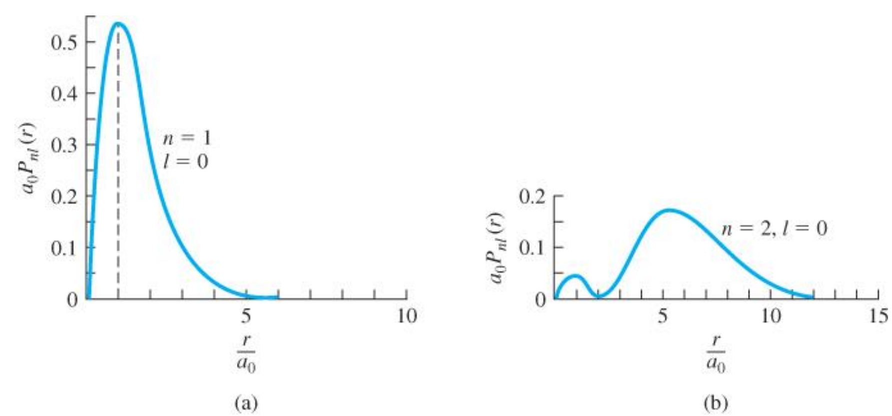


Figure 2.11 | The radial probability density function for the one-electron atom in the (a) lowest energy state and (b) next-higher energy state.
(From Eisberg and Resnick [5].)