Semiconductor Materials and Devices
(반도체 재료 및 소자)

Lecture 3. Introduction to Quantum Mechanics

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‘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

Classical physics:
If the intensity of the light is large enough, the work function of the material will be overcome and an electron will be emitted from the surface independent of the incident frequency.

Quantum physics:
At a constant incident intensity, the maximum kinetic energy of the photoelectron varies linearly with frequency with a limiting frequency ν_0.

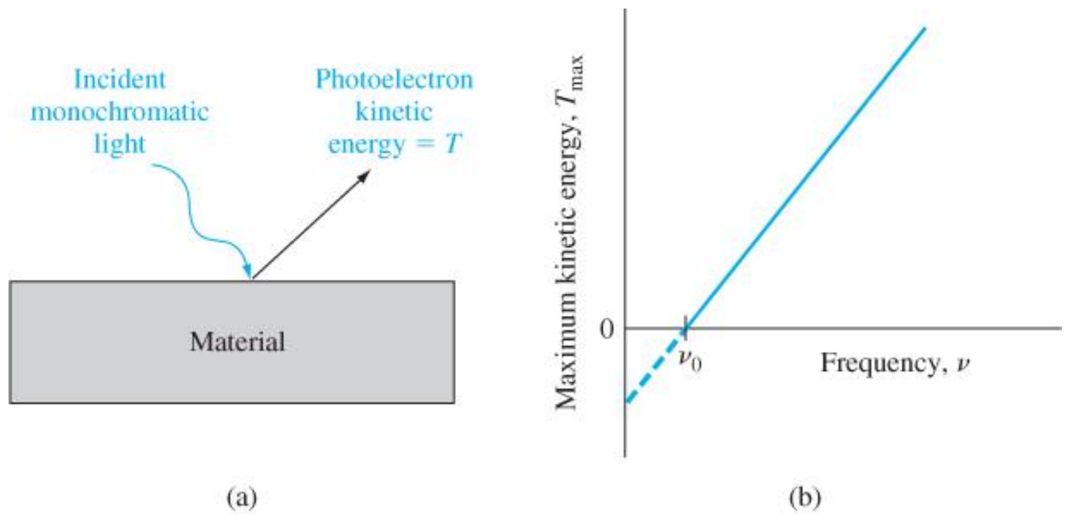


Figure 2.1 | (a) The photoelectric effect and (b) the maximum kinetic energy of the photoelectron as a function of incident frequency.

$$T_{max} = \frac{1}{2} m \upsilon^2 = h\nu - \underline{h\nu_0}$$

work function

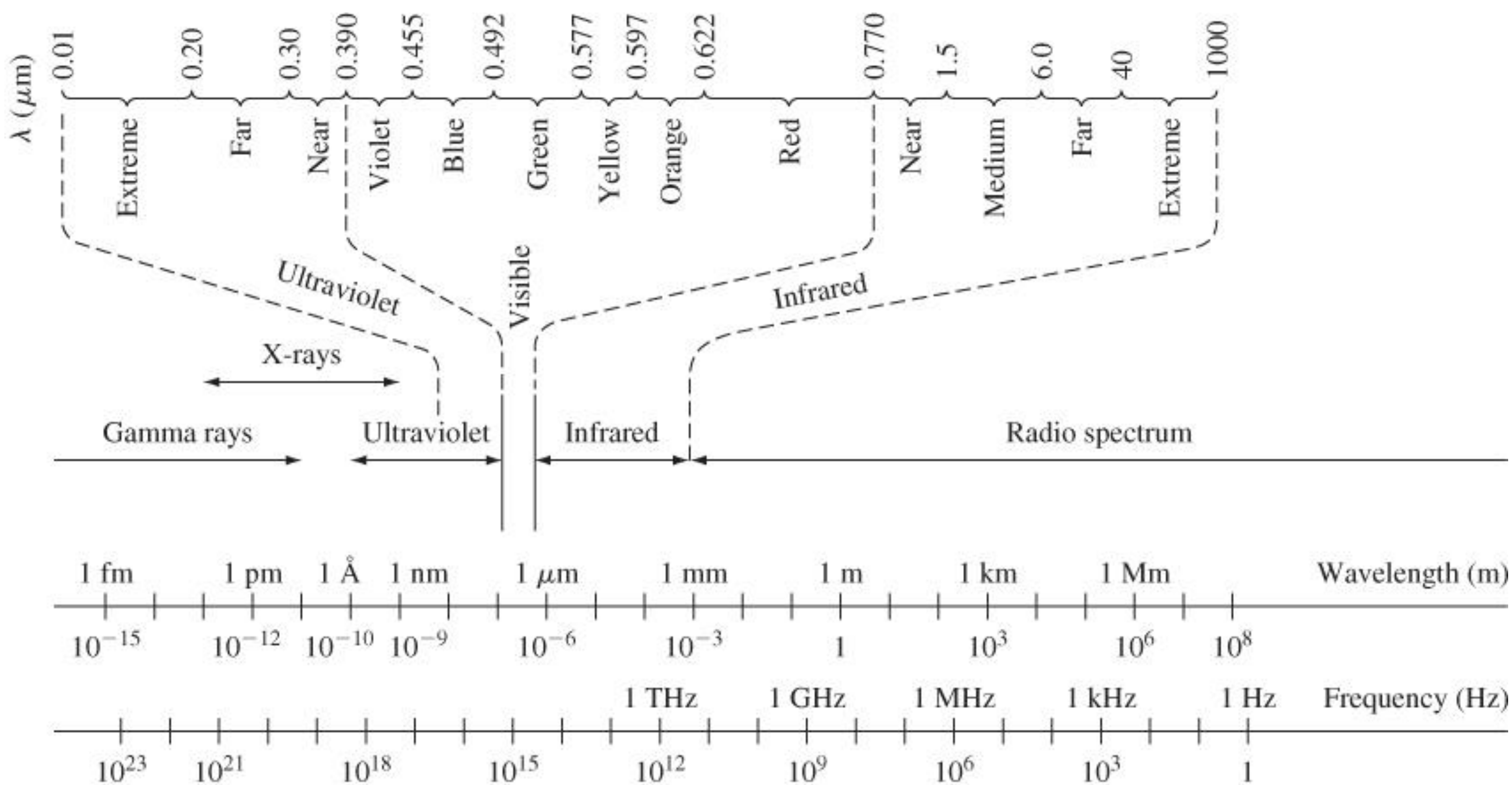
Minimum energy required to remove an electron from the surface.

Wave-Particle Duality : Matter Wave

De Broglie postulated the existence of matter waves.
He suggest that since waves exhibit particle-like behavior, particles should be expected to show wave-like properties. The hypothesis of de Broglie was the existence of a wave-particle duality principle.

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

The electromagnetic frequency spectrum



Schrondinger's wave equation

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

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

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

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

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

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

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

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

Physical Meaning of the Wave Function :

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

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

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

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

: 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

Potential function and wave function

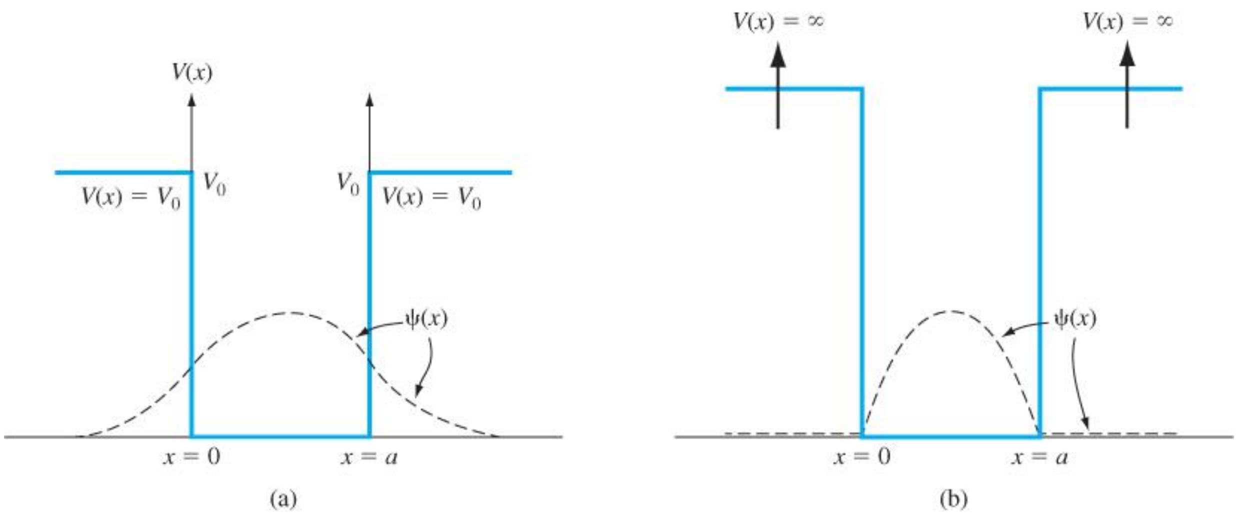


Figure 2.5 | Potential functions and corresponding wave function solutions for the case (a) when the potential function is finite everywhere and (b) when the potential function is infinite in some regions.

In classical mechanics, the position of a particle can be determined precisely, whereas in quantum mechanics, the position of a particle is found in terms of probability!

Electrons in Free Space

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

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

This wave function solution is a traveling wave, which means that a particle moving in free space is represented by a traveling wave.

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

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

$\Psi(x,t)\Psi^*(x,t) = AA^*$: 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 = ħk. Therefore, the uncertainty Δp in its momentum is zero.

Electrons in Free Space

Electrons in the Infinite Potential Well

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

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

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

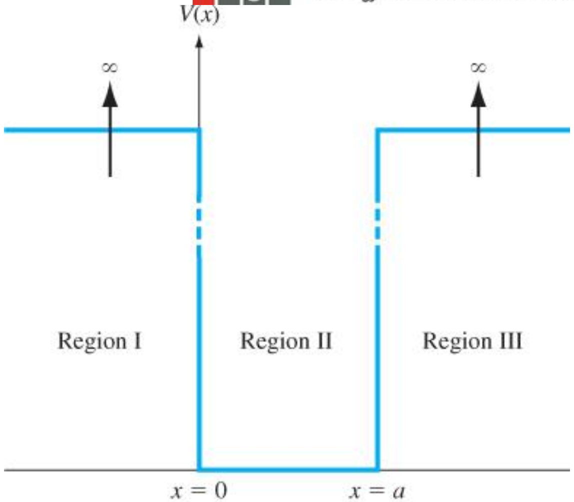


Figure 2.6 | Potential function of the infinite potential well.

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

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

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

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

This solution represents the electron in the infinite potential well and is a standing wave solution.

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

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

Electrons in the Infinite Potential Well

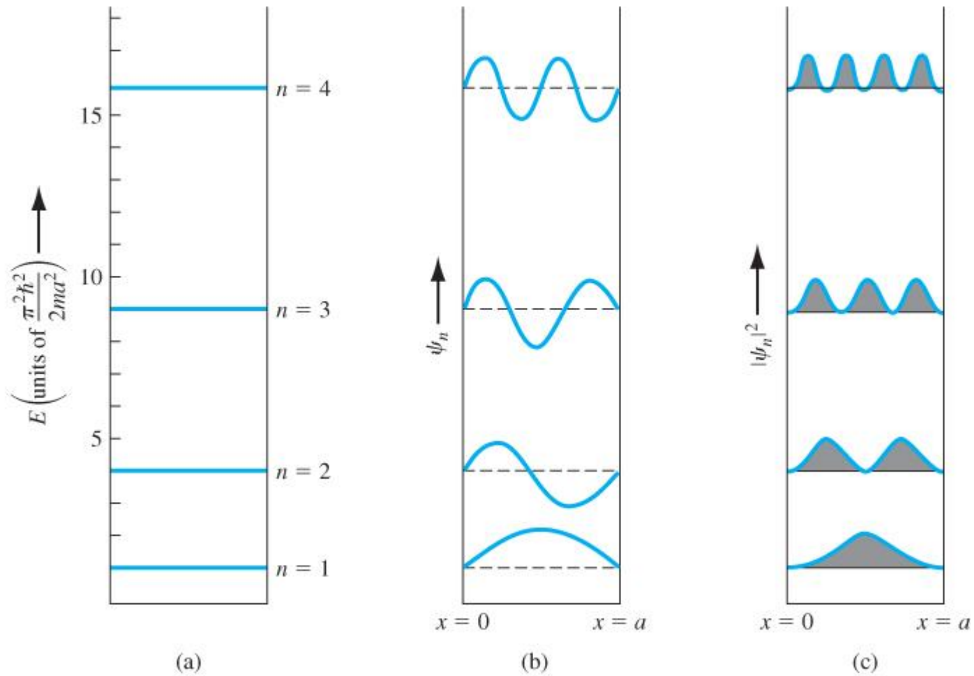


Figure 2.7 | Particle in an infinite potential well: (a) four lowest discrete energy levels, (b) corresponding wave functions, and (c) corresponding probability functions. *(From Pierret [10].)*

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

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

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

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

Electrons in the Infinite Potential Well

The Potential Barrier

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

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

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

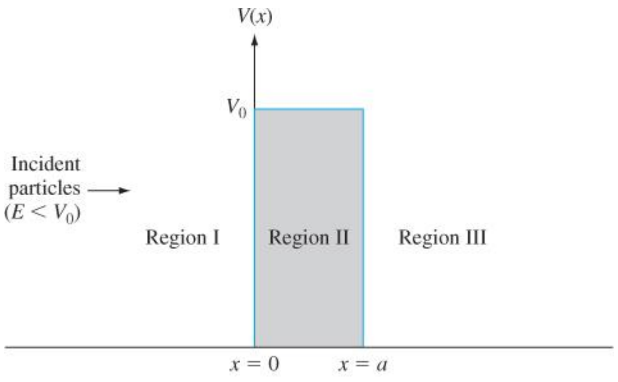


Figure 2.9 | The potential barrier function.

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.

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

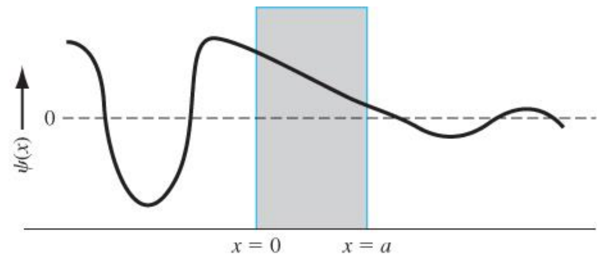


Figure 2.10 | The wave functions through the potential barrier.

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

$$K_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = \sqrt{\frac{2(9.11\times10^{-31})(20-2)(1.6\times10^{-19})}{(1.054\times10^{-34})^2}} \qquad K_2 = 2.17\times10^{10}\ \text{m}^{-1}$$

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

Hydrogen Atom : solving Schrodinger's equation

$$V(r) = \frac{-e^2}{4\pi\epsilon_0 r}$$ Potential function from the coulomb attraction btw the proton and electron

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

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

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

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.

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

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

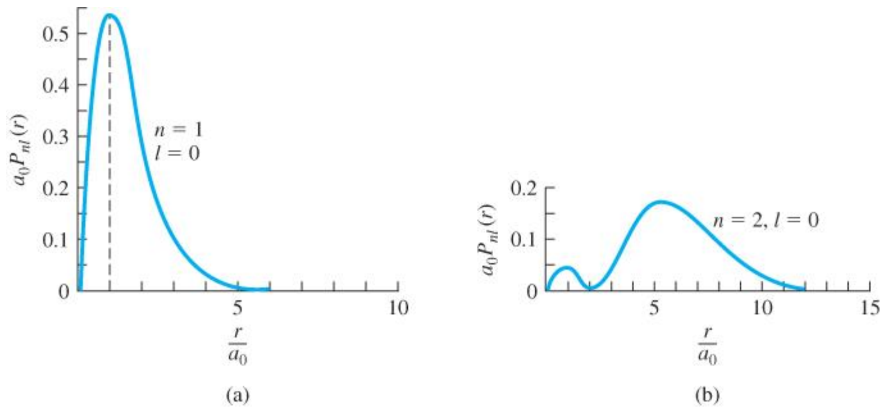


Figure 2.11 | The radial probability density function for the one-electron atom in the (a) lowest energy state and (b) next-higher energy state.
(From Eisberg and Resnick [5].)