Semiconductor Devices

Chapter 2 Introduction to Quantum Mechanics

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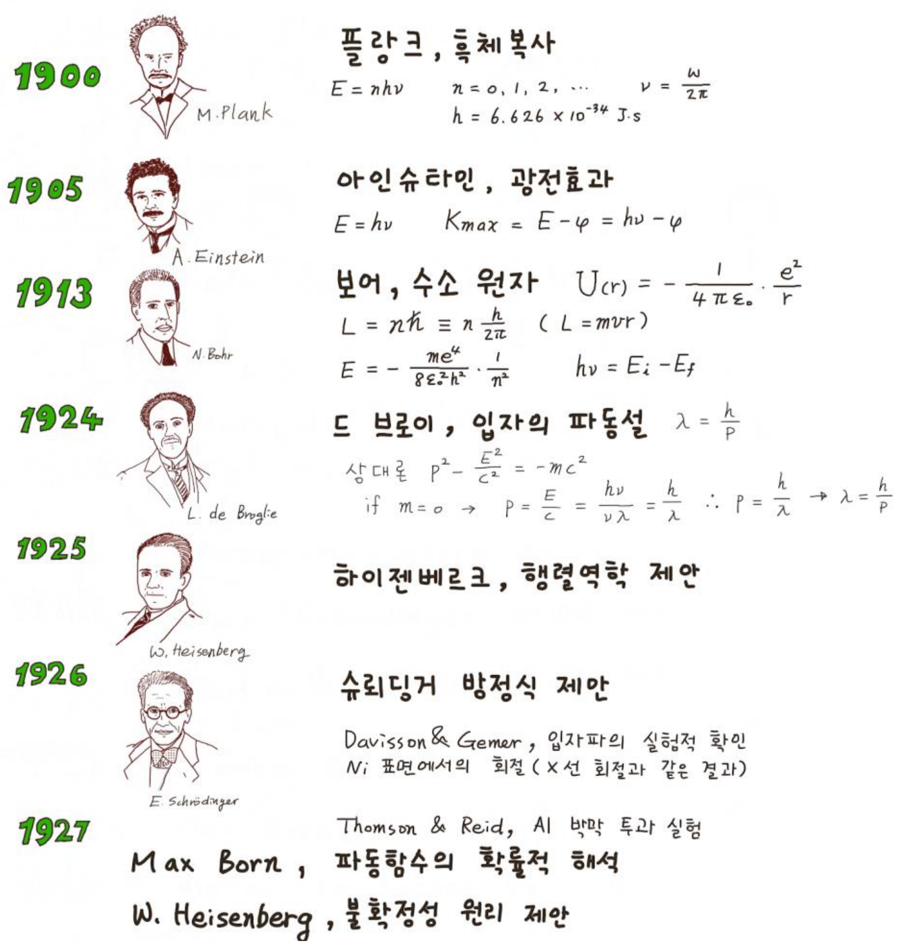
Quantum Mechanics

- Principle of energy quanta (에너지의 양자화 원리)
- Wave-particle duality principle (파동-입자 이중성 원리)
- Uncertainty principle (불확정성의 원리)



Photoelectric Effect (광전효과)

- Albert Einstein (1905) : Light is matter!
- $E = h\nu = hf = \hbar\omega$

$$h = \text{planck constant} = 6.62606 \times 10^{-34} [kgm^2s^{-1}]$$

$$\hbar = \frac{h}{2\pi}$$

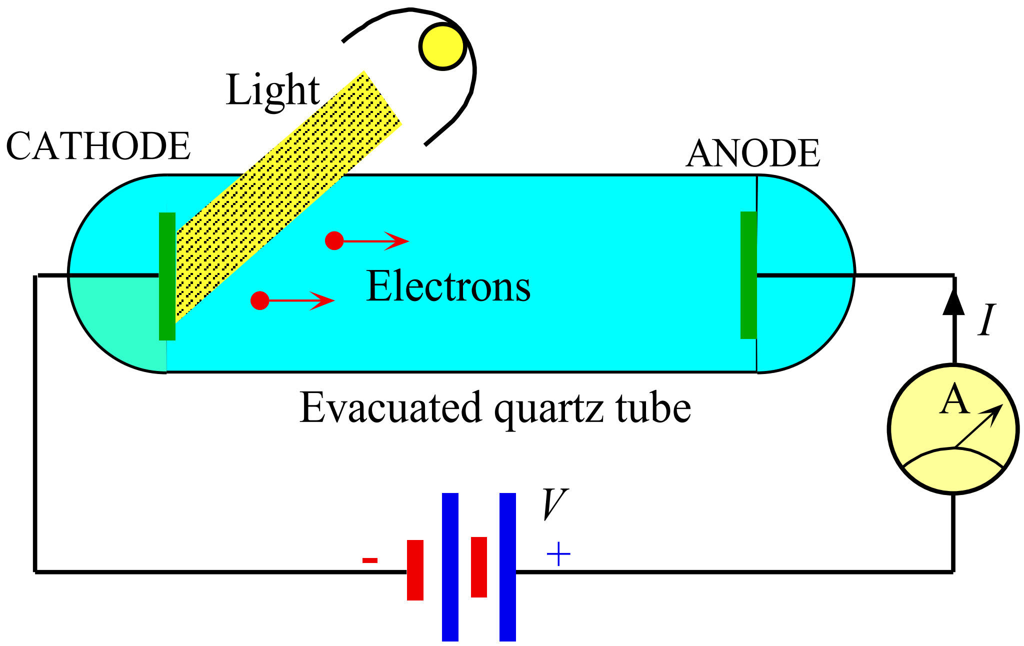


Fig. 3.4: The Photoelectric Effect.

Photoelectric Effect

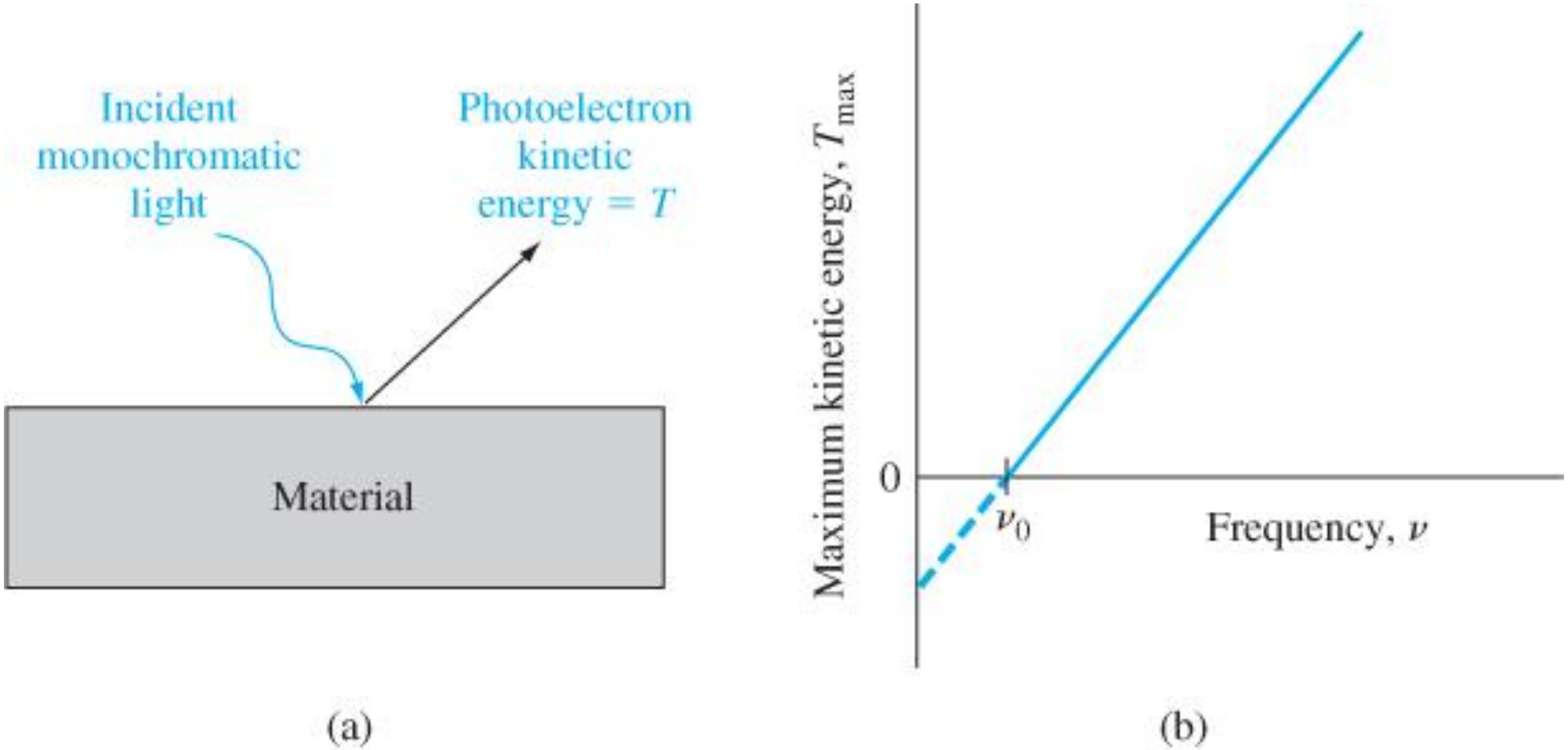


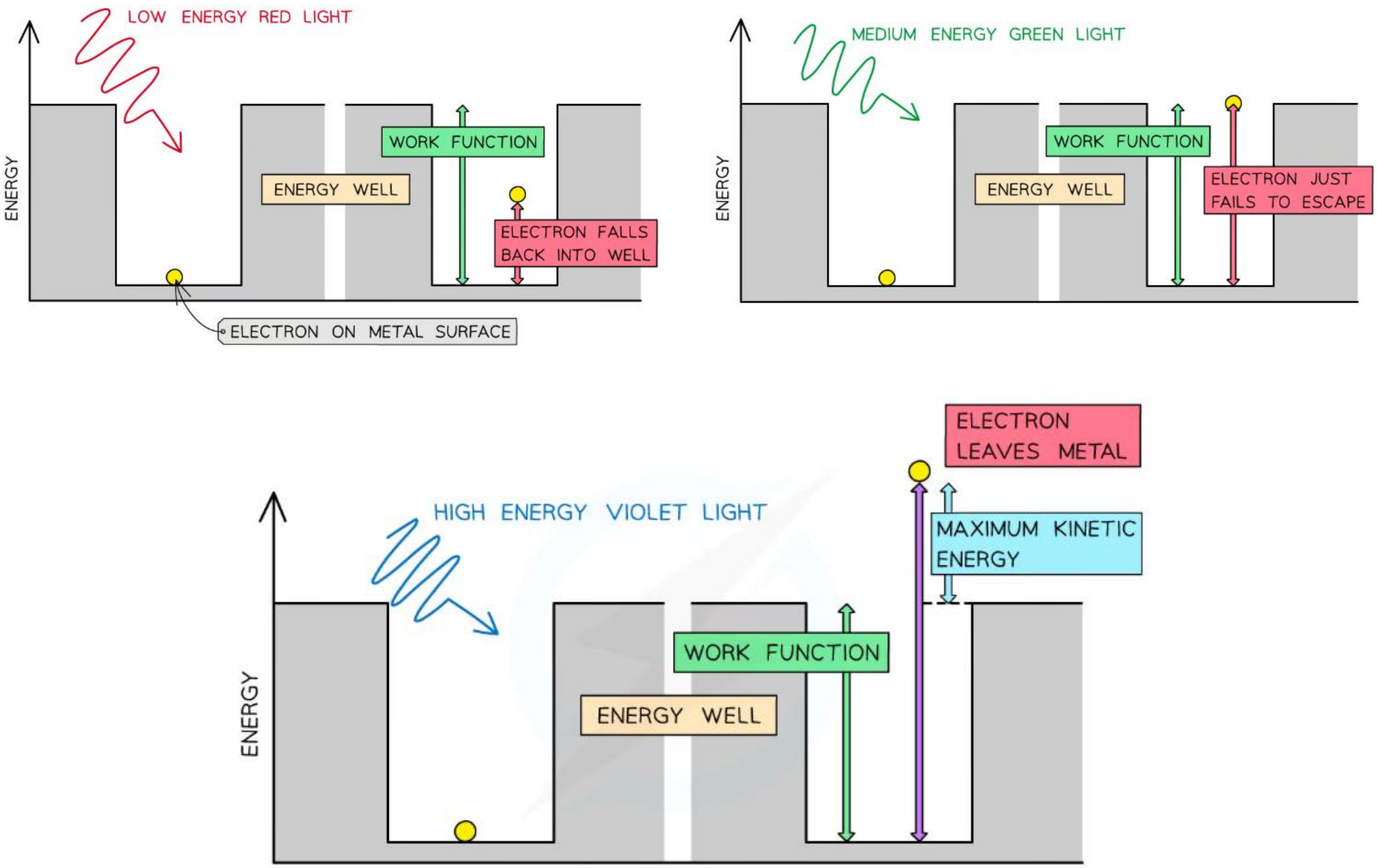
Figure 2.1 | (a) The photoelectric effect and (b) the maximum kinetic energy of the photoelectron as a function of incident frequency.

$$T = \frac{1}{2}mv^2 = h\nu - \Phi = h\nu - h\nu_0 \qquad (2.1)$$

Kinetic energy

Work function

Photoelectric Effect



Wave-Particle duality

- *wave-particle duality principle*

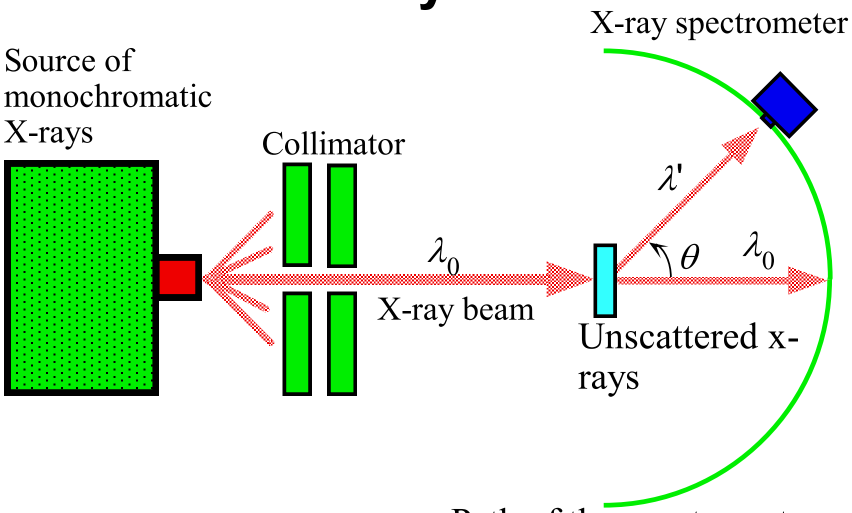
$$p = \frac{h}{\lambda} \tag{2.2}$$

- *de Broglie wavelength*

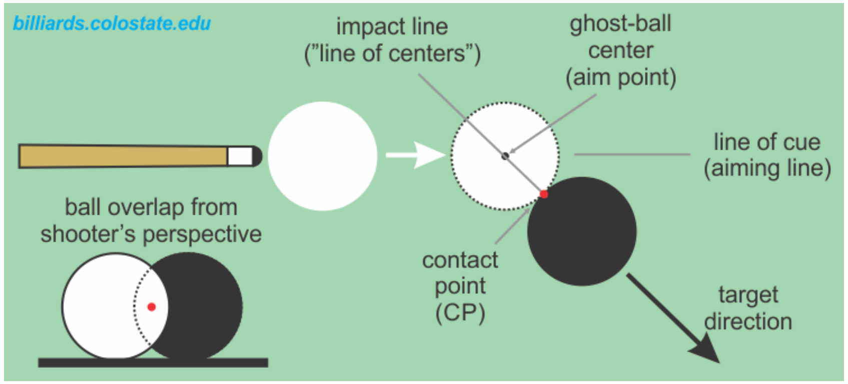
$$\lambda = \frac{h}{p} \tag{2.3}$$

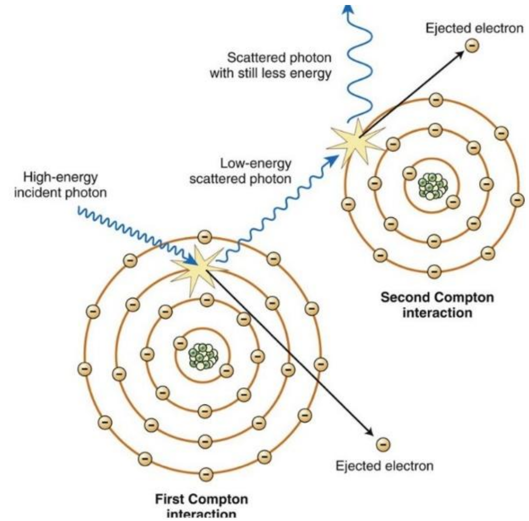
"Matter waves" or "de Broglie waves"

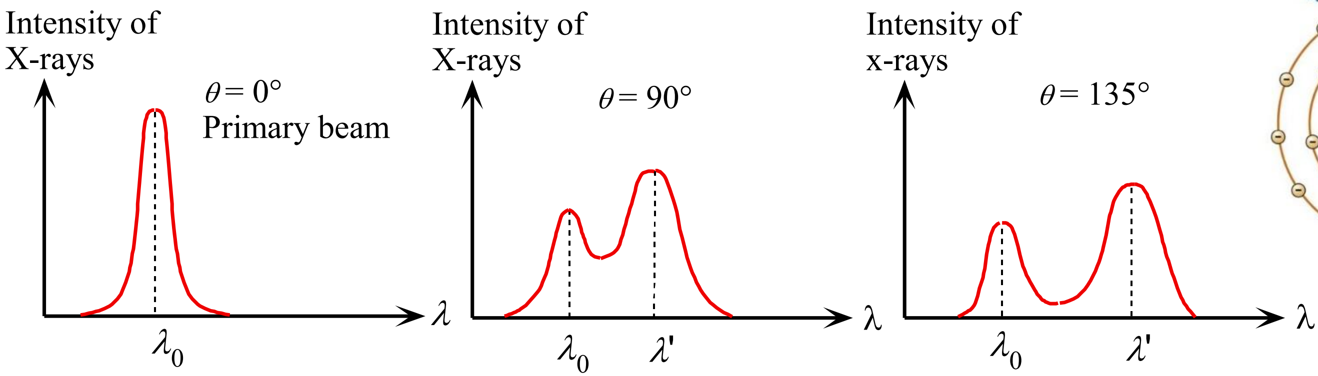
Wave-Particle duality



(a) A schematic diagram of the Compton experiment.







(b) Results from the Compton experiment

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

Fig. 3.10. The Compton experiment and its results.

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Wave-Particle duality

- Davisson & Germer : Light is wave!

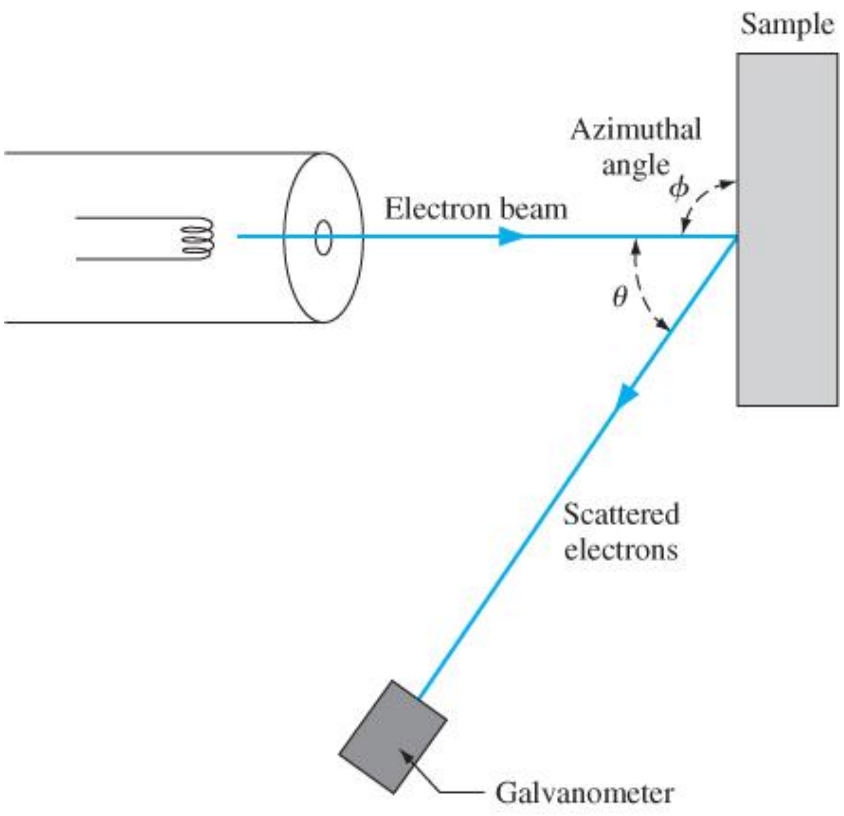


Figure 2.2 | Experimental arrangement of the Davisson–Germer experiment.

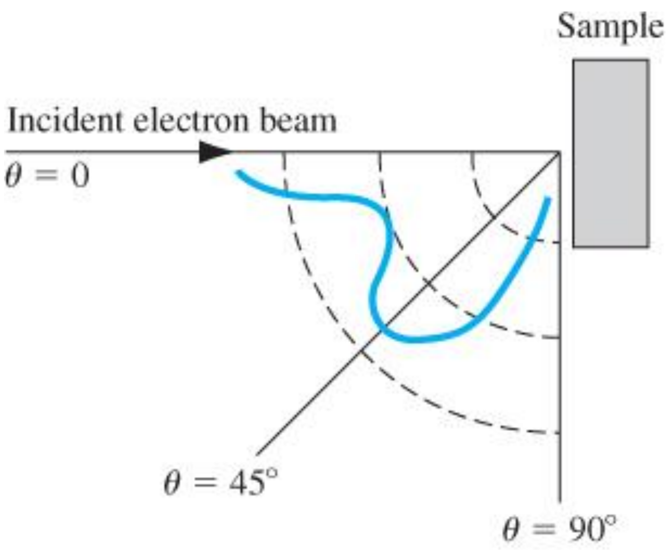


Figure 2.3 | Scattered electron flux as a function of scattering angle for the Davisson–Germer experiment.

Electromagnetic frequency spectrum

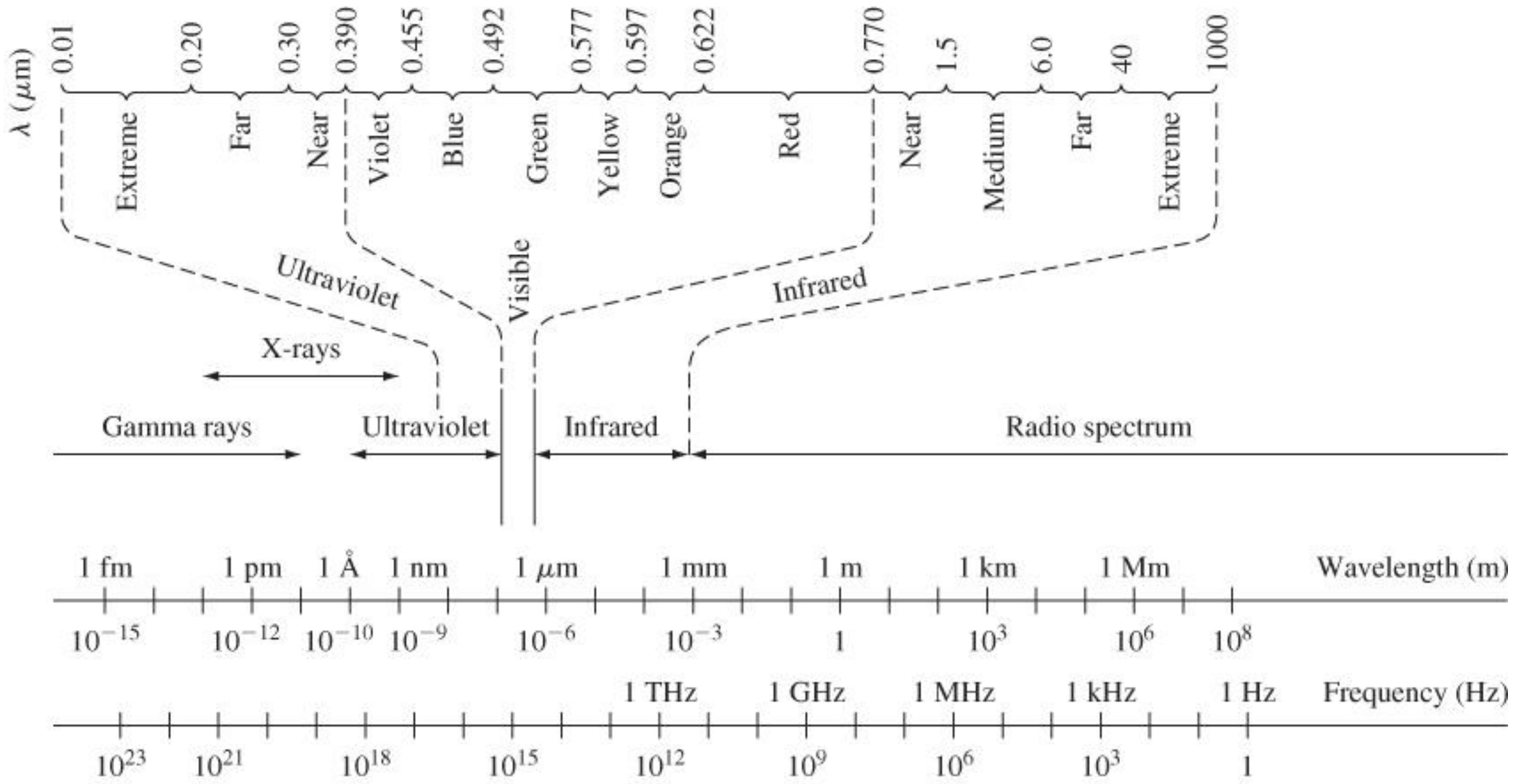


Figure 2.4 | The electromagnetic frequency spectrum.

Uncertainty principle (불확정성의 원리)

- Werner Karl Heisenberg (1927) :

$$\Delta p \Delta x \geq \hbar \qquad (2.4) \qquad \hbar = \frac{h}{2\pi}$$

Uncertainty in momentum **Uncertainty in position**

$$\Delta E \Delta t \geq \frac{\hbar}{2} \qquad (2.5)$$

Uncertainty in energy **Uncertainty in time**

Schrödinger's wave equation

$\Psi(x,t)$ = Wave equation

$V(x)$ = Potential function

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

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

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

Divide by $\psi(x)\phi(t)$

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

Space **Time**

Schrödinger's wave equation

$\Psi(x,t)$ = Wave equation

$V(x)$ = Potential function

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

Constant

Space **Time**

$$j\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt}=\eta$$

$$\frac{1}{\phi(t)}\frac{d\phi(t)}{dt}=\frac{\eta}{j\hbar}=-j\frac{\eta}{\hbar}$$

1st order ODE, e^{λ}

$$\frac{1}{\phi(t)}d\phi(t)=-j\frac{\eta}{\hbar}dt$$

$$ln|\phi(t)|=-j\frac{\eta}{\hbar}t$$

$$E=h\nu=hf=\hbar\omega$$

$$\phi(t)=e^{-j(\frac{\eta}{\hbar})t}=e^{-j\omega t}=e^{-j(\frac{E}{\hbar})t}$$

$$\omega=\frac{\eta}{\hbar}=\frac{E}{\hbar}\qquad \eta=E$$

Schrödinger's wave equation

$\Psi(x,t)$ = Wave equation

$V(x)$ = Potential function

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

⇦ **Constant**

Space **Time**

$$-\frac{\hbar^2}{2m^*}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2}+V(x)=E \quad \Rightarrow \quad \frac{d^2\psi(x)}{dx^2}+\frac{2m^*}{\hbar^2}(E-V(x))\psi(x)=0$$

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

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

Schrödinger's wave equation

$$|\psi(x)|^2$$

Probability density function of finding particle
(확률밀도함수)

$$|\psi(x)|^2 dx$$

Probability of finding particle between x and x+dx
(x와 x+dx 사이에서 전자를 찾을 확률)

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

Total probability
(전체 확률은 항상 1)

Schrödinger's wave equation analysis for free electron

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

2nd order ODE, e^{λ} ⇨

$$\psi(x) = Ae^{+jkx} + Be^{-jkx}$$

$$k = \sqrt{\frac{2m^*E}{\hbar^2}}$$

⇩

$$\phi(t) = e^{-j\omega t}$$

⇦

$$\Psi(x,t) = \psi(x)\phi(t) = Ae^{+j(kx-\omega t)} + Be^{-j(kx+\omega t)}$$

+x 방향으로 진행 **-x 방향으로 진행**

$\Psi(x,t)$ = 진행파 = 시간에 따라 움직이는 파동

❖ Kinetic energy and momentum of free electron

$$k = \sqrt{\frac{2m^*E}{\hbar^2}} \quad ⇨ \quad E_k = \frac{\hbar^2k^2}{2m^*} = \frac{1}{2}m^*v^2 = \frac{p^2}{2m^*} \quad ⇨ \quad p = \hbar k$$

❖ Wavelength of free electron

$$\lambda = \frac{h}{p} \qquad p = \hbar k \quad ⇨ \quad \lambda = \frac{h}{p} = \frac{2\pi\hbar}{p} = \frac{2\pi}{k}$$

Schrödinger's wave equation analysis for free electron

- assume that electron traveling in the +x direction,

$$\Psi(x,t) = Ae^{+j(kx-\omega t)} \Rightarrow |\Psi(x,t)|^2 = Ae^{+j(kx-\omega t)}\, A^* e^{-j(kx-\omega t)} = |A|^2$$

➔ The probability of finding an electron is the same regardless of x's position.
➔ The electron can exist everywhere!

❖ Summary of analysis for free electron

$$\Psi(x,t) = Ae^{+j(kx-\omega t)} + Be^{-j(kx+\omega t)}$$

$$k = \sqrt{\frac{2m^*E}{\hbar^2}} \qquad E_k = \frac{\hbar^2}{2m^*}k^2$$

***y* = a*x*²**

***E-k* diagram**

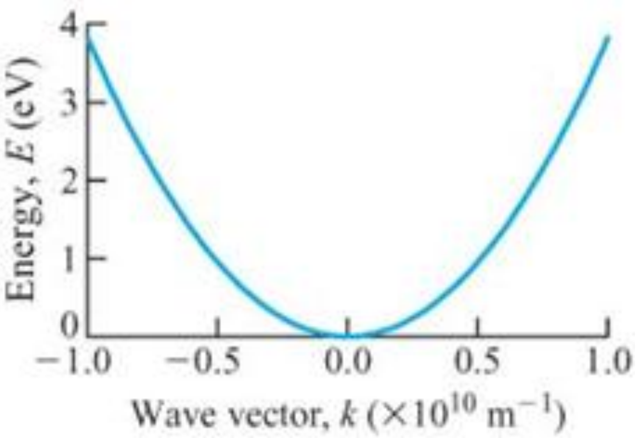


Figure 2.5

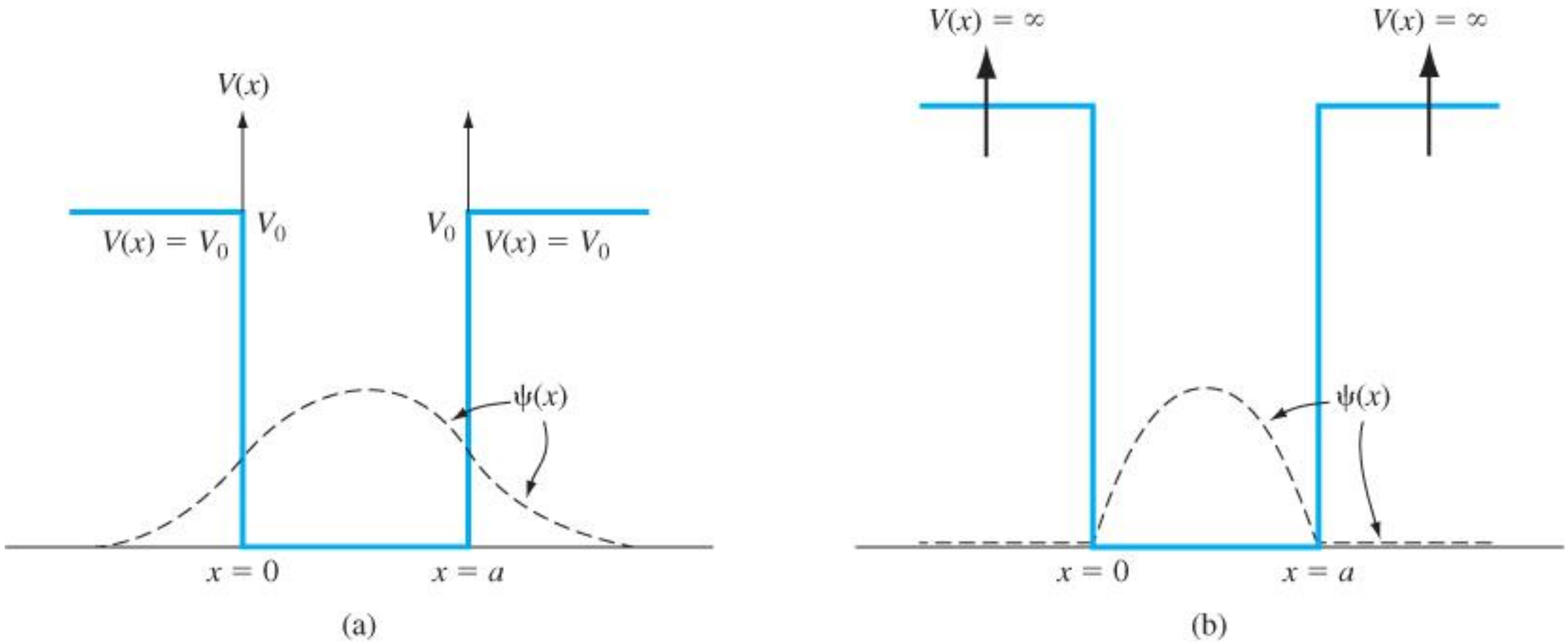


Figure 2.5 | Potential functions and corresponding wave function solutions for the case (a) when the potential function is finite everywhere and (b) when the potential function is infinite in some regions.

Schrödinger's wave equation analysis for infinite potential well

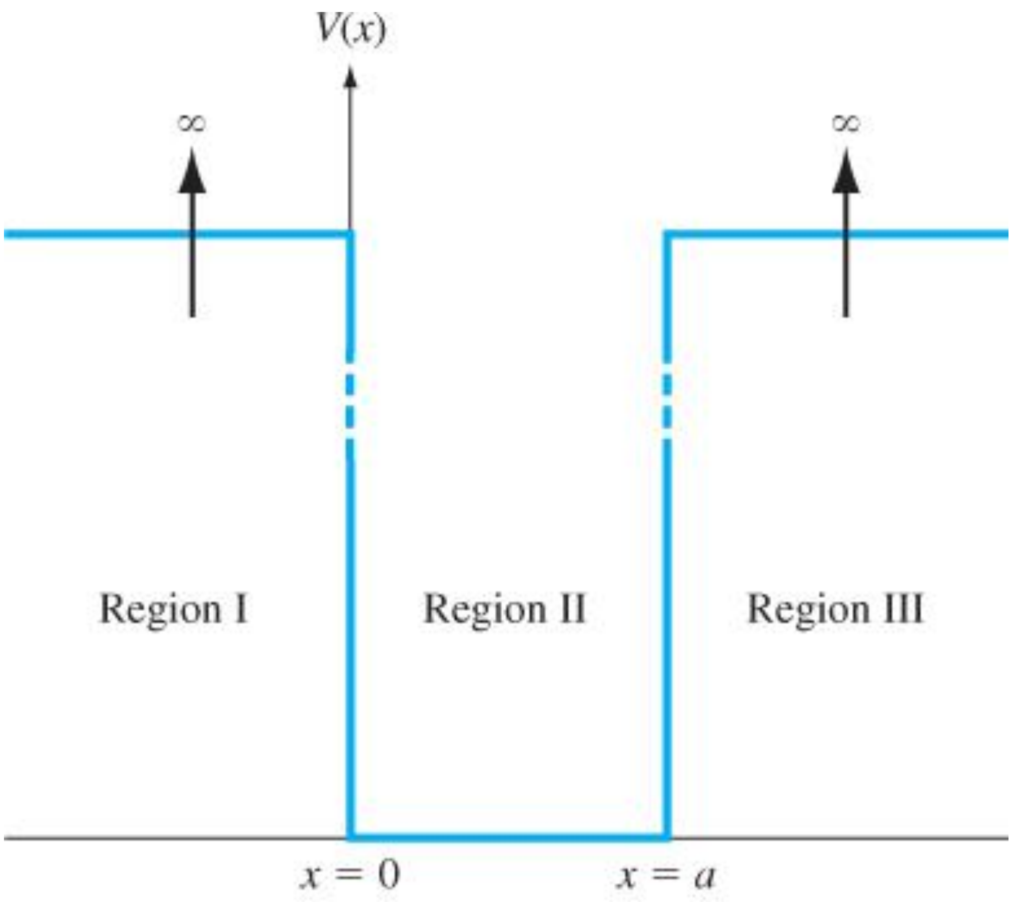


Figure 2.6 | Potential function of the infinite potential well.

Schrödinger's wave equation analysis for infinite potential well

❖ **Boundary conditions**

- Wave function is finite.
- Wave function is continuous.
- Derivative of wave function is also finite and continuous.

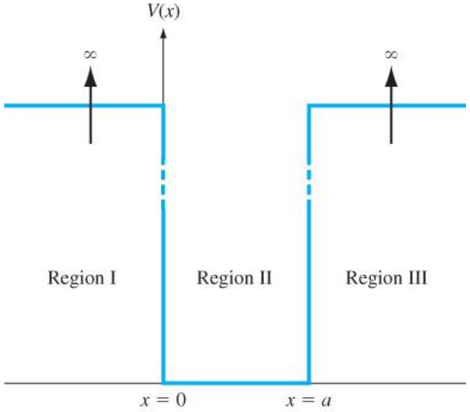


Figure 2.6 | Potential function of the infinite potential well.

$$\psi(x) = \begin{cases} 0 & x < 0, & V(x) = \infty \\ \psi(x) & 0 \le x \le a, & V(x) = 0 \\ 0 & x > a, & V(x) = \infty \end{cases}$$

⇩

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m^*E}{\hbar^2}\psi(x) = 0 \quad \Rightarrow \quad \begin{aligned} \psi(x) &= Ae^{+jkx} + Be^{-jkx} \\ \psi(x) &= A\cos kx + B\sin kx \end{aligned} \qquad k = \sqrt{\frac{2m^*E}{\hbar^2}}$$

Consider boundary conditions

$$\begin{aligned} \psi(x=0) &= 0 = A \\ \psi(x=a) &= 0 = B\sin ka \end{aligned} \quad \Rightarrow \quad \begin{aligned} ka &= n\pi \quad n = 1, 2, 3, \cdots \\ k_n &= \left(\frac{\pi}{a}\right)n, \qquad n = 1, 2, 3, \cdots \end{aligned}$$

***k* is quantized**

$$\psi(x) = \begin{cases} 0 & x < 0 \; or \; x > a \\ B\sin\left(\frac{n\pi}{a}\right)x & 0 \le x \le a \end{cases}$$

Schrödinger's wave equation analysis for infinite potential well

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_0^a |\psi(x)|^2 dx = \int_0^a B^2 \sin^2 k_n x \, dx = \frac{B^2 a}{2} = 1 \quad \Rightarrow \quad B = \sqrt{\frac{2}{a}}$$

$$\boldsymbol{k_n = \left(\frac{\pi}{a}\right) n, \qquad n = 1, 2, 3, \cdots}$$

$$\Psi(x,t) = \psi(x)\phi(t) = \psi(x)e^{-j\omega t} = \begin{cases} 0 & x < 0 \; or \; x > a \\ \left(\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}\right) x\right) e^{-j\omega t} & 0 \le x \le a \end{cases}$$

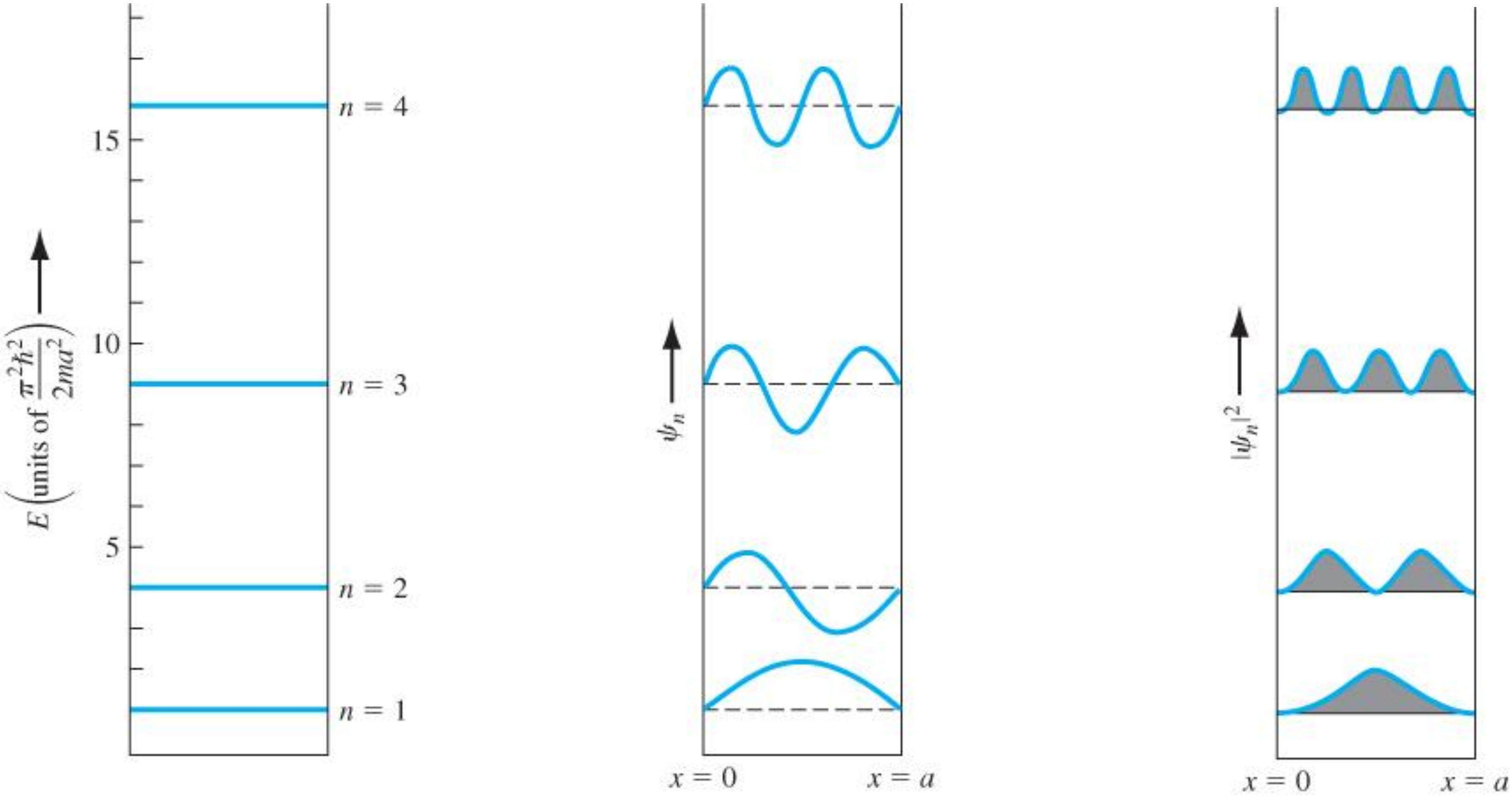
$$E_k = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2 k_n^2}{2m^*} = \frac{\hbar^2 n^2 \pi^2}{2m^* a^2}, \qquad n = 1, 2, 3, \cdots$$

Figure 2.7

$$E_k = \frac{\hbar^2 n^2 \pi^2}{2m^* a^2}$$

$$\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}\right) x$$

$$|\psi(x)|^2 = \frac{2}{a} \sin^2\left(\frac{n\pi}{a}\right) x$$



(a) (b) (c)

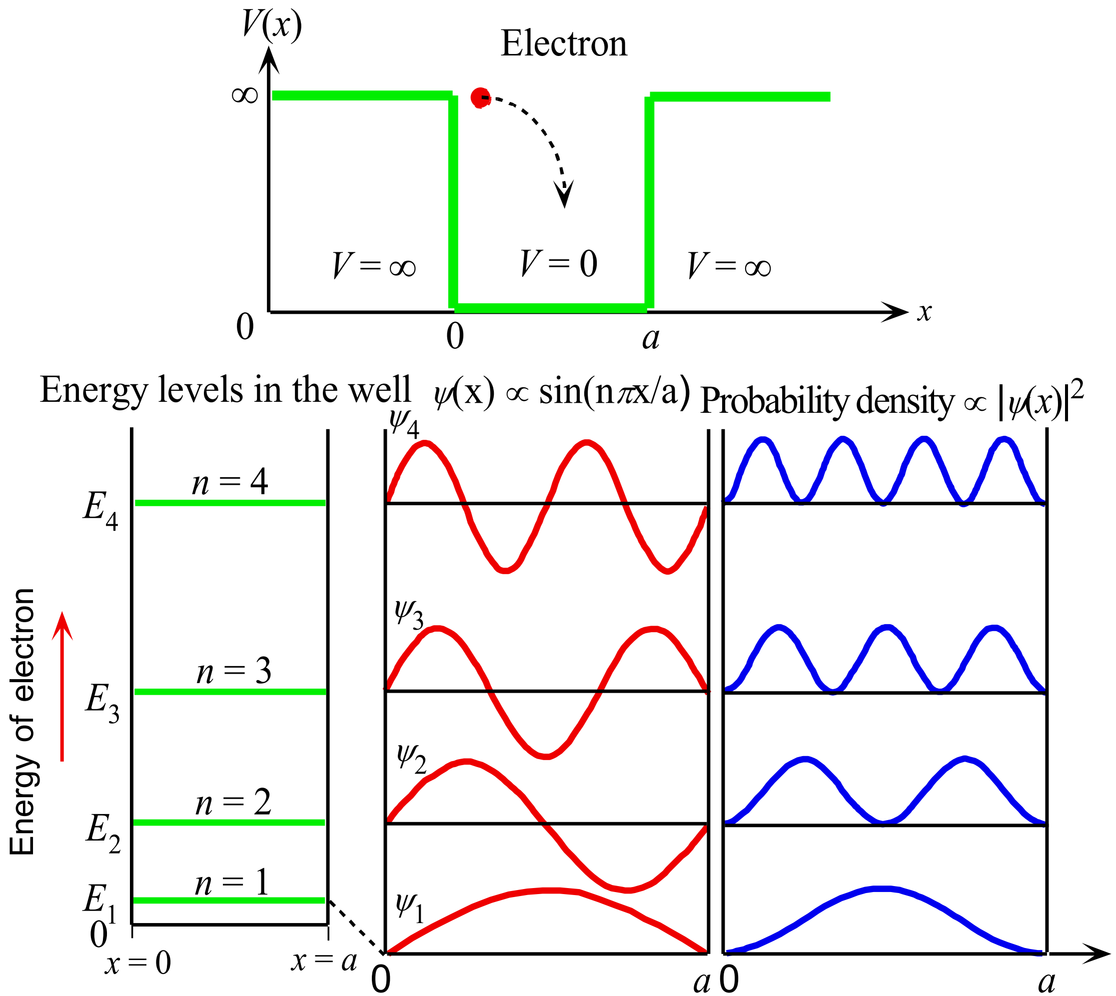


Fig. 3.15: Electron in a one-dimensional infinite PE well. The energy of the electron is quantized. Possible wavefunctions and the probability distributions for the electron are shown.

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Schrödinger's wave equation analysis for stepwise potential barrier

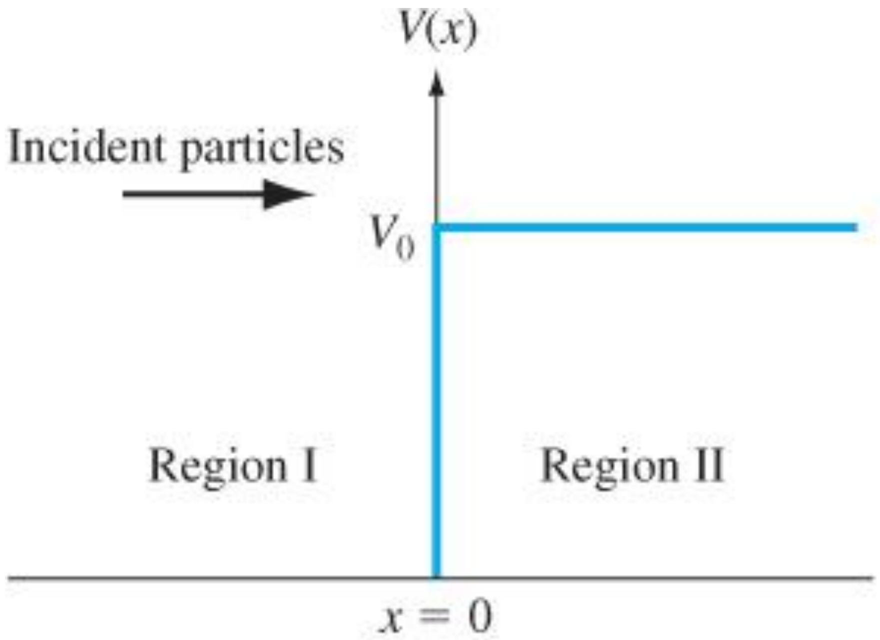

Figure 2.8 | The step potential function.

This result implies that there is a finite probability that the incident particle will penetrate barrier and exist in region II. The probability of a particle penetrating the potential barrier is another difference between classical and quantum mechanics: The quantum mechanical penetration is classically not allowed.

Schrödinger's wave equation analysis for stepwise potential barrier

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m^*E}{\hbar^2}\psi(x) = 0$$

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

$$\psi(x) = Ae^{+jk_1x} + Be^{-jk_1x}$$

$$\psi(x) = Ce^{+jk_2x} + De^{-jk_2x}$$

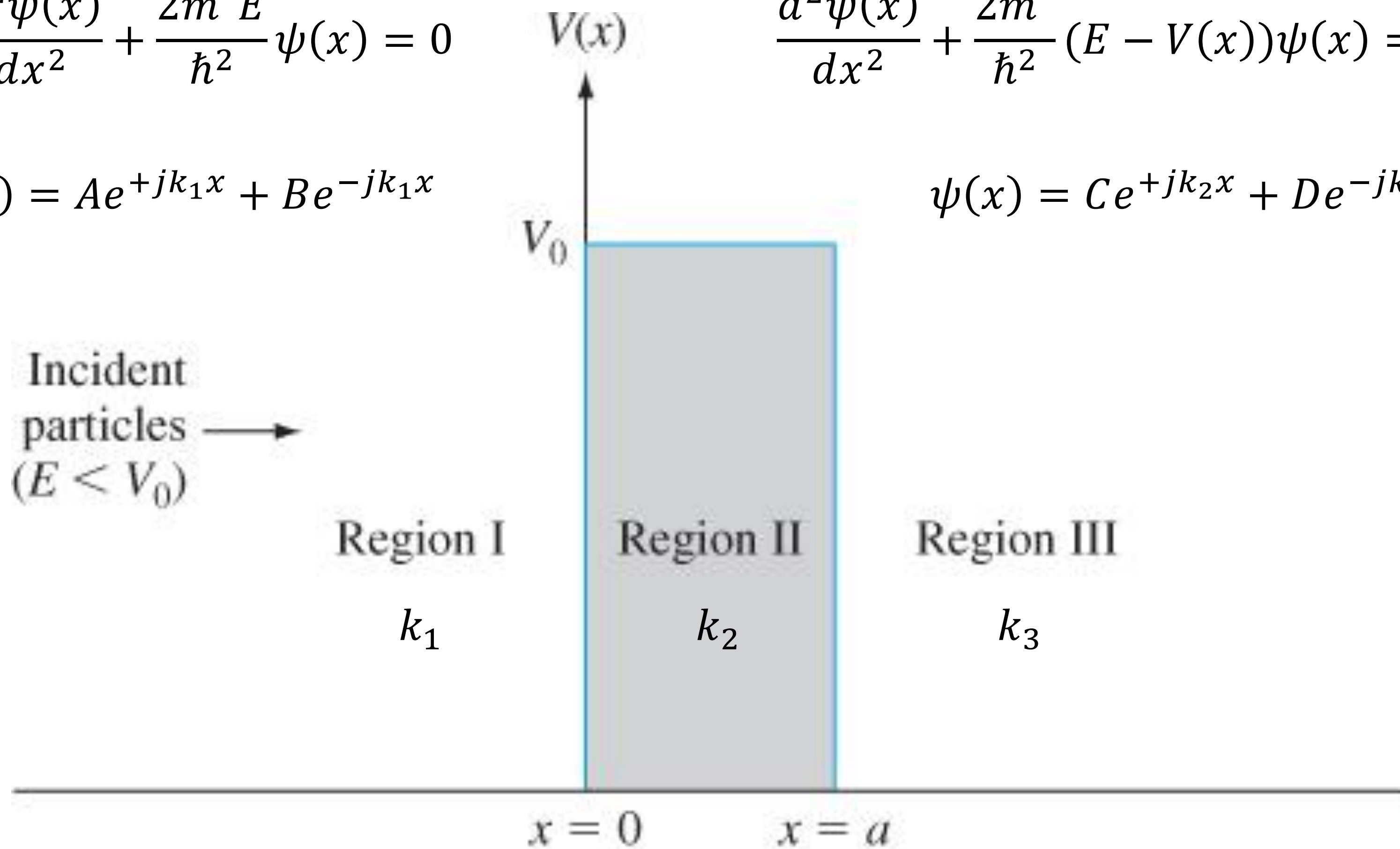

Figure 2.9 | The potential barrier function.

Schrödinger's wave equation analysis for stepwise potential barrier

➔ Tunneling !

$$T \approx 16\left(\frac{E}{V_0}\right)\left(1-\frac{E}{V_0}\right)e^{-2k_2 a} \qquad k_2 = \sqrt{\frac{2m^*(V_0-E)}{\hbar^2}} \qquad (2.63)$$

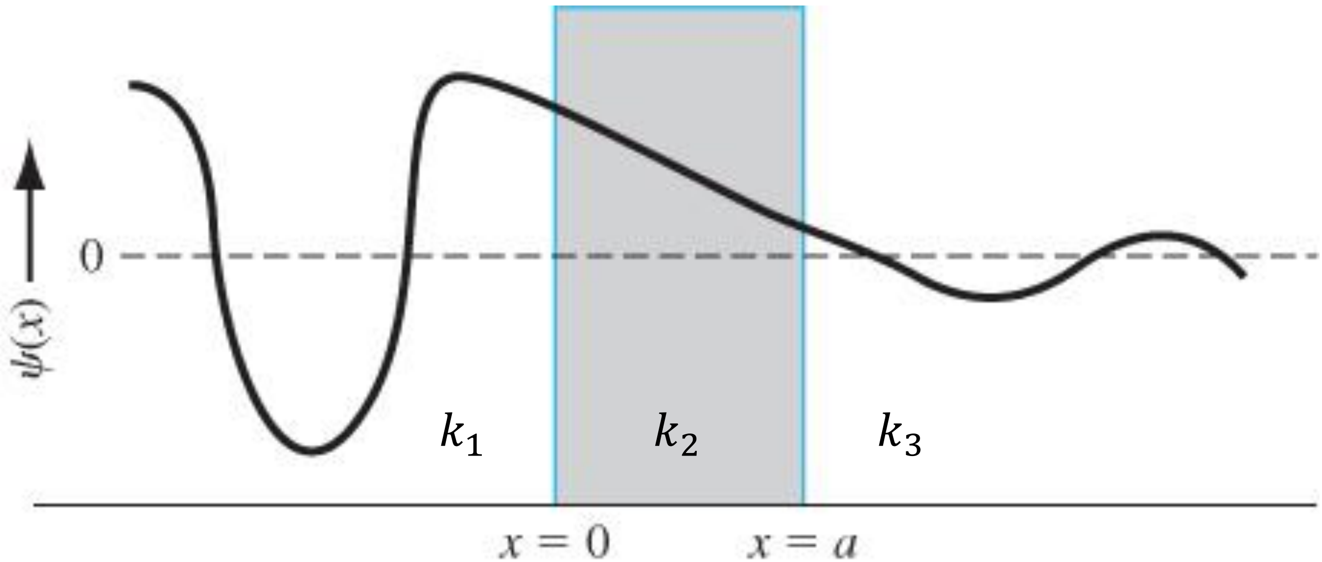

Figure 2.10 | The wave functions through the potential barrier.