

Outline

2.1 Principles of Quantum Mechanics

2.2 Schrodinger's Wave Equation

2.3 Applications of Schrodinger's Wave Equation

2.4 Extensions of the Wave Theory to Atoms

光(電磁波)

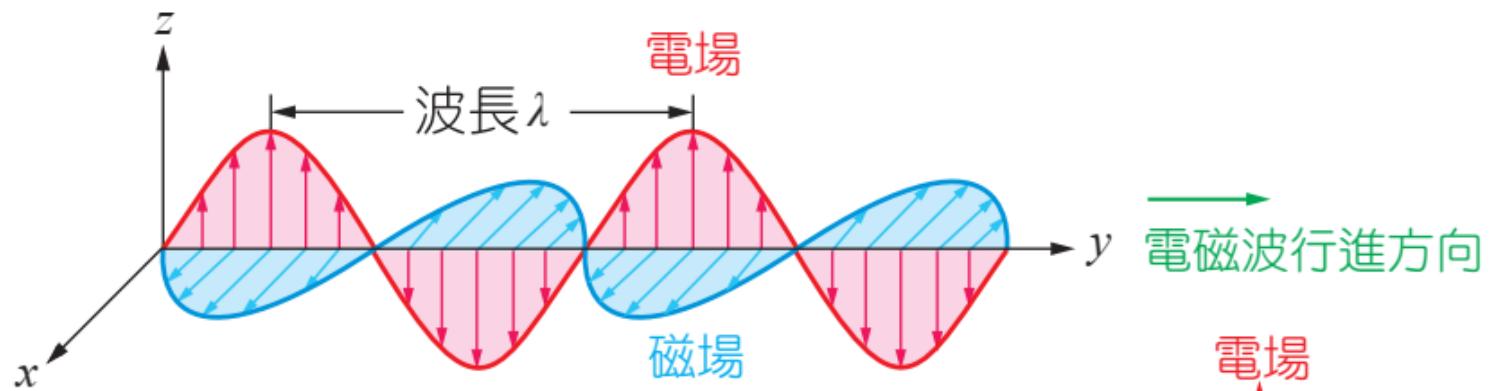
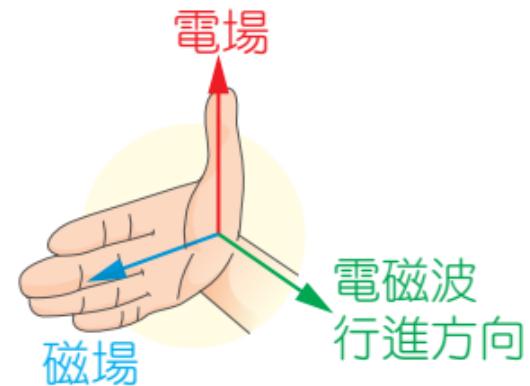


圖 4-21 電磁波示意圖。

電場、磁場及行進方向三者互相垂直，且可用右手（開掌）定則表達三者的關係。



波動

波長

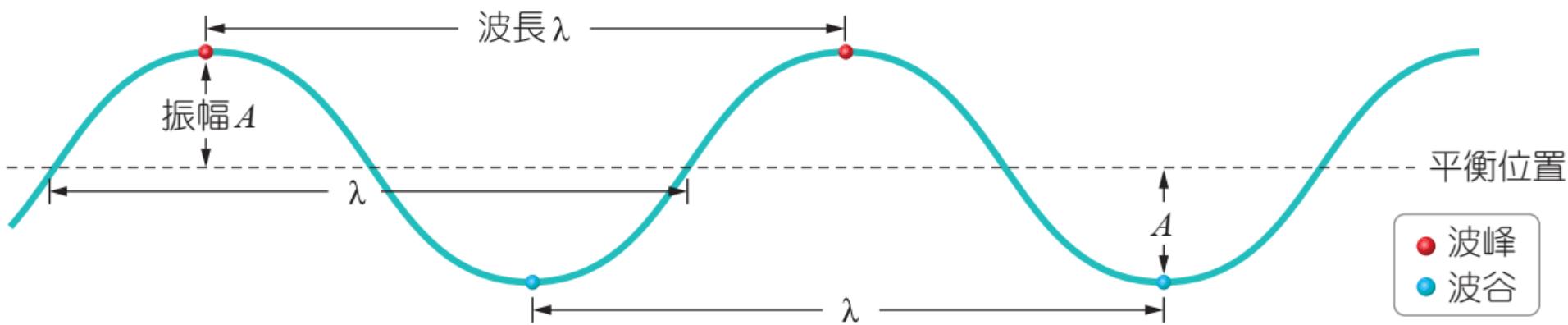
波速 $v = \frac{\lambda}{T} = f\lambda$

↓

週期 頻率

角頻率： $\omega = 2\pi f$

波數： $k = \frac{2\pi}{\lambda}$

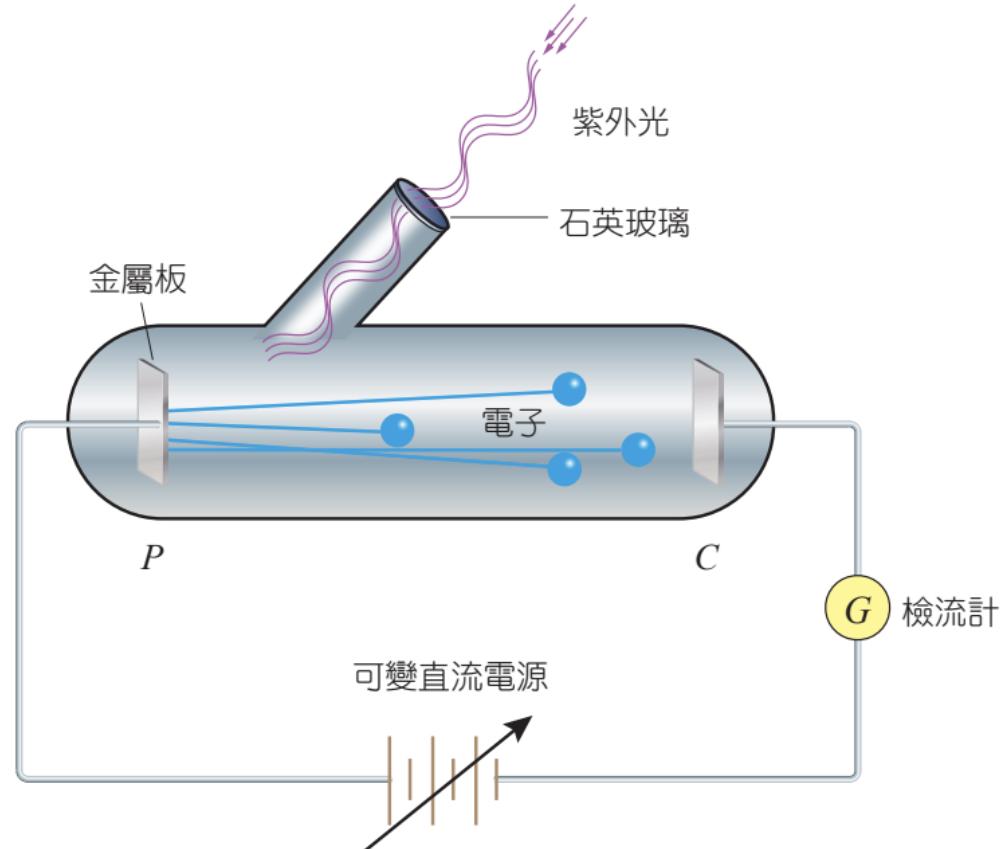


光電效應 Photoelectric Effect

古典物理認為：

- 光是電磁波，光的強度與電磁波的振幅有關
- 只要光強度夠大，金屬上的電子就可以被電磁波搖晃而出
- 電子動能應與光的頻率無關

但光電效應的實驗結果無法以古典物理解釋



黑體輻射 Blackbody Radiation

- Blackbody radiation refers to the EM radiation emitted by a blackbody in the thermodynamic equilibrium
- The spectrum of EM radiation determined by the temperature of blackbody

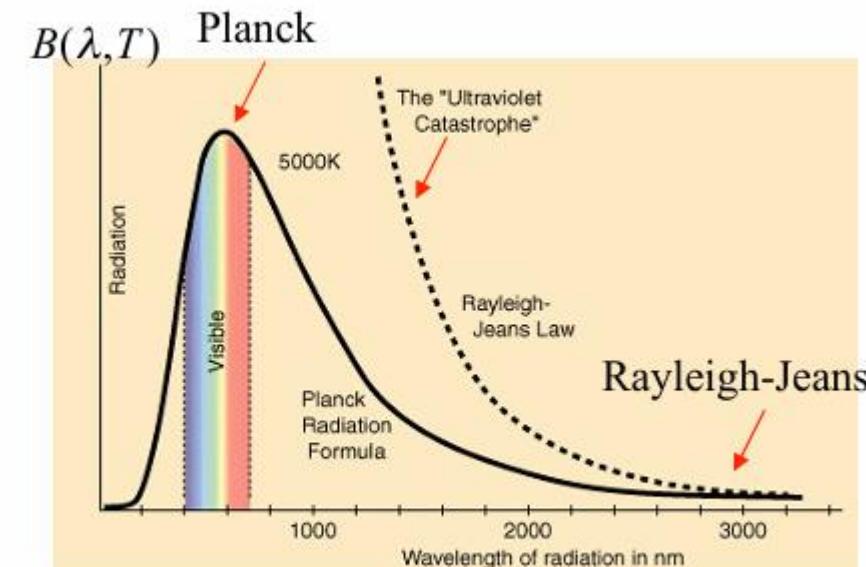
Rayleigh-Jeans law

$$B(\lambda, T) = \frac{8\pi\nu^2}{c^3} * kBT \quad \rightarrow \text{ultraviolet catastrophe (classical physics)}$$

Planck's Radiation law

$$E = nhv$$

$$B(\lambda, T) = \frac{8\pi\nu^2}{c^3} * \frac{hv}{e^{\frac{hv}{k_B T}} - 1}$$

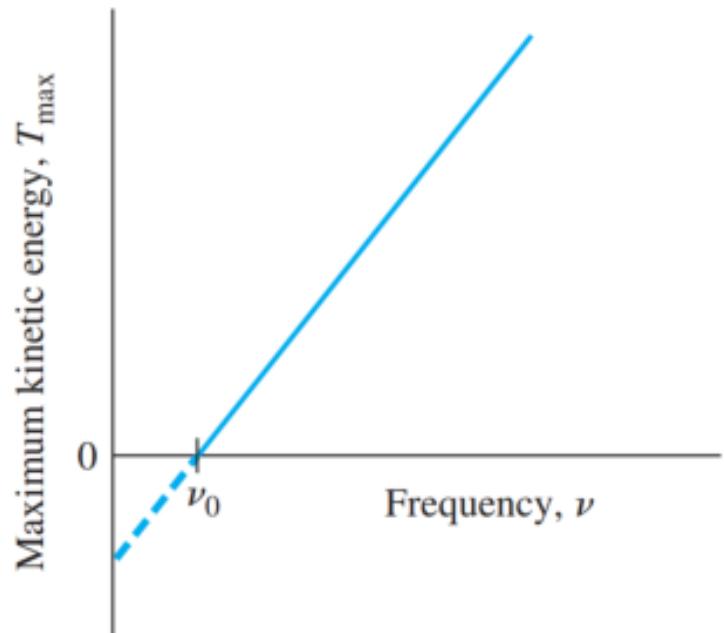


Planck's constant

$$h = 6.625 \times 10^{-34} \text{ J.s}$$

光電效應 Photoelectric Effect

- 1905年愛因斯坦提出光量子說，後來被稱為光子(photon)
- 光子以光速($c = 3 \times 10^8$ m/s)前進，其能量與光的頻率成正比
- 單顆光子的能量為 $E = h\nu$



$$h\nu = W + T_{max}$$

$$\hbar\omega = W + T_{max}$$

- 當入射光頻率是高於材料的特徵頻率時，光電效應才可適用
- 所激發出的動能與入射光頻率成正比
- 出射光強度與最大動能無關，而是與光子數目有關

$h (6.625 \times 10^{-34})$	普朗克常數
$\hbar = h/2\pi$	約化普朗克常數
ν	光子頻率
W	功函數
T_{max}	電子動能

Example 2.1 Photon Energy

Objective: Calculate the photon energy corresponding to a particular wavelength.

Consider an x-ray with a wavelength of $\lambda = 0.708 \times 10^{-8}$ cm.

Example 2.1 Photon Energy

Objective: Calculate the photon energy corresponding to a particular wavelength.

Consider an x-ray with a wavelength of $\lambda = 0.708 \times 10^{-8} \text{ cm}$.

使用物理 m(公尺) k(公斤) s(秒) 制 , $0.708 \times 10^{-8} \text{ cm} = 0.708 \times 10^{-10} \text{ m}$

$$E = h\nu = h \frac{c}{\lambda} = \frac{(6.625 \cdot 10^{-34})(3 \cdot 10^8)}{0.708 \cdot 10^{-10}} = 2.81 \cdot 10^{-15} \text{ J}$$

$$E = \frac{2.81 \cdot 10^{-15}}{1.6 \cdot 10^{-19}} = 1.75 \cdot 10^4 \text{ eV}$$

Note: $1 \text{ eV} = 1.6 \times 10^{-19} \text{ C} \times 1 \text{ V} = 1.6 \times 10^{-19} \text{ Joule}$

物質波 Matter wave

- 1924年德布羅意提出不僅光具有波動粒子的雙重特性，連粒子也具有波動性，並稱之為「物質波」。
- 物質與波動的轉換關係為：

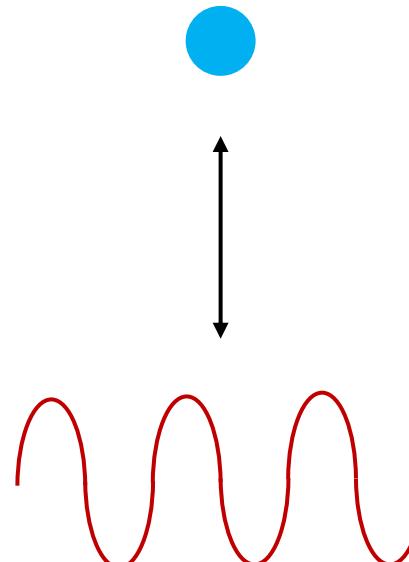
物質波波長 $\lambda = \frac{h}{p}$

Particles: wave-like behavior

物質波動量 $p = \frac{h}{\lambda} = \frac{2\pi}{\lambda} \frac{h}{2\pi} = \hbar k$

Waves: particle-like behavior

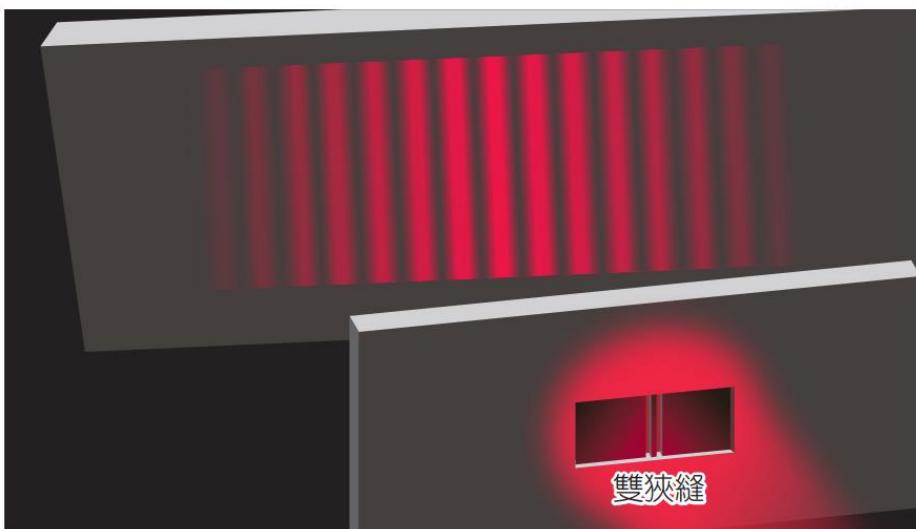
物質波能量 $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$



電子的雙狹縫干涉實驗

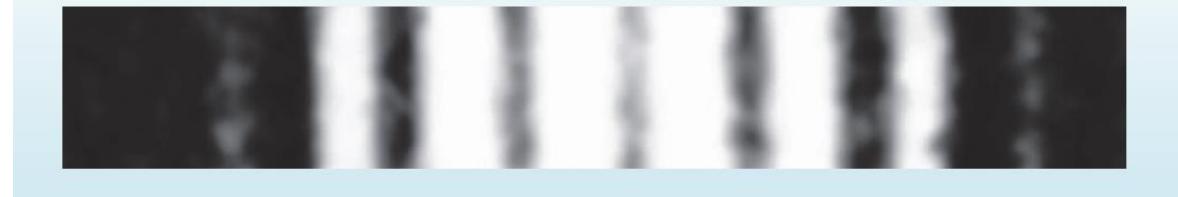
- 雙狹縫干涉實驗是光具波動性的代表性實驗，如果粒子也有波動性，那麼以粒子束取代光源進行雙狹縫干涉實驗應可以得到類似的結果。
- 德國人詹頌(Claus Jönsson, 1930 ~)在1959年完成了這個實驗。證明了粒子具有波動性。

雷射光的雙狹縫干涉



電子的雙狹縫干涉

a 謂頌的電子雙狹縫實驗結果。



Example 2.2 de Broglie wavelength

Objective: Calculate the de Broglie wavelength of a particle.

Consider an electron traveling at a velocity of 10^7 cm/s = 10^5 m/s.

Example 2.2 de Broglie wavelength

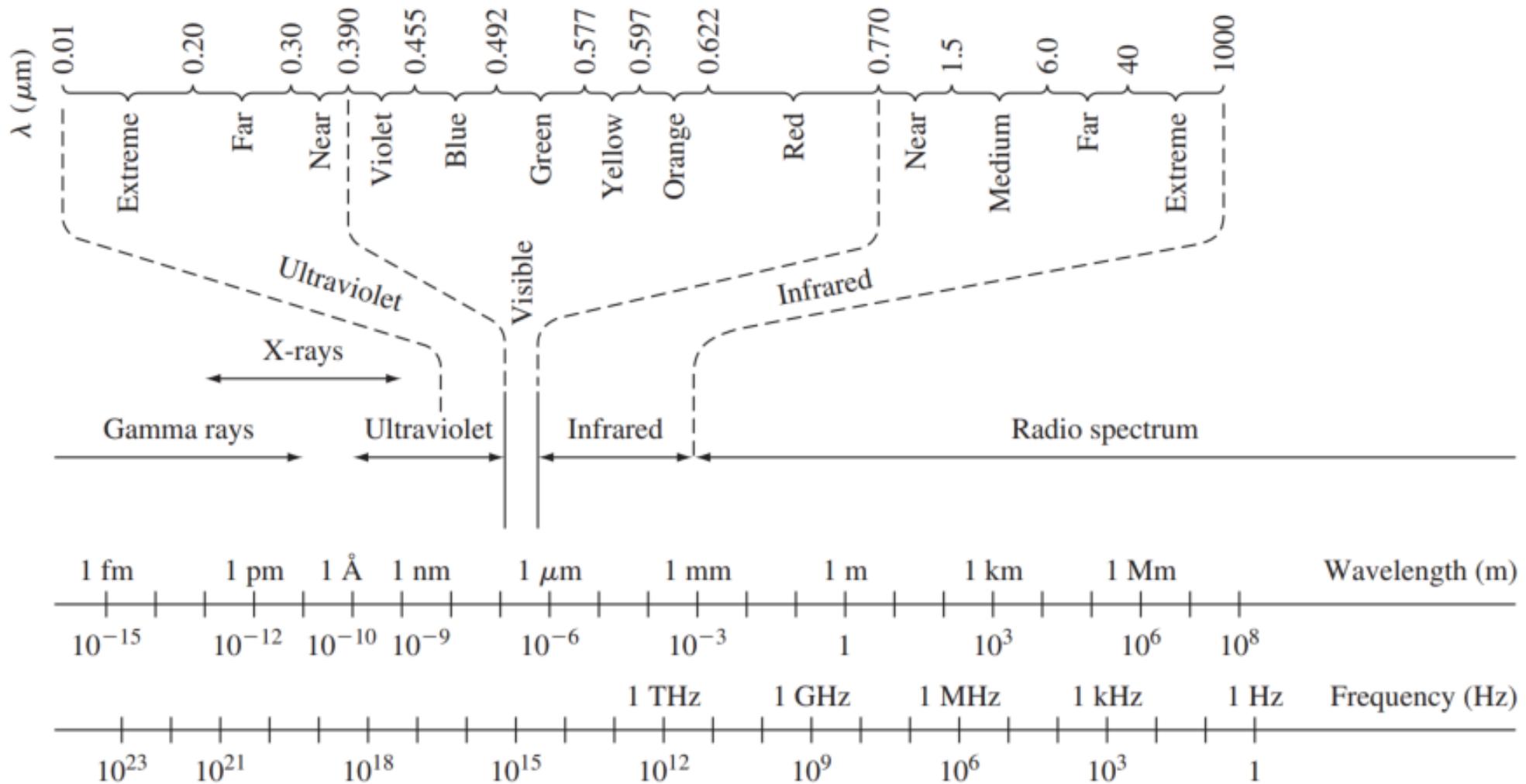
Objective: Calculate the de Broglie wavelength of a particle.

Consider an electron traveling at a velocity of 10^7 cm/s = 10^5 m/s.

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

$$\lambda = \frac{h}{p} = \frac{6.625 \times 10^{-34}}{9.11 \times 10^{-26}} = 7.27 \text{ nm}$$

電磁波頻譜



測不準原理 Uncertainty Principle

- 測不準原理（海森堡） 不可能同時描述粒子的絕對精度、位置和動量不可能同時描述粒子的絕對精度能量和粒子具有此的瞬間時間
- 如果我們試圖更精確地測量粒子的位置（使 Δx 變小），那麼它的動量不確定性 Δp 會變大---**波動性與粒子性**
- 如果我們試圖非常精確地測量一個粒子的能量，那麼你對它在那個能量狀態下存在了多久就會變得模糊---**量子躍遷與自發輻射、量子穿隧效應（掃描穿隧電子顯微鏡 STM）**

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

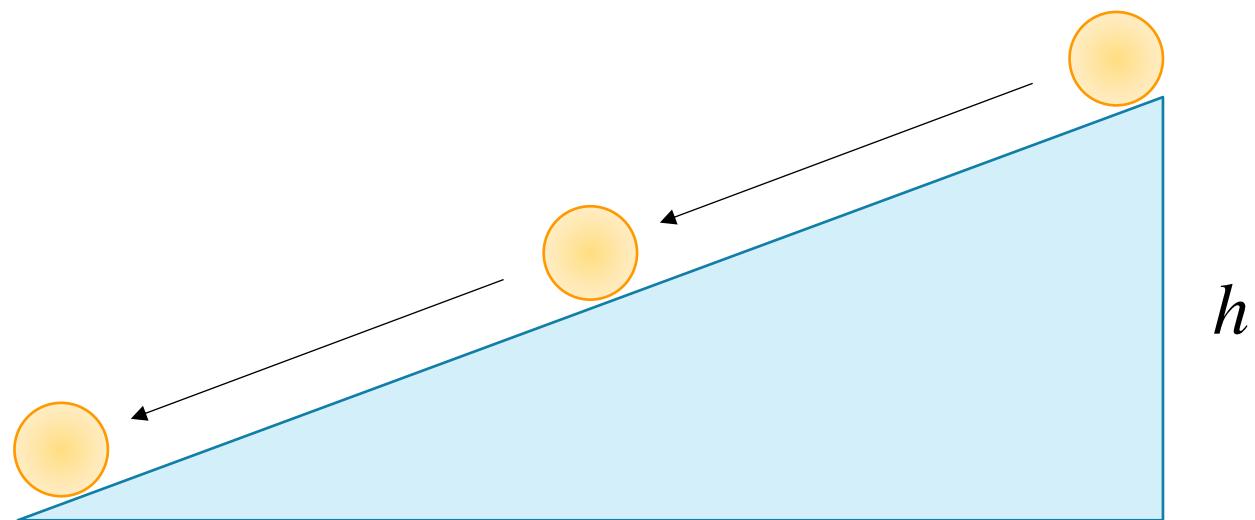
$$\Delta E \cdot \Delta t \geq \hbar$$

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

古典力學能

力學能（總能） = 動能 + 位能 (potential)

$$E = \frac{1}{2}mv^2 + V \quad \text{或表示為} \quad E = \frac{p^2}{2m} + V$$



WARNING

2.2 薛丁格波動方程式

動能 + 位能 總能

$$\left[\frac{\hat{p}^2}{2m} + V \right] \Psi(x, t) = \hat{E} \Psi(x, t)$$

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

波函數的物理意義

量子力學中，物質的位置不確定，而是呈現機率分布的型態

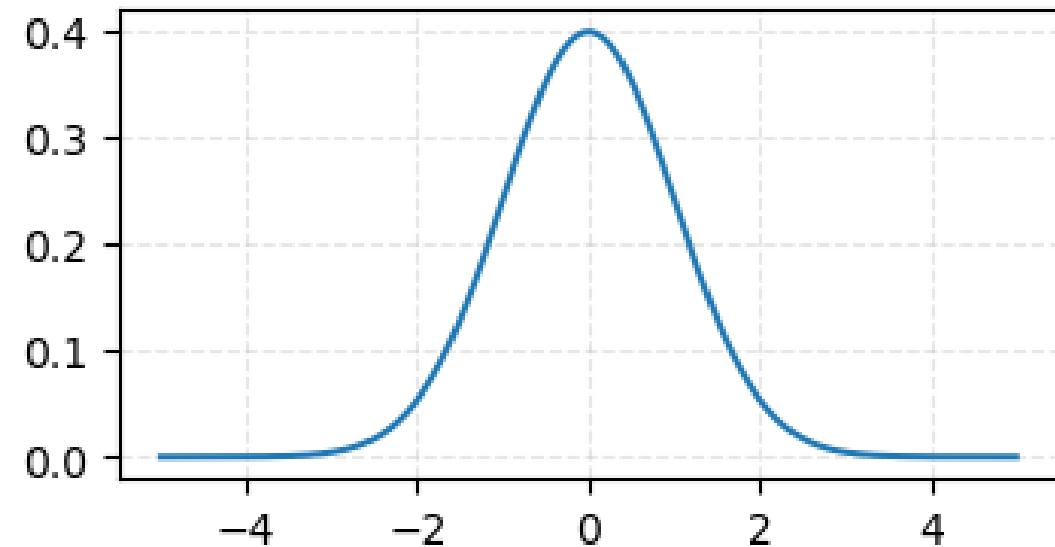
機率密度函數

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

全域機率總和必定為1

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

例：高斯函數



無限位能井 Infinite Potential Well

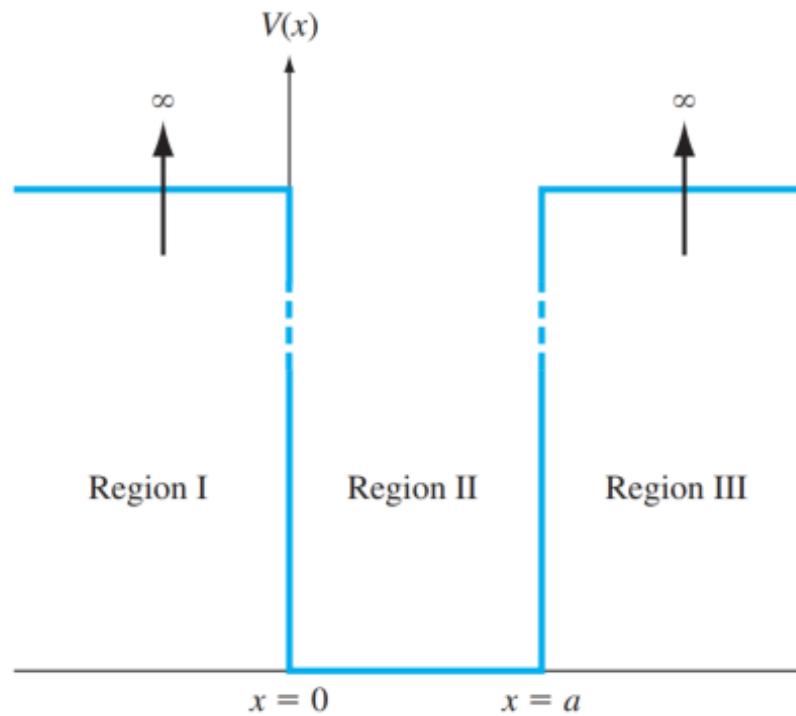
在 $a < x$ 或 $x < 0$ 的區域中： $\psi(x) = 0$

在 $0 < x < a$ 的區域中： $\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$ $n = 1, 2, 3\dots$

能量 $E = n^2 \frac{\hbar^2 \pi^2}{2ma^2}$ $n = 1, 2, 3\dots$

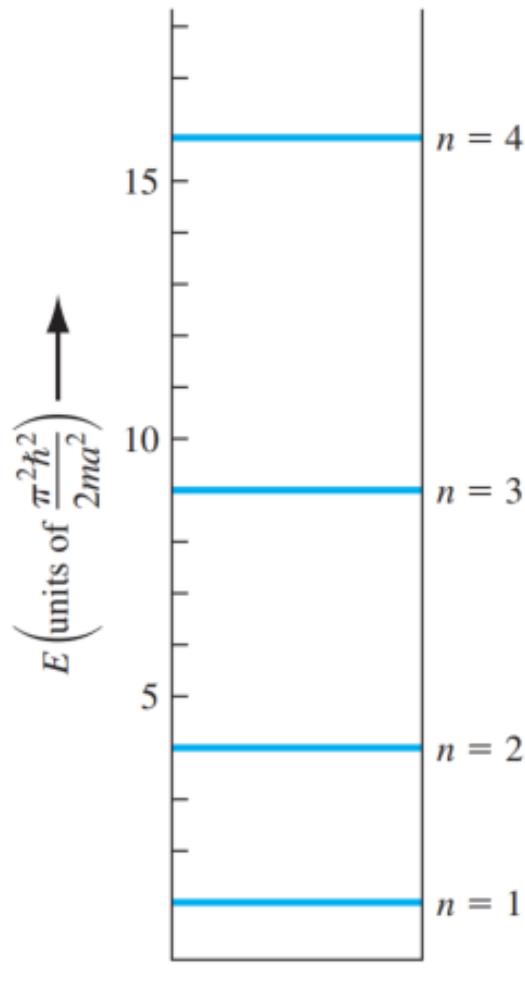
量子數

能量受到 n 的限制，不能是任意值

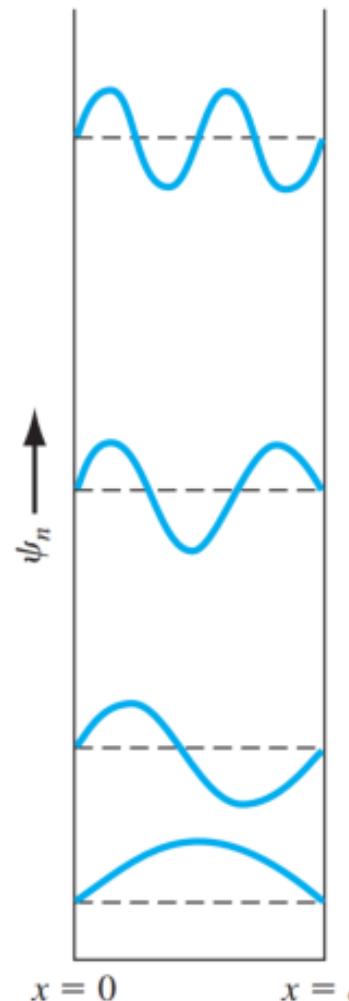


無限位能井 – 能量量子化

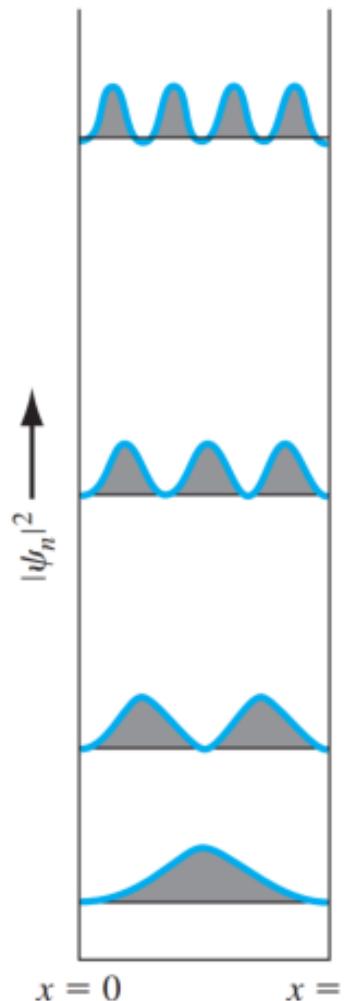
$$E = n^2 \frac{\hbar^2 \pi^2}{2ma^2}$$



$$\Psi(x)$$



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



Example 2.3 Quantization of Energy

Objective: Calculate the first three energy levels of an electron in an infinite potential well.

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

Example 2.3 Quantization of Energy

Objective: Calculate the first three energy levels of an electron in an infinite potential well.

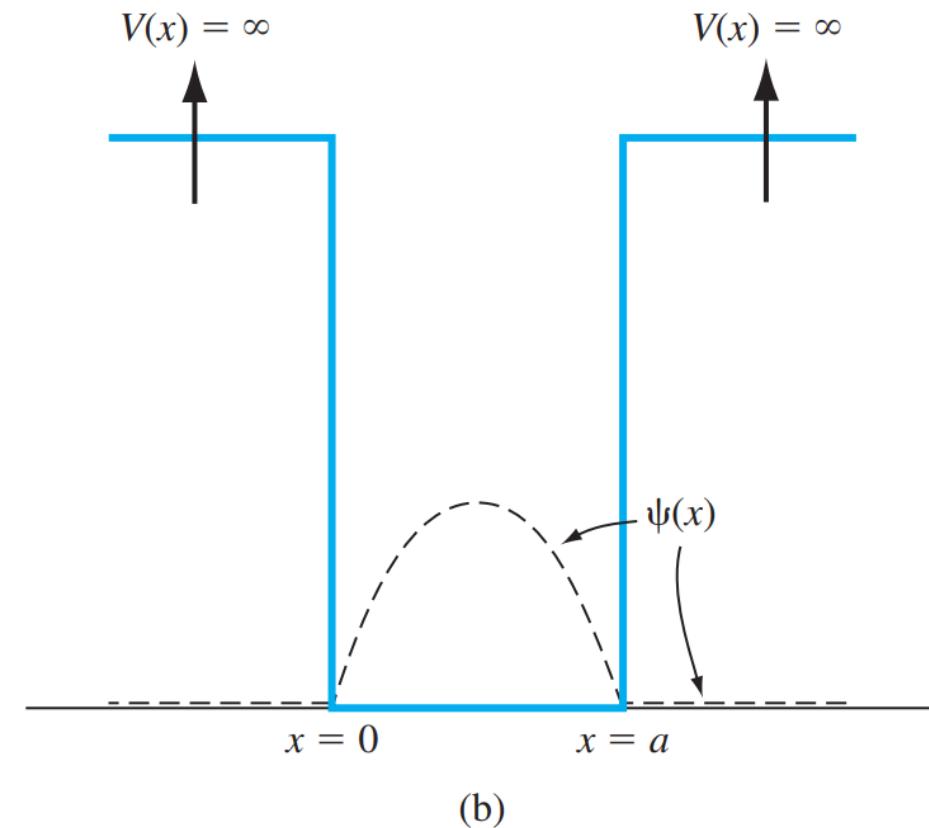
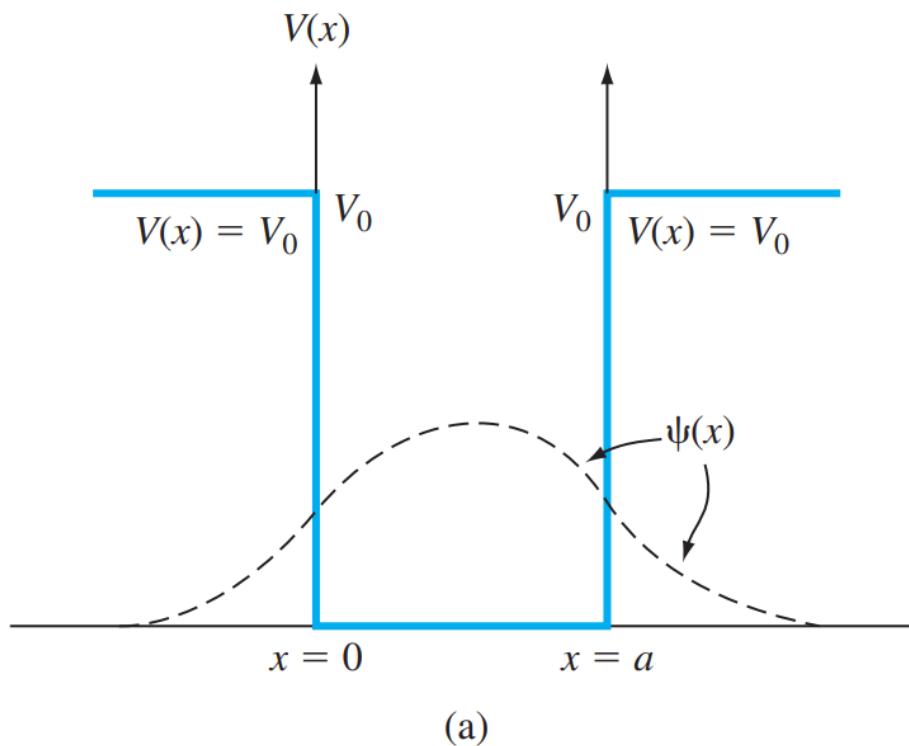
Consider an electron in an infinite potential well of width 5 Å.

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2ma^2} = n^2 \frac{1.054 \cdot 10^{-34} \pi^2}{2 \cdot (9.11 \cdot 10^{-31}) (5 \cdot 10^{-10})^2} = n^2 (2.14 \cdot 10^{-19}) \quad \text{J}$$

$$E_n = \frac{n^2 (2.14 \cdot 10^{-19})}{1.6 \cdot 10^{-19}} = n^2 (1.51) \quad \text{eV}$$

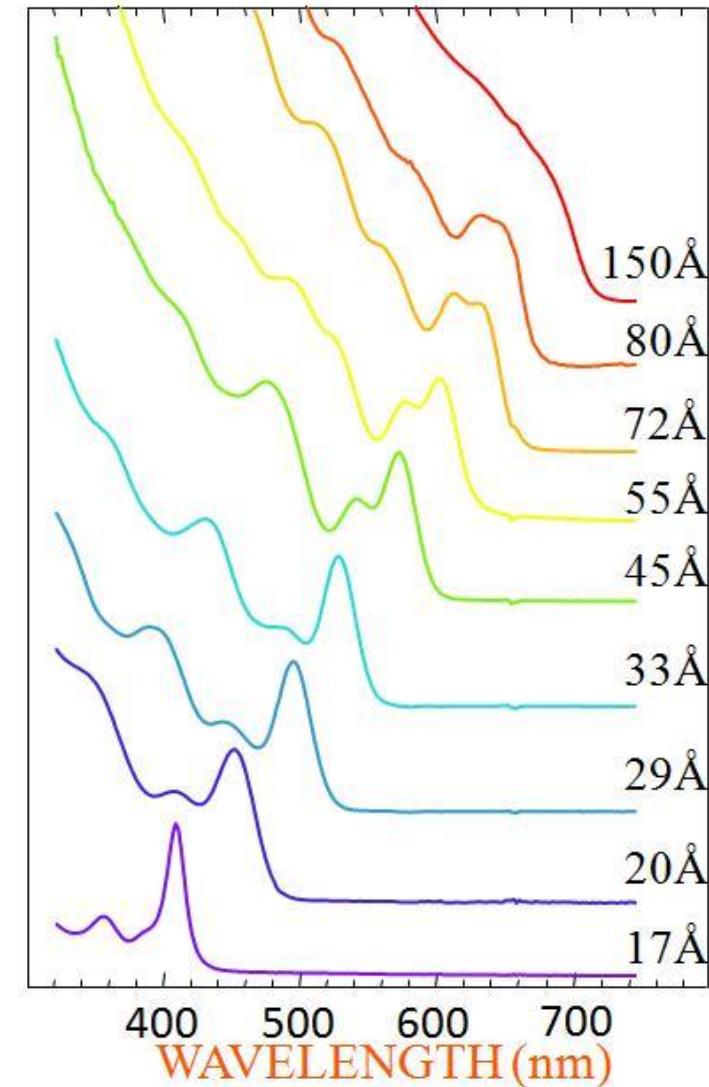
$$E_1 = 1.51 \quad E_2 = 6.04 \quad E_3 = 13.59$$

有限位能井 Finite Potential Well

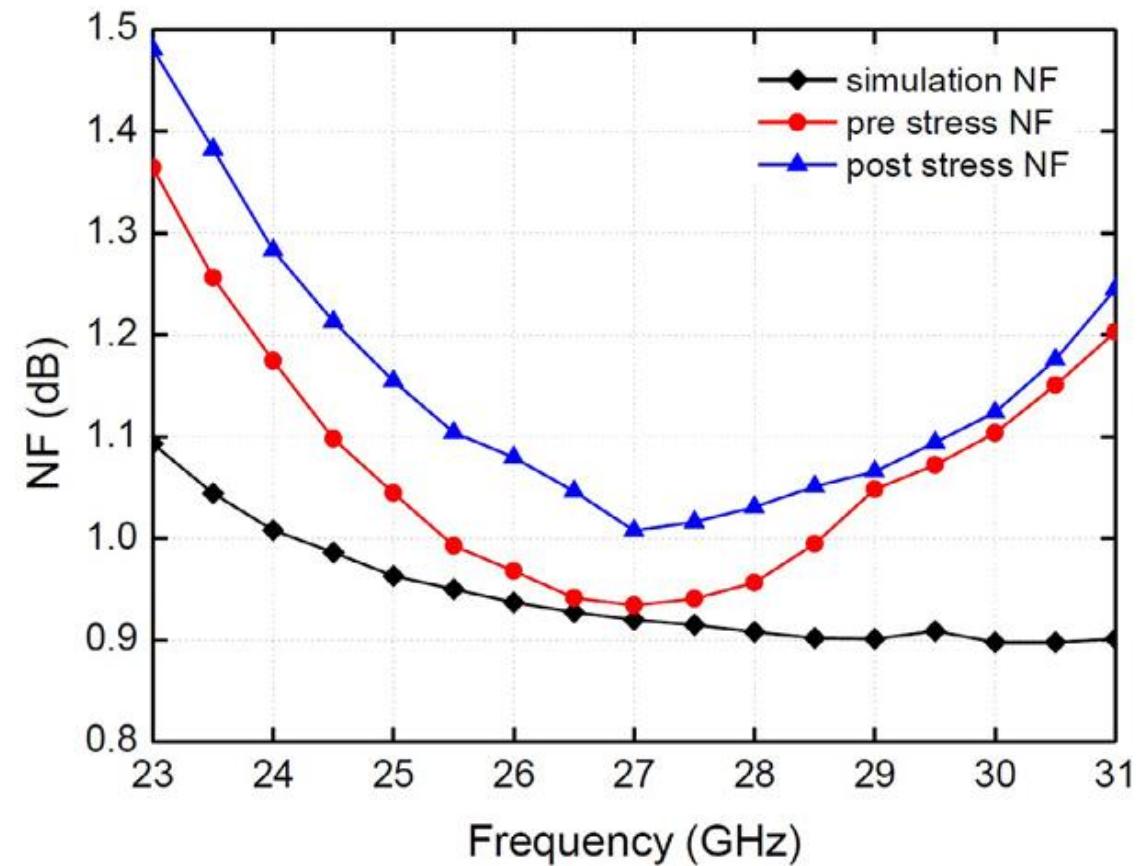
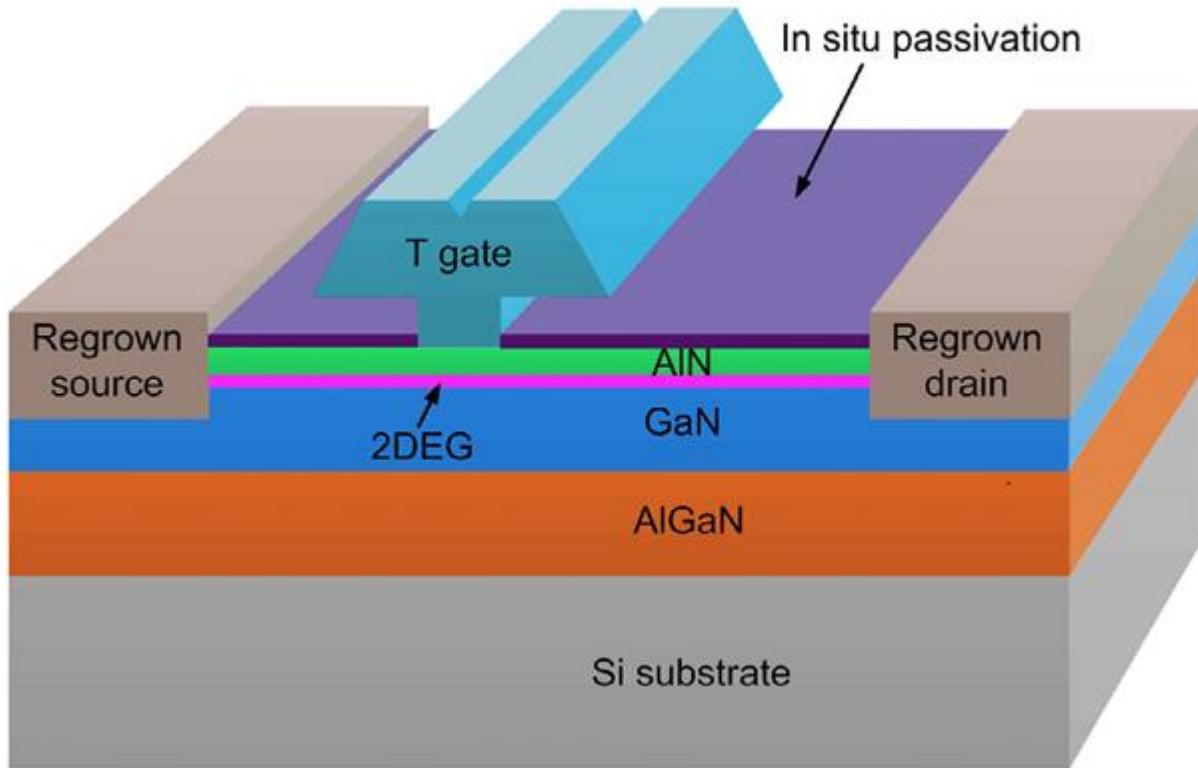


量子點

Quantum Confinement



HEMT

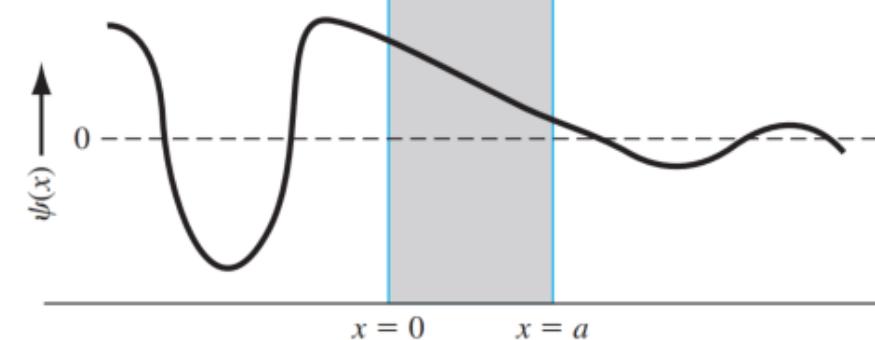
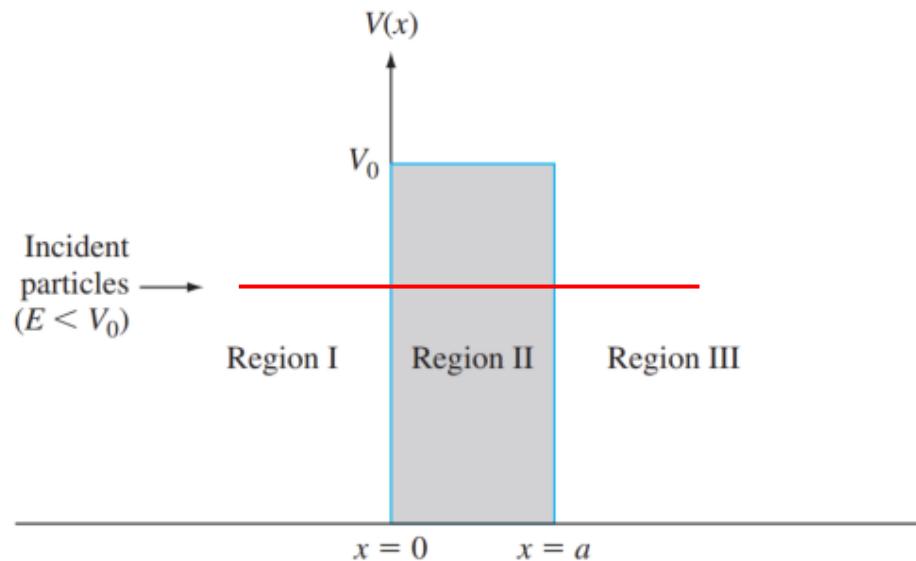


Source: Penghui Zheng et al, A23-31 GHz gallium nitride high-robustness low-noise amplifier with 1.1-24 dB noise figure and 28-dBm saturation output power, Microw Opt Technol Lett. 2020;62:1077–1081

穿隧 Tunneling

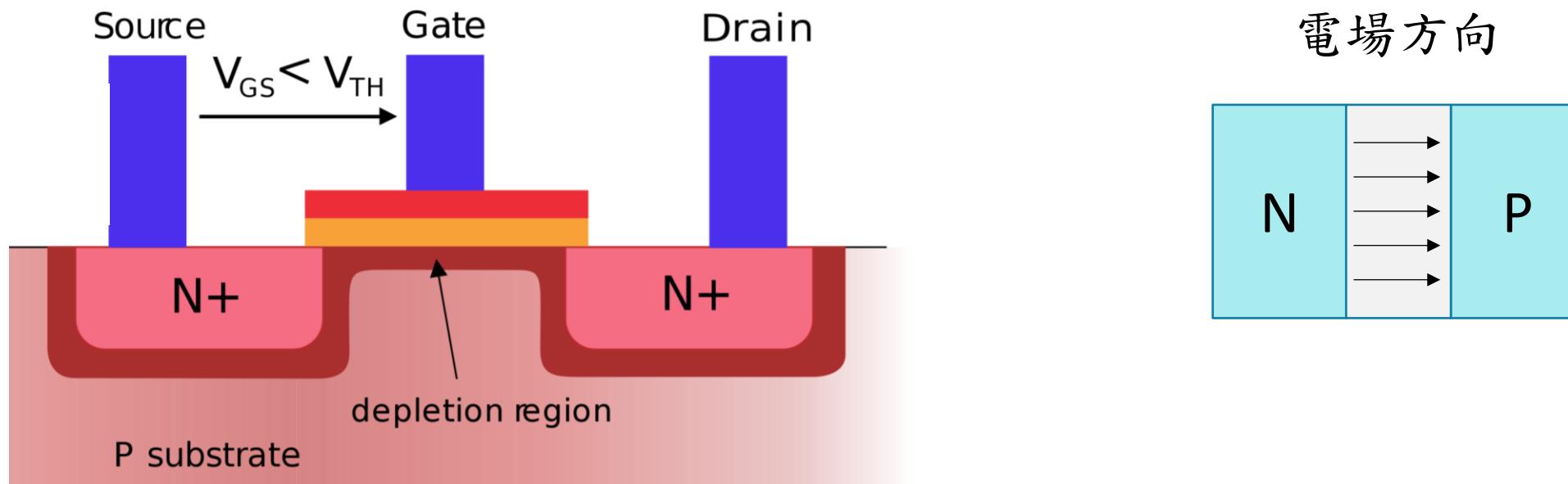
電子穿過障壁的機率為：

$$T = \left[1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(k_2 L) \right]^{-1} \approx 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0} \right) \exp(-2k_2 L) \quad , E \ll V_0$$

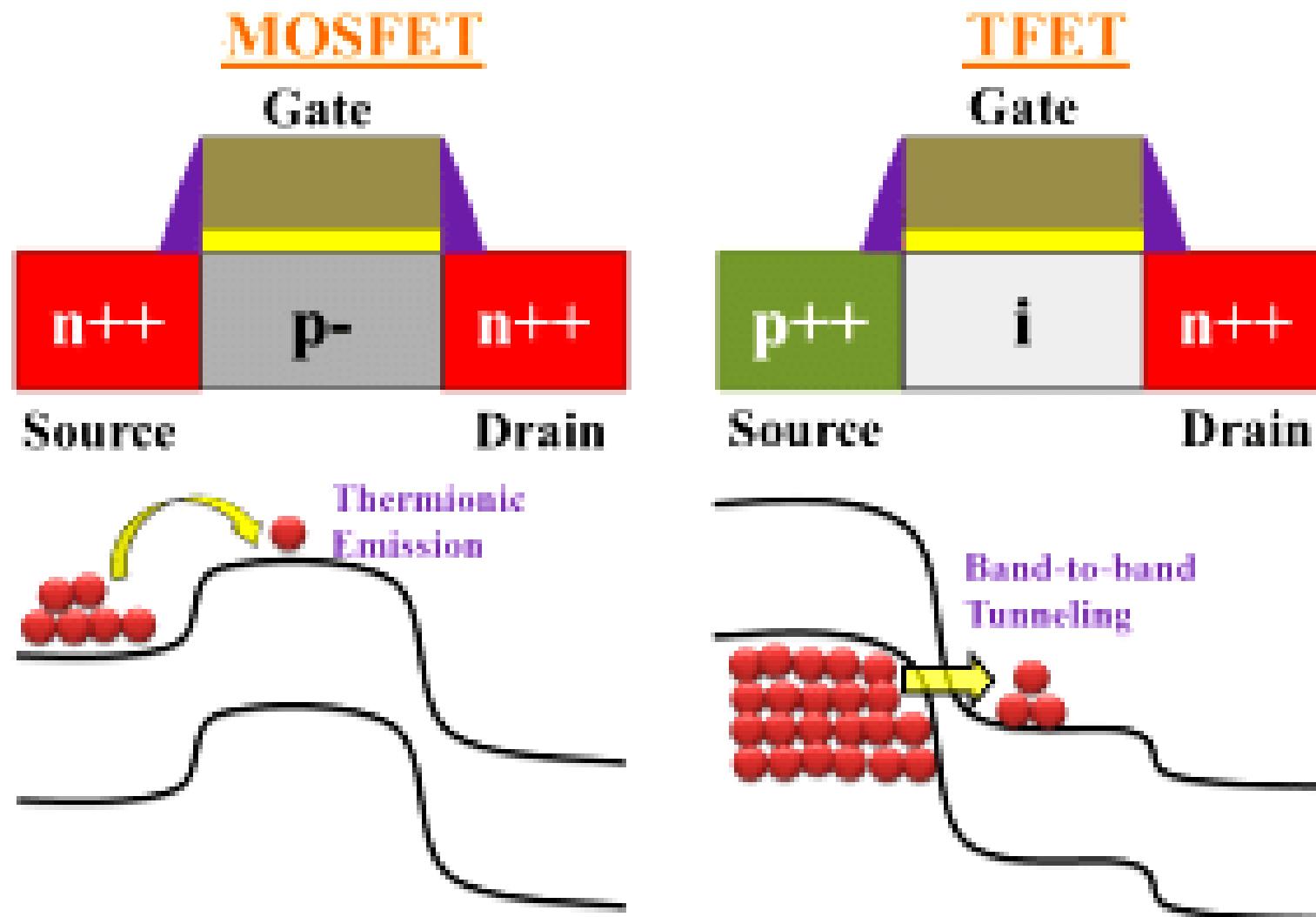


量子穿隧效應

- 當電荷帶有過多的動能，越過位能障壁並產生電流。
- 基於等效質量的差異，電子比電洞發生穿隧的機率更高。
- 穿隧效應對MOSFET的影響：穿隧過氧化層或通道(漏電)。



穿隧電晶體 (Tunneling Field Effect Transistor)



Example 2.5

Objective: Calculate the probability of an electron tunneling through a potential barrier.

Consider an electron with an energy of 2 eV impinging on a potential barrier with $V_0 = 20 \text{ eV}$ and a width of 3 Å.

Example 2.5

Objective: Calculate the probability of an electron tunneling through a potential barrier.

Consider an electron with an energy of 2 eV impinging on a potential barrier with $V_0 = 20 \text{ eV}$ and a width of 3 Å.

$$k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = 2.17 \cdot 10^{10} \text{ m}^{-1}$$

$$T = 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0}\right) \exp(-2k_2 L)$$

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

氫原子的薛丁格方程式(參考用)

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

波函數(極複雜，略)

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_{lm}(\theta, \phi)$$

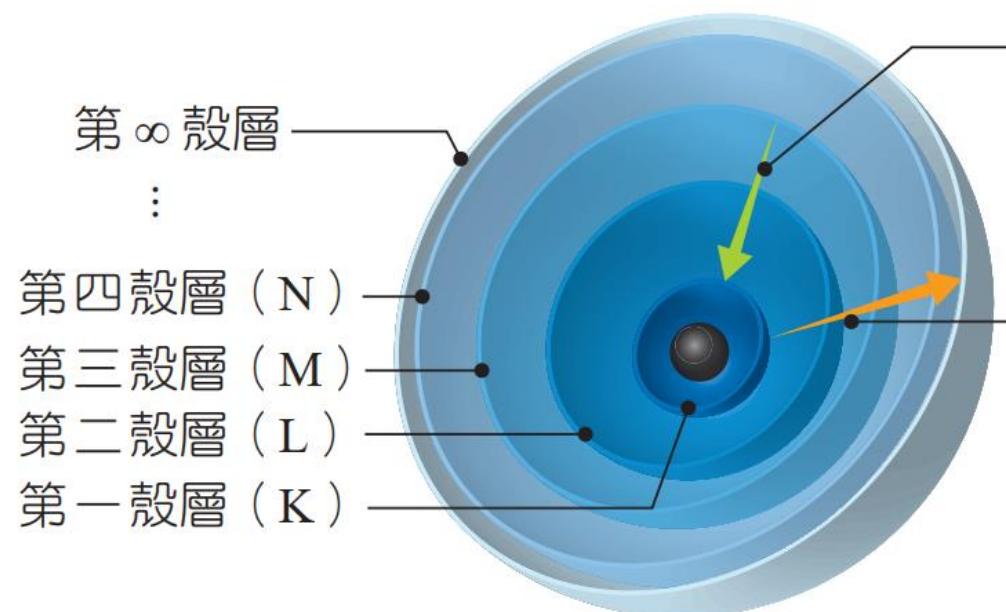
$$R(r) \rightarrow n = 1, 2, 3 \dots$$

$$\Theta(\theta) \rightarrow \ell = n-1, n-2, n-3, \dots, 0$$

$$\Phi(\phi) \rightarrow m = \pm \ell, \pm (\ell-1), \dots, 0$$

能量量子化

$$E_n = \frac{-m_0 e^4}{(4\pi\epsilon_0)^2 2\hbar^2} \frac{1}{n^2} = -13.6 \frac{1}{n^2} \text{ eV}$$

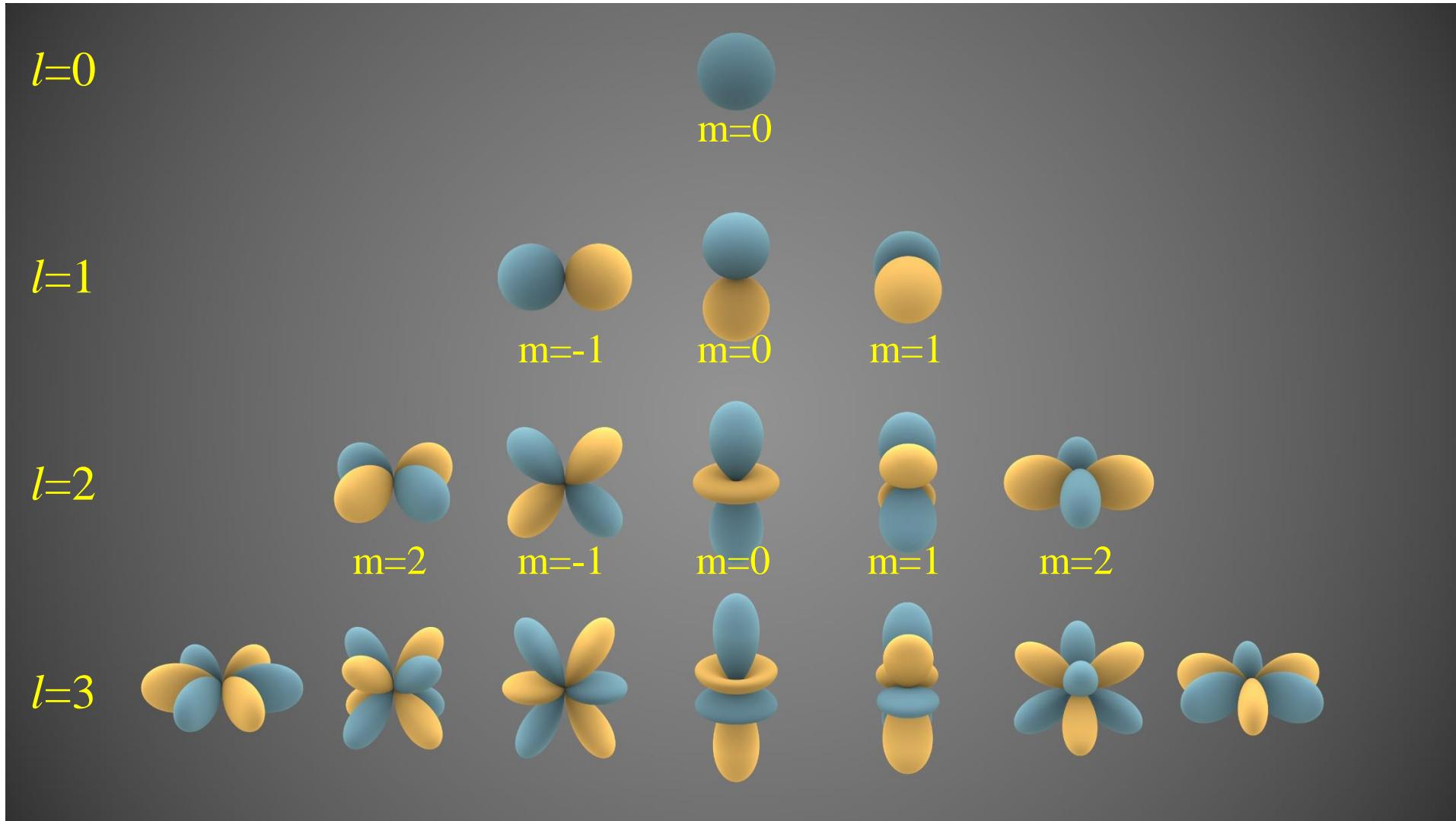


量子態 Quantum States

- 主量子數 n $n = 1, 2, 3\dots$
- 軌道量子數 l $l = 0, 1, 2\dots n-1$
- 軌道磁量子數 m $m = 0, \pm 1, \pm 2\dots \pm l$
- 自旋磁量子數 s $s = \pm 1/2$

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

量子軌域



量子態

$n=1$
 $l=0$
 $m=0$
 $s=1/2$



$n=1$
 $l=0$
 $m=0$
 $s=-1/2$



$n=2$
 $l=0$
 $m=0$
 $s=1/2$



$n=2$
 $l=0$
 $m=0$
 $s=-1/2$



$n=2$
 $l=1$
 $m=-1$
 $s=1/2$



$n=2$
 $l=1$
 $m=-1$
 $s=-1/2$



$n=2$
 $l=1$
 $m=0$
 $s=1/2$



$n=2$
 $l=1$
 $m=0$
 $s=-1/2$



$n=2$
 $l=1$
 $m=1$
 $s=1/2$



$n=2$
 $l=1$
 $m=1$
 $s=-1/2$



結論

■ 波粒二相性

1. 光電效應 → 證明光具有粒子性 $E = h\nu$
2. 電子雙狹縫干涉實驗 → 證明粒子具有波動性 $\lambda = h/p$

■ 薛丁格將古典力學能觀念和物質波結合成薛丁格波動方程式

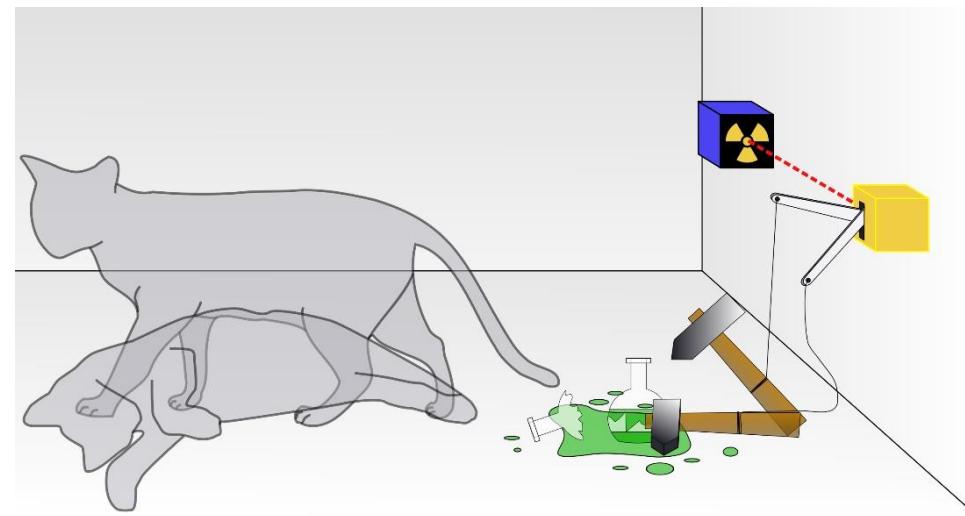
1. 無限位能井
2. 波動的穿隧效應
3. 氢原子模型的量子化和量子態（電子被限制）

薛丁格的貓

把一隻貓關在一個封閉的容器裏，內裝置一台蓋格計數器和少量放射性物質，在一小時內該物質衰變的機率為50%，不衰變的機率為50%。假若衰變事件發生了，則蓋格計數器放電啟動繼電器，使榔頭打破裝有氰化氫的燒瓶。

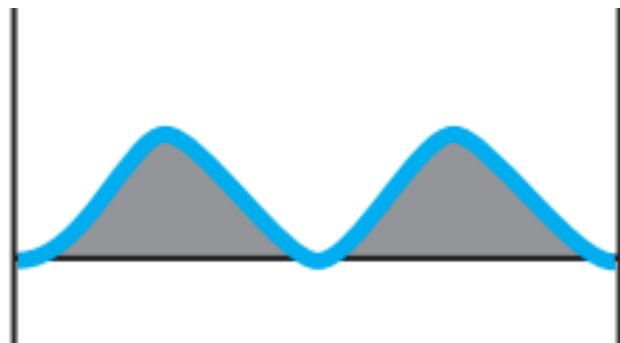
問：一個小時後，貓是死還是活？

答：打開觀察的那一刻才知道，還沒打開前，貓處於既生既死的狀態



波函數坍塌

測量前



測量後(坍塌)

