The Quantum Nature of Light

The Photoelectric Effect

$K_{max} = eV_{stop}$

1° K_{max} does not depend on the intensity.

2° not occur when $f < f_0$, no matter intensity

$\Rightarrow$ Electromagnetic radiation is quantized $\rightarrow$ photons

$$E = hf = \hbar\omega$$

$h = 2\pi\hbar = 6.63\times10^{-34}\,J\cdot s$: Planck constant

hf: energy of a single photon

Total energy: an integer multiple of hf.

So in photoelectric effect:

$$hf = K + W$$

$$K_{max} = hf - W.$$

◎ increase the light intensity increases the number of photons, not the photon energy.

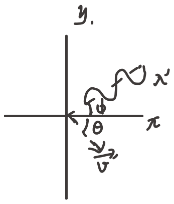
Photons have Momentum

According to theory of relativity:

$$E^2 - c^2p^2 = m^2c^4 = 0$$

$$\therefore p = \frac{hf}{c} = \frac{h}{\lambda} = \hbar k$$

① Compton Scattering



$$\frac{hc}{\lambda} + mc^2 = \frac{hc}{\lambda'} + \gamma mc^2$$

$$\frac{h}{\lambda} = \frac{h}{\lambda'}\cos\phi + \gamma mv\cos\theta$$

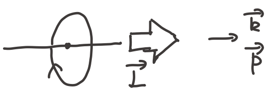
$$0 = \frac{h}{\lambda'}\sin\phi - \gamma mv\sin\theta$$

$$\Rightarrow \Delta\lambda = \frac{h}{mc}(1-\cos\phi).$$

Compton wavelength $\frac{h}{mc}$

① Photons have angular momentum

intrinsic spin angular momentum (either $-\hbar$ or $+\hbar$)



$\mathcal{L}$-State

$\mathcal{R}$-State

Each individual photon exists in either spin state with equal likelihood. (Linearly polarized)

$$|H\rangle = \frac{|R\rangle + |L\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}\right]$$

Matter Waves

Light as a Probability Wave

Probability density of detecting a photon at some point P depends on $I \propto E_0^2$.

$\Rightarrow E_0$ at P $\rightarrow$ probability amplitude (whose square gives the density)

① De Broglie Hypothesis

1° A beam of light is a wave, but it transfers energy and momentum to matter only at points.

2° treat a particle with momentum p:

$$\lambda = \frac{h}{p} \text{ (de Broglie wavelength)}$$

② Electron Diffraction

probability amplitude ψ

probability: $|\psi|^2 = \psi^* \psi$

Sum of amplitudes: $\psi = \psi_1 + \psi_2 + \cdots$

$$\therefore P = |\psi|^2 = |\psi_1|^2 + |\psi_2|^2 + \underbrace{2R(\psi_1^* \psi_2)}_{\text{interference term}}$$

③ Heisenberg's uncertainty principle

$$\Delta x \cdot \Delta p_x \geq \hbar$$
$$\Delta y \cdot \Delta p_y \geq \hbar$$
$$\Delta z \cdot \Delta p_z \geq \hbar$$

wave function $\psi(x,t) = e^{i(kx - wt)}$

Fouirer Transform

$$f(t) = \begin{cases} \frac{1}{\tau}, & -\frac{\tau}{2} \leq t \leq \frac{\tau}{2} \\ 0, & \text{otherwises} \end{cases}$$

$$F(\omega) = \int_{-\infty}^{+\infty} f(t) e^{-i\omega t} dt = \frac{\sin(\frac{\omega\tau}{2})}{\frac{\omega\tau}{2}}$$

Schroedinger's Equation

Classical Particle

$$\psi(x,t) = e^{i(kx-\omega t)}$$

$$p = \frac{h}{\lambda} = \hbar k = -i\hbar \frac{1}{\psi(x,t)} \frac{\partial \psi(x,t)}{\partial x}$$

$$p^2 = -\hbar^2 \frac{1}{\psi(x,t)} \frac{\partial^2 \psi(x,t)}{\partial x^2}$$

We expect $E = \hbar\omega = i\hbar \frac{1}{\psi(x,t)} \frac{\partial \psi(x,t)}{\partial t}$

According to $E = \frac{p^2}{2m}$

$$\Rightarrow i\hbar \frac{1}{\psi(x,t)} \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{1}{\psi(x,t)} \frac{\partial^2 \psi(x,t)}{\partial x^2}$$

In the prescence of potential:

$$E = \frac{p^2}{2m} + U(x)$$

① Schroedinger Equation (1D)

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + U(x,t)\psi(x,t)$$

(a postulate of quantum mechanics)

When $U = U(x)$ is independent of time. $E = \hbar\omega$

$$\psi(x,t) = \phi(x) e^{-\frac{iEt}{\hbar}} \quad \text{(stationary solution)}$$

So: $\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right]\phi(x) = E\phi(x)$

$\Rightarrow$ time-independent Schroedinger's equation.

The wave function $\phi(x)$:

$$\frac{\partial^2 \phi(x)}{\partial x^2} + \frac{2m}{\hbar^2}[E - U(x)]\phi(x) = 0$$

$U(x) = 0$:

$\phi(x) = Ae^{ikx} + Be^{-ikx}$

(左行，右行)

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

for the right-moving $\psi(x,t) = Ae^{i(kx-\omega t)}$

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

① Wave Packets

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

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

$$\therefore V_{ph} = \frac{\hbar k}{2m} = \sqrt{\frac{E}{2m}}$$

(free quantum mechanical particle)

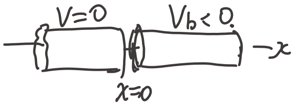
classical speed: $V_{cl} = \sqrt{\frac{2E}{m}} = 2V_{ph}$

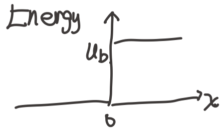
normalize the wave function:

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

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m}t)} dk$$

Reflection from a Potential Step





$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U_b = E$$

Classical electron: $E > qV_b$

Quantum Mechanically:

① Region 1 $(x<0)$: $k = \frac{\sqrt{2mE}}{\hbar}$

$$\psi_1 = Ae^{ikx} + Be^{-ikx}$$

② Region 2 $(x>0)$: $k_b = \frac{\sqrt{2m(E-qV_b)}}{\hbar}$

$$\psi_2 = Ce^{ik_bx} + De^{-ik_bx}$$

Wave functions should be consistent with each other at $x=0$ (Boundary conditions).

① no electron off to the right in region 2. $D=0$

② $A + B = C$. (matching of value)

$Ak - Bk = Ck_b$ (matching of slopes)

$$\therefore R = \frac{|B|^2}{|A|^2} = \left|\frac{k-k_b}{k+k_b}\right|^2 \quad \text{reflection coefficient}$$

$\Rightarrow$ Quantum mechanically, electrons are reflected (with a probability)

Transmission coefficient

$$\frac{|C|^2}{|A|^2} = \frac{4k^2}{|k+k_b|^2} = T \cdot \frac{k}{k_b}$$

$J = nev$

$$T = 1 - R = \frac{4kk_b}{|k+k_b|^2} \quad \text{(why this ?)}$$

$J = nqv$

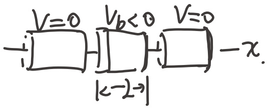
Recall: $T = \frac{|C|^2}{|A|^2}\frac{k_b}{k} = \frac{|C|^2 q\left(\frac{\hbar k_b}{m}\right)}{|A|^2 q\left(\frac{\hbar k}{m}\right)} = \frac{J_{transmitted}}{J_{incident}}$ ($\frac{\hbar k_b}{m} \to P$)

Similarly $R = \frac{J_{reflected}}{J_{incident}}$

So $T = 1 - R$: conservation of current.

Continued.

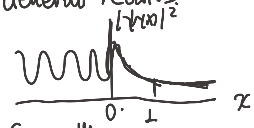
⑩ Tunneling through a Potential Barrier



consider $E<qV_b$

interested in P(electron appearing on the other side of barrier)

General results



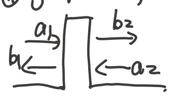
Standing Wave

$T \approx e^{-2kL}$

$k = \frac{\sqrt{2m(qV_b - E)}}{\hbar}$

⑩ Scanning Tunneling Microscope

⑪ S- Matrix



$\psi_1 = a_1 e^{ikx} + b_1 e^{-ikx}$

$\psi_2 = b_2 e^{ikx} + a_2 e^{-ikx}$

$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} r_{11} & t_{12} \\ t_{21} & r_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

$r_{11} = r_{22} = r, \; t_{12} = t_{21} = t$

$|r|^2 + |t|^2 = 1$

⑫ Puzzle

Classical: $\hbar k = p = mv$

$\hbar\omega = E = \frac{p^2}{2m} \Rightarrow v = \frac{\hbar k}{m}$

QM: $Ae^{i(kx-\omega t)}$

$= Ae^{i(kx - \frac{\hbar k^2}{2m}t)}$

$v = \frac{\hbar k}{2m}$

⑬ Wave Packets

$V_{classical} = 2V_{QM}$

Why?

How to normalized?

$\int_{\mathbb{R}} |\psi(x)|^2 dx = \int_{\mathbb{R}} A^2 dx = |A|^2 \infty$

a linear superposition of stationary free-particle

In general, we construct a linear combination

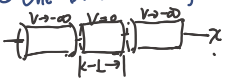
$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m}t)} dk$$

Wave Packet: carries a range of k

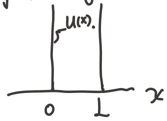
Quantum Wells

confining the wave to a finite region of space leads to quantization of motion.

① One-Dimensional Infinite Potential Well



put a single electron in central cylinder → cannot escape



$U = -eV.$

* For standing waves

$\frac{n\lambda}{2} = L$

$y_n(x) = A\sin\left(\frac{n\pi}{L}x\right)$

② Probability of detection.

$P_n(x) = |\psi_n(x)|^2 = |A|^2 \sin^2\left(\frac{n\pi}{L}x\right)$

$\int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = \int_0^L |\psi_n(x)|^2 dx = 1$

$A = \sqrt{\frac{2}{L}}$ (normalization)

③ Energys: $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mK}}$

$E_n = \frac{h^2}{2m\lambda^2} = \left(\frac{h^2}{8mL^2}\right) n^2$

n: quantum number

n=1: ground state

confined systems must always have a certain minimum energy (Zero-point energy)

Electrons can be excited or de-excited by the absorption or emission of a photon with energy

$\hbar\omega = \frac{hc}{\lambda} = \Delta E = E_{high} - E_{low}$

Wave Function:

By solving Schroedinger's Equation

$\psi_n(x) = e^{i\frac{n\pi}{L}x}$ or $\psi_n(x) = e^{-i\frac{n\pi}{L}x}$

$\psi_n(0) = \psi_n(L) = 0.$

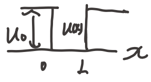
$\Rightarrow \psi_n(x) = A\sin\left(\frac{n\pi}{L}x\right)$

④ Correspondence principle:

At large enough quantum numbers, the predictions of quantum physics merge smoothly with those classical physics

⑤ An Electron in a Finite Well.

wave functions can penetrate the wall into classically forbidden regions.



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

⑥ Schrodinger's Equation in High Dimensions

Assuming $U=0$

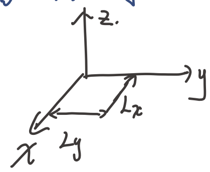
$$E\psi(x,y) = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]\psi(x,y)$$

$$\psi(x,y) = X(x)\cdot Y(y)$$

$$E = -\frac{\hbar^2}{2m}\frac{1}{X(x)}\frac{\partial^2 X(x)}{\partial x^2} - \frac{\hbar^2}{2m}\frac{1}{Y(y)}\frac{\partial^2 Y(y)}{\partial y^2}$$

$$\Rightarrow E = F(x) + G(y),\quad F(x) = E_1 \text{ (constant)}$$
$$G(y) = E - E_1$$

⑦ 2D & 3D Infinite Potential Wells



$$\psi_n(x,y) = \frac{2}{\sqrt{L_x L_y}}\sin\left(\frac{n_x\pi}{L_x}x\right)\sin\left(\frac{n_y\pi}{L_y}y\right)$$

$$E_{n_x,n_y} = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2}\right)$$

The Hydrogen Atom

(i) Mystery of the H-Atom

$$\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r^2} = m\frac{v^2}{r}$$

$$E_C = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r} = -2E_k$$

$$E_{total} = -E_k.$$

(ii) Bohr Model

$L = n\hbar$, $n = 1, 2, 3 \cdots$

Physical meaning of $L = n\hbar$

$$L = mvr = n\hbar.$$

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

$$\therefore \frac{\lambda}{r} = \frac{h}{mvr} = \frac{h}{L}$$

$$\Rightarrow \frac{2\pi r}{\lambda} = \frac{L}{\hbar} = n$$

⇒ The length of orbit, an integer multiple of λ.

Analysis. $L = rmv = n\hbar$

$\Rightarrow v = \frac{n\hbar}{mr}$

$$\frac{mv^2}{r} = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r^2}$$

$$\Rightarrow r_n = n^2 a_B, \quad a_B = \frac{\hbar^2}{\frac{me^2}{4\pi\varepsilon_0}} = 0.529\,\text{Å}$$

⇒ Electron's orbital radius r is quantized

smallest possible radius: a_B (Bohr radius)

The energy: $E_n = \frac{1}{2}mv^2 - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r} = -\frac{E_R}{n^2}$

$$E_R = \frac{me^4/(4\pi\varepsilon_0)^2}{2\hbar^2} = 13.6\,eV \text{ (Rydberg)}$$

(iii) The Hydrogen Spectrum

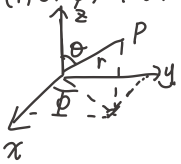
$$\hbar\omega_{nm} = E_R\left(\frac{1}{n^2} - \frac{1}{m^2}\right), \quad m > n$$

$$\frac{1}{\lambda} = \frac{E_R}{hc}\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$$

Uncertainty ?

(iv) Schroedinger's Equation for the H-Atom

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



1° Φ function: quantum number m_ℓ.

where $\Phi_{m_\ell}(\phi) \sim e^{im_\ell\phi}$, $m_\ell = 0, \pm1, \pm2 \cdots$

2° Θ: Legendre polynomials. have quantum number m_ℓ and ℓ.

multiply $\Theta \cdot \Phi$: spherical harmonics

$$Y_\ell^{m_\ell}(\theta, \phi) = \Theta_\ell^{m_\ell}(\theta)\,\Phi_{m_\ell}(\phi)$$

3° $R_{n\ell}(r)$: quantum number n and ℓ.

(v) Hydrogen Wave Function

Labeled by (n, ℓ, m_ℓ)

1°. energy only depends on the principal quantum number $n = 1, 2, 3 \cdots$

2° orbital quantum number $\ell = 0, 1, 2, \cdots, n-1$ a measure of the magnitude of angular momentum. $\ell = 0, 1, 2, 3$ called s, p, d, f.

3°. orbital magnetic quantum number $m_\ell = -\ell, -\ell+1, \cdots, \ell-1, \ell$ → space orientation of $\vec{L}$

(vi) Ground State Wave Function

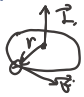
$$\psi_{100}(\vec{r}) = R_{10}(r) = \frac{1}{\sqrt{\pi}\, a_B^{3/2}} e^{-\frac{r}{a_B}}$$

$$dV = 4\pi r^2 dr$$

radial probability density $P(r)dr = |\psi_{100}(\vec{r})|^2 dV$

Angular Momentum and Spin

Classical Loop Model for Electron Orbits



$L_{orb} = mrv$

$$i = \frac{e}{\frac{2\pi r}{v}}$$

$$\mu_{orb} = i(\pi r^2) = \frac{evr}{2}$$

In vector form: $\vec{\mu}_{orb} = -\frac{e}{2m}\vec{L}_{orb} \equiv \gamma \vec{L}_{orb}$

$$\vec{L} = \vec{r}\times\vec{p} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} \qquad L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial \varphi}.$$

$$L_z R(r) = 0$$

$\Delta L_x \Delta L_y$ involves $\Delta z \Delta p_z$. → cannot vanish (uncertainty principle)

① Orbital Angular Momentum

We can measure $L_z = m_l \hbar$, $m_l = 0, \pm1, \cdots \pm l$.

If electron has a definite value of L_z, it cannot have definite values of L_x, L_y.

The allowed magnitude: $L = \sqrt{l(l+1)}\,\hbar$.

$$\therefore \mu_{orb} = |\gamma| L = \frac{e}{2m}\sqrt{l(l+1)}\,\hbar$$

$$\mu_{orb,z} = \gamma L_z = -m_l \frac{e\hbar}{2m} = -m_l \mu_B$$

define Bohr magneton

$$\mu_B = \frac{eh}{4\pi m} = \frac{e\hbar}{2m} = 9.274\times10^{-24}\ J/T.$$

② Spin Dynamics

$$\vec{\tau} = \vec{\mu}\times\vec{B}.$$

$$\vec{\tau} = \frac{d\vec{L}}{dt} = \gamma \vec{L}\times\vec{B}$$

① Larmor frequency $\vec{\omega} = -\gamma\vec{B}$

s.t. $\frac{d\vec{L}}{dt} = \vec{\omega}\times\vec{L}$ (Larmor precession)

$$U_B = -\vec{\mu}\cdot\vec{B} = -\mu B\cos\theta$$

When in a nonuniform magnetic field: $\vec{B}(z) = B(z)\hat{z}$

$$U = -\vec{\mu}\cdot\vec{B}(z) = -\mu_z B(z)$$

$$F_z = -\frac{dU}{dz} = \mu_z\frac{dB}{dz}.$$

③ Spin

Electron Spin: (intrinsic)

for every electron, spin $s = \frac{1}{2}$.

$S_z = m_s\hbar$, $m_s = \pm s = \pm\frac{1}{2}$

m_s: spin magnetic quantum number

$\vec{\mu}_s = g\gamma\vec{S}$, $\gamma = -\frac{e}{2m}$

↳ g-factor $g = 2$

$$\mu_s = g|\gamma|S = \frac{e}{m}\sqrt{s(s+1)}\,\hbar$$

$$\mu_{s,z} = -g m_s \mu_B$$

$(x,y,z)\to(r,\theta,\varphi)$.

$$\begin{cases} x = r\cos\varphi\sin\theta \\ y = r\sin\varphi\sin\theta \\ z = r\cos\theta. \end{cases}$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$$

$$\Rightarrow -\frac{\hbar^2}{2m_e}[\nabla^2]\psi + V(r)\psi = E\psi.$$

角动量 $\vec{L} = \vec{r}\times\vec{p}$ $\begin{cases} \hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \end{cases}$

$$\Rightarrow \begin{cases} \hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right) \\ \hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right) \\ \hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial\varphi}. \end{cases}$$

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2.$$

动能项 → 径向+角向

对易关系: $[\hat{H}, \hat{L}^2] = 0$ $\qquad [\hat{L}^2, \hat{L}_z] = 0$

$\hat{L}_x, \hat{L}_y, \hat{L}_z$ 相互不对易, $[\hat{L}_x^2 + \hat{L}_y^2, \hat{L}_z^2] = 0$

$$\psi = R(r)\ \Theta(\theta)\ \Phi(\varphi)$$

$$\downarrow \qquad \downarrow \qquad \downarrow$$

$$\frac{\hat{p}_r^2}{2m_e} + \hat{V} \qquad \hat{L}_x^2 + \hat{L}_y^2 \qquad \hat{L}_z$$

角向解: $\hat{L}_z$ $\quad -i\hbar\frac{\partial}{\partial\varphi}\Phi_m = L_{z,m}\Phi_m$

$$\Phi_m = e^{-\frac{L_{z,m}}{i\hbar}\varphi}$$

φ: 绕z轴旋转. $e^{-\frac{L_{z,m}}{i\hbar}2\pi} = 1 \Rightarrow L_{z,m} = m\hbar$

$\hat{L}^2$ 角动量本征值 $\lambda = l(l+1)\hbar^2$

基态 $n=1$, $l=m=0$

$$\psi_{100} = \frac{1}{\sqrt{\pi a_B^3}}e^{-\frac{r}{a_B}}$$

电子出现在半径为某个 r 附近的概率

$$dP = |\psi_{100}|^2\cdot 4\pi r^2 dr$$

$$f(r) = \frac{dP}{dr} = \frac{4}{a_B}\cdot\left(\frac{r}{a_B}\right)^2 e^{-\frac{2r}{a_B}}$$

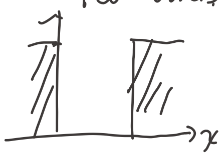
一维无限深方势阱

$\psi(x,t)=\phi(x)e^{-\frac{iEt}{\hbar}}$

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

$\psi_n(x)=\sqrt{\frac{2}{a}}\sin(\frac{n\pi}{a}x)$

$V(x)=\begin{cases}0, & 0\le x\le a\\ \infty & \text{others}\end{cases}$



势阱外 $\psi(x)=0$

势阱内 $\psi_n(x)=\sqrt{\frac{2}{a}}\sin(\frac{n\pi}{a}x)$

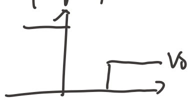
$E_n=\frac{n^2\pi^2\hbar^2}{2ma^2}=\frac{h^2}{8ma^2}n^2$

ψ_1：基态，$\psi_2,\psi_3\cdots$激发态

三维无限深

$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+V\psi=E\psi$

一维单侧无限深



$E<V_0$:

$A\cos kx+B\sin kx$

$x<0$: $\psi=0$

$0\le x\le a$, $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}=E\psi$

$\psi=A\cos(kx)+B\sin(kx)=B\sin(kx)$

$x\ge a$: $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}=(E-V_0)\psi$

$\psi=Ce^{k_2x}+De^{-k_2x}$

$=De^{-k_2x}$

$B\sin(k_1a)=De^{-k_2a}$

$Bk_1\cos(k_1a)=-k_2De^{-k_2a}$

一维δ函数势阱

$V(x)=-\delta(x)V_0$. $E<0$

$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}=E\psi$

$\psi=Ae^{kx}+Be^{-kx}$

$\psi=\begin{cases}Ae^{-kx}, & x>0\\ Ae^{kx}, & x<0\end{cases}$ $k=\frac{\sqrt{-2mE}}{\hbar}$

$A=\sqrt{k}$.

$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}-\delta(x)V_0\psi=E\psi$

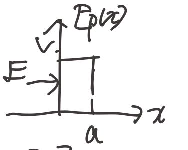
$\therefore \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+(E+\delta(x)V_0)\psi=0$

$\int_{0^-}^{0^+}\left(\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+(E+\delta(x)V_0)\psi\right)=0$

$\frac{\hbar^2}{2m}\left[\frac{\partial\psi}{\partial x}\Big|_{0^+}-\frac{\partial\psi}{\partial x}\Big|_{0^-}\right]+V_0\psi=0$

$-\frac{\hbar^2}{2m}\cdot 2Ak+V_0\psi=0$

$V_0=\frac{\hbar^2}{m}k=\frac{\hbar^2}{m}\frac{\sqrt{-2mE}}{\hbar}$ $E=-\frac{mV_0^2}{2\hbar^2}$



$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi=E\psi$

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