呂浩宇

General Physics (II) Quantum Physics.

1D Schrödinger Equation

complex variable，但只有平方具物理意義

Determining the evolution of the wave function $\Psi(x,t)$, where $\int_a^b |\Psi(x,t)|^2 dx$ gives the probability of finding the particle between $x = [a, b]$ at time t.

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi \qquad \hbar = \frac{h}{2\pi} = 1.054573 \cdot 10^{-34}\ \mathrm{Js} \qquad \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$$

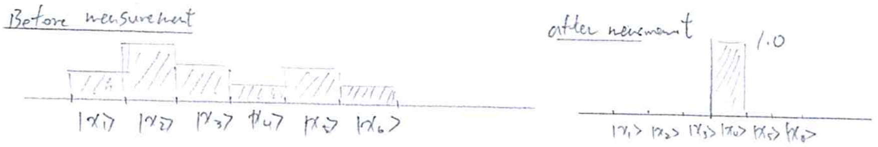
$-\frac{\hbar^2}{2m} + V = E$

For example, given an initial $\Psi(x,0)$, the Schrödinger equation determines $\Psi(x,t)$ for future time t.

Copenhagen Interpretation :

Before making measurement of any physical quantity, $\Psi(x,t)$ tells you the probability for the particle to be in various states. To obtain the physical quantity, we use the "operator" of that physical quantity to operate on the wave function. For example, to obtain momentum, we operate $-i\hbar\frac{\partial}{\partial x}$ on $\Psi(x,t)$. The expectation value of momentum is $-i\hbar\int \Psi^* \frac{\partial}{\partial x}\Psi\, dx$.

When we measure a physical quantity, the wave function collapse to the eigen wave function of the corresponding operator. For example, if we measure position with the operator $\hat{X}$, the wave function collapse to the eigen state $|x\rangle$, which has a definite location x but uncertain momentum.



Conservation of probability :

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = \int_{-\infty}^{\infty}\left(\Psi^*\frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t}\Psi\right) dx$$

Given directly by Schrödinger equation

$$\begin{cases} \dfrac{\partial \Psi}{\partial t} = \dfrac{i\hbar}{2m}\dfrac{\partial^2 \Psi}{\partial x^2} - \dfrac{i}{\hbar}V\Psi \\ \dfrac{\partial \Psi^*}{\partial t} = \dfrac{-i\hbar}{2m}\dfrac{\partial^2 \Psi^*}{\partial x^2} + \dfrac{i}{\hbar}V\Psi^* \end{cases}$$

$$= \int_{-\infty}^{\infty}\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2 \Psi}{\partial x^2} - \frac{\partial^2 \Psi^*}{\partial x^2}\Psi\right) dx$$

$$= \frac{i\hbar}{2m}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right) dx = 0 \quad \text{if} \quad \Psi(x,t) \longrightarrow 0 \text{ at } x = \pm\infty$$

(即粒子出現在無窮遠處之機率為0，為物理合理之假設)

Expectation of position and momentum : $\langle x\rangle$, $\langle p\rangle$

$$\frac{d\langle x\rangle}{dt} = \int x \frac{d}{dt}|\Psi|^2 dx = \frac{i\hbar}{2m}\int x\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right) dx \qquad \text{integration by part}$$

$$= \frac{-i\hbar}{2m}\int\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right) dx \qquad \text{another integration by part for } \frac{\partial \Psi^*}{\partial x}\Psi$$

$$= -\frac{i\hbar}{m}\int \Psi^*\frac{\partial \Psi}{\partial x} dx$$

$$\Rightarrow \underbrace{m\frac{d\langle x\rangle}{dt}}_{\langle v\rangle} = -i\hbar\int\left(\Psi^*\frac{\partial \Psi}{\partial x}\right) dx = \langle p\rangle$$

動量的期望值等於位置的期望值之改變率乘以質量

能量本徵態 (energy eigen state) 問題 : $\Psi = U(t)\,\psi(x)$

$i\hbar\frac{\partial \Psi}{\partial t} = E\Psi$

$$\Rightarrow \psi(x)\, i\hbar\frac{\partial U(t)}{\partial t} = -\frac{\hbar^2}{2m}U(t)\frac{\partial^2 \psi}{\partial x^2} + VU(t)\,\psi(x)$$ 左右同除以 $U(t)\,\psi(t)$

$$\Rightarrow \frac{1}{U}\, i\hbar\frac{\partial U}{\partial t} = \frac{1}{\psi}\frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V$$ 令式子左右皆等於常數 E

$$\Rightarrow i\hbar\frac{\partial U}{\partial t} = EU \quad \text{and} \quad \frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = E\psi$$

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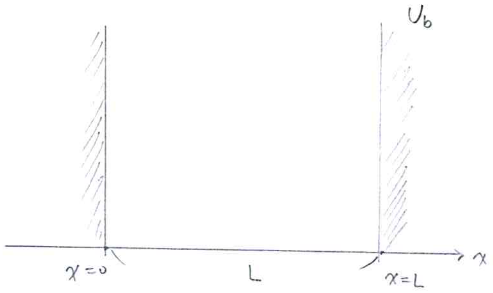
D. 1-dimensional infinite square potential well



先假設 U_0 為有限，再令 U_0 趨近無窮大 ($E < U_0$，因 E 不為無窮大)

time-independent Schrödinger equation at $x > L$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V\psi = \frac{\hbar^2}{2m}k^2\psi + U_0\psi = E\psi$$

$$\Rightarrow k^2 = \left(\frac{E-U_0}{\hbar^2}\right)2m < 0$$

$$\Rightarrow k = \pm i\left(\frac{2m(U_0-E)}{\hbar^2}\right)^{\frac{1}{2}},$$

however, the solution with a negative sign is unphysical since it diverges at $x \longrightarrow \infty$ (i.e., unnormalizable, not in the Hilbert space)

$$\Rightarrow \text{at } x > L,\ \psi \propto e^{-\left(\frac{2m(U_0-E)}{\hbar^2}\right)^{\frac{1}{2}}x}$$ which is vanishing with x.

when $U_0 \longrightarrow \infty$, ψ decays to 0 in infinitely short distance

In addition, we observe that $\frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial x}\right) = \frac{2m}{\hbar^2}(U_0 - E)\psi$ $\Rightarrow$ when $U_0 \to \infty$, $\frac{\partial\psi}{\partial x}$ can have discontinuity at $x = L$

ψ 的斜率隨距離的變化率

(i.e., there is no need of solving the continuity of $\frac{\partial\psi}{\partial x}$ at $x=0, L$)

$\Rightarrow$ In this case, we have the general solution of $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi = E\psi$ for $0 < x < L$, and the constraints:

$$\begin{cases} \text{(i)} & \psi = 0 \text{ at } x = 0 \text{ and } x = L \\ \text{(ii)} & \int_0^L |\psi|^2 dx = \int_0^L \psi^*\psi\, dx = 1 \end{cases}$$ —— conserving total probability.

normalization constant

cannot choose this one otherwise ψ has to be 0 everywhere

$$\Rightarrow \psi(x) = A \sin kx, \quad kL = \cancel{0}, \pm\pi, \pm 2\pi, \pm 3\pi, \cdots$$

$$\Rightarrow k_n = \frac{n\pi}{L}, \quad n = 1, 2, 3, \cdots$$

energy level: $E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2}$

$\cos(2kx) = \cos^2 kx - \sin^2 kx$, $\cos^2 kx + \sin^2 kx = 1$

$$\because \int_0^L \psi^*\psi\, dx = \int_0^L A^2 \sin^2 kx\, dx = \int_0^L \frac{A^2}{2}(1 - \cos(2kx))dx = \frac{A^2}{2}L = 1.0$$

$$\Rightarrow A^2 = \frac{2}{L}$$

$$\Rightarrow \text{wave function}: \psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

※
① the energy of the ground state (zero-point energy) is not zero
② The energy eigen wave functions are mutually orthogonal (i.e., $\int \psi_m(x)^*\psi_n(x)dx = \delta_{mn}$) easy to verify
③ Any other wave function in this infinite well can be expressed as

$$f(x) = \sum_{n=1}^{\infty} C_n \psi_n(x) = \sqrt{\frac{2}{L}}\sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi}{L}x\right)$$ —— Fourier series.

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General Physics (II) Quantum Physics

E. free-electron in 1D compactified space (空間大小為 L)

This is requiring $\begin{cases} \psi(0) = \psi(L) \\ \left.\frac{\partial \psi}{\partial x}\right|_{x=0} = \left.\frac{\partial \psi}{\partial x}\right|_{x=L} \end{cases}$

The general solution (for the time-independent schrödinger equation) is again e^{ikx}

$$\Downarrow$$

$$k_n L = 2n\pi, \quad n = 0, 1, \dots$$

$$\Rightarrow k_n = \frac{2n\pi}{L}$$

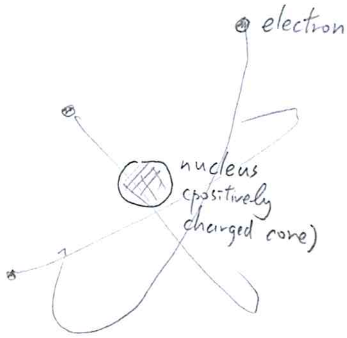
momentum $p_n = \hbar k_n = \frac{2n\pi}{L}\hbar$

Early hypotheses about hydrogen atom

ancient Greek: matter consisted ultimately of indivisible units: **atoms**

(i) Ernest Rutherford's atomic model (1911)

(motivated by the experiment of α-particle (氦原子核) scattered by gold foil (金箔))



Electrons are orbiting the positively charged nucleus, like planets revolving the Sun.

↳ This classical picture is incorrect since:

(i) an orbiting electron will lose energy through synchrotron emission. Thus the orbit will shrink. A classical calculation shows that the electron will fall onto the nucleus in 10^{-10} s.

(ii) why all atoms of an element are the same?

(ii) Rydberg-Ritz formula

1853: Anders Ångström discovered that a set of discrete frequencies was present in the radiation emitted by hydrogen.

1885: Johann Balmer found that these frequencies form a definite pattern

verified by Johannes Rydberg in 1890s

$$\frac{1}{\lambda} = R_y \left(\underbrace{\frac{1}{n^2} - \frac{1}{m^2}}_{\text{positive integers. } n<m} \right) \quad \text{— Rydberg-Ritz formula}$$

Rydberg constant: $1.09737 \cdot 10^7 \, m^{-1}$

"structures" of atoms/molecules are thoroughly characterized by these discrete frequencies.

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(iii) Niels Bohr's model (1913)

verified by Franck-Hertz experiment in 1914

1. Atoms can only exist in certain allowed states that have definite (discrete) energies.
2. Any change in the energy of a system, including emission/absorption of radiation, must take place as transition between states.
3. When there is a transition between two states that have energies E_1, E_2, the frequency of the associated emitted/absorbed photon ν satisfy

$$h\nu = |E_1 - E_2|$$

(i.e, each transition is associated with one photon)

4. The states corresponds to classical circular orbits of electron around the nucleus. The angular momentum is quantized as integral multiple of Planck's constant $\hbar$:

quantum number

$$\underbrace{L}_{\text{電子繞原子核之角動量}} = n\hbar, \quad n = 1, 2, 3, \ldots$$

對於任意帶正電荷 $+Ze$ 之原子核，其最內層電子之軌道滿足

1. $L = n\hbar$ (Bohr's hypothesis) $\Rightarrow r m_e v = n\hbar = L$
2. force balance: $\underbrace{m_e \dfrac{v^2}{r}}_{\text{向心力}} = \underbrace{\dfrac{1}{4\pi\epsilon_0}\dfrac{Ze^2}{r^2}}_{\text{靜電力}}$

$$\Rightarrow \begin{cases} r = \dfrac{L}{m_e v} \\ m_e v^2 = \dfrac{1}{4\pi\epsilon_0}\dfrac{Ze^2}{r} = \dfrac{1}{4\pi\epsilon_0} Ze^2 \dfrac{m_e v}{L} \end{cases} \Rightarrow v = \frac{Ze^2}{4\pi\epsilon_0 L}$$

$$\Rightarrow v_n = \frac{Ze^2}{4\pi\epsilon_0 n\hbar}$$

fine structure constant: $\alpha \equiv \dfrac{e^2}{4\pi\epsilon_0 \hbar c} \sim \dfrac{1}{137}$ (dimensionless)

$$v_n = \frac{Z}{n}\alpha \underbrace{c}_{\text{光速}}, \quad n = 1, 2, \ldots$$

(此表示式方便看出 v_n 為幾倍光速)

$$\Rightarrow R_n = \frac{n\hbar}{m_e v_n} = \frac{n\hbar}{m_e (Z\alpha c/n)} = \frac{n^2}{Z}\underbrace{\left(\frac{\hbar}{mc\alpha}\right)}$$

Bohr radius: $a_0 \equiv \dfrac{\hbar}{mc\alpha} = 0.53 \cdot 10$

Energy $E_n = T + V = \frac{1}{2} m_e v_n^2 - \dfrac{Ze^2}{4\pi\epsilon_0 R_n}$

$$= -\frac{1}{2} m_e \left(\frac{Z\alpha c}{n}\right)^2 = (-13.6\,\text{eV})\frac{Z^2}{n^2}$$

emission/absorption of photon:

should be corrected to the reduced mass $\mu = \dfrac{1}{m_e} + \dfrac{1}{M_{nuc}}$ (原子核質量)

$$h\nu_{n_2 \to n_1} = E_{n_2} - E_{n_1} = \frac{m_e Z^2 \alpha^2 c^2}{2}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

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General Physics (II) Quantum Physics

Niels Bohr did not know about the thesis of de Broglie which was published later. But we can comprehend Bohr's hypothesis of angular momentum based on de Broglie's concept:

$$2\pi R_n = \underset{\text{de Broglie wavelength}}{\overset{\text{整數}}{n}\lambda_n} = nh/P_n = 2\pi \hbar n/P_n$$

(想像 page 12, case 三中 wave function 在 compactify 空間中之情形, wave function 所需滿足的連續性條件)

$$\Rightarrow \quad R_n P_n = L_n = n\hbar$$

↳ 由於波函數須滿足边界或其它連續性條件而有不連續之 quantum number

Bohr's model correctly predicts the radius of hydrogen atom and the energy levels of hydrogen atom. However, it is still incomplete/incorrect. To get the full picture, we need to solve Schrödinger equation in 3D space

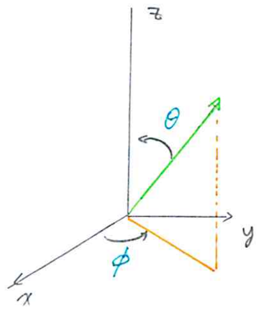
Hydrogen atom and the Schrödinger equation in three dimensions

$$i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 \Psi(\vec{r},t) + V(\vec{r})\Psi(\vec{r},t)$$

$$\vec{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (\text{Laplacian})$$

Since we are interested in the energy eigenstates, we separate the spatial and time dependence as usual:

$$\Psi(\vec{r},t) = \psi(\vec{r})\, e^{-\frac{iEt}{\hbar}}$$



$\Rightarrow$ the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2\underbrace{\mu}_{\text{reduced mass of electron}}}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right]\psi(\vec{r}) + V(r)\psi(\vec{r}) = E\psi(\vec{r})$$

transform to spherical coordinates: $x = r\sin\theta\cos\varphi$, $y = r\sin\theta\sin\varphi$, $z = r\cos\theta$

In atoms, $V(r) = -Ze^2/(4\pi\epsilon_0 r)$

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\right]\psi(\vec{r}) + V(r)\psi(\vec{r}) = E\psi(\vec{r}) \qquad \text{Eq (1)}$$

To solve this equation, we can continue with the technique of separation of variable, to separate the radial and angular dependence of $\psi(\vec{r})$:

$$令 \quad \psi(\vec{r}) = R(r)Y(\theta,\phi) = R(r)F(\theta)\Phi(\phi) \qquad \text{Eq (2)}$$

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Eq (2) 代入 Eq (1)

$$\Rightarrow -\frac{\hbar^2}{2\mu}\Big(\underbrace{\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}}_{\text{只作用在 } R(r) \text{ 上, 不作用在 } Y(\theta,\phi) \text{ 上}}\Big)R(r)Y(\theta,\phi) - \frac{\hbar^2}{2\mu}\frac{1}{r^2}\Big(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Big)R(r)Y(\theta,\phi) = (E-V)R(r)$$

左右同除 $R(r)Y(\theta,\phi)$

$$\Rightarrow -\frac{\hbar^2}{2\mu}\frac{1}{R(r)}\Big(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\Big)R(r) - \frac{\hbar^2}{2\mu}\frac{1}{r^2}\underbrace{\frac{1}{Y(\theta,\phi)}\Big(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Big)Y(\theta,\phi)}_{\text{此處完全沒有 } r \text{ dependence, 故只能為常數, 令其為 } \lambda} = E - V(r)$$

$\Rightarrow$ radial equation

$$-\frac{\hbar^2}{2\mu}\Big(\frac{d^2R(r)}{dr^2}+\frac{2}{r}\frac{dR(r)}{dr}+\lambda\frac{R(r)}{r^2}\Big)+V(r)R(r) = ER(r)$$

形式類似一維位能井問題,
若隨處 $E - V(r) < 0$ (bound state)
則只有在 E 為某些特定值時此
ordinary differential equation 有解
因此能量 quantization 後為不連續

angular equation (注意此式及其結論對任意球對稱之 $V(r)$ 皆成立,
因此式本身無 $V(r)$ 的 dependence)

$$\Big(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Big)Y(\theta,\phi) = \lambda Y(\theta,\phi)$$

$\Big\downarrow$ 代入 $Y(\theta,\phi) \equiv F(\theta)\Phi(\phi)$

$$\Phi\Big(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}\Big)F + \frac{F}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Phi = \lambda F\Phi \Rightarrow \frac{1}{F}\Big(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}\Big)F + \frac{1}{\sin^2\theta}\underbrace{\frac{1}{\Phi}\frac{\partial^2}{\partial\phi^2}\Phi}_{\text{此處沒有 } \theta \text{ 的 dependence, 可令其為常數}} =$$

$$\Rightarrow \frac{d^2\Phi}{d\phi^2} = -m^2\Phi \Rightarrow \Phi \propto e^{im\phi}$$

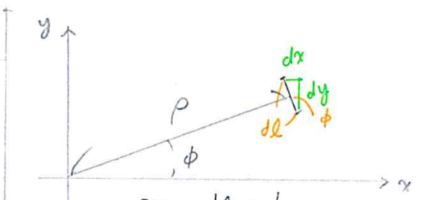
為滿足 $\Phi(\phi) = \Phi(\phi+2\pi)$ —— 回憶之前 1D compactify space 問題

$$\underbrace{\Rightarrow m = 0, \pm 1, \pm 2, \pm 3, \ldots}_{\text{此處為 z-軸角動量只能取ħ的整數倍之一般性原因}}$$

$$\vec{L} = \vec{r}\times\vec{p} : L_x = yP_z - zP_y,\ L_y = zP_x - xP_z,\ L_z = xP_y - yP_x$$

$$P_x = -i\hbar\frac{\partial}{\partial x},\ P_y = -i\hbar\frac{\partial}{\partial y},\ P_z = -i\hbar\frac{\partial}{\partial z}$$

$$\frac{\partial}{\partial\phi} = \frac{\partial}{\partial x}\overbrace{\frac{\partial x}{\partial\phi}}^{-y} + \frac{\partial}{\partial y}\overbrace{\frac{\partial y}{\partial\phi}}^{x} + \frac{\partial}{\partial z}\underbrace{\frac{\partial z}{\partial\phi}}_{0}$$



$$\delta x = -dl\sin\phi$$
$$= -dl\frac{y}{\rho} = -\rho\, d\phi\frac{y}{\rho} = -$$
$$\Rightarrow \frac{\delta x}{\delta\phi} = -y,\ \text{同理},\ \frac{\delta y}{\delta\phi} = x$$

$$\Rightarrow -i\hbar\frac{\partial}{\partial\phi} = +i\hbar y\frac{\partial}{\partial x} \overbrace{- i\hbar x\frac{\partial}{\partial y}}^{xP_y}$$
$$= xP_y - yP_x = L_z$$

$\because \frac{\partial}{\partial\phi}\psi = im\psi$ 故 L_z, 即 z 軸角動量只能為整數

$\Rightarrow$ Bohr's model.

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$$\Rightarrow \frac{d^2F(\theta)}{d\theta^2} + \cot\theta\frac{dF}{d\theta} - \frac{m^2}{\sin^2\theta}F(\theta) = \lambda F(\theta)$$ generalized Legendre equation

此式只有在取 $\lambda = -\ell(\ell+1)$, $\ell = 0, 1, 2, 3, \cdots$ 時有 physical 的解，並同時限制 $m = -\ell, \cdots \ell$

($\cos\theta = \pm 1$ 時，$F(\theta)$ 不為無窮大)

$$\Rightarrow \left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)Y(\theta,\phi) = \ell(\ell+1)Y(\theta,\phi)$$

代 $L_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$, $L_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$, $L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$

轉換成球座標後發現 總角動量

$$L^2 = L_x^2 + L_y^2 + L_z^2$$
$$= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

① 稱 ℓ 為 angular momentum quantum number 或 orbital quantum number (告訴我們總角動量)

② 稱 m 為 orbital magnetic quantum number (告訴我們總角動量在 z-軸之投影)

$\Rightarrow$ radial equation for hydrogen atom:

$$-\frac{\hbar^2}{2m_e}\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{\ell(\ell+1)}{r^2}\right]R(r) - \frac{Ze^2}{4\pi\epsilon_0 r}R(r) = ER(r)$$

只有在 E 為特定值

$$E = -\frac{1}{2}m_e c^2\left(\frac{Ze^2}{4\pi\epsilon_0\hbar c}\right)^2\frac{1}{(n_r+\ell+1)^2} = -\frac{1}{2}\underbrace{m_e c^2}_{\text{電子靜止能量}}(Z\underbrace{\alpha}_{\text{fine-structure constant}})^2\frac{1}{(n_r+\ell+1)^2}$$

radial quantum number: $n_r = 0, 1, 2, \cdots$

principal quantum number: $n \equiv n_r + \ell + 1$. n is a positive integer.

$$\Rightarrow E = -\frac{1}{2}m_e c^2(Z\alpha)^2\frac{1}{n^2}$$ 恰好等於 Bohr model 給出之原子能階

Finally, the Stern-Gerlach experiment (1921–1924) shows that electron carries spin magnetic moment, which is proportional to the intrinsic angular momentum, spin. Similar to orbital angular,

$$S^2 = s(s+1)\hbar^2, \quad \text{here } s = \frac{1}{2}$$

Spin has no classical limit, and S_z can only take values $\pm\frac{\hbar}{2}$

Summary: Hydrogen atom

(i) the energy level of a hydrogen atom is determined by the principal QN: n
(we call all states of a specific QN n a shell)

(ii) for a given n, ℓ can take $0, 1, 2, \cdots n-1$, and m can take $-\ell, -(\ell-1), \cdots, (\ell-1), \ell$.
(we call all states of a specific ℓ under a shell a subshell)

$\Rightarrow$ a. A subshell contains $(2\ell+1)\cdot \underbrace{2}_{\text{spin-up, spin-down}}$ states

b. A shell of principle quantum n contains: $2\cdot(1+3+5+\cdots(2n-1)) = 2n^2$ states

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historically, the subshells are labeled by letters:

$\ell =$	0	1	2	3	4	5
	s	p	d	f	g	h

s: 2 states, spin up/down

p: $2(2\cdot1+1)=6$ states

d: $2\cdot(2\cdot2+1)=10$ states

Pauli exclusion principle: No two electrons confined to the same trap can have the same set of values for their quantum numbers.

full or **fully occupied**: when an energy level cannot be occupied by more electrons because Pauli exclusion principle

empty or **unoccupied**: a energy level is not occupied by any electron

partially occupied: Neither of the above situation is true.

Periodic table (最外層電子的行為類似氫原子)

Ordering according to the number of protons in the atoms that are electrically neutral. Example:

Neon (Ne): noble gas

Sodium (Na): alkali metal

Chlorine (Cl): halogens.

Iron (Fe) (exceptional)

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \underbrace{3d^6\ 4s^2}$

餘下兩電子可把4s全填
能量低於只在d軌域填
電子而不填4s軌域