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Radial Equation

Example : Infinite spherical well

$$V(r)\begin{cases}0 & \text{if } r\le a\\ \infty & \text{if } r>a\end{cases}$$

$\frac{d}{dr}(r^2\frac{dR}{dr}) = r\frac{du}{dr} - u$

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2mr^2}{\hbar^2}[V(r)-E]R=\ell(\ell+1)R \qquad \text{let } u(r)\equiv rR(r)$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\underbrace{\left[V+\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]}_{V_{eff}}u=Eu \quad \text{radial equation}$$

$R=\frac{u}{r}$ $\quad \frac{dR}{dr}=\frac{(r\frac{du}{dr}-u)}{r^2}$, $\quad \frac{d}{dr}(r^2\frac{dR}{dr})=r\frac{d^2u}{dr^2}$

$-\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}$ centrifugal term

$\times\frac{d^2u}{dr^2}-\frac{2mr^2}{\hbar^2}(V-E)\frac{u}{r^2}=\ell(\ell+1)\frac{u}{r^2}$

$$\Rightarrow \frac{d^2u}{dr^2}=\left[\frac{\ell(\ell+1)}{r^2}-k^2\right]u \quad , \quad k\equiv\frac{\sqrt{2mE}}{\hbar}$$

$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}u=Eu \qquad \times\frac{\hbar^2}{2m}$

$\frac{d^2u}{dr^2}-\frac{\ell(\ell+1)}{r^2}u=-\frac{2m}{\hbar^2}Eu$

(i) $\ell=0$

$$\frac{d^2u}{dr^2}=-k^2u \quad , \quad u(r)=A\sin(kr)+B\cos(kr)$$

$R=\frac{u}{r}=\frac{\cos(kr)}{r}$ blows up as $r\to 0 \Rightarrow B=0$

$u(a)=0,\ \sin(ka)=0 \qquad ka=n\pi \qquad E_0=\frac{n^2\pi^2\hbar^2}{2ma^2} \qquad n=1,2,3\cdots$

$$\Rightarrow R(r)=\sqrt{\frac{2}{a}}\frac{\sin(\frac{n\pi r}{a})}{r} \qquad \psi_{n00}=\sqrt{\frac{2}{a}}\frac{\sin(\frac{n\pi r}{a})}{r}\underbrace{\frac{1}{\sqrt{4\pi}}}_{Y_0^0}=\frac{1}{\sqrt{2a\pi}}\frac{\sin(\frac{n\pi r}{a})}{r}$$

(ii) $\ell=+N$

$$\Rightarrow u(r)=Ar\underbrace{j_\ell(kr)}_{\text{spherical bessel function}}+Br\underbrace{n_\ell(kr)}_{\text{spherical neumann function}}$$

$$j_\ell(x)\equiv(-x)^\ell\left(\frac{1}{x}\frac{d}{dx}\right)^\ell\frac{\sin x}{x}$$

$$n_\ell(x)\equiv-(-x)^\ell\left(\frac{1}{x}\frac{d}{dx}\right)^\ell\frac{\cos x}{x}$$

for small x

$$j_0(x)\approx 1 \qquad j_1(x)\approx\frac{x}{3} \qquad j_2(x)\approx\frac{x^2}{15}$$

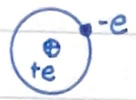
for small r, $x=kr$

$n_\ell(0)=-\infty \Rightarrow B=0 \qquad u(a)=0,\ j_\ell(ka)=0$

$$k=\frac{1}{a}\underbrace{\beta_{n\ell}}_{\text{Nth zero of the }\ell\text{-th of spherical bessel function}} \qquad E_{n\ell}=\frac{\hbar^2}{2ma^2}\beta_{n\ell}^2$$

$$u(r)=Arj_\ell(kr)=rR(r)\ , \quad R(r)=Aj_\ell\left(\frac{\beta_{n\ell}r}{a}\right)$$

The Hydrogen Atom



$V(r) = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$ solve bound states

$$\Rightarrow -\frac{\hbar^2}{2m_e}\frac{d^2u}{dr^2} + \left[-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m_e}\frac{l(l+1)}{r^2}\right]u = Eu$$

$\frac{2m}{\hbar k^2}$ ÷E

Radial Wave Function

let $\kappa \equiv \frac{\sqrt{-2m_e E}}{\hbar}$ $E = -\frac{\hbar^2\kappa^2}{2m}$

$$\Rightarrow \frac{1}{\kappa^2}\frac{d^2u}{dr^2} = \left[1 - \frac{m_e e^2}{2\pi\epsilon_0\hbar^2\kappa}\frac{1}{\kappa r} + \frac{l(l+1)}{(\kappa r)^2}\right]u$$

let $\rho \equiv \kappa r$ $\rho_0 \equiv \frac{m_e e^2}{2\pi\epsilon_0\hbar^2\kappa}$

$$\Rightarrow \frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right]u$$

(i) $\rho \to \infty$

$\frac{d^2u}{d\rho^2} \simeq u$, $u(\rho) = Ae^{-\rho} + \cancel{B}e^{\rho}$ ($B \to 0$)

as $\rho \to \infty$ e^{ρ} blows up

(ii) $\rho \to 0$

$\frac{d^2u}{d\rho^2} \simeq \frac{l(l+1)}{\rho^2}u$

$u(\rho) \simeq C\rho^{l+1} + \cancel{D\rho^{-l}}$ $\to 0$

$\Rightarrow$ let $u(\rho) = \rho^{l+1}e^{-\rho}v(\rho)$

$$\Rightarrow \rho\frac{d^2v}{d\rho^2} + 2(l+1-\rho)\frac{dv}{d\rho} + [\rho_0 - 2(l+1)]v = 0$$

set $v(\rho) = \sum_{j=0}^{\infty} c_j\rho^j$ $\frac{dv}{d\rho} = \sum_{j=0}^{\infty} jc_j\rho^{j-1} = \sum(j+1)c_{j+1}\rho^j$ $\frac{d^2v}{d\rho^2} = \sum_{j=0}^{\infty} j(j+1)c_{j+1}\rho^{j-1}$

$\Rightarrow c_{j+1} = \frac{2(j+l+1)-\rho_0}{(j+1)(j+2l+2)}c_j$, when $j \to \infty$ $c_{j+1} \simeq \frac{2j}{j^2}c_j \simeq \frac{2}{j}c_j = \frac{2\cdot 2}{j(j-1)}c_{j-1}$

$= \frac{2^j}{j!}c_0$

$v(\rho) = c_0\sum\frac{2^j}{j!}\rho^j = c_0e^{2\rho}$, $u(\rho) = c_0\rho^{l+1}e^{\rho}$

$\underbrace{2(l+j_{max}+1)}_{n} = \rho_0 = 2n = \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa}$, $\kappa = \frac{me^2}{4\pi\epsilon_0\hbar^2}\frac{1}{n} \equiv \frac{1}{a_n} = 0.529Å$ Bohr radius

$E = \frac{-\hbar^2\kappa^2}{2m} = -\frac{\hbar^2}{2m}\frac{me^2}{4\pi\epsilon_0\hbar^2}\frac{1}{n^2} = \frac{me^4}{32\pi^2\epsilon_0^2\hbar^2}\frac{1}{n^2} = -13.6eV\frac{1}{n^2}$ Bohr formula

$\rho = \kappa r = \frac{r}{a_n}$

$\psi(r,\theta,\phi) = R_{nl}(r)Y_l^m(\theta,\phi)$

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$$\psi_{100} = R_{10}(r)Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}} R_{10}(r) = \frac{1}{\sqrt{4\pi}} e^{-\frac{r}{a}}$$ 1S orbit

$C_1 = C_0 = 0 \quad v(\rho) = C_0$

$u(\rho) = e^{-\rho}\rho^{l+1}v(\rho) = e^{-\rho}\rho C_0$

$R(r) = \frac{u(\rho)}{r} = \frac{1}{r}e^{-kr}(kr)C_0 = C_0 e^{-\frac{r}{a}}$

$n=2 \quad l=0 \quad m=0$

$\psi_{200}(r,\theta,\phi) = R_{20}(r)Y_0^0(\theta,\phi)$

$C_1 = -C_0,\ C_2 = 0$ $\quad R(u) = \frac{u}{r} = C_0(1-\frac{r}{2a})e^{-\frac{r}{2a}}$

$v(\rho) = C_0 - C_0\rho = C_0(1-\rho)$

$u(\rho) = e^{-\rho}\rho\, C_0(1-\rho)$

$l=1 \quad m=\pm 1$

$C_1 = 0 \quad v(\rho) = C_0 \quad u(\rho) = e^{-\rho}\rho^2 v(\rho)$ $\quad Y_1^0 =$

$R_{20} = e^{-\frac{r}{2a}} r\, C = \frac{C_0}{4a^2} r e^{-\frac{r}{2a}}$ $\quad P_1^0 = \cos\theta$

$\psi_{210} = \frac{C}{4a^2} r e^{-\frac{r}{2a}} \cos\theta$ 2Pz

$\psi_{211} = \frac{C}{4a^2} r e^{-\frac{r}{2a}} \sin\theta\, e^{+i\phi}$ 2Px

$\psi_{21,-1} = \frac{C}{4a^2} r e^{-\frac{r}{2a}} \sin\theta\, e^{-i\phi}$ 2Py

$$\psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n(n+l)!}}\; e^{-\frac{r}{na}} \left(\frac{2r}{na}\right)^l \left(L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right)\right) Y_l^m(\theta,\phi)$$

$$L_q^p(x) = (-1)^p \left(\frac{d}{dx}\right)^p L_{p+q}(x)$$

$$L_q(x) = \frac{e^x}{q!}\left(\frac{d}{dx}\right)^q (e^{-x}x^q)$$

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