中心力场 (作业: 20230514)

1. 球坐标下的角动量平方算符: $\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$;
   (a) 拉普拉斯算符: $\nabla^2 = -\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\hat{L}^2}{\hbar^2 r^2}$;
2. 球坐标下粒子在中心力场运动的哈密顿算符: $\hat{H} = -\frac{\hbar^2}{2mr}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{2mr^2} + V(r)$;
   (a) 对易关系: $[\hat{\vec{L}}, \hat{L}^2] = 0, [\hat{H}, \hat{\vec{L}}] = 0, [\hat{H}, \hat{L}^2] = 0$;
   (b) 中心力场中运动的粒子角动量守恒;
3. 中心力场中粒子的定态薛定谔方程: $\left[-\frac{\hbar^2}{2mr}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{2mr^2} + V(r)\right]\psi(\vec{r}) = E\psi(\vec{r})$;
   (a) 分离变量: $\psi(r,\theta,\varphi) = R(r)Y_{lm}(\theta,\varphi)$;
   (b) 径向方程: $\left[-\frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right]R(r) = ER(r)$, 设 $u = rR$ 得约化的径向方程 $-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u(r) = Eu(r)$;
      i. 有效势: $V_{eff} = V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$;
   (c) 归一化条件: $\int_0^\infty |R|^2 r^2 dr = 1$;
   (d) 波函数: $\psi_{nlm}(\vec{r}) = R_{nl}(r)Y_{lm}(\theta,\varphi)$;
4. 库仑力场中的电子: 设原子核的电荷为 $+Ze$, Z 是原子序数;
   (a) 类氢原子的哈密顿算符: $\hat{H} = -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Ze_s^2}{r}$, 在国际单位制 $e_s = \frac{e}{\sqrt{4\pi\varepsilon_0}}, e_s = e$;
   (b) 电子的径向方程: $\frac{d^2u}{dr^2} + \left[\frac{2m_e}{\hbar^2}\left(E + \frac{Ze_s^2}{r}\right) - \frac{l(l+1)}{r^2}\right]u(r) = 0$;
      i. 设 $\alpha = \left(\frac{8m_e|E|}{\hbar^2}\right)^{\frac{1}{2}}, \beta = \frac{Ze_s^2}{\hbar}\left(\frac{m_e}{2|E|}\right)^{\frac{1}{2}}, \rho = \alpha r$, 方程变为 $\frac{d^2u}{d\rho^2} + \left[\frac{\beta}{\rho} - \frac{1}{4} - \frac{l(l+1)}{\rho^2}\right]u = 0$;
         A. 渐进解: $u(\rho) = e^{-\frac{\rho}{2}}\rho^{l+1}f(\rho)$;
      ii. 合流超几何方程:$\rho\frac{d^2f}{d\rho^2} + (2l+2-\rho)\frac{df}{d\rho} - (l+1-\beta)f = 0$;
         A. 一般形式: $\rho\frac{d^2F}{d\rho^2} + (b-\rho)\frac{dF}{d\rho} - aF = 0, b \notin \mathbb{Z}^- \cup \{0\}$, 解为 $F(\rho) = \sum_{v=0}^{\infty} c_v\rho^v, c_0 = 1, c_{v+1} = \frac{a+v}{(b+v)(v+1)}c_v = \frac{\frac{(a+v)!}{(a-1)!}}{\frac{(b+v)!}{(b-1)!}(v+1)!}$, 即 $F(a,b,\rho) = 1 + \frac{a}{b}\rho + \frac{a(a+1)\rho^2}{b(b+1)2!} + ...$;

iii. 径向波函数: $u(\rho) = e^{-\frac{\rho}{2}}\rho^{l+1}F(l+1-\beta, 2l+2, \rho)$;

A. 截断条件: $a = l+1-\beta = -n_r$, 即主量子数 $n = \beta = l+1+n_r$;

B. 能量: $E_n = -\frac{m_e Z^2 e_s^4}{2n^2\hbar^2}, n \in \mathbb{Z}^*$, 引入波尔半径 $a_0 = \frac{\hbar^2}{m_e e_s^2}$, 则 $E_n = \frac{E_1}{n^2}$;

C. 能级简并度: $d_n = \sum\limits_{l=0}^{n-1}(2l+1) = n^2$;

iv. 归一化因子: $N_{nl} = \frac{2}{(2l+1)1}\sqrt{\frac{(n+1)!Z^3}{(n-l-1)!a_0^3}}$;

v. 基态波函数: $\psi_{100} = R_{10}Y_{00} = \sqrt{\frac{Z^3}{\pi a_0^3}}e^{-\frac{Zr}{a_0}}$;

(c) 前几个定态波函数:

i. $R_{10} = 2\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-\frac{Zr}{a_0}}$;

ii. $R_{20} = \frac{1}{\sqrt{2}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\left(1-\frac{Zr}{2a_0}\right)e^{-\frac{Zr}{2a_0}}$;

iii. $R_{21} = \frac{1}{\sqrt{24}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}}\frac{Zr}{a_0}e^{-\frac{Zr}{2a_0}}$;

5. 氢原子:

(a) 体系的哈密顿量: 考虑原子核运动时, 核和电子组成体系的哈密顿算符为 $\hat{H} = \frac{\hbar^2}{2m_p}\vec{\nabla}_p^{\ 2} - \frac{\hbar^2}{2m_e}\vec{\nabla}_e^{\ 2} - \frac{e_s^2}{|\vec{r_e}-\vec{r_p}|}$, 其中 m_p 是原子核的质量, m_e 是电子的质量, $\vec{r_p}$ 是核的坐标, $\vec{r_e}$ 是电子的坐标;

(b) 体系的薛定谔方程: $i\hbar\frac{\partial\psi(\vec{r_p},\vec{r_e},t)}{\partial t} = \hat{H}\psi(\vec{r_p},\vec{r_e},t)$ 可展开为 $i\hbar\frac{\partial\psi(\vec{r_p},\vec{r_e},t)}{\partial t} = \left[-\frac{\hbar^2}{2M}\vec{\nabla}_R^2 - \frac{\hbar^2}{2\mu}\vec{\nabla}_r^2 - \frac{e_s^2}{\vec{r}}\right]\psi(\vec{r_p},\vec{r_e},t)$;

i. 质心坐标: $\vec{R} = \frac{m_p\vec{r_p}+m_e\vec{r_e}}{M}$, 其中 $M = m_e + m_p$;

ii. 相对坐标: $\vec{r} = \vec{r_e} - \vec{r_p}$;

iii. 约化质量: $\mu = \frac{m_p m_e}{m_p+m_e}$;

(c) 求解方法: 设 $\psi(\vec{R},\vec{r},t) = \chi(t)\phi(\vec{R})w(\vec{r})$, 则方程变为 $\frac{i\hbar}{\chi}\frac{d\chi}{dt} = -\frac{\hbar^2}{2M\phi}\vec{\nabla}_R^2\phi - \frac{\hbar^2}{2\mu w}\vec{\nabla}_r^2 w - \frac{e_s^2}{\vec{r}}$. 分离变量到常数 E_t 得到 $\begin{cases} i\hbar\frac{d\chi}{dt} = E_t\chi \\ -\frac{\hbar^2}{2M\phi}\vec{\nabla}_R^2\phi - \frac{\hbar^2}{2\mu w}\vec{\nabla}_r^2 w - \frac{e_s^2}{\vec{r}} = E_t \end{cases}$,

进一步分离相对坐标 (两项) 到常数 E 得到 $\begin{cases} i\hbar\frac{d\chi(t)}{dt} = E_t\chi(t) \\ -\frac{\hbar^2}{2M}\vec{\nabla}_R^2\phi(\vec{R}) = (E_t - E)\phi(\vec{R}) \\ \left(-\frac{\hbar^2}{2\mu}\vec{\nabla}_r^2 - \frac{e_s^2}{\vec{r}}\right)w(\vec{r}) = Ew(\vec{r}) \end{cases}$;

(d) 氢原子能级: $E_n = -\frac{\mu e_s^4}{2\hbar^2 n^2}, n \in \mathbb{N}^+$, 可由库仑力场中的电子能级令 $Z = 1$ 得到;

i. 氢原子的电离能: $E_\infty - E_1 = -E_1 = \frac{m_e e_s^4}{2\hbar} \approx -13.597eV$;

ii. 氢原子的辐射光频率: $\nu = \frac{E_n - E_{n'}}{2\pi\hbar c} = R_H\left(\frac{1}{n'^2} - \frac{1}{n^2}\right)$, 其中氢的 Rydberg 常数 $R_H = \frac{m_e e_s^4}{4\pi\hbar^3 c}$;