工程数学

Engineering Mathematics

李小飞

光电科学与工程学院

2022 年 2 月 21 日

第四章 氢原子 (6 学时)

Contents

氢原子含一原子核和一核外电子，是二体问题。

哈密顿量为：

$$H=\left[-\frac{\hbar^2}{2m_1}\nabla_1^2+V(\vec{r}_1,t)\right]+\left[-\frac{\hbar^2}{2m_2}\nabla_2^2+V(\vec{r}_2,t)\right]+U(|\vec{r}_1-\vec{r}_2|)$$

其中 V 为，U 为库仑势：

$$U(|\vec{r}_1-\vec{r}_2|)=-\frac{e_s^2}{|\vec{r}_1-\vec{r}_2|}\quad,\quad e_s=\frac{Ze}{\sqrt{4\pi\epsilon_0}}$$

薛定谔方程为:

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r}_1,\vec{r}_2,t)=H(\vec{r}_1,\vec{r}_2,t)\Psi(\vec{r}_1,\vec{r}_2,t)$$

当背景势 V 不显含时间 t，时空可分离变量。解得时间函数:

$$f(t)=e^{-iEt/\hbar}$$

空间函数服从定态薛定谔方程:

$$\left[-\frac{\hbar^2}{2m_1}\nabla_1^2+V_1-\frac{\hbar^2}{2m_2}\nabla_2^2+V_2+U_{1,2}\right]\Psi(\vec{r}_1,\vec{r}_2)=E\Psi(\vec{r}_1,\vec{r}_2)$$

相对坐标

设背景势 V=0，简化为:

$$\left[-\frac{\hbar^2}{2m_1}\nabla_1^2-\frac{\hbar^2}{2m_2}\nabla_2^2+U(|\vec{r}_1-\vec{r}_2|)\right]\Psi(\vec{r}_1,\vec{r}_2)=E\Psi(\vec{r}_1,\vec{r}_2)$$

引入相对坐标和质心坐标，令:

$$\begin{cases}\vec{r}(x,y,z)=\vec{r}_1-\vec{r}_2\\ \vec{R}(X,Y,Z)=\dfrac{m_1\vec{r}_1+m_2\vec{r}_2}{m_1+m_2}\end{cases}$$

$$\begin{cases}M=m_1+m_2\\ m=\dfrac{m_1m_2}{m_1+m_2}\end{cases}$$

对坐标函数: $\begin{cases} \vec{r}_1 = f_1(\vec{r}, \vec{R}) \\ \vec{r}_2 = f_2(\vec{r}, \vec{R}) \end{cases}$

求导:

$$\frac{d}{dx_1} = \frac{\partial}{\partial X}\frac{\partial X}{\partial x_1} + \frac{\partial}{\partial x}\frac{\partial x}{\partial x_1} = \frac{m_1}{M}\frac{\partial}{\partial X} + \frac{\partial}{\partial x}$$

$$\frac{d^2}{dx_1^2} = \frac{m_1^2}{M^2}\frac{\partial^2}{\partial X^2} + \frac{2m_1}{M}\frac{\partial^2}{\partial X \partial x} + \frac{\partial^2}{\partial x^2}$$

$$\nabla_1^2 = \frac{m_1^2}{M^2}\nabla_R^2 + \frac{2m_1}{M}\left(\frac{\partial^2}{\partial X \partial x} + \frac{\partial^2}{\partial Y \partial y} + \frac{\partial^2}{\partial Z \partial z}\right) + \nabla^2$$

$$\nabla_2^2 = \frac{m_2^2}{M^2}\nabla_R^2 - \frac{2m_2}{M}\left(\frac{\partial^2}{\partial X \partial x} + \frac{\partial^2}{\partial Y \partial y} + \frac{\partial^2}{\partial Z \partial z}\right) + \nabla^2$$

结合在一起，得:

$$\frac{1}{m_1}\nabla_1^2 + \frac{1}{m_2}\nabla_2^2 = \frac{1}{M}\nabla_R^2 + \frac{1}{m}\nabla^2$$

代回简化后的方程，得:

$$\left[-\frac{\hbar^2}{2M}\nabla_R^2 - \frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right]\Psi(\vec{R},\vec{r}) = E\Psi(\vec{R},\vec{r})$$

相对和质心坐标可分离变量,

令：$\Psi(\vec{R},\vec{r})=\psi(\vec{R})\Psi(\vec{r})$, 代入上方程，得方程（1）：

$$-\frac{\hbar^2}{2M}\nabla_R^2\psi(\vec{R})=E_c\psi(\vec{R}).....(1)$$

这是二体的质心运动方程，解为自由粒子平面波：

$$\psi(\vec{R},t)=-\frac{1}{(2\pi\hbar)^{3/2}}e^{-\frac{i}{\hbar}(E_ct-\vec{p}\cdot\vec{R})}$$

方程（2）：

$$\left[-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r})\right]\Psi(\vec{r})=E\Psi(\vec{r}).....(2)$$

这是二体相对运动方程，核与核外电子相对质心的运动方程。是核外电子相对于核的运动方程的近似！

无限深势求解

1. 量子无限深势阱

薛定谔方程基础

薛定谔方程分离变量

2. 量子谐振子与厄密方程

3. 厄密多项式及性质

大氣大為 求實求真

U 为库仑势:

$$U(\vec{r}) = -\frac{e_s^2}{r} \quad , \quad r = \sqrt{x^2 + y^2 + z^2}$$

与角量无关。方程 (2) 应改用球坐标系描述。

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + U(r)\right]\Psi(\vec{r}) = E\Psi(\vec{r}).....(2)$$

问题的关键在如何把 (x, y, z) 的 ∇^2 用 (r, θ, φ) 坐标系进行描述

球坐标拉普拉斯算子

已知 (x,y,z) 坐标系下的拉普拉斯算子为

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

求 (r, θ, φ) 坐标系下的拉普拉斯算子

解: 坐标的变换关系为:

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

对函数 $u(x,y,z)$，进行 r,θ,φ 求导，有：

$$
\begin{cases}
\dfrac{\partial u}{\partial r} = \dfrac{\partial u}{\partial x}\dfrac{\partial x}{\partial r} + \dfrac{\partial u}{\partial u}\dfrac{\partial y}{\partial r} + \dfrac{\partial u}{\partial z}\dfrac{\partial z}{\partial r} \\
\dfrac{\partial u}{\partial \theta} = \dfrac{\partial u}{\partial x}\dfrac{\partial x}{\partial \theta} + \dfrac{\partial u}{\partial u}\dfrac{\partial y}{\partial \theta} + \dfrac{\partial u}{\partial z}\dfrac{\partial z}{\partial \theta} \\
\dfrac{\partial u}{\partial \varphi} = \dfrac{\partial u}{\partial x}\dfrac{\partial x}{\partial \varphi} + \dfrac{\partial u}{\partial y}\dfrac{\partial y}{\partial \varphi} + \dfrac{\partial u}{\partial z}\dfrac{\partial z}{\partial \varphi}
\end{cases}
$$

$$
\begin{bmatrix} \dfrac{\partial u}{\partial r} \\ \dfrac{\partial u}{\partial \theta} \\ \dfrac{\partial u}{\partial \varphi} \end{bmatrix} = \begin{bmatrix} \sin\theta\cos\varphi & \sin\theta\sin\varphi & \cos\theta \\ r\cos\theta\cos\varphi & r\cos\theta\sin\varphi & -r\sin\theta \\ -r\sin\theta\sin\varphi & r\sin\theta\cos\varphi & 0 \end{bmatrix} \begin{bmatrix} \dfrac{\partial u}{\partial x} \\ \dfrac{\partial u}{\partial y} \\ \dfrac{\partial u}{\partial z} \end{bmatrix}
$$

$$\begin{bmatrix} \dfrac{\partial u}{\partial r} \\ \dfrac{\partial u}{\partial \theta} \\ \dfrac{\partial u}{\partial \varphi} \end{bmatrix} = \begin{bmatrix} \sin\theta\cos\varphi & \sin\theta\sin\varphi & \cos\theta \\ \cos\theta\cos\varphi & \cos\theta\sin\varphi & -\sin\theta \\ -\sin\varphi & \cos\varphi & 0 \end{bmatrix} \begin{bmatrix} \dfrac{\partial u}{\partial x} \\ \dfrac{1}{r}\dfrac{\partial u}{\partial y} \\ \dfrac{1}{r\sin\theta}\dfrac{\partial u}{\partial z} \end{bmatrix}$$

$$\begin{bmatrix} \dfrac{\partial u}{\partial r} \\ \dfrac{\partial u}{\partial \theta} \\ \dfrac{\partial u}{\partial \varphi} \end{bmatrix} = \begin{bmatrix} e_r & e_\theta & e_\varphi \end{bmatrix} \begin{bmatrix} \dfrac{\partial u}{\partial x} \\ \dfrac{1}{r}\dfrac{\partial u}{\partial y} \\ \dfrac{1}{r\sin\theta}\dfrac{\partial u}{\partial z} \end{bmatrix}$$

$$\to \nabla = e_r \frac{\partial}{\partial r} + \frac{1}{r} e_\theta \frac{\partial}{\partial \theta} + \frac{1}{r\sin\theta} e_\varphi \frac{\partial}{\partial \varphi}$$

$$
\begin{aligned}
\nabla^2 &= \nabla \cdot \nabla \\
&= (e_r \frac{\partial}{\partial r} + \frac{1}{r} e_\theta \frac{\partial}{\partial \theta} + \frac{1}{r \sin\theta} e_\varphi \frac{\partial}{\partial \varphi}) \cdot (e_r \frac{\partial}{\partial r} + \frac{1}{r} e_\theta \frac{\partial}{\partial \theta} + \frac{1}{r \sin\theta} e_\varphi \frac{\partial}{\partial \varphi}) \\
&= \frac{\partial^2}{\partial r^2} + (\frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}) + (\frac{1}{r}\frac{\partial}{\partial r} + \frac{\cos\theta}{r^2 \sin\theta}\frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \varphi^2}) \\
&= \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial}{\partial r}) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}(\sin\theta \frac{\partial}{\partial \theta}) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \varphi^2}
\end{aligned}
$$

tips：利用单位矢的正交归一性和微分性质进行计算（见讲义 15 页）

直角坐标 (x, y, z):

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

球坐标 (r, θ, φ)：

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

令角向部分为:

$$L^2 = -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

有:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) - \frac{1}{r^2}L^2$$

角向算符与角动量算符

角向算子:

$$L^2 = -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

角动量算子:

$$L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

角动量的径向和切向分量

$$p_r^2 = -\hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}), \quad p_\perp^2 = \frac{L^2}{r^2}$$

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

矩阵形式:

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} r\sin\theta\cos\varphi \\ r\sin\theta\sin\varphi \\ r\cos\theta \end{bmatrix} = re_r$$

动量算子:

$$\hat{p} = -i\hbar\nabla = -i\hbar(e_r\frac{\partial}{\partial r} + \frac{1}{r}e_\theta\frac{\partial}{\partial\theta} + \frac{1}{r\sin\theta}e_\varphi\frac{\partial}{\partial\varphi})$$

角动量: $\vec{L} = \vec{r} \times \vec{p}$

算子为:

$$\hat{L} = \hat{r} \times \hat{p} = -i\hbar r e_r \times \nabla$$

$$\hat{L} = -i\hbar(e_\varphi \frac{\partial}{\partial\theta} - \frac{1}{\sin\theta} e_\theta \frac{\partial}{\partial\varphi})$$

角动量的 Z 分量:

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial\varphi}$$

$$\hat{L}^2 = -\hbar^2(e_\varphi \frac{\partial}{\partial\theta} - \frac{1}{\sin\theta} e_\theta \frac{\partial}{\partial\varphi}) \cdot (e_\varphi \frac{\partial}{\partial\theta} - \frac{1}{\sin\theta} e_\theta \frac{\partial}{\partial\varphi})$$

$$\hat{L}^2 = -\hbar^2(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta}(\sin\theta \frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2})$$

无限深势求解

1. 量子无限深势阱
   - 薛定谔方程基础
   - 薛定谔方程分离变量
2. 量子谐振子与厄密方程
3. 厄密多项式及性质

球坐标氢原子方程

球坐标下的哈密顿量（折合质量 m 计为 μ）：

$$H=-\frac{\hbar^2}{2\mu r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})+\frac{\hbar^2}{2\mu r^2}L^2-\frac{e_s^2}{r}=\frac{1}{2\mu}p_r^2+\frac{1}{2\mu r^2}L^2-\frac{e_s^2}{r}$$

球坐标氢原子定态方程：

$$\left[\frac{1}{2\mu}p_r^2+\frac{1}{2\mu}p_\perp^2-\frac{e_s^2}{r}\right]\Psi(r,\theta,\varphi)=E\Psi(r,\theta,\varphi)$$

方程可做动量的径向/切向分离……

为了与数学方程统一，采用角向算符 L^2（与角动量算符差一个 $\hbar^2$）：

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

球坐标系下的方程形式变为：

$$\left[-\frac{\hbar^2}{2\mu r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) - \frac{\hbar^2}{2\mu r^2}L^2 - \frac{e_s^2}{r}\right]\Psi = E\Psi$$

数学上的径向/角向分离，令：

$$\Psi = R(r)Y(\theta,\varphi)$$

代回原方程，得：

$$-\frac{L^2 Y}{Y} = \frac{1}{R}\frac{\partial}{\partial r}(r^2\frac{\partial R}{\partial r}) + \frac{2\mu r^2}{\hbar^2}(E + \frac{e_s^2}{r}) = \lambda$$

氢原子的空间方程在球坐标系下分离成两个方程:

(1) 角向方程:

$$L^2 Y = -\lambda Y$$

(2) 径向方程:

$$\frac{d}{dr}(r^2\frac{dR}{dr}) + \frac{2\mu r^2}{\hbar^2}(E + \frac{e_s^2}{r})R = \lambda R$$

分别求解径向/角向方程...

1、求基向量 $(e_r, e_\theta, e_\varphi)$ 点积和叉积的运算规律

2、求如下偏分

$$\frac{\partial}{\partial\theta}e_\theta, \qquad \frac{\partial}{\partial\theta}e_r$$

3、角向算子与角动量算子有什么区别？

Contents

1. 量子无限深势阱

2. 量子谐振子与厄密方程

- 相互作用势
- 量子谐振子方程
- 厄密方程

3. 厄密多项式及性质

经纬度分离变量

角向方程:

$$L^2Y = -\lambda Y \to L^2Y = -l(l+1)Y$$

代入角向算子:

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]Y = -l(l+1)Y$$

可进一步进行经/纬度变量分离，令:

$$Y(\theta,\varphi) = \Theta(\theta)\Phi(\varphi)$$

代回上方程。得:

$$\Phi \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \Theta\frac{1}{\sin^2\theta}\frac{d^2\Phi}{d\varphi^2} + l(l+1)\Theta\Phi = 0$$

整理得:

$$\frac{\sin^2\theta}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \sin^2\theta l(l+1) = -\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2} = \lambda$$

分离变量，得 (1) 经度方程:

$$\frac{d^2\Phi}{d\varphi^2} + \lambda\Phi = 0, (0 < \varphi < 2\pi)$$

(2) 纬度方程:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \left[l(l+1) - \frac{\lambda}{\sin^2\theta}\right]\Theta = 0$$

解经度方程

经度方程是周期性边界条件固有值问题:

$$\frac{d^2\Phi}{d\varphi^2} + \lambda\Phi = 0, 0 < \varphi < 2\pi$$

$$\Phi(0) = \Phi(2\pi), \Phi'(0) = \Phi'(2\pi)$$

特征方程有两虚根，对应固有值和固有函数为:

$$\lambda = m^2, \quad (m = 0, 1, 2, \cdots)$$

$$\Phi(\varphi) = A\cos m\varphi + B\sin m\varphi$$

写指数形式

$$\Phi_m(\varphi) = A_m e^{im\varphi}$$

求归一化系数:

$$\int_0^{2\pi} |\Phi_m(\varphi)|^2 d\varphi = 1$$

$$\int_0^{2\pi} A_m e^{im\varphi} A_m e^{-im\varphi} d\varphi = 1$$

$$A_m^2 \int_0^{2\pi} 1 d\varphi = 1$$

$$A_m^2 2\pi = 1$$

$$A_m = \frac{1}{\sqrt{2\pi}}$$

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$$

解纬度方程

把固有值代回纬度方程，得 n 阶连带勒让德方程：

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left[l(l+1)-\frac{m^2}{\sin^2\theta}\right]\Theta=0$$

解:微分展开，再整理，得：

$$\frac{d^2\Theta}{d\theta^2}+\frac{\cos\theta}{\sin\theta}\frac{d\Theta}{d\theta}+\left[l(l+1)-\frac{m^2}{\sin^2\theta}\right]\Theta=0$$

令： $x=\cos\theta,\ y(x)=y(\cos\theta)=\Theta(\theta)$, 有，做微分计算：

$$\frac{dx}{d\theta}=-\sin\theta$$

$$\frac{d\Theta}{d\theta}=\frac{dy}{dx}\frac{dx}{d\theta}=-\sin\theta\frac{dy}{dx}$$

$$\frac{d^2\Theta}{d\theta^2} = -\sin^2\theta\frac{d^2y}{dx^2} - \cos\theta\frac{dy}{dx}$$

代回方程（注意 $\cos\theta = x$，$\sin\theta = 1 - x^2$），

得标准连带勒让德方程：

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + \left[l(l+1) - \frac{m^2}{1-x^2}\right]y = 0$$

令 m=0，得 (0 阶) 勒让德方程：

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + l(l+1)y = 0$$

大气大为 求实求真

$$(1-x^2)\frac{d^2y}{dx^2}-2x\frac{dy}{dx}+l(l+1)y=0$$

解：令方程有级数解，

$$y=\sum_{k=0}^{\infty}a_k x^k$$

求导，并代回上方向，得：

$$\sum_{k=0}^{\infty}\left\{(k+1)(k+2)a_{k+2}+[l(l+1)-k(k+1)]a_k\right\}x^k=0$$

系数项为零：

$$(k+1)(k+2)a_{k+2}+[l(l+1)-k(k+1)]a_k=0$$

得递推式:

$$a_{k+2} = -\frac{l(l+1)-k(k+1)}{(k+1)(k+2)}a_k$$

k 为偶数:

$$y_1(x) = a_0\left[1-\frac{l(l+1)}{2}x^2+\frac{l(l+1)(l+3)(l-2)}{4!}x^4+\cdots\right]$$

k 为奇数:

$$y_2(x) = a_1\left[x-\frac{(l-1)(l+2)}{3!}x^3+\frac{(l+2)(l+3)(l-1)(l-3)}{5!}x^5+\cdots\right]$$

方程的级数解:

$$y(x) = y_1(x)+y_2(x)$$

逆向递推式为 (l=n):

$$a_{k-2} = -\frac{(k-1)k}{(n-k+2)(n+k-1)}a_k$$

注意到级数解应只含有限多项，取最高项 k=n

$$a_{n-2} = -\frac{(n-1)n}{2(2n-1)}a_n$$

令最高项系数:

$$a_n = \frac{(2n)!}{2^n(n!)^2}$$

有:

$$a_{n-2} = -\frac{(2n-2)!}{2^n(n-1)!(n-2)!}$$

一般式:

$$a_{n-2m} = (-1)^m \frac{(2n-2m)!}{2^n m!(n-m)!(n-2m)!}$$

得勒让德方程的多项式解:

$$P_n(x) = \sum_{m=0}^{[n/2]} (-1)^n \frac{(2n-2m)!}{2^n m!(n-m)!(n-2m)!} x^{n-2m}$$

称为勒让德多项式。

取 x=$\cos\theta$, 得下表:

$P_0(x) = 1$	
$P_1(x) = x$	$P_1(\cos\theta) = \cos\theta$
$P_2(x) = \frac{1}{2}(3x^2 - 1)$	$P_2(\cos\theta) = \frac{1}{4}[3\cos 2\theta + 1]$
$P_3(x) = \frac{1}{2}(5x^3 - 3x)$	$P_3(\cos\theta) = \frac{1}{8}[5\cos 3\theta + 3\cos\theta]$
$P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3)$	$P_4(\cos\theta) = \frac{1}{64}[35\cos 4\theta + 20\cos 2\theta + 9]$

性质 1: 勒让德多项式具有如下微分形式:

$$P_n(x)=\frac{1}{2^n n!}\frac{d^n}{dx^n}\left(x^2-1\right)^n, \quad (n=0,1,2,3,\cdots\cdots)$$

证明: 由二项式定理，有:

$$\left(x^2-1\right)^n=\sum_{m=0}^{n} C_n^m(-1)^m\left(x^2\right)^{n-m}=\sum_{m=0}^{n}\frac{(-1)^m n!}{m!(n-m)!}x^{2n-2m}$$

求 n 次导,

$$\frac{d^n}{dx^n}\left(x^2-1\right)^n=\sum_{m=0}^{n}\frac{(-1)^m n!}{m!(n-m)!}\frac{d^n}{dx^n}\left(x^{2n-2m}\right)$$

当 $2n-2m<n$ 时，上次的右边导数为零，即非零的最高项为 $[n/2]$，有：

$$\frac{d^n}{dx^n}\left(x^2-1\right)^n=\sum_{m=0}^{[n/2]}\frac{(-1)^m n!}{m!(n-m)!}\frac{d^n}{dx^n}\left(x^{2n-2m}\right)$$

$$\frac{1}{2^n n!}\frac{d^n}{dx^n}\left(x^2-1\right)^n=\frac{1}{2^n n!}\sum_{m=0}^{[n/2]}\frac{(-1)^m n!}{m!(n-m)!}\frac{d^n}{dx^n}\left(x^{2n-2m}\right)=P_n(x)$$

证毕！

性质 2:勒让德多项式具有如下母函数:

$$w(x,z) = \left(1 - 2zx + z^2\right)^{-1/2}$$

证明:即要证

$$\left(1 - 2zx + z^2\right)^{-1/2} = \sum_{n=0}^{\infty} P_n(x) z^n$$

由二项式定理有:

$$(1+v)^p = \sum_{k=0}^{\infty} \frac{p(p-1)\cdots(p-k+1)}{k!} v^k$$

取 $p=-1/2$，得:

$$(1+v)^{-1/2}=\sum_{k=0}^{\infty}(-1)^k\frac{(2k)!}{2^{2k}(k!)^2}v^k$$

取 $v=-2zx+z^2=-z(2x-z)$，有:

$$v^k=(-1)^kz^k(2x-z)^k=(-1)^kz^k\sum_{m=0}^{k}C_k^m(2x)^{k-m}(-z)^m$$

代回上式，得:

$$\left(1-2zx+z^2\right)^{-\frac{1}{2}}=\sum_{k=0}^{\infty}\frac{(2k)!}{2^{2k}(k!)^2}\sum_{m=0}^{k}(-1)^mC_k^m(2x)^{k-m}z^{k+m}$$

令： $k-m=n$，即要证明上式右边的系数就是 $P_n(x)$!

$$
\begin{aligned}
\sum_{k+m=n} & 2^{2k}(k!)^2(-1)^m C_k^m (2x)^{k-m} \\
&= \sum_{m=0}^{n} (-1)^m \frac{(2n-2m)!}{2^{2(n-m)}(n-m)!} \frac{1}{m!(n-2m)!} (2x)^{n-2m} \\
&= \sum_{m=0}^{n} (-1)^m \frac{(2n-2m)!}{2^n m!(n-m)!(n-2m)!} x^{n-2m} \\
&= P_n(x)
\end{aligned}
$$

证毕!

性质 3:勒让德多项式具有如下递推关系:

$$(n+1)P_{n+1}(x)-(2n+1)xP_n(x)+nP_{n-1}(x)=0$$

证明:对于母函数的形式级数:

$$w(x,z)=(1-2zx+z^2-1/2)=\sum_{n=0}^{\infty}P_n(x)z^n$$

求关于 z 的偏导:

$$\frac{\partial w}{\partial z}=\sum_{n=1}^{\infty}nP_n(x)z^{n-1}=\sum_{n=0}^{\infty}(n+1)P_{n+1}z^n$$

$$\frac{\partial w}{\partial z} = (x-z)(1-2zx+z^2)-3/2$$

$$(1-2zx+z^2)\frac{\partial w}{\partial z} = (x-z)(1-2zx+z^2)-1/2$$

$$(1-2zx+z^2)\frac{\partial w}{\partial z} - (x-z)w = 0$$

$$(1-2zx+z^2)\sum_{n=0}^{\infty}(n+1)P_{n+1}z^n - (x-z)\sum_{n=0}^{\infty}P_n(x)z^n = 0$$

整理，得

$$\sum_{n=1}^{\infty}[(n+1)P_{n+1} - (2n+1)xP_n + nP_{n-1}]z^n = 0$$

系数项等于零，得证!

性质 4:勒让德多项式具有正交性:

证明:勒让德多项式满足勒让德方程

$$\left(1-x^2\right)P_n''(x)-2xP_n'(x)+n(n+1)P_n(x)=0$$

等价形式:

$$\left[\left(1-x^2\right)P_n'(x)\right]'+n(n+1)P_n(x)=0\cdots(1)$$

同理:

$$\left(1-x^2\right)P_m'(x)'+m(m+1)P_m(x)=0\cdots(2)$$

(1) 式 $\times P_m$, (2) 式 $\times P_n$, 所得两式相减并积分:

$$[n(n+1)-m(m+1)]\int_{-1}^{1}P_mP_ndx=\int_{-1}^{1}\left(P_m\left[\left(1-x^2\right)P_n'\right]'-P_n\left[\left(1-x^2\right)P_m'\right]'\right)dx$$

上式右端分部积分,

$$
\begin{aligned}
&=\left(P_m\left[\left(1-x^2\right) P_n'\right]-P_n\left[\left(1-x^2\right) P_m'\right]\right)\Big|_{-1}^{1} \\
&\quad-\int_{-1}^{1}\left[\left(1-x^2\right) P_m' P_n'-\left(1-x^2\right) P_n' P_m'\right] d x \\
&=0
\end{aligned}
$$

因此,

$$
[n(n+1)-m(m+1)] \int_{-1}^{1} P_m P_n d x=0
$$

有:

$$
\int_{-1}^{1} P_m P_n d x=0, \cdots(n \neq m)
$$

证毕!

性质 5: 勒让德多项式具有归一性

$$\int_{-1}^{1} P_n P_n dx = \frac{2}{2n+1}$$

证明: 有递推公式

$$[nP_n - (2n-1)xP_{n-} + (n-1)P_{n-2}] = 0$$

$$nP_n^2 = (2n-1)xP_nP_{n-1} - (n-1)P_nP_{n-2}$$

$$\int_{-1}^{1} nP_n^2 dx = \int_{-1}^{1} (2n-1)xP_nP_{n-1} dx$$

递推式写成 $xP_n = AP_{n+1} + BP_{n-1}$ 代入上式，得积分递推式

$$\int_{-1}^{1} P_n^2 dx = \frac{2n-1}{2n+1}\int_{-1}^{1} P_{n-1}^2 dx$$

反复递推:

$$\int_{-1}^{1} P_n^2 dx = \frac{1}{2n+1} \int_{-1}^{1} P_0^2 dx = \frac{2}{2n+1}$$

证毕!

例 1: 利用勒让德多项式正交性计算积分:

$$\int_{-1}^{+1} x^2 P_n(x)dx$$

解: 由 $P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n$, 得:

$$P_0(x) = 1, P_1(x) = x, P_2(x) = \frac{1}{2}(3x^2-1)$$

x^2 的勒让德多项式展开式:

$$x^2 = \frac{2}{3}P_2 + \frac{1}{3}P_0$$

原式为:

$$\int_{-1}^{+1} x^2 P_n dx = \int_{-1}^{+1} (\frac{2}{3}P_2 + \frac{1}{3}P_0)P_n dx$$

分情况讨论:

(1) $n=0$,

$$\int_{-1}^{+1} x^2 P_n dx = \int_{-1}^{+1} \frac{1}{3} P_0 P_0 dx = \frac{1}{3}\frac{2}{2n+1} = \frac{2}{3}$$

(2) $n=2$,

$$\int_{-1}^{+1} x^2 P_n dx = \int_{-1}^{+1} \frac{2}{3} P_2 P_2 dx = \frac{2}{3}\frac{2}{2n+1} = \frac{4}{15}$$

(3) $n \neq 0, 2$

$$\int_{-1}^{+1} x^2 P_n dx = 0$$

Tips:

$$1 = P_0$$

$$x = P_1$$

$$x^2 = \frac{1}{3}(2P_2 + P_0)$$

$$x^3 = \frac{1}{5}(2P_3 + 3P_1)$$

1. 量子无限深势阱

2. 量子谐振子与厄密方程

相互作用势

量子谐振子方程

厄密方程

3. 厄密多项式及性质

求實求真 大氣大為

勒让德方程:

$$(1-x^2)\frac{d^2y}{dx^2}-2x\frac{dy}{dx}+l(l+1)y=0$$

解为勒让德多项式

$$P_l(x)=\frac{1}{2^l l!}\frac{d^l}{dx^l}\left(x^2-1\right)^l,\quad (l=0,1,2,3,\cdots\cdots)$$

连带勒让德方程:

$$(1-x^2)\frac{d^2y}{dx^2}-2x\frac{dy}{dx}+\left[l(l+1)-\frac{m^2}{1-x^2}\right]y=0$$

解为连带勒让德多项式

$$P_l^m(x)=(1-x^2)^{m/2}\frac{d^m}{dx^m}P_l(x),\quad (m\le l, l=0,1,2,3,\cdots\cdots)$$

解法细节：

把勒让德多项式 $P_l(x)$ 代入勒让德方程，然后对勒让德方程逐级求导, m 次后得连带勒让德方程

$$(1-x^2)\,P_l''(x)-2xP_l'(x)+l(l+1)P_l(x)=0$$

$$(1-x^2)\,P_l^3(x)-2(1+1)xP_l''(x)+(l(l+1)-1(1+1)P_l'(x)=0$$

$$(1-x^2)\,P_l^4(x)-2(2+1)xP_l^3(x)+(l(l+1)-2(2+1)P_l''(x)=0$$

$$\cdots\cdots$$

$$(1-x^2)\,P_l^{m+2}(x)-2(m+1)xP_l^{m+1}(x)+(l(l+1)-m(m+1)P_l^m(x)=0$$

即：连带勒让德多项式 $P_l^m(x)$ 是连带勒让德方程的解

连带勒让德多项式性质:

(1) 正交性:

$$\int_{-1}^{1} P_m^k P_n^k dx = 0, \cdots (n \neq m)$$

(2) 归一性:

$$\int_{-1}^{1} P_n^k P_n^k dx = \frac{(n+k)!}{(n-k)!} \frac{2}{2n+1}$$

(3) 递推式:

$$(n+1-k) P_{n+1}^k - (2n+1) x P_n^k + (n+k) P_{n-1}^k = 0$$

氢原子角向方程:

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]Y=-l(l+1)Y$$

其解为球谐函数:

$$Y(\theta,\varphi)=\Theta(\theta)\Phi(\varphi)$$

经度解函数为:

$$\Phi_m(\varphi)=\frac{1}{\sqrt{2\pi}}e^{im\varphi}$$

纬度解函数为:

$$\Theta(\theta)=P_n^m(\cos\theta),\quad (m\le n, n=1,2,3,\cdots\cdots)$$

角向函数归一化

$$Y_{lm}(\theta,\varphi) = A_{lm}P_l^m(cos\theta)e^{im\varphi}$$

求归一化系数

$$\iint |Y_{lm}|^2 d\sigma = 1$$

$$\iint A_{lm}^2 |P_l^m(cos\theta)|^2 |\Phi(\varphi)|^2 d\sigma = 1$$

$$A_{lm}^2 2\pi \int_0^\pi |P_l^m(cos\theta)|^2 \sin\theta d\theta = 1$$

$$A_{lm}^2 2\pi \frac{(l+m)!}{(l-m)!}\frac{2}{2l+1} = 1$$

$$A_{lm} = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}$$

大气大局 求实求真

1、将 $x = \cos x$ 代入勒让德多项式，写出前 4 个勒让德多项式表达式

2、计算积分

$$\int_{-1}^{1} (x^2 + x) P_n(x) dx, \qquad \int_{-1}^{1} x^k P_n(x) dx, \quad (k < n) \qquad \int_{-1}^{1} x^n P_n(x) dx$$

Contents

1. 量子无限深势阱

2. 量子谐振子与厄密方程

3. 厄密多项式及性质

- 生成函数
- 性质
- 归一化系数

径向方程:

$$\frac{d}{dr}(r^2\frac{dR}{dr}) + \frac{2\mu r^2}{\hbar^2}(E + \frac{e_s^2}{r}) = \lambda R$$

解:取 $\lambda = l(l+1)$

$$\frac{d}{dr}(r^2\frac{dR}{dr}) + \frac{2\mu r^2}{\hbar^2}(E + \frac{e_s^2}{r})R = l(l+1)R$$

$$\frac{d^2R}{dr^2} + \frac{2}{r^2}\frac{dR}{dr} + \frac{2\mu}{\hbar^2}(E + \frac{e_s^2}{r})R - \frac{l(l+1)}{r^2}R = 0$$

令 $\xi = \alpha r, U(\xi) = R(\xi/\alpha), \alpha = \sqrt{-\frac{8\mu E}{\hbar^2}}, \beta = \frac{2\mu e_s^2}{\alpha\hbar^2},$

进行伸缩变换......, 得:

$$\frac{d^2U}{d\xi^2} + \frac{2}{\xi}\frac{dU}{d\xi} - [\frac{1}{4} - \frac{\beta}{\xi} + \frac{l(l+1)}{\xi^2}]U = 0 \cdots (1)$$

考虑方程解的渐近行为:

(1) $r \to \infty, \xi \to \infty$, 有方程:

$$\frac{d^2U}{d\xi^2} - \frac{1}{4}U = 0$$

特征方程有两互异实根，通解为:

$$U = C_1 exp(\frac{1}{2}\xi) + C_2 exp(-\frac{1}{2}\xi)$$

考虑到有界性，有特解:

$$U_\infty = Cexp(-\frac{1}{2}\xi)$$

(2) $r \to 0, \xi \to 0$，有欧拉方程:

$$\frac{d^2U}{d\xi^2} + \frac{2}{\xi}\frac{dU}{d\xi} + [\frac{\beta}{\xi} - \frac{l(l+1)}{\xi^2}]U = 0$$

通解为:

$$U = C_1\xi^{-(l+1)} + C_2\xi^l$$

考虑到有界性，有特解:

$$U_0 = C\xi^l$$

作常数变异，令方程的解为:

$$U = H(\xi)\xi^l exp(-\frac{1}{2}\xi)$$

问题变为求多项式 $H(\xi)$

对上式求导，并把结果代回原方程 (1)，得

$$\xi H'' + [2(l+1) - \xi]H' - [\beta - (l+1)]H = 0$$

标准的广义拉盖方程为

$$xH'' + [m+1-x]H' + nH = 0$$

对比以上两方程，发现当

$$m = 2l+1, \qquad n = -\beta + (l+1)$$

时，方程正是广义拉盖方程，问题转化为求广义拉盖方程

1. 量子无限深势阱

2. 量子谐振子与厄密方程

3. 厄密多项式及性质

生成函数

性质

归一化系数

解拉盖方程

取 $m=0$, 得一般的拉盖方程，取标准形式:

$$xy'' + [1-x]y' + ny = 0$$

解: 设方程有级数解

$$y = \sum_{k=0}^{\infty} c_k x^k$$

求导，代回上方程，得

$$\sum_{k=0}^{\infty}[(n-k)c_k + (k+1)^2 c_{k+1}]x^k = 0$$

得系数递推式:

$$c_{k+1} = -\frac{n-k}{(k+1)^2}c_k, \qquad (k=0,1,2,\cdots)$$

反复递推，有：

$$c_k = (-1)^k \frac{n(n-1)\cdots(n-k+1)}{(k!)^2} c_0, \qquad (k = 1, 2, \cdots, n)$$

当 $k = n$ 时，最高项系数为：

$$c_n = (-1)^n \frac{1}{n!} c_0,$$

级数解转化为多项式解 (拉盖多项式)，取

$$c_0 = n!, c_n = (-1)^k$$

拉盖多项式的系数为：

$$c_k = (-1)^k \frac{(n!)^2}{(k!)^2 (n-k)!}, \qquad (k = 0, 1, 2, \cdots, n)$$

拉盖多项式:

$$
\begin{aligned}
L_n(x) &= \sum_{k=0}^{n} c_k x^k = \sum_{k=0}^{n} (-1)^k \frac{(n!)^2}{(k!)^2(n-k)!} x^k \\
&= \sum_{k=0}^{n} (-1)^k \frac{(n!)}{(k!)(n-k)!} \frac{n!}{k!} x^k \\
&= \sum_{k=0}^{n} (-1)^k C_n^k \frac{n!}{k!} x^k, \qquad (k = 0, 1, 2, \cdots, n)
\end{aligned}
$$

$$
\begin{aligned}
L_0(x) &= 1 \\
L_1(x) &= 1 - x \\
L_2(x) &= 2 - 4x + x^2 \\
L_3(x) &= 6 - 18x + 9x^2 - x^3
\end{aligned}
$$

课堂作业:

求 x, x^2, x^3 的拉盖尔多项式展开式

拉盖多项式的性质

性质 1: 拉盖多项式微分形式

$$L_n(x) = e^x \frac{d^n}{dx^n}(x^n e^{-x})$$

证明: 由高阶导数莱布尼兹公式

$$(u \cdot v)^{(n)} = \sum_{k=0}^{n} C_n^k u^{(k)} V^{(n-k)},$$

得:

$$\begin{aligned}(e^{-x} \cdot x^n)^{(n)} &= \sum_{k=0}^{n} C_n^k [e^{-x}]^{(k)} [(x^n)^{(n-k)}] \\ &= \sum_{k=0}^{n} C_n^k [(-1)^k e^{-x}][C_n^k \frac{n!}{k!} x^k]\end{aligned}$$

$$
\begin{aligned}
e^x \frac{d^n}{dx^n}(e^{-x} \cdot x^n) &= e^x \sum_{k=0}^{n} C_n^k [(-1)^k e^{-x}][C_n^k \frac{n!}{k!} x^k] \\
&= \sum_{k=0}^{n} (-1)^k C_n^k \frac{n!}{k!} x^k \\
&= L_n(x)
\end{aligned}
$$

证毕！

性质 2: 拉盖多项式生成函数

$$w(t,x) = \frac{e^{-xt/(1-t)}}{1-t}$$

证明: 对函数在 $t=0$ 做泰勒展开

$$\begin{aligned} w(t,x) &= \sum_{n=0}^{\infty} \frac{d^n w}{dt^n}\Big|_{t=0} \frac{t^n}{n!} \\ &= \sum_{n=0}^{\infty} e^x \frac{d^n}{dx^n}\left(e^{-x}\cdot x^n\right)\frac{t^n}{n!} \\ &= \sum_{n=0}^{\infty} L_n \frac{t^n}{n!} \end{aligned}$$

性质 3: 拉盖多项式递推式

$$
\begin{aligned}
L_{n+1} &= (2n+1-x)L_n - n^2 L_{(}n-1) \\
L_1 &= (1-x)L_0
\end{aligned}
$$

证明: 对 w 函数就 t 求偏导,

$$
\begin{aligned}
\frac{\partial w}{\partial t} &= [\frac{1}{(1-t)^2} - \frac{x}{(1-t)^3}]e^{-xt/(1-t)} \\
(1-t)^2\frac{\partial w}{\partial t} &= [1-t-x]w, \cdots\cdots(1)
\end{aligned}
$$

对 w 函数的展开式就 t 求偏导，

$$\frac{\partial w}{\partial t} = \sum_{n=1}^{\infty} L_n \frac{t^{n-1}}{(n-1)!}$$
$$= \sum_{n=0}^{\infty} L_(n+1) \frac{t^{n}}{(n)!}$$
$$= \sum_{n=2}^{\infty} L_(n-1) \frac{t^{n-2}}{(n-2)!}$$

代入 (1) 式的左边，有:

$$(1-t)^2 \frac{\partial w}{\partial t} = \sum_{n=0}^{\infty} L_{n+1} \frac{t^n}{(n)!} - 2\sum_{n=1}^{\infty} L_n \frac{t^n}{(n-1)!} + \sum_{n=2}^{\infty} L_{n-1} \frac{n(n-1)}{(n)!} t^n$$

(1) 式的右边，有:

$$
\begin{aligned}
[1-t-x]w &= (1-x)w - tw \\
&= \sum_{n=0}^{\infty}(1-x)L_n\frac{t^n}{n!} - \sum_{n=0}^{\infty}L_n\frac{t^{n+1}}{n!} \\
&= \sum_{n=0}^{\infty}(1-x)L_n\frac{t^n}{n!} - \sum_{n=1}^{\infty}L_{n-1}\frac{t^n}{(n-1)!}
\end{aligned}
$$

(1) 式的左边 = 右边，整理得递推式!

性质 4: 拉盖多项式归一性

证明: 有递推式

$$
\begin{aligned}
L_{n+1} &= (2n+1-x)L_n - n^2 L_(n-1) \\
L_n &= (2n-1-x)L_{n-1} - (n-1)^2 L_(n-2) \\
L_n^2 &= (2n-1-x)L_n L_{n-1} - (n-1)^2 L_n L_(n-2) \\
L_{n-1}L_{n+1} &= (2n+1-x)L_{n-1}L_n - n^2 L_(^2 n-1) \\
\int_0^\infty e^{-x} L_n^2 dx &= n^2 \int_0^\infty e^{-x} L_{n-1}^2 dx \\
&= (n!)^2 \int_0^\infty e^{-x} L_0^2 dx \\
&= (n!)^2
\end{aligned}
$$

性质 5: 拉盖多项式正交性

证明: 拉盖多项式满足拉盖方程:

$$xL_n'' + [1-x]L_n' + nL_n = 0$$

$$[xe^{-x}L_n']' + ne^{-x}L_n = 0$$

$$[xe^{-x}L_m']' + me^{-x}L_m = 0$$

$$L_m[xe^{-x}L_n']' + ne^{-x}L_mL_n = 0$$

$$L_n[xe^{-x}L_m']' + me^{-x}L_nL_m = 0$$

$$\begin{aligned}(m-n)\int_0^{\infty} e^{-x}L_nL_m dx &= \int_0^{\infty}[L_n[xe^{-x}L_m']' - L_m[xe^{-x}L_n']']dx \\ &= -\int_0^{\infty}[L_n'[xe^{-x}L_m']dx + L_m'[xe^{-x}L_n']dx \\ &= \int_0^{\infty}[xe^{-x}L_m'L_n' - xe^{-x}L_n'L_m']dx = 0\end{aligned}$$

1. 量子无限深势阱

2. 量子谐振子与厄密方程

3. 厄密多项式及性质

生成函数

性质

归一化系数

大气大为 求实求真

广义拉盖方程多项式

量子力学定义广义拉盖多项式为:

$$L_n^0(x) = \frac{1}{n!}L_n(x) = \frac{1}{n!}\sum_{k=0}^{n}(-1)^k C_n^k \frac{n!}{k!}x^k$$

$$L_n^m(x) = \frac{1}{n!}\sum_{k=0}^{n}(-1)^k C_n^k \frac{(n+m)!}{(m+k)!}x^k$$

微分形式:

$$L_n^m(x) = \frac{x^{-m}e^x}{n!}\frac{d^n}{dx^n}(x^{m+n}e^{-x})$$

递推式:

$$(n+1)L_{n+1}^{m} = (2n+1+m-x)L_{n}^{m} - (n+m)L_{n-1}$$

正交性:

$$\int_0^{\infty} e^{-x} x^m L_n^m L_k^m dx = 0, \qquad (k \neq n)$$

归一性:

$$\int_0^{\infty} e^{-x} x^m [L_n^m]^2 dx = \frac{(n+m)!}{n!}$$

归一性推论:

$$\int_0^{\infty} e^{-x} x^{m+1} [L_n^m]^2 dx = \frac{(n+m)!}{n!}(2n+m+1)$$

氢原子径向解:

$$R_{nl}(r) = N_{nl}R(r) = N_{nl}\xi^l L_{n-l-1}^{2l+1}(\xi)e^{-\xi/2}, \qquad (\xi = \alpha r)$$

能量固有值:

$$n = \beta = \frac{2\mu e_s^2}{\alpha\hbar^2}$$
$$E_n = -\frac{1}{n^2}\frac{\mu e_s^4}{2\hbar^2} = \frac{E_1}{n!}$$

氢原子的解:

$$\Psi(r,\theta,\varphi) = R_{nl}(r)Y_{lm}(\theta,\varphi)$$

求归一化系数 N_{nl}

$$\iiint \Psi(r,\theta,\varphi)d\tau = 1$$

$$\iiint |N_{nl}R(r)Y_{lm}(\theta,\varphi)|^2 r^2 \sin\theta dr d\theta d\varphi = 1$$

$$\int_0^\infty N_{nl}^2 R^2(r) r^2 dr = 1$$

$$\frac{1}{\alpha^3}\int_0^\infty N_{nl}^2 R^2(\xi)\xi^2 d\xi = 1$$

$$\frac{1}{\alpha^3}\int_0^\infty N_{nl}^2 \xi^{2l+2}[L_{n-l-1}^{2l+1}(\xi)]^2 e^{-\xi} d\xi = 1$$

$$\frac{1}{\alpha^3}\int_0^\infty N_{nl}^2 \xi^{M+1}[L_N^M(\xi)]^2 e^{-\xi} d\xi = 1$$

$$\frac{1}{\alpha^3} N_{nl}^2 \frac{(N+M)!}{N!}(2N+M+1) = 1$$

$\rightarrow$

$$N_{nl}^2 \frac{2n(n+1)!}{\alpha^3 (n-l-1)!} = 1$$

$$N_{nl} = \sqrt{\alpha^3 \frac{(n-l-1)!}{2n(n+1)!}}$$

作业

1、证明拉盖多项式的正交性

2、求方程的解

$$\frac{d^2U}{d\xi^2}+\frac{2}{\xi}\frac{dU}{d\xi}+[\frac{\beta}{\xi}-\frac{l(l+1)}{\xi^2}]U=0$$

3、计算积分:

$$\int_0^\infty e^{-x}(L_1(x))^2dx, \qquad \int_0^\infty e^{-x}(L_2(x))^2dx,$$

Thanks for your attention!

A & Q