

- Bessel 方程:

1. Helmholtz 方程在柱坐标下变量分离:

$$\nu \text{ 阶 Bessel 方程: } x^2 y'' + xy' + (x^2 - \nu^2) y = 0$$

ν 阶 Bessel 方程的通解为: $y(x) = C J_\nu(x) + D N_\nu(x)$, $0 < |x| < +\infty$.

$$J_\nu(x) = \sum_{k=0}^{+\infty} \frac{(-1)^k}{k! \Gamma(k+\nu+1)} \left(\frac{x}{2}\right)^{2k+\nu}$$

$$N_\nu(x) = \begin{cases} \frac{J_\nu(x) \cos \nu\pi - J_{-\nu}(x)}{\sin \nu\pi}, & \nu \text{ 不是整数} \\ \lim_{\nu \rightarrow m} N_\nu(x), & \nu \text{ 是非负整数} \end{cases}$$

若 m 不是整数, 通解也可表示成 $y(x) = A J_\nu(x) + B J_{-\nu}(x)$.

2. Bessel 函数:

2.1 递推和微分公式:

$$(x^\nu J_\nu)' = x^\nu J_{\nu-1}$$

$$(x^{-\nu} J_\nu)' = -x^{-\nu} J_{\nu+1} \Rightarrow x^{-(\nu-1)} J_\nu = -\{x^{-(\nu-1)} J_{\nu-1}\}', \quad J_0' = -J_1$$

$$2J_\nu' = J_{\nu-1} - J_{\nu+1} \Rightarrow J_\nu = J_{\nu-2} - 2J_\nu'$$

$$2\nu x^{-1} J_\nu = J_{\nu-1} + J_{\nu+1} \Rightarrow J_\nu = 2(\nu-1)x^{-1} J_{\nu-1} - J_{\nu-2}$$

2.2 零点和衰减振荡性 (P116).

考虑积分 $\int x^\mu J_\nu(x) dx$, 利用 $(x^{-\nu} J_\nu)' = -x^{-\nu} J_{\nu+1}$

$$\int x^\mu J_\nu dx = \int x^{\mu+\nu-1} x^{-\nu+1} J_\nu dx$$

$$= -x^{\mu+\nu-1} x^{-\nu+1} J_{\nu-1}(x) - (\mu+\nu-1) \int x^{\mu+\nu-2} x^{-\nu+1} J_{\nu-1}(x) dx$$

$$= -x^\mu J_{\nu-1}(x) + (\mu+\nu-1) \int x^{\mu-1} J_{\nu-1}(x) dx$$

每分部积分一次, 幂次降 1, Bessel 函数阶数降 1. n 次后:

$$\int x^{\mu-n} J_{\nu-n}(x) dx, \text{ 若 } (\mu-n) \pm (\nu-n) = 1 \text{ 即, } \mu-\nu=1 / \mu+\nu=2n+1.$$

此积分可表示为有限形式, 能用初等函数积出.

若 $\mu \pm \nu \neq$ 奇数时, 该积分就比较难:

$$\text{e.g. } \int_0^x z^\nu J_\nu(z) dz = 2^{\nu-1} \sqrt{\pi} \Gamma(\nu + \frac{1}{2}) z [J_\nu(z) H_{\nu-1}(z) - J_{\nu-1}(z) H_\nu(z)].$$

$$\nu \text{ 阶 Struve 函数: } H_\nu(z) = \sum_{k=0}^{+\infty} \frac{(-1)^k}{\Gamma(k+\frac{3}{2}) \Gamma(\nu+k+\frac{3}{2})} \left(\frac{z}{2}\right)^{2k+\nu+1}$$

这类积分化到 J_1, J_0 . $\int J_0 dx$ 即可.

3. Bessel 方程的固有值问题 (P117)

① $N_\nu(x)$ 在 $x=0$ 无界, 故一般不考虑; 同时注意有界性条件.

② 第二类边界条件有固有值 $\lambda=0$ (S-L 定理).

③ 固有函数系 $\{J_\nu(w_{1n}r)\}$, $\{J_\nu(w_{2n}r)\}$, $\{J_\nu(w_{3n}r)\}$ 分别是满足相应边界条件的函数区间里的加权为 r 的完备正交函数系.

④ 模平方: $N_{\nu kn} = \int_0^a r J_\nu^2(w_{kn}r) dr$ 会结, 可记可不记.

题目: 15.11; 16.

二. Legendre 方程.

1. Helmholtz 方程在球坐标下的变量分离及 Legendre 方程的导出

m 阶伴随 Legendre 方程: $[(1-x^2)y']' + (\lambda - \frac{m^2}{1-x^2})y = 0$.

$m=0 \Rightarrow$ Legendre 方程.

$\lambda = l(l+1)$, $l \neq n$ (非负整数), Legendre 方程不存在 $x=\pm 1$ 都有界的解

$l=n$ (非负整数). $P_n(x) \doteq \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{(-1)^k (2n-2k)!}{2^n k! (n-k)! (n-2k)!} x^{n-2k}$

$Q_n(x) \doteq P_n(x) \int \frac{dx}{(1-x^2)(P_n(x))^2}$, $x \rightarrow \pm 1$ 时, $Q_n(x) \rightarrow \infty$.

$y(x) = C P_n(x) + D Q_n(x)$.

2. Legendre 函数:

Rodrigues 公式: $P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2-1)^n$. Remember!

性质:

① $P_n(-x) = (-1)^n P_n(x)$.

$$\left[P_n'(x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{(-1)^k (2n-2k)! (n-2k)}{2^n k! (n-k)! (n-2k)!} x^{n-2k-1} \right]$$

② 特殊点函数值:

★ $2^m m! = (2m)!!$

$$P_n(0) = \begin{cases} 0, & n=2m+1 \geq 1 \\ \frac{(-1)^m (2m-1)!!}{(2m)!!}, & n=2m \geq 2 \\ 1, & n=0. \end{cases}$$

$$P_n'(0) = \begin{cases} 0, & n=2k \\ \frac{(-1)^k (2k+1)!!}{(2k)!!}, & n=2k+1, \end{cases} \quad k=0, 1, 2, \dots$$

$P_n(1) = 1, P_n(-1) = (-1)^n$.

③ 零点分布: $P_n(x)$ 在 $(-1, 1)$ 内有且仅有 n 个互不相同单零点

递推公式:

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

$nP_n(x) - xP_n'(x) + P_{n-1}'(x) = 0 \rightarrow$ 计算 $x^n P_n(x)$.

$nP_{n-1}(x) - P_n'(x) + xP_{n-1}'(x) = 0$; $P_{n+1}'(x) - P_{n-1}'(x) = (2n+1)P_n(x) \rightarrow$ 计算 $P_n(x)$.

含有 Legendre 多项式的积分:

$$\textcircled{1} n \geq 2, I = \int_0^1 P_n(x) dx = \begin{cases} 0, & n = 2k \\ \frac{(-1)^k (2k-1)!!}{(2k+2)!!}, & n = 2k+1 \end{cases}$$

② $m \geq 1, n \geq 1$:

$$L_{m,n} = \int_0^1 x^m P_n(x) dx = \frac{m}{m+n+1} \int_0^1 x^{m-1} P_{n-1}(x) dx$$

$$L_{m,n} = \begin{cases} \frac{m!}{(m-n)!!(m+n+1)!!}, & m > n. \\ \frac{m!(n-m+1)!!}{(m+n+1)!!} \int_0^1 P_{n-m}(x) dx, & m \leq n. \end{cases}$$

$$\begin{aligned} \text{证: } m > n, L_{m,n} &= \frac{m(m-1)\dots[m-(n-1)]}{(m+n+1)(m+n-1)\dots[m+n+1-2(n-1)]} \int_0^1 x^{m-n} P_0(x) dx \\ &= \frac{m!}{(m-n)!} \frac{(n-m+1)!!}{(m+n+1)!!} \int_0^1 x^{m-n} dx = \frac{m!}{(m-n)!} \frac{(n-m+1)!!}{(m+n+1)!!} \frac{1}{m-n+1} \\ &= \frac{m!}{(m-n)!!(m+n+1)!!} \end{aligned}$$

$$\begin{aligned} m \leq n, L_{m,n} &= \frac{m(m-1)\dots[m-(m-1)]}{(m+n+1)\dots[m+n+1-2(m-1)]} \int_0^1 x^0 P_{n-m}(x) dx \\ &= \frac{m!(n-m+1)!!}{(m+n+1)!!} \int_0^1 P_{n-m}(x) dx. \end{aligned}$$

$$\textcircled{3} \int_{-1}^1 x^m P_n(x) dx. \quad \left[\int_{-1}^1 P_n(x) P_m(x) dx = 0, n \neq m \right]$$

$$n \int_{-1}^1 x^m P_n dx = \int_{-1}^1 x^m [x P_n' - P_{n-1}'] dx$$

$$= [x^{m+1} P_n - x^m P_{n-1}] \Big|_{-1}^1 - \int_{-1}^1 (m+1) x^m P_n dx + \int_{-1}^1 m x^{m-1} P_{n-1} dx$$

$$= [(-1)^{n+m+1} - (-1)^{m+n-1}] - \int_{-1}^1 (m+1) x^m P_n dx + \int_{-1}^1 m x^{m-1} P_{n-1} dx$$

$$\Rightarrow \int_{-1}^1 x^m P_n dx = \frac{m}{n+m+1} \int_{-1}^1 x^{m-1} P_{n-1} dx$$

④ I. $m < n$, 为 0

$$\text{II. } m \geq n, \int_{-1}^1 x^m P_n dx = \frac{m!}{(m-n)!} \frac{(m-n+1)!!}{(m+n+1)!!} \int_{-1}^1 x^{m-n} dx$$

$$= \frac{m! [1 + (-1)^{m-n}]}{(m-n)!!(m+n+1)!!}$$

④ 设 $f_k(x)$ 为任意一个 k 次多项式, 当 $k < l$ 时都有: $\int_{-1}^1 f_k(x) P_l(x) dx = 0$.

3. 轴对称 Laplace 方程球面边值问题: $u(r, \theta) = \sum_{n=0}^{+\infty} [C_n r^n + D_n r^{-(n+1)}] P_n(\cos \theta)$
 (P_{100}).

题目: 8

三. 解氢原子.

$$\hat{H} = -\frac{\hbar^2}{2\mu} \nabla^2 + V(r), \quad \hat{H}\psi = E\psi$$

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

设 $\psi = R(r) Y(\theta, \phi)$

径向函数 角向函数

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

$$\frac{1}{R} \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] + \frac{2\mu r^2}{\hbar^2} [E - V(r)] = l(l+1) \quad \dots (2)$$

1) 给出角向解:

归一化的球谐函数:

$$Y_{lm}(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos \theta) e^{im\phi} \quad \begin{cases} l = 0, 1, 2, \dots \\ m = 0, \pm 1, \pm 2, \dots, \pm l \end{cases}$$

$$L^2 = - \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right], \quad L^2 Y_{lm}(\theta, \phi) = l(l+1) Y_{lm}(\theta, \phi)$$

$$L_z = -i \frac{\partial}{\partial \phi}, \quad L_z Y_{lm}(\theta, \phi) = m Y_{lm}(\theta, \phi)$$

$$\begin{cases} L^2 Y_{lm}(\theta, \phi) = l(l+1) \hbar^2 Y_{lm}(\theta, \phi) \\ L_z Y_{lm}(\theta, \phi) = m \hbar Y_{lm}(\theta, \phi) \end{cases}$$

球谐函数是算符 L^2 和 L_z 在坐标表象下共同的特征函数

2) 径向归一化的径向函数

$$R_{nl}(r) = \sqrt{\left(\frac{2Z}{na}\right)^3 \frac{(n-l-1)!}{2n(n+l)!}} \exp\left(-\frac{Z}{an}r\right) \left(\frac{2Z}{an}r\right)^l L_{n-l-1}^{2l+1}\left(\frac{2Z}{an}r\right)$$

(confluent hypergeometric function)

因为拉盖尔多项式是超几何函数的特例, 故 $R_{nl}(r)$ 也可用后者表示

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_{lm}(\theta, \phi) = N_{nl} \exp\left(-\frac{Z}{an}r\right) \left(\frac{2Z}{an}r\right)^l L_{n-l-1}^{2l+1}\left(\frac{2Z}{an}r\right) Y_{lm}(\theta, \phi) \quad \begin{cases} n = 1, 2, 3, \dots \\ l = 0, 1, 2, \dots, n-1 \\ m = 0, \dots, \pm l \end{cases}$$