Review

严格对角化

基矢 | ★ 如何选
　　 | ★ 其它 $\psi=\sum_n C_n \phi_n(x)$

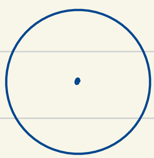
Lanczos 方法

可以处理大的系统 } 三对角矩阵, | $N\sim 10^8$ 不占内存

$q_0\to q_1\to q_2\to\cdots q_N$ 　　 $O(N^2)$

精确对角化中的对称性.

e.g.



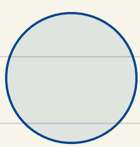
有角动量守恒, 或其它守恒量.

一个实用的例子: <u>柱对称的量子点, 能级</u>, 80, 90年 还十分重要.

p.s. 有自旋轨道耦合; 和 拓扑绝缘体有关.

这里利用 Bessel 函数 求解
其它的基矢选择 可能要选择一些特殊函数.

首先我们考虑一个简单的情形



$$H=-\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}\right)+u(x,y)$$

$u(x,y)$ 有旋转对称性

需要我们求解 $H\psi(x,y)=E\psi(x,y)$.

我们选择极坐标来处理这个问题.

$$H = -\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}\right) + u(r)$$

$$= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}\right) + u(r)$$

我们使用边界条件 $\psi(R,\theta) = 0$，则方程可以分离变量.

$$\psi(r,\theta) = \varphi_n(r) e^{in\theta} \leftarrow \text{单值性}$$

$$\Rightarrow \quad H\psi = E\psi$$

$$\Rightarrow \begin{cases} -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{n^2}{r^2}\right)\varphi_n(r) = E_n \varphi_n(r) \\ \varphi_n(R) = 0. \quad \varphi_n(0) \text{ 有界}. \end{cases}$$

（$\uparrow$ 一个一维的方程.）

无量纲化. 取 $r = \lambda x$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\left(\frac{1}{\lambda^2}\frac{\partial^2}{\partial x^2} + \frac{1}{\lambda^2 x}\frac{\partial}{\partial x} - \frac{n^2}{\lambda^2 x^2}\right)\varphi_n = E_n \varphi_n.$$

取 $\lambda^2 = \frac{\hbar^2}{2mE_n}$

$$\Rightarrow \quad -\left(\frac{\partial^2}{\partial x^2} + \frac{1}{x}\frac{\partial}{\partial x} - \frac{n^2}{x^2}\right)\varphi_n = \varphi_n.$$

$$\Rightarrow \quad x^2\varphi_n'' + x\varphi_n' + (x^2 - n^2)\varphi_n = 0$$

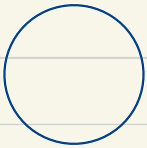
> Bessel function
>
> $x^2 f'' + x f' + (x^2 - \nu^2) f = 0$
>
> f_ν: $J_\nu(x)$ 和 $Y_\nu(x)$
>
> （J_ν: 第一类；Y_ν: 第二类）

$$\psi_n\left(\sqrt{\frac{k}{2mE}}\,x\right)=0 \quad \text{at } r=R \iff J_n\left(\frac{R}{\sqrt{\frac{\hbar^2}{2mE}}}\right)=0$$

求解出本征值

$$\Rightarrow \frac{R}{\sqrt{\frac{\hbar^2}{2mE}}} = x_{nj}, \qquad J_n(x_{nj})=0$$

★



=> 可以求解，按 n 分类.

★ Bessel function 可以做为基矢

$$\psi_{jn} = \sum_{k=1}^{\infty} C_{nk} J_n\left(\frac{x_{nk} r}{R}\right)$$

可以在 $r=R$ 时，天然满足 $\psi_{jn}(r=R)=0$，以及角动量守恒的条件.

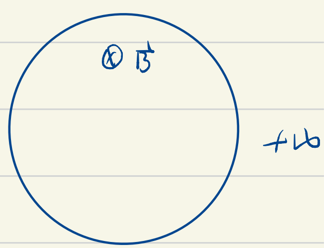
Bessel function 正交性.

$$\int_0^R J_n\left(x_{nj}\frac{r}{R}\right) J_n\left(x_{nk}\frac{r}{R}\right) r\,dr = \begin{cases} 0, & j\neq k \\ \frac{R^2}{2} J_{n+1}^2(x_{nj}) \end{cases}$$

$$H = \begin{pmatrix} M+\frac{1}{2}k_x^2+\frac{1}{2}k_y^2, & \alpha(k_x-ik_y) \\ \alpha(k_x+ik_y), & -M-\frac{1}{2}(k_x^2+k_y^2) \end{pmatrix} \qquad k_x=-i\frac{\partial}{\partial x},\quad k_y=-i\frac{\partial}{\partial y}$$

如果加磁场 $\vec{k} \to \vec{k}-e\vec{A}$

重要性
① 具有旋转对称性.
② 2x2 矩阵
③ SOC，磁场



选择 $\vec{A}=\frac{B}{2}(-y,x)$ 的对称规范，极坐标 $\begin{cases} y=r\sin\theta \\ x=r\cos\theta \end{cases}$

① $$(\vec{k}-e\vec{A})^2=\vec{k}^2+e^2\vec{A}^2-e(\vec{k}\cdot\vec{A}+\vec{A}\cdot\vec{k})$$

$\begin{cases} P_xA_x=[P_x,A_x]+A_xP_x \\ P_yA_y=[P_y,A_y]+A_yA_x \end{cases}$

$$=-\nabla^2+e^2\vec{A}^2-ie(\vec{\nabla}\cdot\vec{A}+\vec{A}\cdot\vec{\nabla})$$

$$=-\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right)+\frac{e^2B^2r^2}{4}-ie\left[-y\frac{\partial}{\partial x}+x\frac{\partial}{\partial y}\right]$$

$$=-\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right)+\frac{e^2B^2r^2}{4}+ieB\frac{\partial}{\partial\theta}$$

② $$k_x-ik_y-eA_x+ieA_y=e^{-i\theta}\left[-i\left(\frac{\partial}{\partial r}-i\frac{1}{r}\frac{\partial}{\partial\theta}\right)+\frac{iBre}{2}\right]$$

$$\begin{cases} H_{11}=M-\frac{1}{2}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}-\frac{B^2e^2}{4}r^2-ieB\frac{\partial}{\partial\theta}\right) \\ H_{12}=\alpha e^{-i\theta}\left((-i)\left(\frac{\partial}{\partial r}-i\frac{1}{r}\frac{\partial}{\partial\theta}\right)+i\frac{Ber}{2}\right) \\ H_{21}=H_{12}^* \\ H_{22}=-M+\frac{1}{2}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}-\frac{B^2e^2}{4}r^2-ieB\frac{\partial}{\partial\theta}\right) \end{cases}$$

$\Rightarrow$ 引起角动量的混合.

而 $$\psi(r,\theta)=\begin{pmatrix} \varphi_n(r)e^{in\theta} \\ \varphi_{n+1}(r)e^{i(n+1)\theta} \end{pmatrix}$$

作业. Liu, Guo, Wang ; Physica. B 407 2334–2339 (2012)
eq.1 → eq.20 推导.