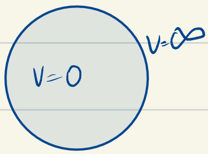
Review

Bessel function $J_n(x)$，作为一组完备基.

对称性.



$$\psi(r,\theta) = \varphi(r)\, e^{in\theta}$$

自旋轨道耦合

$\vec{L}\cdot\vec{S}$

$$\mathcal{H} = \begin{pmatrix} M_z - \frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right) - \frac{e^2B^2r^2}{4} - ieB\frac{\partial}{\partial\theta} & \alpha e^{-i\theta}\left[(-i)\left(\frac{\partial}{\partial r} - i\frac{1}{r}\frac{\partial}{\partial\theta}\right) + i\frac{Br}{2}\right] \\ \alpha e^{i\theta}\left[(-i)\left(\frac{\partial}{\partial r} + i\frac{1}{r}\frac{\partial}{\partial\theta}\right) - \frac{iBr}{2}\right] & -M_z + \frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right) - \frac{e^2B^2r^2}{4} - ieB\frac{\partial}{\partial\theta} \end{pmatrix}$$

$$\psi = \begin{pmatrix} \phi_\uparrow^n e^{in\theta} \\ \phi_\downarrow^{n+1} e^{i(n+1)\theta} \end{pmatrix}$$

$$\Rightarrow \left[M_z - \frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{n^2}{r^2}\right) - \frac{e^2B^2r^2}{4} + eBn\right]\phi_\uparrow^n + \alpha\left((-i)\left(\frac{\partial}{\partial r} + \frac{n+1}{r}\right) + \frac{iBer}{2}\right)\phi_\downarrow^{n+1} = E\phi_\uparrow^n \quad \langle 1\rangle$$

$$\alpha\left[(-i)\left(\frac{\partial}{\partial r} - \frac{n}{r}\right) - \frac{iBer}{2}\right]\phi_\uparrow^n + \left[-M_z - \frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{(n+1)^2}{r^2}\right) - \frac{e^2B^2r^2}{4} + eB(n+1)\right]\phi_\downarrow^{n+1} = E\phi_\downarrow^{n+1} \quad \langle 2\rangle$$

边界条件 $r\in[0,R]$.

$$\begin{cases} \phi_\uparrow^{n} = \sum_l C_{nl} J_n(\nu_{nl} \frac{r}{R}) \\ \phi_\downarrow^{n+1} = \sum_l d_{nl} J_{n+1}(\nu_{n+1,l} \frac{r}{R}) \end{cases}$$

J_n 是 ∇^2 的本征态.
拉普拉斯算子

使用右边同样的方法，我们可以将方程 <1><2> 转化一个矩阵求本征值问题。

P.S.

$$H|\psi\rangle = E|\psi\rangle$$

$$|\psi\rangle = \sum_n C_n |\varphi_n\rangle$$

$$\Rightarrow \quad H|\psi\rangle = \sum_n C_n H |\varphi_n\rangle$$

$$E|\psi\rangle = \sum_n C_n E |\varphi_n\rangle$$

左乘 $\langle \varphi_m|$

$$\Rightarrow \quad \sum_n \langle \varphi_m | H | \varphi_n \rangle \cdot C_n = E C_m$$

$$\sum_n H_{mn} C_n = E C_m$$

能带的计算.

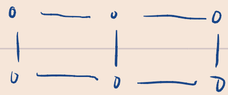
从一个简单的例子.

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + V\cos(x)\right]\psi(x) = E\psi(x)$$

Mathieu 方程. "Equation world"

作业.

计算 2D, 3D 晶体的 Bloch 能带, 求出费米面.



$$V(\vec{r}) = \sum_n \frac{e^2}{4\pi\varepsilon|\vec{r} - \vec{R}_n|}$$

一个猜测

$$\psi = \sum_{n=-\infty}^{\infty} C_n e^{i(k+n)x} \Rightarrow \sum_n \frac{(k+n)^2}{2} C_n e^{i(k+n)x} + \sum_n \frac{V}{2}(C_{n+1} + C_{n-1}) e^{i(k+n)x}$$

$$= E \sum_n C_n e^{i(k+n)x}$$

$$\Rightarrow \frac{(k+n)^2}{2} C_n + \frac{V}{2}(C_{n+1} + C_{n-1}) = E C_n \quad (*)$$ 要求 $\sum |C_n|^2$ 有限

$$\psi = \sum_n C_n e^{i(k+n)x} \Rightarrow \psi(x+R) = \sum_n C_n e^{i(k+n)x} e^{i(k+n)2\pi} \quad (R = 2\pi)$$

$$= \left[\sum_n C_n e^{ikx}\right] e^{ik2\pi}$$

$$= \psi(x) e^{ik2\pi}$$

而 $-\pi < k2\pi < \pi \Rightarrow |k| < \frac{1}{2}$

⇑ 第一布里渊区.

只需要考虑第一布里渊区中的波矢 k 即可。

Bloch 定理.

> 对于一个具有平移对称性的 Hamiltonian
>
> $$H(\vec{x}+\vec{R}) = H(\vec{x}), \text{ 而 } \vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 + \cdots$$
>
> 则满足方程 $H\psi(\vec{x}) = E\psi(\vec{x})$ 的解一定满足
>
> $$\psi_k(\vec{x}+\vec{R}) = \psi_k(\vec{x}) e^{i\vec{k}\cdot\vec{R}} \text{ 或 } \psi_k(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} u_k(\vec{x}), \quad u_k(\vec{x}+\vec{R}) = u_k(\vec{x})$$

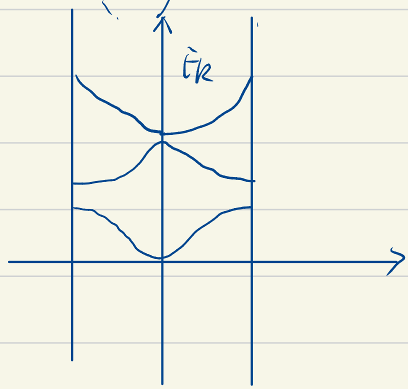
一个方便的选择是平面波展开

$$\psi(\vec{x}) = \sum_{\vec{G}_n} e^{i\vec{k}\cdot\vec{x}} C_n e^{i\vec{G}_n\cdot\vec{x}}$$

$\vec{G}_n$：倒格矢.

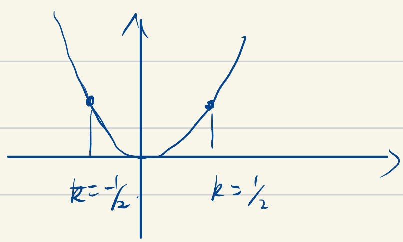
(*)式的矩阵形式

$$\begin{pmatrix} \ddots & & & & & 0 \\ & \frac{(k-1)^2}{2} & V/2 & & & \\ & V/2 & \frac{k^2}{2} & V/2 & & \\ & & V/2 & \frac{(k+1)^2}{2} & V/2 & \\ & & & V/2 & \frac{(k+2)^2}{2} & \\ 0 & & & & & \ddots \end{pmatrix}$$



为什么在布里渊区的边界存在能隙呢?

$V\cos(x)$ 联系着 k 和 $k\pm1$ 的态. 当 $k=\frac{1}{2}$ 时, 是一个共振散射.



黄昆.

简并的态的子空间上. $\begin{pmatrix} \frac{k^2}{2} & V/2 \\ V/2 & \frac{k^2}{2} \end{pmatrix} \Rightarrow \Delta = \pm\frac{V}{2}$ (能隙)