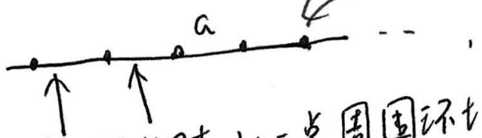
Lecture. 2.

1. Bloch 态与布里渊区.

填原子或原子团



在无限长时,此二点周围环境相同.

$$U(r)=U(r+a)$$

$$H=\frac{p^2}{2m}+U(r).$$

$$H\psi=E\psi.$$

(1) ψ 也是平移算符本征态.

定义: $T_a\psi(r)=\psi(r+a)$; $T_a^{-1}\psi(r)=\psi(r-a)$

$$T_aH\psi=T_aE\psi=ET_a\psi.$$

↳ $T_aHT_a^{-1}T_a\psi$.

$$T_aHT_a^{-1}\phi(r)=T_aH\phi(r-a)=T_a\left(\frac{p^2}{2m}+U(r)\right)\phi(r-a)$$

$$=\left(\frac{p^2}{2m}+U(r+a)\right)\phi(r)$$

$$=H\phi(r)$$

$$\phi(r)\to T_a\psi$$

$$\Rightarrow T_aH\psi=\underline{HT_a\psi=ET_a\psi}$$

晶格动量(crystal momentum

(2) Bloch 定理:

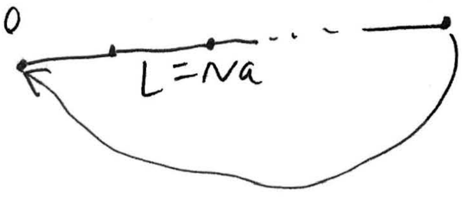
$$\psi(r)=e^{ik\cdot r}u_{nk}(r).$$

带指标

$u_{nk}(r)=u_{nk}(r+a)$,周期部分.

(1D). 证明: 施加周期边条件.

$$\psi|_{r=0}=\psi|_{r=L}.$$



$\psi = \sum_k C_k e^{ik\cdot r} \to$ 具有所需周期性.

$k = \frac{2\pi}{L} m, \; m = 0, \pm 1, \pm 2, \cdots$

$H\psi = E\psi$

$\Rightarrow \quad \sum_k C_k \left(\frac{p^2}{2m} + U(r) \right) e^{ikr} = E \sum_k C_k e^{ikr}$

$\frac{1}{L} \int dr \, e^{-ik'\cdot r}$

$C_k \frac{\hbar^2 k^2}{2m} \delta_{kk'} + \sum_k U(k-k') C_k = E C_{k'}$.

$U(k-k') = \frac{1}{L} \int d^d r \, e^{i(k-k')\cdot r} \, U(r)$

$\because U(r) = U(r+a)$.

$U(r)$ 的 Fourier 分量 为 $U(r) = \sum_G e^{iG\cdot r} u_G$.

$G = \frac{2\pi}{a} \cdot n, \; n = 0, \pm 1, \cdots$.

$\Rightarrow U(k-k') = \sum_G u_G \, \delta_{k-k', G}$.

$\frac{\hbar^2 k'^2}{2m} C_{k'} + \sum_G u_G C_{k'+G} = E C_{k'}$

↓ 矩阵形式

$$\begin{pmatrix} (\quad) & & \\ & (\quad) & \\ & & (\quad) \end{pmatrix} \begin{pmatrix} C_{k_1+\frac{2\pi}{a}0} \\ C_{k_1+\frac{2\pi}{a}1} \\ \vdots \\ \hline \vdots \\ \hline \vdots \end{pmatrix}$$

$k_1 \in \frac{2\pi}{Na}\cdot m,\ m=0,1,\cdots,N-1.$

每个小块:

$$\begin{pmatrix} \quad & \quad \\ \quad & \quad \end{pmatrix}\begin{pmatrix} C_{k_1+\frac{2\pi}{a}0} \\ C_{k_1+\frac{2\pi}{a}} \\ C_{k_1+\frac{2\pi}{a}(-1)} \\ \vdots \end{pmatrix}$$

k_1 值固定而 $G=\frac{2\pi}{a}\cdot n$, n 值可变.

总体本征值 = 小块本征值的集合(并集).

将小块本征值从小到大排列,每个本征值将有两个指标:

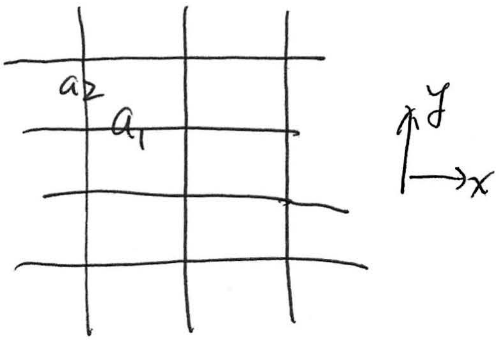
(1) k_1 (2). 用于标记小块本征值的 m'.

$E = E_{m'k}$ → 晶格动量.

带指标

$L \to +\infty$, $k \in [0, \frac{2\pi}{a})$. 布里渊区.

推广至二维正方晶格:



$k_x \in [0, \frac{2\pi}{a_1})$, $k_y \in [0, \frac{2\pi}{a_2})$.

其它情况请参考任一固体物理教材.

(3) 布里渊区周期性.

1维:

$k=0$, $k=\frac{2\pi}{a}$ 或者 k 与 $k+G$ ~~...~~ 代表同一本征态

$$T_a \psi_{m,k}(r) = T_a e^{ikr} u_{m,k}(r)$$
$$= e^{ikr} e^{ika} u_{m,k}(r+a)$$
$$= e^{ika} \psi_{m,k}(r).$$

$G\cdot a = 2\pi\cdot n.$

$$T_a \psi_{m,k+G}(r) = e^{ikr} e^{ika} e^{iGr} e^{iG\cdot a} u_{m,k+G}(r)$$
$$= e^{ika} e^{i(k+G)r} u_{m,k+G}(r)$$
$$= e^{ika} \psi_{m,k+G}(r)$$

$\psi_{m,k}$ 与 $\psi_{m,k+G}$ 有同一本征值.

故为同一本征态.

2. 规范选择.

(1) $H \psi_{m,k}(r) = E \psi_{m,k}(r)$ ← 去规范变换.

$\psi_{m,k}(r) \rightarrow e^{i\varphi(k)} \psi_{m,k}(r)$. 也均满足.

或 $u_{m,k}(r) \rightarrow e^{i\varphi(k)} u_{m,k}(r)$ 也均满足.

固体中电子的贝利相 → A_R, 贝利联络.

$$\phi_B = \int dR \langle \phi(R) | i\partial_R | \phi(R) \rangle$$

$R \rightarrow k$, $|\phi(R)\rangle \rightarrow |u_{m,k}\rangle$.

$$\Rightarrow A_k = \langle u_{m,k} | i\partial_k | u_{m,k} \rangle.$$

$$|u_{mk}\rangle \to e^{i\varphi(k)}|u_{mk}\rangle$$

$$A_k \to \langle u_{mk}|e^{-i\varphi(k)}\, i\partial_k\left(e^{i\varphi(k)}|u_{mk}\rangle\right)$$

$$= \langle u_{mk}|e^{-i\varphi(k)}\left(i\partial_k e^{i\varphi(k)}\right)|u_{mk}\rangle$$

$$+ \langle u_{mk}|e^{-i\varphi(k)}\, e^{i\varphi(k)}\, i\partial_k|u_{mk}\rangle$$

$$= A_k - \partial_k\varphi(k).$$

A_k 与规范有关.

(2) 贝利曲率（二维或三维）

$$\phi_B = \oint A_k\cdot dk$$

$$= \iint \nabla\times A_k\cdot ds. \quad \leftarrow \text{Stokes 定理.}$$

$$\Omega = \nabla\times A_k$$

规范无关:

$$|u_{mk}\rangle \to e^{i\varphi(k)}|u_{mk}\rangle$$

$$A_k \to A_k - \nabla\varphi(k)$$

$$\Omega \to \nabla\times A_k - \nabla\times\nabla\varphi(k)$$

$$= \nabla\times A_k$$

$$= \Omega$$

3) 计算 Ω

$$H\psi = E\psi$$

$$H e^{ikr}|u_{mk}\rangle = E e^{ikr}|u_{mk}\rangle$$

$$e^{-ikr} H e^{ikr}|u_{mk}\rangle = E_{mk}|u_{mk}\rangle$$

定义: $H_k = e^{-ikr} H e^{ikr}$

$$= e^{-ikr}\frac{p^2}{2m}e^{ikr} + U(r)$$

可证. $= \frac{(p+\hbar k)^2}{2m} + U(r)$

$$H_k|u_{mk}\rangle = E_{mk}|u_{mk}\rangle$$

$|u_{mk}\rangle$ 为 H_k 本征态.

单位分解 $\hat{I} = \sum_{m'} |u_{m'k}\rangle\langle u_{m'k}|$, 完备性.

k值固定

缩写 $\partial_\ell = \partial_{k_\ell}$.

$$\partial_\ell(H_k|u_{m'k}\rangle) = \partial_\ell(E_{m'k}|u_{m'k}\rangle)$$

$$(\partial_\ell H_k)|u_{m'k}\rangle + H_k\partial_\ell|u_{m'k}\rangle = (\partial_\ell E_{m'k})|u_{m'k}\rangle + E_{m'k}\partial_\ell|u_{m'k}\rangle$$

$\langle u_{mk}|$ $\langle u_{mk}|$

并且 $m \neq m'$.

$$\langle u_{mk}|\partial_\ell H_k|u_{m'k}\rangle + \underbrace{\langle u_{mk}|H_k}_{\langle u_{mk}|E_{mk}}\partial_\ell|u_{m'k}\rangle = 0 + E_{m'k}\langle u_{mk}|\partial_\ell|u_{m'k}\rangle$$

$$(E_{m'k}-E_{mk})\,\langle u_{m'k}|\partial_l|u_{mk}\rangle = \langle u_{mk}|\partial_l H_k|u_{m'k}\rangle$$

$$\Rightarrow \langle u_{m'k}|\partial_l|u_{mk}\rangle = \frac{\langle u_{mk}|\partial_l H_k|u_{m'k}\rangle}{E_{m'k}-E_{mk}.} \qquad (*1)$$

同时

$$\langle u_{m'k}|u_{mk}\rangle = \delta_{mm'}. \quad (由正交归一).$$

$$\partial_l(\langle u_{m'k}|u_{mk}\rangle) = 0$$

$$\Rightarrow \langle \partial_l u_{m'k}|u_{mk}\rangle = -\langle u_{m'k}|\partial_l|u_{mk}\rangle. \qquad (*2)$$

当$m=m'$时.

$$\langle \partial_l u_{mk}|u_{mk}\rangle = -\langle u_{mk}|\partial_l|u_{mk}\rangle$$

$\Rightarrow \langle u_{mk}|\partial_l|u_{mk}\rangle$ 为纯虚.

故, $A_k = \langle u_{mk}|i\partial|u_{mk}\rangle$ 为实数.

全反对称张量. $\varepsilon_{123}=1$, $\varepsilon_{213}=-1$, . . .

$$\Omega_i = \varepsilon_{ijl}\,\partial_j (A_k)_l \quad (求和规则: 重复指标代表求和).$$

$$= \varepsilon_{ijl}\,\partial_j\langle u_{m'k}|i\partial_l|u_{m'k}\rangle$$

$$= \varepsilon_{ijl}\, i\langle \partial_j u_{m'k}|\partial_l|u_{m'k}\rangle$$

$i^2=-1.$

插入 $I = \sum_b |u_{bk}\rangle\langle u_{bk}|$

$$= i\,\varepsilon_{ijl}\sum_b \langle \partial_j u_{m'k}|u_{bk}\rangle\langle u_{bk}|\partial_l|u_{m'k}\rangle.$$

$(*2)$

$$= -i\,\varepsilon_{ijl}\sum_b \langle u_{m'k}|\partial_j|u_{bk}\rangle\langle u_{bk}|\partial_l|u_{m'k}\rangle.$$

$\varepsilon_{ijl} = \begin{cases} 0, & 若有二指标相同. \\ \pm 1, & 按照排列, \end{cases}$

$\varepsilon_{123}=1$,

相邻位二指标交换则改符号,

比如$\varepsilon_{213}=-1$,

$\varepsilon_{132}=-1$,

. . .

$$= \begin{cases} b=m' \text{时}. \ \Omega_i \propto \langle u_{bk} | \partial_j | u_{bk} \rangle \times \langle u_{bk} | \partial | u_{bk} \rangle = 0. \\ \\ \text{故 } b \neq m'. \end{cases}$$

$$\Omega_i = -i\, \varepsilon_{ijl} \sum_{b \neq m'} \langle u_{m'k} | \partial_j | u_{bk} \rangle \langle u_{bk} | \partial_l | u_{m'k} \rangle.$$

$\Downarrow (*1)$. $(*1)$

$$= -i\, \varepsilon_{ijl} \sum_{b \neq m'} \frac{\langle u_{m'k} | \partial_j H_k | u_{bk} \rangle \langle u_{bk} | \partial_l H_k | u_{m'k} \rangle}{(E_{bk} - E_{m'k})(E_{m'k} - E_{bk})}$$

$$= i\, \varepsilon_{ijl} \sum_{b \neq m'} \frac{\langle u_{m'k} | \partial_j H_k | u_{bk} \rangle \langle u_{bk} | \partial_l H_k | u_{m'k} \rangle}{(E_{bk} - E_{m'k})^2}.$$

$\uparrow$

常用计算公式.

注意 $H_k = e^{-ikr} H e^{ikr}$.