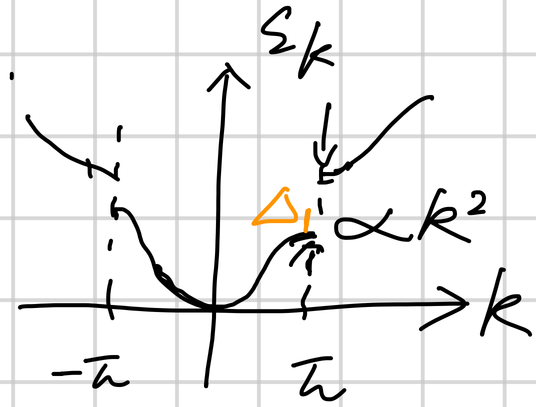
能带理论(上) 紧束缚近似、瓦尼尔函数

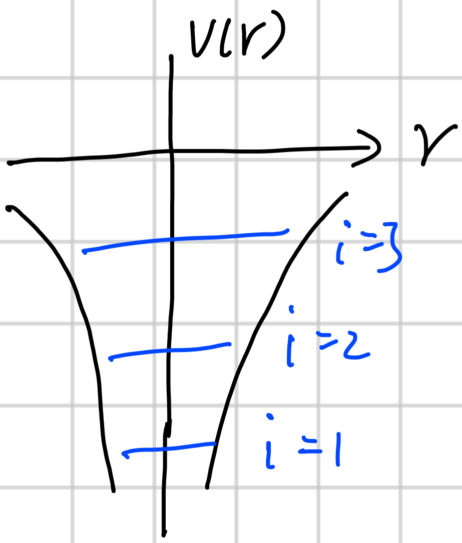


(1) 近自由电子近似：自由电子气(出发点)

(2) 局域电子出发 ⇒ 紧束缚近似
(tight-binding approximation)

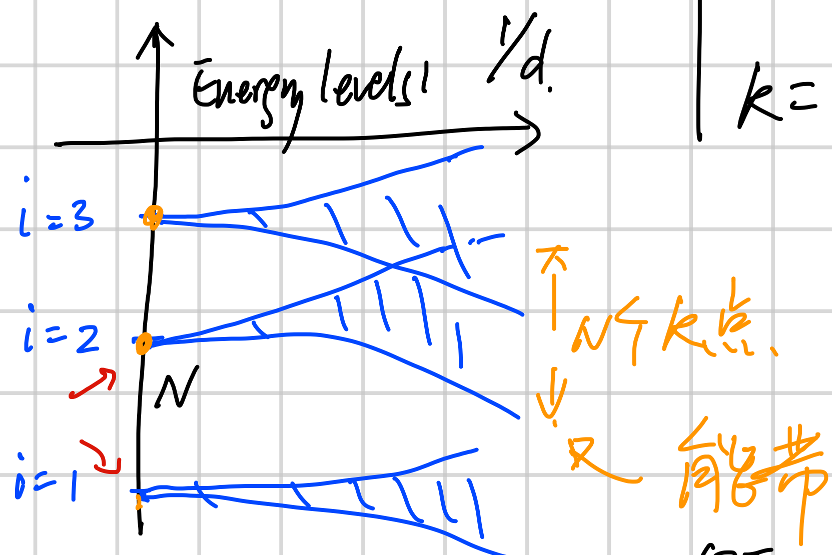
$\Delta_n = 2|V_n|$

$k = \frac{2\pi}{a} \cdot n$



原子极限

⇒



N个原子彼此靠近

$\left(\frac{2\pi}{Na} \cdot n\right)$ $n=1:1:N$

(3) TBA：适用于3d电子(铁、钴、镍) 关联强、磁性

(4) 原子轨道的线性叠加

(i) 第m个原子，$\vec{R}_m$，定义单原子轨道 $\varphi_i(\vec{r}-\vec{R}_m)$

$$\Big[\underbrace{-\frac{\hbar^2}{2m}\nabla^2 + V_{at}(\vec{r}-\vec{R}_m)}_{\text{原子势场}}\Big]\underbrace{\varphi_i(\vec{r}-\vec{R}_m)}_{\text{原子轨道}} = \underbrace{\varepsilon_i}_{\text{能量}}\varphi_i(\vec{r}-\vec{R}_m)$$

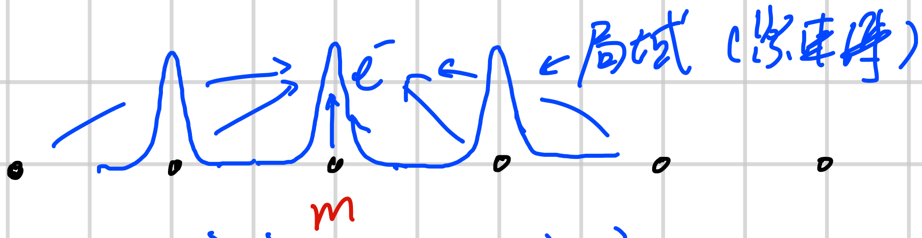
N个原子：N个完全简并的 $\{\varphi_i(\vec{r}-\vec{R}_m)\}$，$m=1,2,\cdots,N$.
(已归一)

(ii) 晶体轨道的紧束缚近似(TBA)

↳ N个原子轨道的线性叠加

$$\psi_{\vec{k}}^{(i)}(\vec{r}) = \sum_{m=1}^{N} \varphi_i(\vec{r}-\vec{R}_m) \cdot e^{i\vec{k}\cdot\vec{R}_m} \cdot \frac{1}{\sqrt{N}}$$ 布洛赫波

$$\left\{ \int \overline{\varphi_i}(\vec{r}-\vec{R}_m) \cdot \varphi_i(\vec{r}-\vec{R}_n)\, d\vec{r} = \delta_{m,n} \right.$$ 正交归一基



(近似正交归一)

$$\langle \varphi_i(\vec r-\vec R_n) | \varphi_i(\vec r-\vec R_m)\rangle \approx 0$$

U(1)

Proof: 布洛赫波 $\hat T_R \psi_k(r) = e^{i\vec k\cdot\vec R}\psi_k(\vec r)$

$$\psi_k^{(i)}(\vec r+\vec R_n) = \sum_m \varphi_i(\vec r+\vec R_n-\vec R_m)\, e^{i\vec k\cdot\vec R_m}\cdot\frac{1}{\sqrt N}$$

$(\vec R_{\tilde m} = \vec R_m - \vec R_n)$

$$= \sum_{\tilde m} \varphi_i(\vec r-\vec R_{\tilde m})\, e^{i\vec k\cdot\vec R_{\tilde m}} e^{i\vec k\cdot\vec R_n}\cdot\frac{1}{\sqrt N}$$

$$= e^{i\vec k\cdot\vec R_n}\sum_{\tilde m} \varphi_i(\vec r-\vec R_{\tilde m})\, e^{i\vec k\cdot\vec R_{\tilde m}}\cdot\frac{1}{\sqrt N}.$$

$$= e^{i\vec k\cdot\vec R_n}\cdot\psi_k^{(i)}(\vec r)$$

(iii) 能带形成

- 单电子 Schrödinger Eq. (晶格周期势中)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec r)\right]\psi(\vec r) = \varepsilon\psi(\vec r)$$

$$V(\vec r) = \sum_{m=1}^{N} V_{at}(\vec r-\vec R_m) \qquad (V(\vec r+\vec R_n) = V(\vec r))$$

$\Rightarrow$ $\Delta V = V(\vec r) - V_{at}(\vec r-\vec R_l)$ (l处的ΔV)

$$\Rightarrow \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{at}(\vec r-\vec R_m)+\Delta V\right]\psi(\vec r) = \varepsilon\psi(\vec r)$$

$$\psi_k(\vec r) = \sum_m e^{i\vec k\cdot\vec R_m}\varphi_i(\vec r-\vec R_m)\cdot\frac{1}{\sqrt N}$$

$$\sum_m \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{at}(\vec r-\vec R_m)+\Delta V\right]\varphi_i(\vec r-\vec R_m)\cdot e^{i\vec k\cdot\vec R_m}\cdot\frac{1}{\sqrt N} = \sum_m \varepsilon\varphi_i(\cdots)$$

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$$\sum_m \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{at}(\vec{r}-\vec{R}_m)\right]\left[\frac{1}{\sqrt{N}} e^{i\vec{k}\cdot\vec{R}_m}\varphi_i(\vec{r}-\vec{R}_m)\right]$$

$$+ \sum_m (\Delta V - \varepsilon_k)\frac{1}{\sqrt{N}} e^{i\vec{k}\cdot\vec{R}_m}\varphi_i(\vec{r}-\vec{R}_m) = 0$$

左乘 $\overline{\varphi_i}(\vec{r})$

$$\sum_m \frac{1}{\sqrt{N}} e^{i\vec{k}\cdot\vec{R}_m}\varepsilon_i \underbrace{\langle\varphi_i(\vec{r})|\varphi_i(\vec{r}-\vec{R}_m)\rangle}_{=\delta_{m,0}\ (\mathrm{TBA})}$$

$$+ \sum_m \langle\varphi_i(\vec{r})|\Delta V - \varepsilon|\varphi_i(\vec{r}-\vec{R}_m)\rangle \frac{1}{\sqrt{N}} e^{i\vec{k}\cdot\vec{R}_m} = 0$$

$$\Rightarrow \frac{1}{\cancel{\sqrt{N}}}(\varepsilon_i - \varepsilon_k) + \sum_m \langle\varphi_i(\vec{r})|\Delta V|\varphi_i(\vec{r}-\vec{R}_m)\rangle \frac{1}{\cancel{\sqrt{N}}} e^{i\vec{k}\cdot\vec{R}_m} = 0$$

② 引入
$$\begin{cases} J_0 = -\langle\varphi_i(\vec{r})|\Delta V_0|\varphi_i(\vec{r})\rangle \\ J_m = -\langle\varphi_i(\vec{r})|\Delta V_m|\varphi_i(\vec{r}-\vec{R}_m)\rangle \neq 0 \\ \quad = -\int \varphi_i^*(\vec{r})\,\Delta V(\vec{r})\,\varphi_i(\vec{r}-\vec{R}_m)\,dr \end{cases}$$

③ 能带
$$\left(\varepsilon_k = \varepsilon_i - J_0 - \sum_m{}' J_m e^{i\vec{k}\cdot\vec{R}_m}\right) \quad \#$$

④ 讨论: a. 求解本质? b. J_0, J_m 代表什么? → 交叠积分. 势 → 跳跃

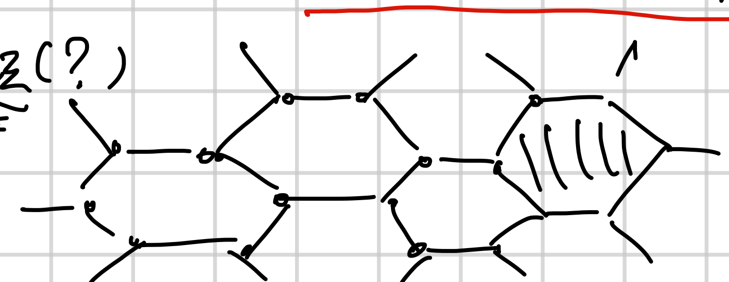
$\langle\varphi_i|H|\psi_k\rangle = \varepsilon_k\langle\varphi_i|\psi_k\rangle$

$\forall i$

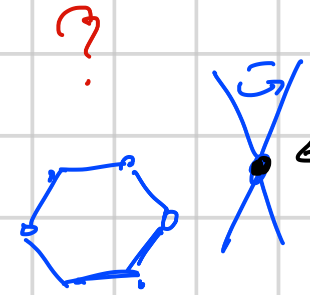
$|\psi_k\rangle$ 为 H 的"本征态". 傅利叶变换对角化哈密顿量.

$$\ulcorner H\psi_k(\vec{r}) = \varepsilon_k\psi_k(\vec{r}) \urcorner \ ?$$

(2) 问题(?)



$\Leftarrow$

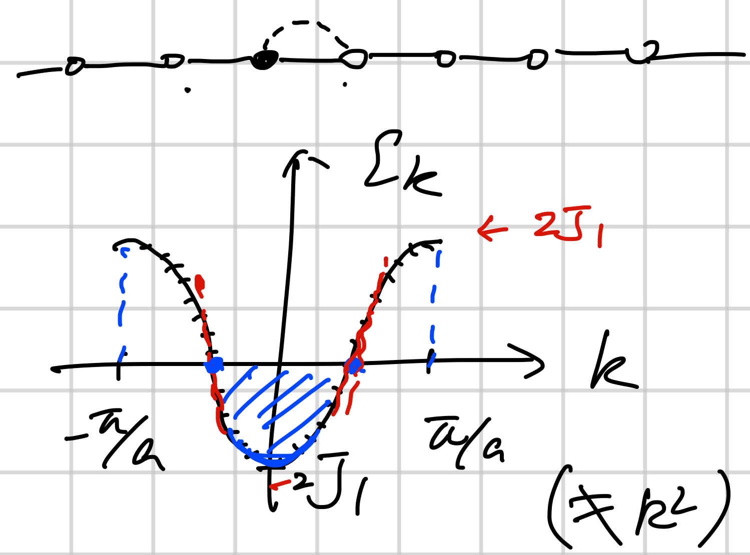


← 态密度 → 想办法.

Dirac fermion

⑩ 应用 ($J_m \neq 0$ if $m = N.N.$)

一维晶格（半满）



1D: $\varepsilon = \varepsilon_i - J_0 - \sum_m J_m e^{i\vec{k}\cdot\vec{R}_m}$

$$= (\varepsilon_i - J_0) - J_1 (e^{ik\cdot a} + e^{-ika})$$

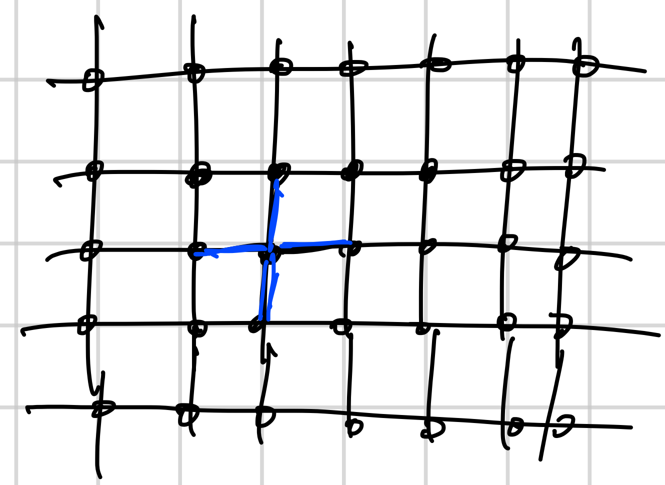
$$= (\underbrace{\varepsilon_i - J_0}_{0}) - J_1 \cdot 2\cos(ka)$$

$(k_l = \frac{2\pi}{Na}\cdot l)$

2D: $\varepsilon = \varepsilon_i - J_0 - \sum_m J_m e^{i\vec{k}\cdot\vec{R}_m}$

$$= \underbrace{\varepsilon_i - J_0}_{0} - \Sigma (e^{ik_xa} + e^{-ik_xa}) J_1 + (e^{ik_ya} + e^{-ik_ya}) J_1$$

$$= [-2\cos(k_xa) - 2\cos(k_ya)] J_1$$



[作业: $\varepsilon_k \sim (k_x, k_y)$ surface plot.
(1) ↳ 分析态密度. $\rho(\varepsilon)$ → von Hove singularity]
→ 热力学.

⑪ 瓦尼尔函数 ⇒ $\varphi_i(\vec{r} - \vec{R}_m)$ 原型.

$$\psi_{nk}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_m a_n(\vec{r} - \vec{R}_m) e^{i\vec{k}\cdot\vec{R}_m}$$

[作业2] 正交归一基矢 (利用Bloch波的正交归一性)

瓦尼尔函数局域. $a_n(\vec{r} - \vec{R}_m) = \frac{1}{\sqrt{N}} \sum_k e^{-i\vec{k}\cdot\vec{R}_m} \psi_{nk}(\vec{r})$

↑ 仅仅依赖于 $(\vec{r} - \vec{R}_m)$