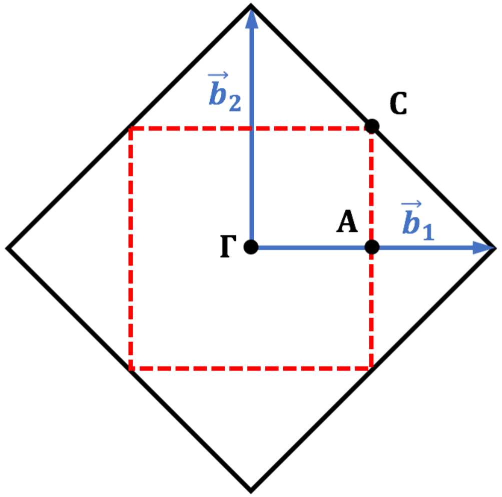
Chapter 4.1: 课后作业

1. 对于边长为a的二维正方晶格，证明：

自由电子在第一布里渊区边界（如右图所示）C点处的动能是A点处动能的2倍。



2. 对于一维近自由电子模型，$k = \pm\frac{2\pi}{a}$状态简并微扰的能量为E_+和E_-，求出对应的波函数ψ_+和ψ_-，并说明它们都代表驻波。（假设$V_n = V_n^*$）

Chapter 4.1: 课后作业-答案

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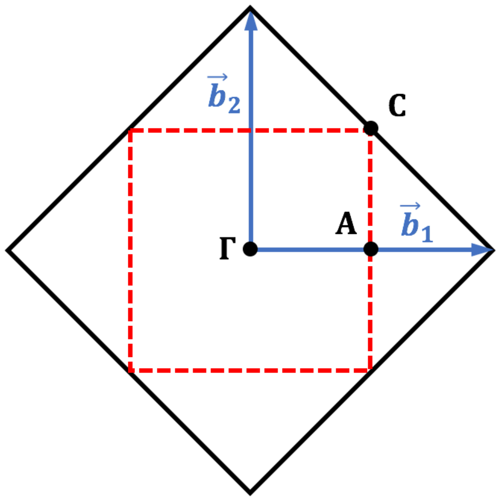


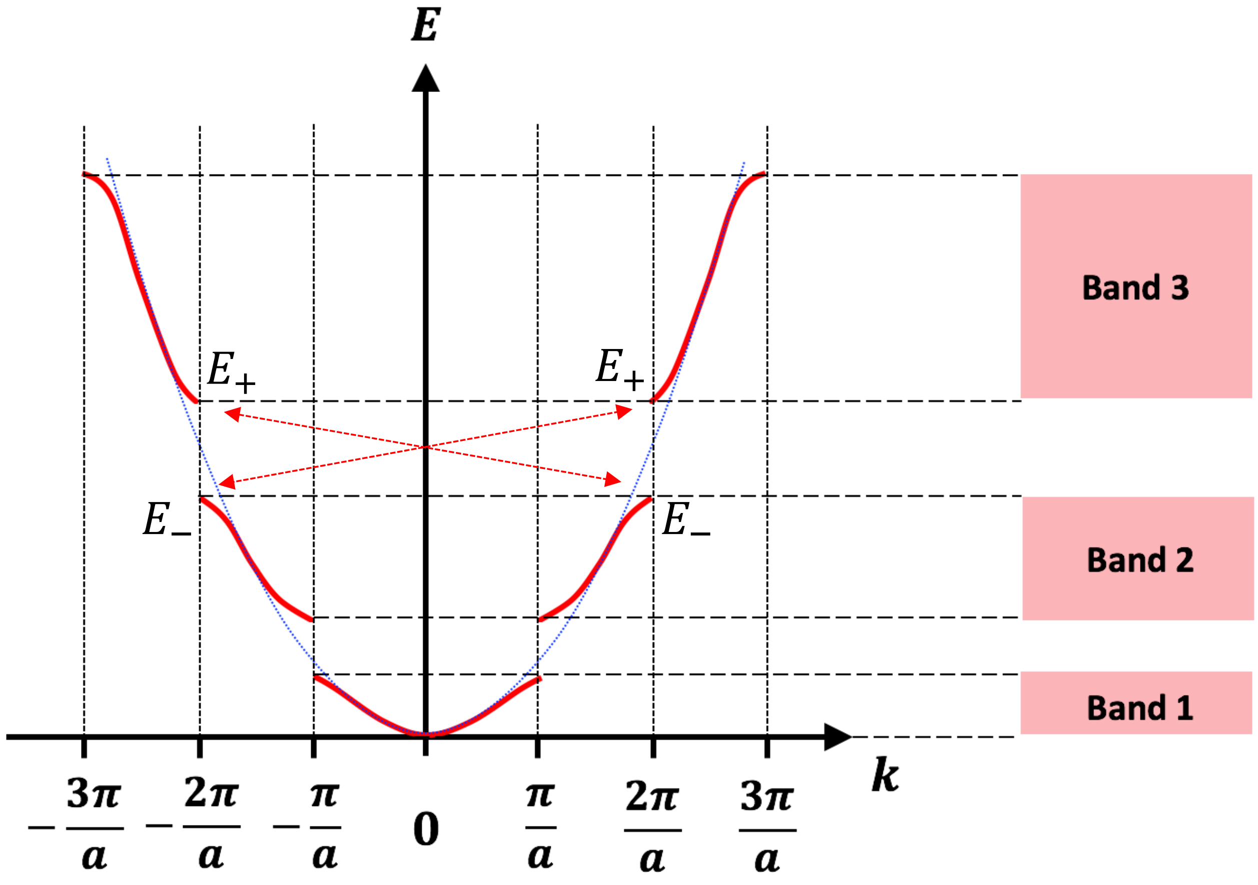
$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 (k_x^2 + k_y^2)}{2m}$$

$$A(\frac{\pi}{a}, 0) \longrightarrow E(A) = \frac{\hbar^2 \pi^2}{2ma^2}$$

$$C(\frac{\pi}{a}, \frac{\pi}{a}) \longrightarrow E(C) = \frac{\hbar^2 \pi^2}{ma^2}$$

$$\longrightarrow E(C) = 2E(A)$$

2. 对于一维近自由电子模型，$k=\pm\frac{2\pi}{a}$状态简并微扰的能量为E_+和E_-，求出对应的波函数ψ_+和ψ_-，并说明它们都代表驻波。（假设$V_n=V_n^*$）



2. 对于一维近自由电子模型，$k=\pm\frac{2\pi}{a}$ 状态简并微扰的能量为E_+和E_-，求出对应的波函数ψ_+和ψ_-，并说明它们都代表驻波。（假设$V_n=V_n^*$）

$$\hat{H}_0|\varphi_k\rangle=\varepsilon_k|\varphi_k\rangle \qquad \hat{H}_0|\varphi_{k'}\rangle=\varepsilon_{k'}|\varphi_{k'}\rangle$$

$$|\psi\rangle=\alpha|\varphi_k\rangle+\beta|\varphi_{k'}\rangle$$

$$|\varphi_k\rangle=\frac{1}{\sqrt{Na}}\mathrm{e}^{i\frac{2\pi}{a}x} \qquad |\varphi_{k'}\rangle=\frac{1}{\sqrt{Na}}\mathrm{e}^{-i\frac{2\pi}{a}x}$$

把$|\psi\rangle$带入$(\hat{H}_0+\hat{H}')|\psi\rangle=E|\psi\rangle$: $\longrightarrow$ $\begin{cases}(\varepsilon_k-E)\alpha+V_2^*\beta=0 & (1)\\ V_2\alpha+(\varepsilon_{k'}-E)\beta=0 & (2)\end{cases}$

$$V_2=\langle\varphi_{k'}|\hat{H}'|\varphi_k\rangle \qquad V_2^*=\langle\varphi_k|\hat{H}'|\varphi_{k'}\rangle$$

$$\longrightarrow \begin{vmatrix}\varepsilon_k-E & V_2^*\\ V_2 & \varepsilon_{k'}-E\end{vmatrix}=0 \longrightarrow \begin{cases}E_+=\varepsilon_k+|V_2|\\ E_-=\varepsilon_k-|V_2|\end{cases}$$

Chapter 4.1: 课后作业-答案

把E_+E_-带回(1)(2)并利用 $\alpha^2+\beta^2=1$ $\longrightarrow$ $\begin{cases} \alpha=\beta=\dfrac{1}{\sqrt{2}} \\ \alpha=-\beta=\dfrac{1}{\sqrt{2}} \end{cases}$

$$\longrightarrow \begin{cases} |\psi_+\rangle=\dfrac{1}{\sqrt{2}}(|\varphi_k\rangle+|\varphi_{k'}\rangle)=\dfrac{2}{\sqrt{2Na}}\cos\left(\dfrac{2\pi}{a}x\right) \\ |\psi_-\rangle=\dfrac{1}{\sqrt{2}}(|\varphi_k\rangle-|\varphi_{k'}\rangle)=\dfrac{2i}{\sqrt{2Na}}\sin\left(\dfrac{2\pi}{a}x\right) \end{cases}$$

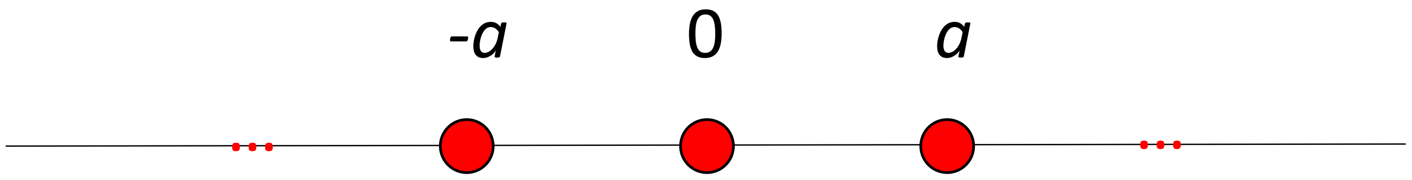
Chapter 4.2: 课后作业

考虑一维单原子链（原子间距为a, 链长为Na）, 对于原子的s能级, 利用紧束缚模型, 求:

1. 原子链能带的色散关系$E(k)$;
2. 能带的态密度$g(E)$;
3. 能带的宽度.

Chapter 4.2: 课后作业-答案

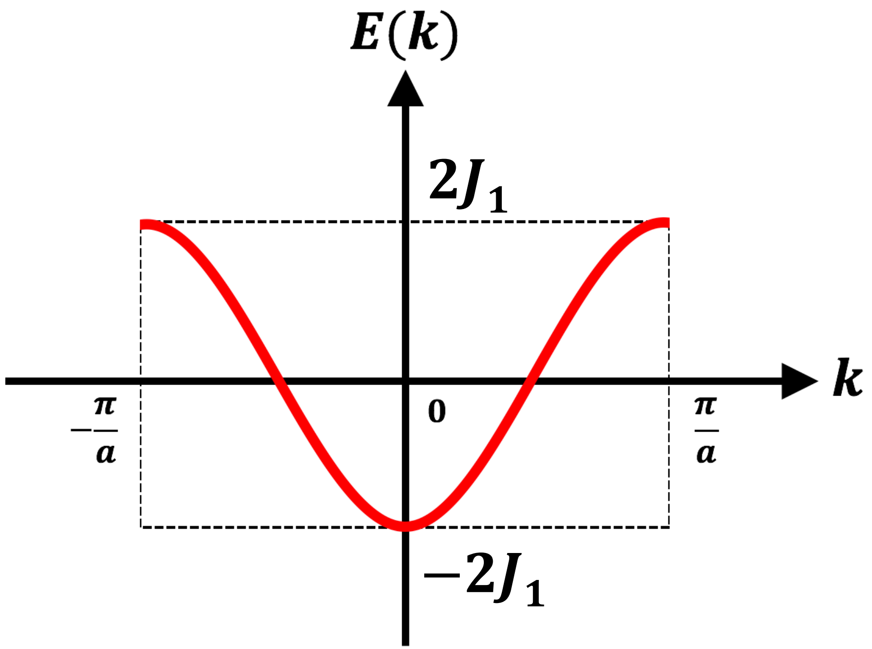
1. $\boldsymbol{E_k = \varepsilon - J_0 - \sum_{j=\mathrm{nbs}} J_1(\vec{a}_j)e^{-i\vec{k}\cdot\vec{a}_j} = \varepsilon - J_0 - J_1\left(e^{-ika} + e^{ika}\right) = \varepsilon - J_0 - 2J_1\cos(ka)}$



Chapter 4.2: 课后作业-答案

2. 波矢密度: $\frac{\mathrm{d}n}{\mathrm{d}k} = \frac{Na}{2\pi}$ $\qquad$ $\frac{\mathrm{d}E}{\mathrm{d}k} = 2aJ_1\sin(ka)$

→ (不计自旋) $g(E) = \frac{\mathrm{d}n}{\mathrm{d}E} = 2\times\frac{dn}{dk}\frac{\mathrm{d}k}{\mathrm{d}E} = 2\times\frac{dn}{dk}\left(\frac{\mathrm{d}E}{\mathrm{d}k}\right)^{-1} = \frac{N}{2\pi J_1\sin(ka)} = \frac{N}{\pi\sqrt{4J_1^2-(E_k-\varepsilon+J_0)^2}}$



3. 带宽: $E_{\pi/a} - E_0 = 4J_1$

Chapter 4.4: 课后作业

考虑原胞数为N的一维晶格, 电子能带为

$$E(k) = \frac{\hbar^2}{ma^2}\left[\frac{7}{8} - \cos(ka) + \frac{1}{8}\cos(2ka)\right]$$

求:

1. 能带宽度;
2. 电子在波矢k状态时的速度;
3. 电子在带底和带顶时的有效质量。

Chapter 4.4: 课后作业-答案

1. 先求能量极值点位置: $\dfrac{\mathrm{d}E}{\mathrm{d}k}=0$ $\longrightarrow$ $\sin(ka)=0$ $\longrightarrow$ $ka=0,\dfrac{\pi}{a}(\text{或}-\dfrac{\pi}{a})$

带宽: $\boldsymbol{E_{\pi/a}-E_0=\dfrac{2\hbar^2}{ma^2}}$

2. $$v_k=\frac{1}{\hbar}\frac{\mathrm{d}E}{\mathrm{d}k}=\frac{\hbar}{ma}\left[\sin(ka)-\frac{1}{4}\sin(2ka)\right]$$

3. $$m^*=\hbar^2\left(\frac{\mathrm{d}^2E}{\mathrm{d}k^2}\right)^{-1}$$ $\longrightarrow$

带顶$(k=\frac{\pi}{a})$: $m^*=-\frac{2}{3}m$

带底$(k=0)$: $m^*=2m$