固体物理第十次作业

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1. **(15.1) ‡ Nearly Free Electron Model**

Consider an electron in a weak periodic potential in one dimension $V(x) = V(x+a)$. Write the periodic potential as

$$V(x) = \sum_G e^{iGx} V_G$$

where the sum is over the reciprocal lattice $G = 2\pi n/a$, and $V_G^* = V_{-G}$ assures that the potential $V(x)$ is real.

(a) Explain why for k near to a Brillouin zone boundary (such as k near π/a) the electron wave function should be taken to be

$$\psi = Ae^{ikx} + Be^{i(k+G)x}$$

where G is a reciprocal lattice vector such that $|k|$ is close to $|k+G|$.

(b) For an electron of mass m with k exactly at a zone boundary, use the above form of the wave-function to show that the eigenenergies at this wave vector are

$$E = \frac{\hbar^2 k^2}{2m} + V_0 \pm |V_G|$$

where G is chosen so $|k| = |k+G|$.

▷ Give a qualitative explanation of why these two states are separated in energy by $2|V_G|$.

▷ Give a sketch (don't do a full calculate) of the energy as a function of k in both the extended and the reduced zone schemes.

(c) *Now Consider k close to, but not exactly at, the zone boundary. Give an expression for the energy $E(k)$ correct to order $(\delta k)^2$ where δk is the wavecector difference from k to the zone boundary wavevector.

▷ Calculate the effective mass of an electron at this wavevector.

(a) 在布里渊区边界处，由于波矢 k 与波矢 $k+G$ 对应的能量十分接近，则需要利用兼并微扰理论求解，两个基矢分别为：$|k\rangle$ 与 $|k+G\rangle$，则 Hamiltonian 本征态可以写为：

$$|\psi\rangle = A\,|k\rangle + |k+G\rangle\,.$$

则坐标表象下波函数为：

$$\psi = \langle x|\psi\rangle = Ae^{ikx} + Be^{i(k+G)x}.$$

(b) ▷ 考虑电子波矢恰好在布里渊区边界处，则对应波矢 k 与波矢 $k+G$ 的电子能量相等，等于 $E_0 = \frac{\hbar^2 k^2}{2m} + V_0$。但是由于势场的微扰，兼并能级被打开，也就是说两个态的

能量出现差值 $2|V_G|$。

定量计算: 在两个态 $|k\rangle$ 与 $|k'\rangle = |k+G\rangle$ 基底下, Hamiltonian 可以写为:

$$H = \begin{pmatrix} \frac{\hbar^2(-\pi/a)^2}{2m} + V_0 & V_G^* \\ V_G & \frac{\hbar^2(\pi/a)^2}{2m} + V_0 \end{pmatrix}$$

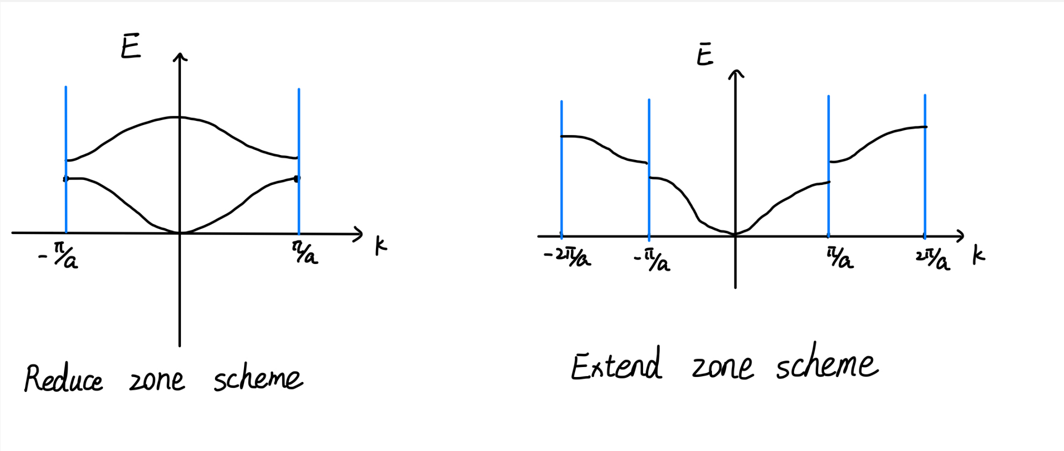
则 Hamiltonian 本征值满足:

$$\begin{vmatrix} \frac{\hbar^2(-\pi/a)^2}{2m} + V_0 - E & V_G^* \\ V_G & \frac{\hbar^2(\pi/a)^2}{2m} + V_0 - E \end{vmatrix} = 0.$$

则可以解得:

$$E = \frac{\hbar^2(\pi/a)^2}{2m} + V_0 \mp |V_G| = \frac{\hbar^2k^2}{2m} + V_0 \pm |V_G|.$$

▷ 色散关系如下图:



(c) 假设波矢为: $k = -\pi/a + \delta k$, 则两波矢 k 与 $k+G$ 为基底对应的 Hamiltonian 为:

$$H = \begin{pmatrix} \frac{\hbar^2}{2m}(-\pi/a + \delta k)^2 + V_0 & V_G^* \\ V_G & \frac{\hbar^2}{2m}(\pi/a + \delta k)^2 + V_0 \end{pmatrix}$$

则本征值 E 满足:

$$\begin{vmatrix} \frac{\hbar^2}{2m}((\pi/a)^2 + (\delta k)^2 - 2\pi(\delta k)/a) + V_0 - E & V_G^* \\ V_G & \frac{\hbar^2}{2m}((\pi/a)^2 + (\delta k)^2 + 2\pi(\delta k)/a) + V_0 - E \end{vmatrix} = 0$$

可以解得:

$$E = \frac{\hbar^2}{2m}((\pi/a)^2 + (\delta k)^2) + V_0 \pm \sqrt{|V_G|^2 + \frac{\pi^2\hbar^4(\delta k)^2}{m^2a^2}}.$$

当 $\delta k \to 0$ 时, 本征值近似得:

$$E = \frac{\pi^2\hbar^2}{2ma^2} + V_0 + \frac{\hbar^2(\delta k)^2}{2m} \pm |V_G| \left(1 + \frac{\pi^2\hbar^4(\delta k)^2}{2|V_G|^2m^2a^2}\right)$$

▷ 有效质量满足:

$$\frac{\hbar^2(\delta k)^2}{2m^*} = \frac{\hbar^2(\delta k)^2}{2m} \pm \frac{\pi^2\hbar^4(\delta k)^2}{2|V_G|m^2a^2}.$$

则可以解得：

$$m^* = \frac{|V_G|m^2a^2}{m|V_G|a^2 \pm \pi^2\hbar^2}$$

2. **(15.3) Tight Binding Bloch Wavefunctions**

Analogous to the wavefunction introduced in Chapter 11, consider a tight-binding wave ansatz of the form

$$|\psi\rangle = \sum_R e^{i\mathbf{k}\cdot\mathbf{R}}\,|\mathbf{R}\rangle$$

where the sun is over the points $\mathbf{R}$ of a lattice, and $|\mathbf{R}\rangle$ is the ground-state wavefunction of an electron bound to a nucleus on site $\mathbf{R}$. In real space this ansatz can be expressed as

$$\psi(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}\varphi(\mathbf{r}-\mathbf{R}).$$

Show that this wavefunction is of the form required by Bloch's theorem (i.e., show it is a modified plane wave).

该波函数可以写为：

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\sum_{\vec{R}} e^{-i\vec{k}\cdot(\vec{r}-\vec{R})}\varphi(\vec{r}-\vec{R}) = e^{i\vec{k}\cdot\vec{r}}u_{\vec{k}}(\vec{r}).$$

接下来只需验证 $u_{\vec{k}}(\vec{r})$ 的周期性。

$$\begin{aligned}
u_{\vec{k}}(\vec{r}+\vec{a}) =& \sum_{\vec{R}} e^{-i\vec{k}\cdot(\vec{r}+\vec{a}-\vec{R})}\varphi(\vec{r}+\vec{a}-\vec{R}) \\
=& \sum_{\vec{R}'=\vec{R}-\vec{a}} e^{-i\vec{k}\cdot(\vec{r}-\vec{R}')}\varphi(\vec{r}-\vec{R}') \\
=& \sum_{\vec{R}} e^{-i\vec{k}\cdot(\vec{r}-\vec{R})}\varphi(\vec{r}-\vec{R}) \\
=& u_{\vec{k}}(\vec{r}).
\end{aligned}$$

即这个波函数满足 Bloch 定理要求的形式。

3. **(15.4) *Nearly Free Electrons in Two Dimensions**

Consider the nearly free electron model for a square lattice with lattice constant a. Suppose the periodic potential is given by

$$V(x,y) = 2V_{10}[\cos(2\pi x/a) + \cos(2\pi y/a)] + 4V_{11}[\cos(2\pi x/a)\cos(2\pi y/a)]$$

(a) Use the nearly free electron model to find the energies of states at wavevector $\mathbf{G} = (\pi/a, 0)$.
(b) Calculate the energies of the states at wavevector $\mathbf{G} = (\pi/a, \pi/a)$. (Hint: You should write down a 4 by 4 secular determinant, which looks difficult, but actually factors nicely. Make use of adding together rows or columns of the determinant before trying to evaluate it!)

(a) 注意到倒格矢为 $\mathbf{G} = (\pi/a, 0)$ 的波矢与 $(0, \pm\pi/a)$ 的波矢不满足动量守恒的 Laue 公式，所以只需考虑一维情况，位于 $(\pm\pi/a, 0)$ 处的两个态能量简并，需利用简并微扰理论计算，则能量为：

$$E = \frac{\hbar^2(\pi/a)^2}{2m} \pm |V_G|.$$

其中，$|V_G|$ 为：

$$|V_G| = \left| \frac{1}{a^2} \int_{-a/2}^{a/2} \int_{-a/2}^{a/2} e^{i\pi x/a} V(x,y) e^{i\pi x/a} \, dx \, dy \right| = |V_{10}|.$$

则能量为：

$$E = \frac{\hbar^2(\pi/a)^2}{2m} \pm |V_{10}|.$$

(b) 注意到倒格矢为 $\mathbf{G} = (\pi/a, \pi/a)$ 的波与 $(\pi/a, -\pi/a)$ 和 $(-\pi/a, \pm\pi/a)$ 能量简并，且满足动量守恒 $\vec{k}' - \vec{k} = \vec{G}$，则需要在四维基底 $(\pm\pi/a, \pm\pi/a)$ 上展开 Hamiltonian，可以计算：

$$\begin{aligned}
\langle(\pi/a, \pi/a)| \hat{H} |(\pi/a, \pi/a)\rangle &= \frac{\hbar^2 2(\pi/a)^2}{2m} = \epsilon_0 \\
\langle(\pi/a, \pi/a)| \hat{H} |(\pi/a, -\pi/a)\rangle &= V_{10} \\
\langle(\pi/a, \pi/a)| \hat{H} |(-\pi/a, \pi/a)\rangle &= V_{10} \\
\langle(\pi/a, \pi/a)| \hat{H} |(-\pi/a, -\pi/a)\rangle &= V_{11} \\
\langle(\pi/a, -\pi/a)| \hat{H} |(-\pi/a, \pi/a)\rangle &= V_{11} \\
\langle(\pi/a, -\pi/a)| \hat{H} |(-\pi/a, -\pi/a)\rangle &= V_{10} \\
\langle(-\pi/a, \pi/a)| \hat{H} |(-\pi/a, -\pi/a)\rangle &= V_{10}
\end{aligned}$$

则矩阵为：

$$H = \begin{pmatrix} \epsilon_0 & V_{10} & V_{10} & V_{11} \\ V_{10} & \epsilon_0 & V_{11} & V_{10} \\ V_{10} & V_{11} & \epsilon_0 & V_{10} \\ V_{11} & V_{10} & V_{10} & \epsilon_0 \end{pmatrix}.$$

特征值满足：

$$\begin{vmatrix} \epsilon_0 - E & V_{10} & V_{10} & V_{11} \\ V_{10} & \epsilon_0 - E & V_{11} & V_{10} \\ V_{10} & V_{11} & \epsilon_0 - E & V_{10} \\ V_{11} & V_{10} & V_{10} & \epsilon_0 - E \end{vmatrix} = 0$$

整理可得：

$$(\epsilon_0 - E - V_{11})^2(\epsilon_0 - E + V_{11} + 2V_{10})(\epsilon_0 - E + V_{11} - 2V_{10}) = 0$$

即对应倒格矢 $\mathbf{G} = (\pi/a, \pi/a)$ 的能量为：

$$\begin{aligned} E_1 =& E_2 = \frac{2\hbar^2(\pi/a)^2}{2m} - V_{11}, \\ E_3 =& \frac{2\hbar^2(\pi/a)^2}{2m} + V_{11} + 2V_{10}, \\ E_4 =& \frac{2\hbar^2(\pi/a)^2}{2m} + V_{11} - 2V_{10}. \end{aligned}$$

4. **(15.5) Decaying Waves**

As we saw in this chapter, in one dimension, a periodic potential opens a band gap such that there are no plane-wave eigennstates between energies $\epsilon_0(G/2) - |V_G|$ and $\epsilon_0(G/2) + |V_G|$ with G a reciprocal lattice vector. However, at these forbidden energies, decaying (evanescent) waves still exist. Assume the form

$$\psi(x) = e^{ikx - \kappa x}$$

with $0 < \kappa \leq k$ and κ real. Find κ as a function of energy for $k = G/2$. For what range of V_G and E is your result valid?

对于该形式的波，可令 $k' = k + i\kappa$，则波函数可以写为：$\psi(x) = e^{ik'x}$，则对于布里渊区边界处的态的能量，满足：

$$\begin{vmatrix} \frac{\hbar^2}{2m}(-G/2 + i\kappa)^2 - E & V_G^* \\ V_G & \frac{\hbar^2}{2m}(G/2 + i\kappa)^2 - E \end{vmatrix} = 0$$

则可以解得：

$$E = \frac{\hbar^2}{2m}(G^2/4 - \kappa^2) \pm \sqrt{|V_G|^2 - \frac{\hbar^4 \kappa^2 G^2}{4m^2}}.$$

则可以解得：

$$\kappa^2 = -\frac{2m}{\hbar^2}\left(E + \frac{\hbar^2 G^2}{8m}\right) + \sqrt{\frac{m}{\hbar^2}\left(2EG^2 + \frac{4m|V_G|^2}{\hbar^2}\right)}$$

满足 $\kappa^2 > 0$，可得：

$$mE\hbar^2 G^4 + 4m^2(|V_G|^2 - E^2) > \frac{\hbar^4 G^4}{16}.$$

即 $|V_G|^2 > \left(E - \frac{\hbar G^2}{8m}\right)^2$