

Home Problem Set #3

1. Describe the energy for

(a) a free electron

$$\text{No potential} \rightarrow E = \frac{\hbar^2 k^2}{2m} \text{ (continuous energy)}$$

(b) a strongly bound electron

$$E_n = \frac{\hbar^2 k^2}{2ma^2} n^2 \quad (n=1, 2, 3, \dots) \text{ (discrete energy)}$$

(c) an electron in a periodic potential (i.e., in a crystal)

Why do we get these different band schemes?

주기적인 potential에 의해 energy band 형성

(allowed energy band, forbidden energy band 존재)

다른 energy band scheme를 보이는 이유

각각의 경우 Schrodinger equation을 풀 때

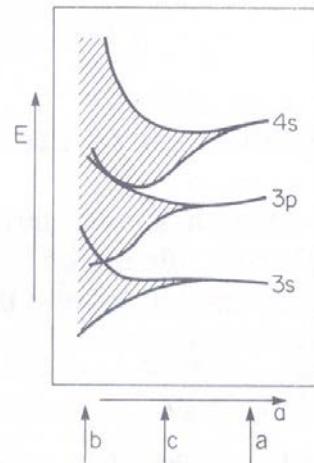
boundary condition, potential이 다르다.

이에 따라 각각의 해가 다른 모습을 보이는 것이다.

다른 설명으로는 interatomic distance를 이용한 것이다.

하나의 고립된 atom에 속하는 전자는 discrete energy를 가진다.

Atom이 서로 근접하여 영향을 미치고 하나의 system이 되는 경우 Pauli exclusion principle에 의해 energy state가 나누어져 있지만 그 차이가 매우 작아 연속적인 것으로 생각할 수 있다.



2. Answer the following questions.

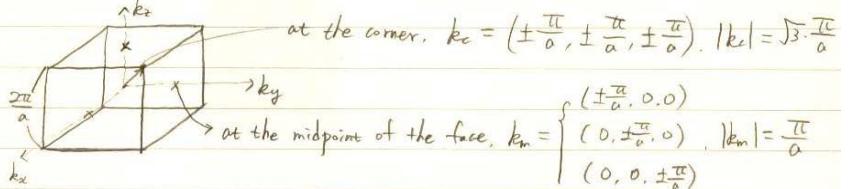
(a) Calculate how much the kinetic energy of a free electron at the corner of the first Brillouin zone of a simple cubic lattice (three dimensions!) is larger than that of an electron at the midpoint of the face.

(b) Construct the first four Brillouin zones for a simple cubic lattice in two dimensions.

(a) Simple cubic lattice : reciprocal lattice は b_1, b_2, b_3 で simple cubic です。
reciprocal lattice の 1st fundamental vector b_1, b_2, b_3 が $\frac{2\pi}{a}$ です。 (real lattice parameter a)

in reciprocal space,

first Brillouin zone

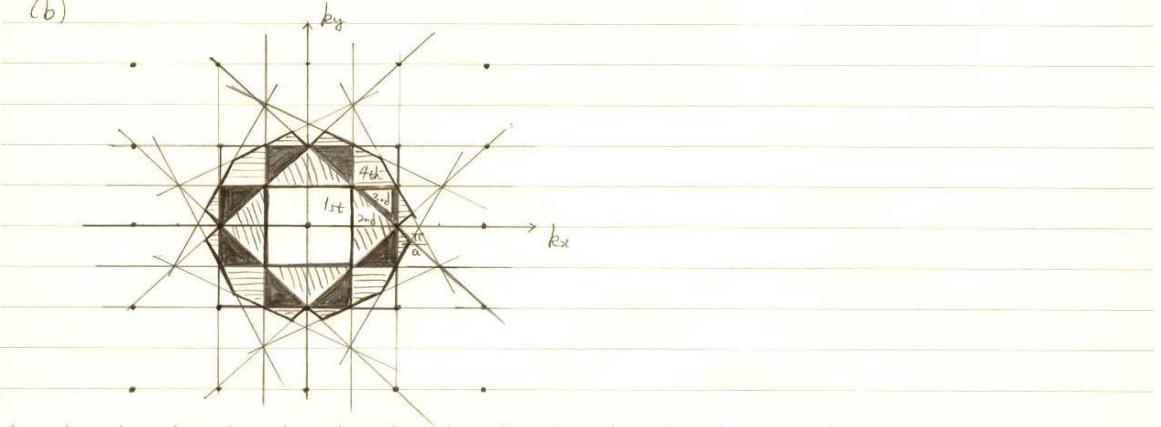


(for free electron)

$$\therefore E_c = \frac{\hbar^2 |k_c|^2}{2m} = \frac{3\hbar^2 \pi^2}{2ma^2}, \quad E_m = \frac{\hbar^2 |k_m|^2}{2m} = \frac{\hbar^2 \pi^2}{2ma^2}$$

$\therefore E_c : E_m \approx \frac{\hbar^2 \pi^2}{ma^2}$ であるからこれが 3:1 である。 $(E_c : E_m = 3:1)$

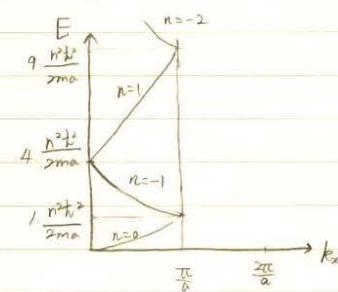
(b)



3. Answer the following questions.

- Calculate the shape of the free electron bands for the cubic primitive crystal structure for $n = 1$ and $n = -2$ (See Fig. 5.6).
- Calculate the main lattice vectors in reciprocal space of an fcc crystal.
- If $\mathbf{b}_1 \cdot \mathbf{t}_1 = 1$ is given (see equation (5.14)), does this mean that \mathbf{b}_1 is parallel to \mathbf{t}_1 ?

9(a) Fig. 5.6



$$E = \frac{\hbar^2}{2m} (k_x + n \frac{2\pi}{a})^2, \quad n=0, \pm 1, \pm 2, \dots$$

$$n=1, \quad E = \frac{\hbar^2}{2m} (k_x + \frac{2\pi}{a})^2 \quad \begin{cases} k_x=0, \quad E=4 \frac{n^2 \hbar^2}{2ma^2} \\ k_x=\frac{\pi}{a}, \quad E=9 \frac{n^2 \hbar^2}{2ma^2} \end{cases}$$

$$n=-2, \quad E = \frac{\hbar^2}{2m} (k_x - 2 \cdot \frac{2\pi}{a})^2 \quad \begin{cases} k_x=0, \quad E=16 \frac{n^2 \hbar^2}{2ma^2} \\ k_x=\frac{\pi}{a}, \quad E=9 \frac{n^2 \hbar^2}{2ma^2} \end{cases}$$

(b) FCC crystal of main lattice vector (in real space)

$$\vec{t}_1 = \frac{a}{2}(i+j), \quad \vec{t}_2 = \frac{a}{2}(j+l), \quad \vec{t}_3 = \frac{a}{2}(l+i) \quad (a: \text{lattice parameter})$$

$(i, j, l \stackrel{\text{def}}{=} \frac{1}{2}\hat{x}, \frac{1}{2}\hat{y}, \frac{1}{2}\hat{z} \text{ unit vector, Miller notation } \stackrel{\text{def}}{=} \frac{1}{h} \frac{1}{k} \frac{1}{l})$

in reciprocal space,

$$\vec{b}_1 = \frac{\vec{t}_1 \times \vec{t}_2}{V}, \quad \vec{b}_2 = \frac{\vec{t}_2 \times \vec{t}_3}{V}, \quad \vec{b}_3 = \frac{\vec{t}_3 \times \vec{t}_1}{V} \quad (V = \vec{t}_1 \cdot \vec{t}_2 \times \vec{t}_3)$$

$$V = \left(\frac{a}{2}\right)^3 \cdot \begin{vmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix} = \left(\frac{a}{2}\right)^3 \cdot (1+1) = \frac{a^3}{4}$$

$$\therefore \vec{b}_1 = \frac{4}{a^3} \cdot \left(\frac{a}{2}\right)^2 \cdot \begin{vmatrix} i & j & l \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix} = \frac{1}{a} (i+j-l)$$

$$\vec{b}_2 = \frac{4}{a^3} \cdot \left(\frac{a}{2}\right)^2 \cdot \begin{vmatrix} i & j & l \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} = \frac{1}{a} (-i+j+l), \quad \vec{b}_3 = \frac{4}{a^3} \cdot \left(\frac{a}{2}\right)^2 \cdot \begin{vmatrix} i & j & l \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{vmatrix} = \frac{1}{a} (i-j+l)$$

간단하게 표현, $b_1 = \frac{1}{a}(11\bar{1}), \quad b_2 = \frac{1}{a}(\bar{1}11), \quad b_3 = \frac{1}{a}(1\bar{1}1) \rightarrow \text{brr of main lattice vector}$
(in reciprocal space)

(c) $b_i \cdot t_j = 1$

이 시기 $b_i \parallel t_j$, 즉 의미하지 않는다. b_i 는 정의에 따라 \vec{t}_1 과 \vec{t}_2 에 수직인 방향이며

$\vec{t}_1 \circ \vec{t}_2$ 와 \vec{t}_3 에 수직한 평면 $\vec{b}_i \parallel \vec{t}_1 \circ \vec{t}_2$ 에 수직한 평면이다. 나머지 경우, $|b_i| \cdot |t_j| \cos \theta = 1$ 만

만족시키면 된다.