Chapter 7.
Energy band

free electron model : Heat capacity, thermal conductivity, electric conductivity, magnetic susceptibility, electrodynamics of metal

문제점 : metal, semiconductor, semimetals, insulators

Hall coefficient + magnetoresistance

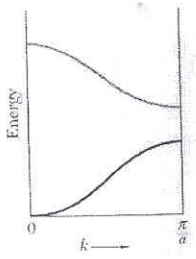
Good conductor Good insulator

1K에서 good conductor, good insulator의 차이는 대단하다.

Good conductor의 저항 : 10^{-10} ohm · cm

Good insulator의 저항 : 10^{22} ohm · cm

Range는 10^{32}정도



→ no wavelike electron orbitals exist

이런 region은 energy gap 또는 band gap이라 한다.

electron의 wave와 crystal ion core 사이의 interaction

약간씩 차있거나 약간씩 모자라면 어떻게 되나?

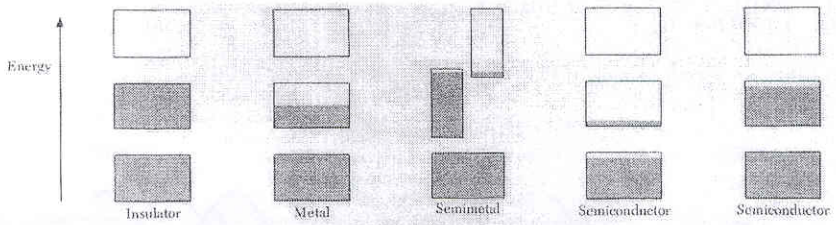


Figure 1 Schematic electron occupancy of allowed energy bands for an insulator, metal, semimetal, and semiconducter. The vertical extent of the boxes indicates the allowed energy regions; the shaded areas indicate the regions filled with electrons. In a **semimetal** (such as bismuth) one band is almost filled and another band is nearly empty at absolute zero, but a pure **semiconductor** (such as silicon) becomes an insulator at absolute zero. The left of the two semiconductors shown is at a finite temperature, with carriers excited thermally. The other semiconductor is electron-deficient because of impurities.

Nearly free electron model

$$\varepsilon_k = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$$

$$k_x,\ k_y,\ k_z = 0,\ \pm\frac{2\pi}{L},\ \frac{4\pi}{L},\ \cdots$$

$$\Psi_k(\vec{r}) = \exp(i\vec{k}\cdot\vec{r})$$

왜 gap이 나타나나?

Bragg reflection은 crystal 내에서 파동이 진행

$$(\vec{k}+\vec{G})^2 = k^2$$

$$\therefore\ k^2 + 2\vec{k}\cdot\vec{G} + G^2 = k^2$$

$$\therefore |\vec{k}| = \pm\left|\frac{1}{2}\vec{G}\right|$$

$$k = \frac{1}{2}G = \pm\frac{\pi}{a}$$

G는 reciprocal lattice vector이다.

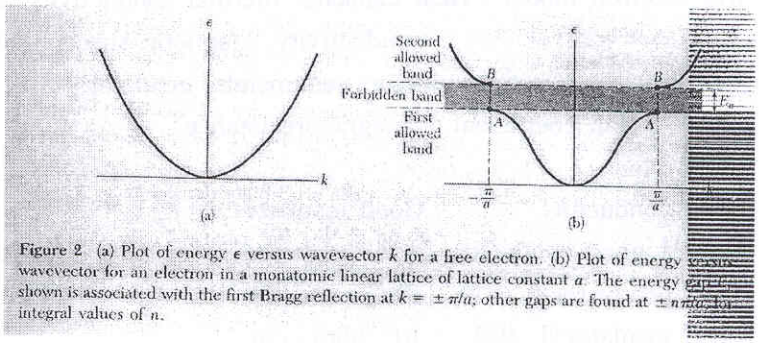


Figure 2 (a) Plot of energy ϵ versus wavevector k for a free electron. (b) Plot of energy versus wavevector for an electron in a monatomic linear lattice of lattice constant a. The energy gap shown is associated with the first Bragg reflection at $k = \pm\pi/a$; other gaps are found at $\pm n\pi/a$ for integral values of n.

$\frac{\pi}{a}$에서의 wave는 traveling wave가 아니다.

equally →, ←로 구성이 되어있다.

time independent state는 standing wave로 형성되어있다.

two traveling waves $\exp\left(\pm\frac{i\pi x}{a}\right)$

$$\Psi(+) = \exp\left(\frac{i\pi x}{a}\right) + \exp\left(-\frac{i\pi x}{a}\right) = 2\cos\frac{\pi x}{a}$$

$$\Psi(-) = \exp\left(\frac{i\pi x}{a}\right) - \exp\left(-\frac{i\pi x}{a}\right) = 2i\sin\frac{\pi x}{a}$$

Origin of the Energy gap

$$\rho(+) = |\Psi(+)|^2 \propto \cos^2\frac{\pi x}{a}$$

$$\rho(-) = |\Psi(-)|^2 \propto \sin^2\frac{\pi x}{a}$$

$\rho(+)$: traveling wave보다 낮다. E_g보다 낮다.

$\rho(-)$: traveling wave보다 높다. E_g보다 높다.

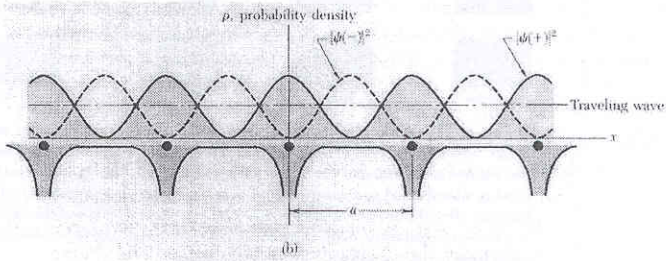


Figure 3 (a) Variation of potential energy of a conduction electron in the field of the ion a linear lattice. (b) Distribution of probability density ρ in the lattice for $|\psi(-)|^2 \propto \sin$

Magnitude of the energy gap at $k = \frac{\pi}{a}$

$$U(x) = U\cdot\cos\frac{2\pi x}{a}$$

first order energy difference between tow standing wave

$$E_g = \int dx\ U(x)\left[\,|\Psi(+)|^2 - |\Psi(-)|^2\,\right]$$

$\Psi(+) = \sqrt{2}\cos\frac{\pi x}{a}$ 이므로

$$\int_{+0}^{a} |\Psi(+)|^2 dx = \int_0^a 2\cos^2\frac{\pi x}{a}\,dx = a$$

unit length당 1로 normalize하자.

$$E_g = \int dx\ U(x)\,[\,|\Psi(+)|^2 - |\Psi(-)|^2\,]\cdot$$

$$= 2\int_0^a dx\ U\cdot\cos\frac{2\pi x}{a}\left(\cos^2\frac{\pi x}{a} - \sin^2\frac{\pi x}{a}\right)\cdot$$

$$= 2\int_0^a dx\ U\cdot\frac{1+\cos\frac{4\pi x}{a}}{2}\cdot$$

$$= U$$

unit length 당 에너지 차이

Bloch function

periodic potential일 때는 Sch. eq.의 답이 다음과 같다.

$$\Psi_k(\vec{r}) = u_k(\vec{r})\exp(i\vec{k}\cdot\vec{r})$$

$$u_k(\vec{r}) = u_k(\vec{r}+T)$$

$$u(x) = u(x+sa)$$

$$\Psi(x+a) = C\Psi(x)$$

$$\therefore\ \Psi(x+Na) = \Psi(x) = C^N\Psi(x)$$

$$C = \exp\left(i\frac{2\pi s}{N}\right) \qquad s = 0,\ 1,\ 2,\ \cdots,\ N-1$$

$$\Psi(x) = u_k(x)\cdot\exp\left(i\frac{2\pi s x}{Na}\right) \qquad k = \frac{2\pi s}{Na}$$

$$= u_k(x)\cdot\exp(ikx)$$

Kronig-Penney model

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi + u(x)\Psi = \varepsilon\Psi$$

$0 < x < a$, $u = 0$라 하면

$$\Psi = Ae^{iKx} + Be^{-iKx}$$

$$\varepsilon = \frac{\hbar^2 K^2}{2m}$$

$-b < x < 0$

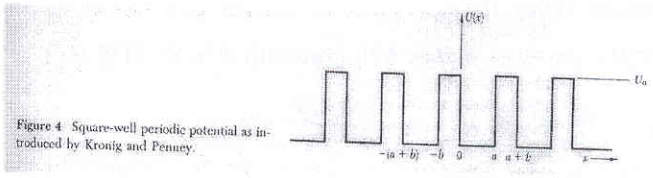


Figure 4 Square-well periodic potential as introduced by Kronig and Penney.

$\Psi = Ce^{Qx} + Dd^{-Qx}$ with

$$-\frac{\hbar^2 Q^2}{2m} + u_0 = \varepsilon$$

$$u_0 - \varepsilon = \frac{\hbar^2 Q^2}{2m}$$

$a < x < a+b$

$\Psi(a < x < a+b) = \Psi(-b < x < 0) \cdot e^{ik(a+b)}$

$x = 0$에서 continuous

$A + B = C + D$

$ik(A - B) = Q(C - D)$

$x = a$에서 continuous

$Ae^{iKa} + Be^{-iKa} = (Ce^{-Qb} + De^{Qb})\, e^{ik(a+b)}$

$ik(Ae^{iKa} - Be^{-iKa}) = Q(Ce^{-Qb} - De^{Qb})\, e^{ik(a+b)}$

$A + B - C - D = 0$

$iKA - iKB - QC + QD = 0$

$e^{iKa}A + e^{-iKa}B - e^{-Qb} \cdot e^{ik(a+b)}C - e^{Qb} \cdot e^{ik(a+b)}D = 0$

$ike^{iKa}A - ike^{-iKa}B - Qe^{-Qb} \cdot e^{ik(a+b)}C + Qe^{Qb} \cdot e^{ik(a+b)}D = 0$

determinant zero

$[(Q^2 - K^2)/2QK] \sinh Qb \cdot \sin Ka + \cosh Qb \cdot \cos Ka = \cos k(a+b)$

periodic delta ft.

$b = 0$, $u_0 = \infty$ ($u_0 \cdot b$가 constant되도록 하면서)

$\varepsilon = \frac{\hbar^2 K^2}{2m}$, $u_0 - \varepsilon = \frac{\hbar^2 Q^2}{2m}$ 이므로

$Q \gg K$ and $Qb \ll 1$

$\sinh Qb = Qb$
$\cosh Qb = 1$

$\frac{Q^2 ba}{2} = P$라 하자.

$$\frac{(Q^2-K^2)}{2QK}\cdot\sinh Qb\cdot\sin Ka+\cosh Qb\cdot\cos Ka=\cos k(a+b)$$

$$\frac{1}{2}Q^2b\sin Ka+K\cos Ka=K\cos k(a+b)$$

$$\frac{P}{Ka}\sin Ka+\cos Ka=\cos ka$$

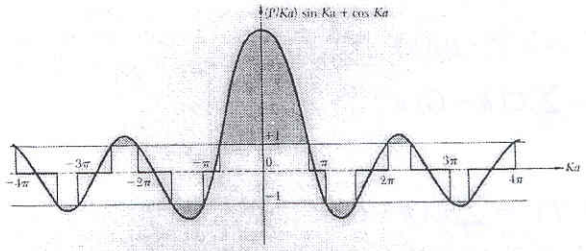


Figure 5 Plot of the function $(P/Ka)\sin Ka+\cos Ka$, for $P=3\pi/2$. The allowed values of the energy ϵ are given by those ranges of $Ka=(2m\epsilon/\hbar^2)^{1/2}a$ for which the function lies between ±1. For other values of the energy there are no traveling wave or Bloch-like solutions to the wave equation, so that forbidden gaps in the energy spectrum are formed.

Wave equation of electron in a periodic potential

Assume $U(x)=U(x+a)$

$$U(x)=\sum_G U_G e^{iGx}$$
$$=\sum_{G>0}U_G(e^{iGx}+e^{-iGx})$$
$$=2\sum_{G>0}U_G\cos Gx$$

$$\left(\frac{p^2}{2m}+U(x)\right)\Psi(x)=\left(\frac{1}{2m}p^2+\sum_G U_G e^{iGx}\right)\Psi(x)=\varepsilon\Psi(x)$$

$$\Psi(x)=\sum_k C(k)\,e^{ikx}$$

$$\frac{p^2}{2m}\Psi(x)=\frac{1}{2m}\left(-i\hbar\frac{d}{dx}\right)^2\Psi(x)=\frac{\hbar^2}{2m}\sum_k k^2C(k)\,e^{ikx}$$

Potential energy term

$$\left(\sum_G u_G e^{iGx}\right)\Psi(x)=\sum_G\sum_k U_G e^{iGx}C(k)\,e^{ikx}$$

The eq. in obtained as the sum

$$\sum_k\frac{\hbar^2}{2m}k^2C(k)\,e^{ikx}+\sum_G\sum_k U_G e^{iGx}\cdot C(k)\,e^{ikx}=\varepsilon\sum_k C(k)\,e^{ikx}$$

$$\therefore\sum_k\left(\frac{\hbar^2k^2}{2m}-\varepsilon\right)C(k)\,e^{ikx}+\sum_G\sum_k U_G\,C(k)\,e^{i(G+k)x}=0$$

모든 k에 대해 성립 [∴DIAGONAL!]

$$\left(\frac{\hbar^2k^2}{2m}-\varepsilon\right)C(k)+\sum_G U_G\,C(k-G)=0$$

$$\lambda_k=\frac{\hbar^2k^2}{2m}$$

Infinite #. to be determined

실제로는 2~4개 정도면 충분하다.

Restatement of the Bloch theorem

$$\Psi_k(x) = \sum_G C(k-G)\, e^{i(k-G)x}$$
$$= \left(\sum_G C(k-G)\, e^{-iGx}\right) e^{ikx}$$
$$= e^{ikx} \cdot u_k(x)$$
$$u_k(x) \equiv \sum_G C(k-G)\, e^{-iGx}$$

$$u_k(x+T) = \sum_G C(k-G) e^{-iG(x+T)}$$
$$= \sum_G C(k-G) e^{-iGx}$$
$$= u_k(x)$$

k의 의미

Crystal momentum of an electron

◦ $\Psi_k(\vec{r}+\vec{T}) = e^{i\vec{k}\cdot(\vec{T}+\vec{r})} u_k(\vec{r}+\vec{T})$

$$= e^{ikT} \cdot \Psi_k(\vec{r})$$

e^{ikT} : phase factor

◦ 만약 potential이 zero이면

위의 eq은 $(\lambda_k - \varepsilon) C(k) = 0$

$\therefore\ C(k) \neq 0$ all other $C(\vec{k}-\vec{G}) = 0$

Solution of the Central equation

$$(\lambda_k - \varepsilon) C(k) + \sum_G U_G C(k-G) = 0$$

만약 $U(x)$가 하나의 component만 있다면

$U_g = U_{-g}$만 있다. $\qquad (\lambda_k - \varepsilon) C(k) + U_{-G} C(k+G) + U_G C(k-G) = 0$

$$\begin{matrix}
\lambda_{k-2g}-\varepsilon & u & 0 & 0 & 0 \\
u & \lambda_{k-g}-\varepsilon & u & 0 & 0 \\
0 & u & \lambda_k-\varepsilon & u & 0 \\
0 & 0 & u & \lambda_{k+g}-\varepsilon & u \\
0 & 0 & 0 & u & \lambda_{k+2g}-\varepsilon
\end{matrix}$$

$$U_G C(k-G) + (\lambda_k - \varepsilon) C(k) + U_{-G} C(k+G) = 0$$

start $3g$, $3g-g=2g$, $3g-2g=g$

$$u\,C(k-3g)+(\lambda_{k-2g}-\varepsilon)\,C(k-2g)+u\,C(k-g)=0$$

$$u\,C(k-2g)+(\lambda_{k-g}-\varepsilon)\,C(k-g)+u\,C(k)=0$$

$$u\,C(k-g)+(\lambda_{k}-\varepsilon)\,C(k)+u\,C(k+g)=0$$

$$u\,C(k)+(\lambda_{k+g}-\varepsilon)\,C(k+g)+u\,C(k+2g)=0$$

infinite series지만 몇 개만 해도 충분하다.

eigen value ε_{nk} $\quad n$: 1, 2, …

k는 wave vector를 의미한다.

대부분의 경우 k는 first B.Z에서 택한다.

Exactly 풀 수 있는 경우를 생각하자.

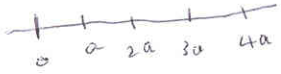
Kronig-Penney model에 의해 periodic delta-function potential을 생각하자.

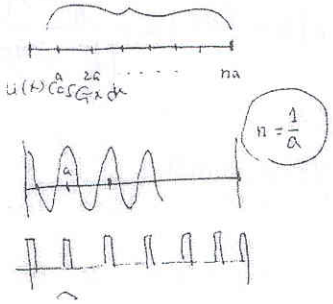
$$U(x)=2\sum_{G>0}U_G\cos Gx=Aa\sum_s\delta(x-sa)$$

a : lattice spacing

단위 길이에 $n=\frac{1}{a}$의 potential이 있다 가정

$0<s<\frac{1}{a}$인 integer





Fourier component

$L=na=1$, $G=\frac{2\pi}{a}$ 이므로

$$\begin{aligned}U_G&=\frac{1}{L}\int_0^L dx\,U(x)\cos Gx\\&=\frac{1}{L}\int_0^L dx\,Aa\sum\delta(x-sa)\cos Gx\\&=\int_0^1 dx\,Aa\sum\delta(x-sa)\cos Gx\\&=Aa\sum_s\cos Gsa\\&=Aa\cdot\sum_s 1\\&=Aa\cdot n\\&=A\end{aligned}$$

Bloch eq.

$$(\lambda_k - \varepsilon)C(k) + \sum_G U_G\, C(k-G) \;=\; 0$$

$$\therefore \quad (\lambda_k - \varepsilon)C(k) + \sum_G AC(k-G)$$

$$= (\lambda_k - \varepsilon)C(k) + \sum_n AC\left(k - \frac{2n\pi}{a}\right) \;=\; 0$$

Let $f(k) = \sum_n C\left(k - \frac{2n\pi}{a}\right)$

$$(\lambda_k - \varepsilon)C(k) + A\,f(k) \;=\; 0$$

$$\therefore \; C(k) \;= \frac{A\,f(k)}{\lambda_k - \varepsilon} \qquad\qquad \lambda_k = \frac{\hbar^2 k^2}{2m}$$

$$= \frac{\frac{2mA}{\hbar^2} f(k)}{k^2 - \frac{2m}{\hbar^2}\varepsilon}$$

for any n

$$f(k) = f\left(k - \frac{2n\pi}{a}\right)$$

$$C\left(k - \frac{2n\pi}{a}\right) = \frac{\frac{2mA}{\hbar^2} f\left(k - \frac{2n\pi}{a}\right)}{\left(k - \frac{2n\pi}{a}\right)^2 - \frac{2m}{\hbar^2}\varepsilon}$$

양쪽을 sum하자.

$$\frac{\hbar^2}{2mA} = \sum_n \frac{1}{\left(k-\frac{2n\pi}{a}\right)^2 - \frac{2m}{\hbar^2}\varepsilon} \qquad LET\ \frac{2m\varepsilon}{\hbar^2} = K^2$$

$$= \sum_n \frac{1}{\left(-k+\frac{2n\pi}{a}\right)^2 - K^2}$$

$$= \sum \frac{1}{\left(\frac{2n\pi}{a}-k+K\right)\left(\frac{2n\pi}{a}-k-K\right)}$$

$$= \sum \frac{1}{-2K}\left[\frac{1}{\frac{2n\pi}{a}-k+K} - \frac{1}{\frac{2n\pi}{a}-k-K}\right]$$

$$= \sum -\frac{1}{2K}\left[\frac{1}{\frac{2}{a}\left(n\pi+\frac{(K-k)a}{2}\right)} - \frac{1}{\frac{2}{a}\left(n\pi-\frac{(K+k)a}{2}\right)}\right]$$

$$= -\frac{1}{2K}\cdot\frac{a}{2}\left[\cot\frac{(K-k)a}{2} + \cot\frac{(K+k)a}{2}\right]$$

그런데

$$\cot(\alpha+\beta)+\cot(\alpha-\beta) = \frac{\cos(\alpha+\beta)}{\sin(\alpha+\beta)} + \frac{\cos(\alpha-\beta)}{\sin(\alpha-\beta)}$$

$$= \frac{\sin(\alpha-\beta)\cos(\alpha+\beta)+\cos(\alpha-\beta)\sin(\alpha+\beta)}{\sin(\alpha+\beta)\sin(\alpha-\beta)}$$

$$= \frac{\sin 2\alpha}{-\frac{1}{2}(\cos 2\alpha - \cos 2\beta)} = -\frac{2\sin 2\alpha}{\cos 2\alpha - \cos 2\beta}$$

이므로

$$\frac{\hbar^2}{2mA} = -\frac{a}{4K}\cdot(-2)\cdot\frac{\sin Ka}{\cos Ka-\cos ka}$$

$$= \frac{a^2}{4Ka}\cdot\frac{\sin Ka}{\cos Ka-\cos ka} \qquad \text{factor 2 다르다.}$$

$$\therefore -\frac{\hbar^2}{2mA} = \frac{a^2}{4Ka}\frac{\sin Ka}{\cos Ka-\cos ka}$$

$$-\sin Ka\cdot\frac{2mA}{\hbar^2}\left(\frac{a^2}{4Ka}\right) = \cos Ka-\cos ka$$

$$-\sin Ka\cdot\frac{mAa}{2K\hbar^2} = \cos Ka-\cos ka$$

$$\therefore\ \cos ka = \frac{mAa}{2K\hbar^2}\sin Ka + \cos Ka$$

Kronig-Penney 결과와 같다.

Empty lattice approximation
first B.Z으로 가져와 approximate하자.

$$\varepsilon(k_x,\ k_y,\ k_z) = \frac{\hbar^2}{2m}(\vec{k}+\vec{G})^2$$

$$= \frac{\hbar^2}{2m}\left[(k_x+G_x)^2+(k_y+G_y)^2+(k_z+G_z)^2\right]$$

Simple cubic인 경우에서 시작하자.

$\frac{\hbar^2}{2m}=1$ 귀찮으니까

Band	$Ga/2\pi$	$\varepsilon(0,\ 0,\ 0)$	$\varepsilon(k,\ 0,\ 0)$
1	000	0	k_x^2
2, 3	100, $\bar{1}00$	$\left(\frac{2\pi}{a}\right)^2$	$\left(k_x\pm\frac{2\pi}{a}\right)^2$
4, 5, 6, 7	010, $0\,\bar{1}0$, 001, $00\,\bar{1}$	$\left(\frac{2\pi}{a}\right)^2$	$k_x^2+\left(\frac{2\pi}{a}\right)^2$
8, 9, 10, 11	110, 101, $1\,\bar{1}0$, $10\,\bar{1}$	$2\cdot\left(\frac{2\pi}{a}\right)^2$	$\left(k_x+\frac{2\pi}{a}\right)^2+\left(\frac{2\pi}{a}\right)^2$
12, 13, 14, 15	$\bar{1}10$, $\bar{1}01$, $\bar{1}\,\bar{1}0$, $\bar{1}0\,\bar{1}$	$2\cdot\left(\frac{2\pi}{a}\right)^2$	$\left(k_x-\frac{2\pi}{a}\right)^2+\left(\frac{2\pi}{a}\right)^2$
16, 17, 18, 19	011, $0\,\bar{1}1$, $01\,\bar{1}$, $0\,\bar{1}\,\bar{1}$	$2\cdot\left(\frac{2\pi}{a}\right)^2$	$k_x^2+2\cdot\left(\frac{2\pi}{a}\right)^2$

Approximate Solution near a zone boundary

wave vector at zone boundary : $\left(\frac{1}{2}G\right)$

$k=\pm\frac{1}{2}G$ or $k=\frac{3}{2}G$

K.E는 서로 같다.

$$\Psi_k(x) = \sum_G C(\vec{k}-\vec{G})\,e^{i(\vec{k}-\vec{G})x}$$

$$= C(\tfrac{1}{2}G-G)\,e^{i(\frac{1}{2}G-G)x} + C(\tfrac{3}{2}G-G)\,e^{i(\frac{3}{2}G-G)x}$$

$C(\frac{G}{2})$, $C(-\frac{G}{2})$만 생각하자.

$$= C\left(-\frac{1}{2}G\right)e^{-\frac{i}{2}Gx} + C\left(\frac{1}{2}G\right)e^{\frac{i}{2}Gx}$$

Equation은

$$(\lambda_k-\varepsilon)C(k)+\sum_G U_G\,C(k-G) = 0$$

$k=\pm\frac{1}{2}G$에서 문제 푼다.

$$(\lambda-\varepsilon)C\left(\frac{1}{2}G\right)+U\,C\left(-\frac{1}{2}G\right) = 0$$

$$(\lambda-\varepsilon)C\left(-\frac{1}{2}G\right)+U\,C\left(\frac{1}{2}G\right) = 0$$

이 두 개의 방정식은 nontrivial solution을 갖는다.

$$\begin{vmatrix} \lambda-\varepsilon & U \\ U & \lambda-\varepsilon \end{vmatrix}=0$$

$$\therefore \quad (\lambda-\varepsilon)^2=U^2$$

$$\therefore \quad \varepsilon=\lambda\pm U=\frac{\hbar^2}{2m}\left(\frac{1}{2}G\right)^2\pm U$$

두 개의 solution을 가지고 있다.
하나는 아래, 하나는 위에

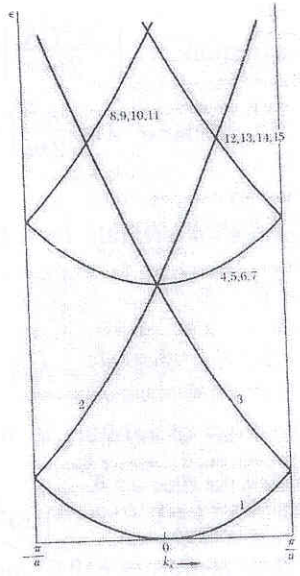
$$\frac{C\left(-\frac{1}{2}G\right)}{C\left(\frac{1}{2}G\right)}=\frac{\varepsilon-\lambda}{U}=\pm 1$$

Fourier expansion of $\Psi(x)$ at the zone boundary

$$\Psi(x)=e^{iGx/2}\pm e^{-iGx/2}$$

Zone boundary 근처에서는 어떻게 되나?

$$\Psi(x)=C(k)e^{ikx}+C(k-G)e^{i(k-G)x}$$



k near $\frac{1}{2}G$

$$(\lambda_k-\varepsilon)C(k)+UC(k-G)=0$$

$$(\lambda_{k-G}-\varepsilon)C(k-G)+UC(k)=0$$

$$\begin{vmatrix} \lambda_k-\varepsilon & u \\ u & \lambda_{k-G}-\varepsilon \end{vmatrix}=0$$

where $\quad (\lambda_k-\varepsilon)(\lambda_{k-G}-\varepsilon)-U^2$

$$=\varepsilon^2-\varepsilon(\lambda_{k-G}+\lambda_k)+\lambda_k\cdot\lambda_{k-G}-U^2$$

$$=0$$

이 energy는 두 개의 근을 갖고 있다.

$$\varepsilon=\frac{1}{2}(\lambda_{k-G}+\lambda_k)\pm\left[\frac{1}{4}(\lambda_{k-G}-\lambda_k)^2+U^2\right]^{1/2}$$

$k-\frac{1}{2}G=K$라 하자. $k-G=K-\frac{1}{2}G$이므로

$$\lambda_{k-G}=\frac{\hbar^2}{2m}\left(K-\frac{1}{2}G\right)^2, \quad \lambda_k=\frac{\hbar^2}{2m}\left(K+\frac{1}{2}G\right)^2$$

$$\lambda_{k-G}+\lambda_k=\frac{\hbar^2}{2m}\left\{2K^2+\frac{1}{2}G^2\right\}$$

$$\lambda_{k-G}-\lambda_k=\frac{\hbar^2}{2m}\left\{\left(K-\frac{1}{2}G\right)^2-\left(K+\frac{1}{2}G\right)^2\right\}$$

$$=\frac{\hbar^2}{2m}\{2KG\}$$

$$\varepsilon = \frac{1}{2}\frac{\hbar^2}{2m}\left\{2K^2+\frac{1}{2}G^2\right\} \pm \left[\frac{1}{4}\cdot\frac{\hbar^4}{4m^2}\cdot 4K^2G^2+U^2\right]^{1/2}$$

$$= \frac{\hbar^2}{2m}\left\{K^2+\frac{1}{4}G^2\right\} \pm U\left\{1+\left(\frac{\hbar^2 KG}{2mU}\right)^2\right\}^{1/2}$$

$$\cong \frac{\hbar^2}{2m}\left\{K^2+\frac{1}{4}G^2\right\} \pm U\left\{1+\frac{1}{2}\cdot\frac{\hbar^4K^2G^2}{4m^2U^2}\right\}^{1/2}$$

$$\lambda = \frac{\hbar^2}{2m}\left(\frac{1}{2}G\right)^2 = \frac{\hbar^2G^2}{8m} \text{ 이므로}$$

$$= \frac{\hbar^2}{2m}\left\{K^2+\frac{1}{4}G^2\right\} \pm U\left\{1+\frac{1}{8}\cdot\frac{\hbar^4K^2G^2}{m^2U^2}\frac{8m}{\hbar^2G^2}\lambda\right\}^{1/2}$$

$$= \frac{\hbar^2}{2m}\left\{K^2+\frac{1}{4}G^2\right\} \pm U\left\{1+\frac{\hbar^2K^2\lambda}{mU^2}\right\}$$

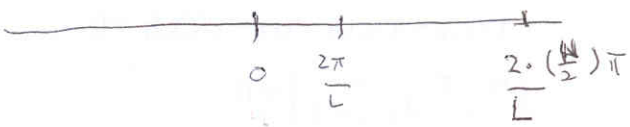
$$= \frac{\hbar^2}{2m}\left\{K^2+\frac{1}{4}G^2\right\} \pm U\left\{1+\frac{2\lambda}{U^2}\cdot\frac{\hbar^2K^2}{2m}\right\}$$

in a region of $\left|\frac{\hbar^2GK}{2m}\right| \ll |U|$

where $\lambda = \frac{\hbar^2}{2m}\left(\frac{1}{2}G\right)^2$

Number of orbitals in a band

$k = 0,\ \pm\frac{2\pi}{L},\ \pm\frac{4\pi}{L},\ \cdots,\ \frac{N\pi}{L}$



$\frac{1}{2}N$개 $\times 2 = N$개

# of orbitals in a band

$$\frac{N\pi}{L} = \frac{\pi}{\left(\frac{L}{N}\right)} = \frac{\pi}{a}$$

각각의 primitive cell은 independent 값을 포함하고 있다.

각각의 energy band에는 $2N$개의 independent orbital이 있다.

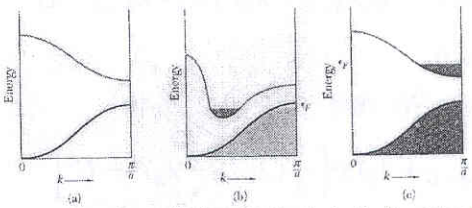


Figure 11 Occupied states and band structures giving (a) an insulator, (b) a metal or a semimetal because of band overlap, and (c) a metal because of electron concentration. In (b) the overlap need not occur along the same directions in the Brillouin zone. If the overlap is small, with relatively few states involved, we speak of a semimetal.

Metals and Insulators>>

odd number even number