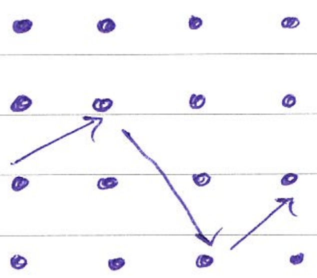
Waves in periodic structures

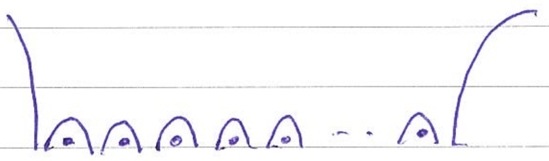
From classical point of view, it is very difficult to understand why the mean free path of electrons can be very large!



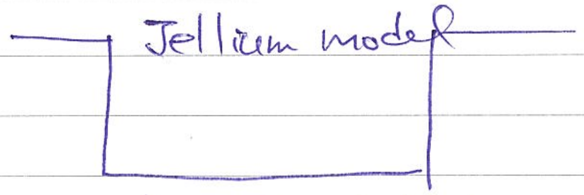
Bloch (1928) provided the solution to this puzzle in his thesis by pointing out that in the presence of a periodic potential, an electron can maintain the coherence of its wave function as if it does not suffer any scattering from the lattice.

This is summarized in the Bloch theorem and the corresponding lattice effect is the most important correction to the Sommefeld free electron theory.

The difference in treating ions in two theories can be summarized as:



≃ periodic potential



ion = smooth background
(Sommefeld theory)

What is found by Bloch is actually a general phenomenon for any waves in a periodic structure.

Generally, the wave function $\psi(\vec{r})$ satisfies

$$\hat{H}(\vec{r})\,\psi(\vec{r}) = \lambda\,\psi(\vec{r})$$

with $\hat{H}(\vec{r}+\vec{R}) = \hat{H}(\vec{r})$. $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

$\vec{a}_i$ = primitive vectors of the crystal.

examples:

1. Electromagnetic waves in a photonic crystal

$$\nabla\times\vec{E} = \frac{-1}{c}\frac{\partial\vec{B}}{\partial t}, \quad \nabla\cdot\vec{D} = 4\pi\rho$$

$$(\vec{J}_{free} = 0)$$

$$\nabla\times\vec{H} = \frac{1}{c}\frac{\partial\vec{D}}{\partial t} + \cancelto{0}{\frac{4\pi}{c}\vec{J}}, \quad \nabla\cdot\vec{B} = 0$$

$$\vec{D} = \epsilon\vec{E}, \quad \vec{B} = \mu\vec{H}$$

$$\therefore \nabla\times\left(\frac{1}{\epsilon}\vec{D}\right) = \frac{-1}{c}\frac{\partial}{\partial t}(\mu\vec{H}) \Rightarrow \frac{1}{\mu}\nabla\times\frac{\vec{D}}{\epsilon} = \frac{-1}{c}\frac{\partial\vec{H}}{\partial t}$$

take $\nabla\times$ & using $\nabla\times\vec{H} = \frac{1}{c}\frac{\partial\vec{D}}{\partial t} + \frac{4\pi}{c}\vec{J}$

$$\Rightarrow \frac{1}{c^2}\frac{\partial^2\vec{D}}{\partial t^2} + \nabla\times\left(\frac{1}{\mu(\vec{r})}\nabla\times\frac{\vec{D}}{\epsilon(\vec{r})}\right) = 0$$

$$\vec{D} = \vec{D}(\vec{r})e^{i\omega t} \Rightarrow \underbrace{\nabla\times\left(\frac{1}{\mu(\vec{r})}\nabla\times\frac{1}{\epsilon(\vec{r})}\right)}_{\hat{H}}\vec{D}(\vec{r}) = \lambda\,\vec{D}(\vec{r})$$

$$\lambda = \omega^2/c^2$$

$\therefore$ if $\epsilon(\vec{r}+\vec{R}) = \epsilon(\vec{r})$, $\mu(\vec{r}+\vec{R}) = \mu(\vec{r})$, $\hat{H}(\vec{r}+\vec{R}) = \hat{H}(\vec{r})$.

2. Elastic waves in crystals

$$\underset{\hat{H}}{D(\vec{k})} \cdot \epsilon(k) = \lambda \; \epsilon(k)$$

$$\lambda = M\omega^2$$

$$D(\vec{k}) = \sum_{R} D(\vec{R}) \, e^{-i\vec{k}\cdot\vec{R}}$$

$$D(\vec{k}+\vec{G}) = D(\vec{k})$$ periodic k space

Elastic wave in a medium
(phononic crystal, acoustic waves
in a medium)

$$\rho(r)\frac{\partial^2 u_\alpha}{\partial t^2} = \frac{\partial}{\partial x_\alpha}\left(\lambda(r)\frac{\partial u_\beta}{\partial x_\beta}\right) + \frac{\partial}{\partial x_\beta}\left[\mu(r)\left(\frac{\partial u_\alpha}{\partial x_\beta}+\frac{\partial u_\beta}{\partial x_\alpha}\right)\right]$$

$$\underbrace{\lambda(\vec{r}+\vec{R}) = \lambda(\vec{r}),\ \mu(\vec{r}+\vec{R}) = \mu(\vec{r})}_{\text{Lamé coefficient}} \quad \rho(\vec{r}+\vec{R}) = \rho(\vec{r})$$

$$u_\alpha = u_\alpha(\vec{r})\, e^{i\omega t}$$

$$\underbrace{-\frac{1}{\rho(r)}\left\{\frac{\partial}{\partial x_\alpha}\left[\lambda(r)\frac{\partial u_\beta}{\partial x_\beta}\right] + \frac{\partial}{\partial x_\beta}\left[\mu(r)\left(\frac{\partial u_\alpha}{\partial x_\beta}+\frac{\partial u_\beta}{\partial x_\alpha}\right)\right]\right.}_{\hat{H}_{\alpha\beta}u_\beta} = \omega^2 u_\alpha$$

3. Schrödinger equation

$$\underbrace{\left[-\frac{\hbar^2}{2m}\nabla^2 + U(r)\right]}_{\hat{H}(r)} \psi(\vec{r}) = \epsilon\,\psi(\vec{r})$$

$$U(\vec{r}+\vec{R}) = U(\vec{r})$$

Naively, one would think that since

$$\hat{H}(\vec r+\vec R) = \hat{H}(\vec r), \qquad \psi(\vec r+\vec R) = \psi(\vec r)$$

This is not correct as one can see for the free Schrödinger equation, $U=0$

$$\psi(\vec r) = e^{i\vec k\cdot\vec r}. \qquad \psi(\vec r+\vec R) = e^{i\vec k\cdot\vec R}\, e^{i\vec k\cdot\vec r}$$

$$\neq e^{i\vec k\cdot\vec r} = \psi(\vec r)\,!$$

The probability density, $|\psi(\vec r)|^2$, however, satisfies $|\psi(\vec r+\vec R)|^2 = |\psi(\vec r)|^2$.

Bloch proves: There exists a $\vec k$ such that

Bloch theorem: $\psi(\vec r+\vec R) = e^{i\vec k\cdot\vec R}\psi(\vec r)$

so that we can label ψ by $\vec k$

$$\psi_k(\vec r+\vec R) = e^{i\vec k\cdot\vec R}\psi_k(\vec r) \qquad ①$$

alternative form: $\psi_k(\vec r) = e^{i\vec k\cdot\vec r}\, u_k(\vec r)$ ②

$u_k(\vec r)$: Bloch function, & $\underline{u_k(\vec r+\vec R) = u_k(\vec r)}$

② implies ①: $\psi_k(\vec r+\vec R) = e^{i\vec k\cdot\vec R}\left[e^{i\vec k\cdot\vec r}\underbrace{u_k(\vec r+\vec R)}_{u_k(\vec r)}\right]$

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

① implies ②: set $u_k(\vec r) = e^{-i\vec k\cdot\vec r}\psi_k(\vec r)$

$$\psi_k(\vec r) = e^{i\vec k\cdot\vec r}\, e^{-i\vec k\cdot\vec r}\psi_k(\vec r) = e^{i\vec k\cdot\vec r}\, u_k(\vec r)$$

$$u_k(\vec r+\vec R) = e^{i\vec k\cdot\vec R}\, e^{-i\vec k\cdot\vec r}\psi_k(\vec r+\vec R) = e^{-i\vec k\cdot\vec r}\psi_k(\vec r) = u_k(\vec r)$$

To prove the Bloch theorem, we first construct the translational operator $\hat{T}_R$

$$\hat{T}_R \psi(\vec{r}) \equiv \psi(\vec{r}+\vec{R}) = \left[1 + \vec{R}\cdot\vec{\nabla} + \frac{1}{2!}(\vec{R}\cdot\vec{\nabla})^2 + \cdots\right] \psi(\vec{r})$$

$$= e^{\vec{R}\cdot\vec{\nabla}} \psi(\vec{r})$$

$$\therefore \hat{T}_R = e^{\frac{i}{\hbar}\vec{R}\cdot\vec{P}}$$

Now, from $\hat{H}(\vec{r})\psi(\vec{r}) = \lambda\psi(\vec{r})$, we get

$$\hat{H}(\vec{r}+\vec{R})\psi(\vec{r}+\vec{R}) = \lambda\psi(\vec{r}+\vec{R})$$

$$= \lambda\hat{T}_R\psi(\vec{r})$$

$$\therefore \quad \hat{H}(\vec{r}+\vec{R})\hat{T}_R\psi(\vec{r}) = \lambda\hat{T}_R\psi(\vec{r})$$

$$\hat{T}_R^{-1}\hat{H}(\vec{r}+\vec{R})\hat{T}_R\psi(\vec{r}) = \lambda\psi(\vec{r})$$

Hence $H(\vec{r}) = T_R^{-1}\hat{H}(\vec{r}+\vec{R})\hat{T}_R$.

That is, under translation, $\hat{H}$ transforms as

$$\hat{H}(\vec{r}+\vec{R}) = T_R H(\vec{r}) T_R^{-1} \qquad --- \text{③}$$

For periodic structures, $\hat{H}(\vec{r}+\vec{R}) = \hat{H}(\vec{r})$

∴ Eq. ③ implies $T_R\hat{H}(\vec{r})T_R^{-1} = \hat{H}(\vec{r})$

$$\therefore \quad T_R\hat{H}(\vec{r}) = \hat{H}(\vec{r})T_R$$

$$[T_R, \hat{H}(\vec{r})] = 0 \qquad -- \text{④}$$

Eq. ④ implies $\hat{H}$ & T_R can be diagonalized simultaneously. That is, one can find a set of eigenfunctions such that

$$T_R \psi(\vec{r}) = C(\vec{R}) \psi(\vec{r})$$
$$\hat{H}(\vec{r}) \psi = \lambda \psi(\vec{r})$$

To find $C(\vec{R})$, we note that

$$T_{R'} T_R = T_{R+R'}$$

$$\because T_{R'} T_R \psi(\vec{r}) = C(\vec{R}') C(\vec{R}) \psi(\vec{r})$$
$$T_{R+R'} \psi(\vec{r}) = C(\vec{R}+\vec{R}') \psi(\vec{r})$$

$$\therefore C(\vec{R}+\vec{R}') = C(\vec{R}') C(\vec{R})$$

$\because \vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$, $\vec{a}_i$ = primitive lattice vectors

$$\therefore C(\vec{R}) = [C(\vec{a}_1)]^{n_1} [C(\vec{a}_2)]^{n_2} [C(\vec{a}_3)]^{n_3}$$

In addition $T_{-R} = T_R^{+}$ $\therefore$ $C(-\vec{R}) = C(\vec{R})^*$

$$\because C(\vec{R}) C(-\vec{R}) = C(0) = 1$$
$$\therefore |C(\vec{R})|^2 = 1$$

$\therefore$ It's always possible to write

$C(\vec{a}_i) = e^{2\pi i x_i}$ x_i being some numbers

$$\therefore C(\vec{R}) = e^{2\pi i (n_1 x_1 + n_2 x_2 + n_3 x_3)}$$

Let $\vec{g}_i$ be primitive reciprocal lattice vectors

$$\vec{g}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$$

$$\therefore \; 2\pi(n_1 x_1 + n_2 x_2 + n_3 x_3)$$

$$= \underbrace{(n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3)}_{\vec{R}} \cdot \underbrace{(x_1\vec{g}_1 + x_2\vec{g}_2 + x_3\vec{g}_3)}_{''\vec{k}}$$

$$\equiv \vec{k}\cdot\vec{R}$$

$$\therefore \; C(\vec{R}) = e^{i\vec{k}\cdot\vec{R}}$$

Hence $\psi(\vec{r}+\vec{R}) = T_R\,\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{R}}\,\psi(\vec{r})$

there exists $\vec{k}$ such that

<u>Crystal momentum</u> v.s. <u>momentum</u>

From the above derivation, it is clear that $\because [T_R, H] = 0$

$C(R)$ is a constant of motion : $\frac{dT_R}{dt} = \frac{i}{\hbar}[T_R, H] = 0$

$\therefore$ What is conserved is $\underline{e^{i\vec{k}\cdot\vec{R}}}$!

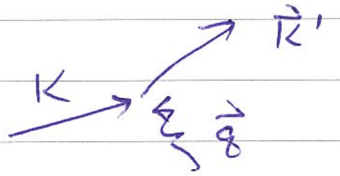
Hence $\hbar\vec{k}$ (for electronic systems) is not the real momentum. Just as $\vec{k}$ for phonons, $\vec{k}$ is termed as <u>crystal momentum</u>!

It is clear that $\psi_k(\vec{r})$ is not an eigenstate to momentum:

$$\frac{\hbar}{i}\nabla\psi_k = \frac{\hbar}{i}\nabla\left[e^{i\vec{k}\cdot\vec{r}}u_k(\vec{r})\right] = \hbar\vec{k}\,\psi_k(\vec{r}) + e^{i\vec{k}\cdot\vec{r}}\frac{\hbar}{i}\nabla u_k(\vec{r})$$

As long as momentum conservation is concerned, one allows $\hbar\vec{G}$ difference and this is the umklapp process for electrons.

e.g. $\hbar\vec{k}' = \hbar\vec{k} + \hbar\vec{q} + \hbar\vec{G}$



Structure of reciprocal lattice

- The Bloch theorem implies that $\vec{k}$ is a good label for electrons.

If we further impose the periodic boundary condition, $\psi(\vec{r}+N_i\vec{a}_i) = \psi(\vec{r})$ $i = 1, 2, 3$

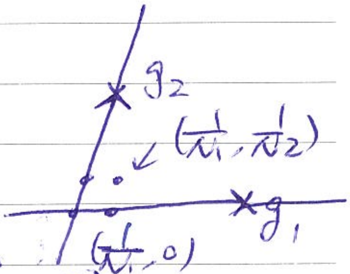
$$\because \psi(\vec{r}+N_i\vec{a}_i) = e^{i\vec{k}\cdot N_i\vec{a}_i}\psi(\vec{r})$$

$$\therefore e^{i\vec{k}\cdot N_i\vec{a}_i} = 1 \quad \text{for } i = 1, 2, 3$$

Therefore, if we write $\vec{k} = x_1\vec{g}_1 + x_2\vec{g}_2 + x_3\vec{g}_3$,

we get $2\pi x_i N_i = 2\pi m_i$

$$\therefore x_i = \frac{m_i}{N_i} \quad m_i = \text{integers}$$



$$\vec{k} = \frac{m_1}{N_1}\vec{g}_1 + \frac{m_2}{N_2}\vec{g}_2 + \frac{m_3}{N_3}\vec{g}_3$$

$\therefore$ Each allowed $\vec{k}$ occupies $\Delta^3\vec{k} = \frac{\vec{g}_1}{N_1}\cdot\left(\frac{\vec{g}_2}{N_2}\times\frac{\vec{g}_3}{N_3}\right)$

i.e. $\Delta^3\vec{k} = \frac{1}{N}\ \vec{g}_1\cdot(\vec{g}_2\times\vec{g}_3)$

Since the volume of a primitive cell of the reciprocal lattice $= \vec{g}_1\cdot(\vec{g}_2\times\vec{g}_3)$

$\therefore$ # of allowed $\vec{k}$ in a primitive cell of the reciprocal lattice $= N =$ # of sites of the crystal!

Furthermore, because $\vec{g}_1\cdot(\vec{g}_2\times\vec{g}_3) = \frac{(2\pi)^3}{v}$, $v = V/N$

(using $\vec{g}_1 = 2\pi\frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}$, $\vec{g}_2 = 2\pi\frac{\vec{a}_3\times\vec{a}_1}{\vec{a}_2\cdot(\vec{a}_3\times\vec{a}_1)}$, $\vec{g}_3 = 2\pi\frac{\vec{a}_1\times\vec{a}_2}{\vec{a}_3\cdot(\vec{a}_1\times\vec{a}_2)}$), we find

$$\Delta^3\vec{k} = \frac{1}{N}\times\frac{(2\pi)^3}{v} = \frac{(2\pi)^3}{V}$$

which is exactly the same form as that for free electrons.

$$\therefore \sum_{\substack{k \\ \in \text{primitive} \\ \text{cell}}} F(\vec{k}) = \frac{V}{(2\pi)^3}\sum_{k} F(\vec{k})\ \Delta^3\vec{k}$$

$$= V\int\frac{d^3\vec{k}}{(2\pi)^3}\ F(\vec{k})$$

$$= V\int_0^1\int_0^1\int_0^1\frac{dx_1\,dx_2\,dx_3}{(2\pi)^3}\ F(x_1, x_2, x_3)$$

$$\vec{k} = x_1\vec{g}_1 + x_2\vec{g}_2 + x_3\vec{g}_3$$

Energy bands

∴ For a given k, $\hat{H}\psi_k = \lambda \psi_k$.

In the case of electrons, we set $\psi_k = e^{i\vec{k}\cdot\vec{r}} u_k(r)$

$$\hat{H}\psi_k = e^{i\vec{k}\cdot\vec{r}}\left[\frac{\hbar^2}{2m}\left(\frac{1}{i}\nabla+\vec{k}\right)^2 + U(\vec{r})\right] u_k(\vec{r})$$

∴ $u_k(\vec{r})$ satisfies

$$\left[\frac{\hbar^2}{2m}\left(\frac{1}{i}\vec{\nabla}+\vec{k}\right)^2 + U(\vec{r})\right] u_k(\vec{r}) = \varepsilon\, u_k(\vec{r}) \quad \text{-- ④}$$

with the boundary condition $u_k(\vec{r}) = u_k(\vec{r}+\vec{R})$ -- ⑤

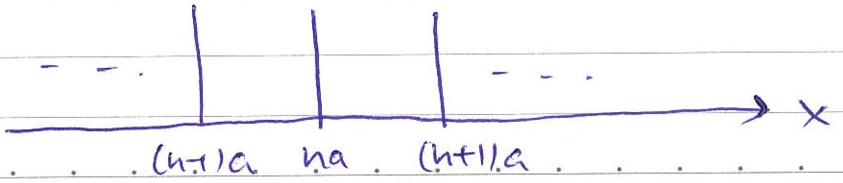
This is the remarkable advantage that the Bloch theorem implies: one only needs to solve the problem in a unit cell!!

It thus reduces the effort of dealing 10^{23} atoms in a crystal to the effort of dealing one!

As an example, we consider the classic example: periodic potential in 1D.

A Kronig-Penny model

$$U(x) = g\sum_{n=-\infty}^{\infty}\delta(x-na) \qquad g>0 \text{ (repulsive)}$$



Between $\begin{cases} (n-1)a \ \& \ na, \\ na \ \& \ (n+1)a \end{cases}$ $U=0$

$\psi(x)$ is a combination of e^{iqx} & e^{-iqx}.
with $\frac{\hbar^2 q^2}{2m} = \varepsilon$

We set

$(n-1)a \leq x < na$

$$\psi(x) = A_{n-1} e^{iq(x-na)} + B_{n-1} e^{-iq(x-na)}$$

$na \leq x < (n+1)a$

$$\psi(x) = A_n e^{iq(x-(n+1)a)} + B_n e^{-iq(x-(n+1)a)}$$

Boundary conditions at $x = na$

$$\psi(na^-) = \psi(na^-) \quad \text{-- ⑥}$$

$$\frac{d}{dx}\psi\Big|_{x=na^+} - \frac{d}{dx}\psi\Big|_{x=na^-} = \underbrace{\frac{2m}{\hbar^2} g}_{\equiv\ \lambda} \psi(na) \quad \text{-- ⑦}$$

⑥, ⑦ implies

$$A_{n-1} + B_{n-1} = A_n e^{-iqa} + B_n e^{iqn}$$

$$iq(A_n e^{-iqa} - B_n e^{iqa}) - iq(A_{n-1} - B_{n-1}) = \lambda(A_{n-1} + B_{n-1})$$

Hence, we can write

$$\begin{pmatrix} 1 & 1 \\ \lambda+iq & \lambda-iq \end{pmatrix} \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix} = \begin{pmatrix} e^{-iqa} & e^{iqa} \\ iq e^{-iqa} & -iq e^{iqa} \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix}$$

$$\therefore \begin{pmatrix} A_n \\ B_n \end{pmatrix} = T \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix} \quad \text{----} ⑧$$

T= transfer matrix (essentially translational operator)

$$T = \begin{pmatrix} e^{-iqa} & e^{iqa} \\ +iq e^{-iqa} & -iq e^{iqa} \end{pmatrix}^{-1} \begin{pmatrix} 1 & 1 \\ \lambda + iq & \lambda - iq \end{pmatrix}$$

$$= \frac{-1}{2iq} \begin{pmatrix} -iq e^{iqa} & -e^{iqa} \\ -iq e^{-iqa} & e^{-iqa} \end{pmatrix} \begin{pmatrix} 1 & 1 \\ \lambda + iq & \lambda - iq \end{pmatrix}$$

$$= \frac{-1}{2iq} \begin{pmatrix} -2iq e^{iqa} - \lambda e^{iqa} & -\lambda e^{iqa} \\ \lambda e^{-iqa} & -2iq e^{-iqa} + \lambda e^{-iqa} \end{pmatrix}$$

Now, Bloch theorem implies $\psi(x+a) = \psi(x) e^{ika}$ for $(n-1)a < x < na$

$$\therefore A_n \left[e^{iq(x+a-(n+1)a)} + e^{-iq(x+a-(n+1)a)} \right] = \left[A_{n-1} e^{iqx} + B_{n-1} e^{-iqx} \right] e^{ika}$$

$$\therefore A_n = e^{ika} A_{n-1}, \quad B_n = e^{ika} B_{n-1}$$

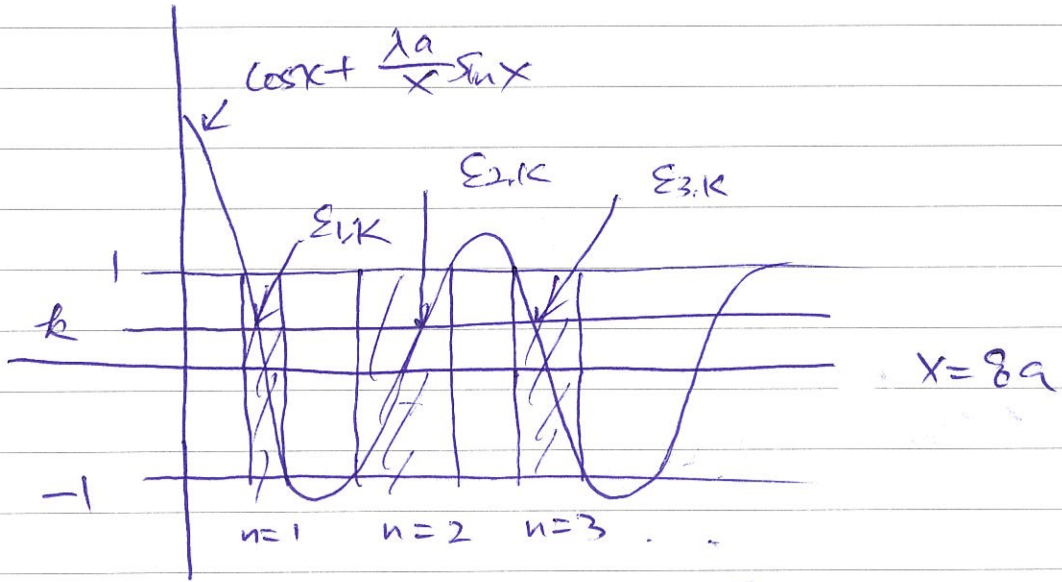
$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = e^{ika} \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix} \quad \text{--} ⑨$$

Eqs ⑧ & ⑨ simply implies the eigenvalue of T is e^{ika}!

Similarly, the eigenvalue of T^{-1} is e^{-ika}!

From $\det(T - e^{iKa}\mathbb{I}) = 0$, one finds

$$\cos Ka = \cos qa + \frac{\lambda}{2q}\sin qa$$



$\because -1 \le \cos Ka \le 1$, one sees that there are many allowed $\varepsilon = \frac{\hbar^2 K^2}{2m}$ for a given K. They can generally be labelled as $\varepsilon_n(K)$.

As K varies, $\varepsilon_n(K)$ changes continuously. Therefore, they form so-called energy bands.

Futhermore, since only $\cos Ka$ matters, $K+G$ & K have the same value of $\cos Ka$ $(G = \frac{2\pi m}{a})$.

$$\varepsilon_n(K+G) = \varepsilon_n(K) \quad --- \quad ⑩$$

For the wavefunction, Eq ⑨ implies

$$\psi_{k+G} = \psi_k \quad --- ⑪$$

The meaning of eqs. ⑪ & ⑫ is that k is a label of electronic state. and k+G labels the same electronic state!

Fourier analysis One can under this by looking into the Fourier analysis of $\psi(\vec r)$.

In general, $\psi(\vec r) = \sum_{q} \psi_{\vec q}\, e^{i\vec q\cdot\vec r}$ (no restriction on $\vec q$)

$$U(\vec r) = \sum_{G} U_G\, e^{i\vec G\cdot\vec r}$$

$$(\because U^*(x) = U(x) \quad \therefore U^*_{-G} = U_G)$$

$$U(\vec r)\,\psi(\vec r) = \sum_{G}\sum_{K} U_G\, \psi_q\, e^{i\vec G\cdot\vec r}\, e^{i\vec q\cdot\vec r}$$

$$= \sum_{q}\Big[\sum_{G} U_G\, \psi_{\vec q - G}\Big] e^{i\vec q\cdot\vec r}$$

$\nearrow$

$\vec q = \vec q + \vec G$

$$\because \frac{\hbar^2}{2m}\nabla^2\psi(\vec r) = \sum_{q} \varepsilon_q^0\, \psi_q\, e^{i\vec q\cdot\vec r} \qquad \varepsilon_q^0 = \frac{\hbar^2 q^2}{2m}$$

$$\therefore \hat H\psi = \varepsilon\psi \Rightarrow \sum_{q}\Big[\varepsilon_q^0\psi_q + \sum_{G} U_G\,\psi_{q-G}\Big] e^{i\vec q\cdot\vec r} = \varepsilon\sum_{q}\psi_q\, e^{i\vec q\cdot\vec r}$$

$$\therefore (\varepsilon_q^0 - \varepsilon)\,\psi_q + \sum_{G} U_G\,\psi_{q-G} = 0$$

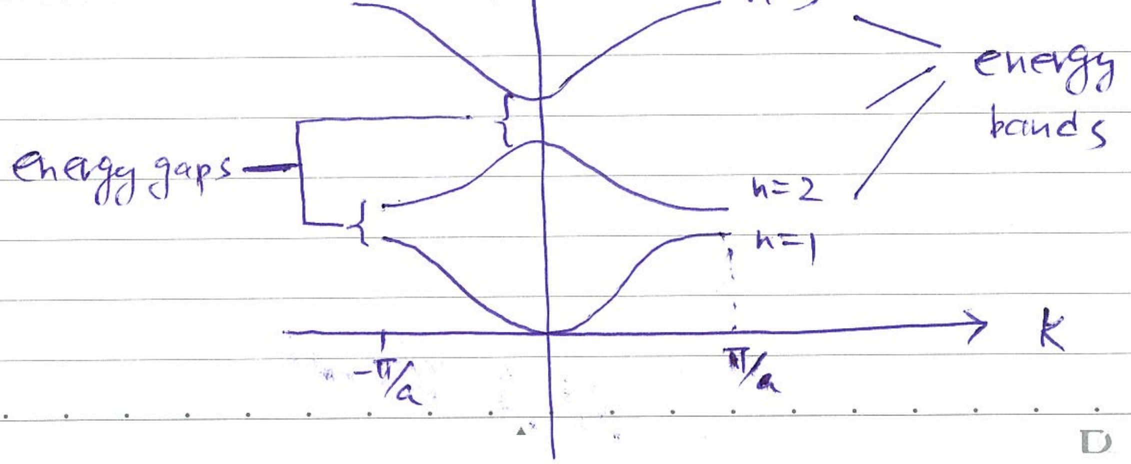
It is clear that for a given k, k only couples to $k \pm G$, $k \pm 2G$, $k \pm 3G$, ...

Hence, $\psi(\vec{r}) = \sum_{G} \psi_{\vec{k}-G}\, e^{i(\vec{k}-\vec{G})\cdot\vec{r}}$ --- ⑫

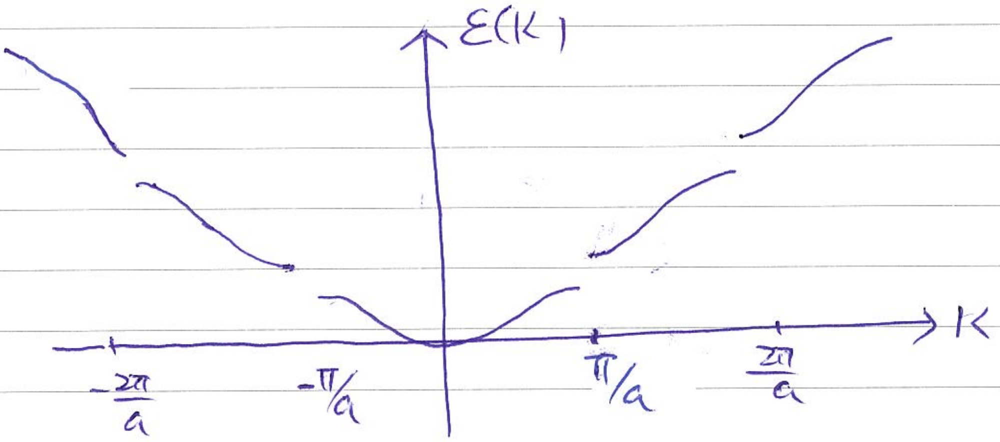
When one changes $\vec{k} \to \vec{k}+\vec{G}'$, it only shift G to $G-G'$. Since G is a dummy variable, it describes the same wave function!

This is similar to the case of phonons. one can restrict the label of k to the 1st Brillouin zone or not restrict the label. This results in 3 different ways of indexing (labeling) / describing the energy bands. Note that $\vec{k}$ is only a label and it doesn't mean $\hbar\vec{k}$ is the momentum of the electrons. Unlike phonons which doesn't have definition of real momentum, the electron's momentum can exceed the 1st Brillouin zone. In some sense, $\hbar(\vec{k}+\vec{G})$ has meaning it doesn't exist for phonons.

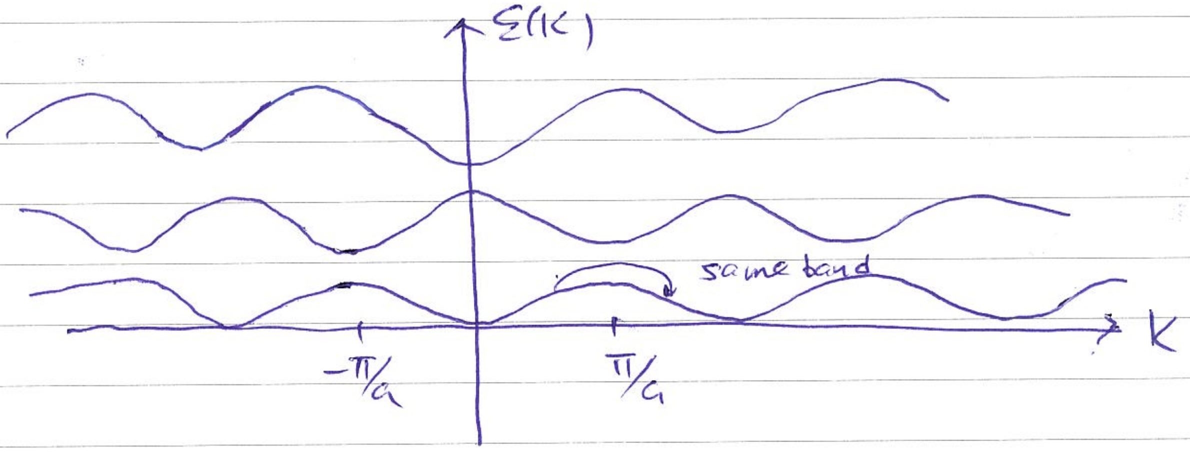
1. Reduced-zone scheme



2. extended-zone scheme



3. repeated-zone scheme



Density of states & Van Hove singularities

For many properties of crystals, it is the Energy. $\mathcal{E}_n(K)$ that plays the dominant role.

It is therefore useful to define the density of states (DOS) for the nth band

spin's degree of freedom

by $g_n(\mathcal{E}) = \frac{2}{V}\sum_{K} \delta(\mathcal{E}-\mathcal{E}_n(K))$

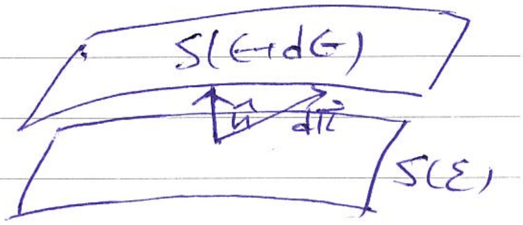
$$= 2\int \frac{d^dK}{(2\pi)^d}\, \delta(\mathcal{E}-\mathcal{E}_n(K))$$

$g_n(\varepsilon)$ can be casted into an integral over the surface $\varepsilon_n(k)=\varepsilon$ by noting that

$$\delta(\varepsilon-\varepsilon_n(\vec{k})) = \frac{\theta(\epsilon-\varepsilon_n(\vec{k}))-\theta(\epsilon-\epsilon_n(\vec{k})-d\epsilon)}{d\epsilon}$$

$\because\ d^d\vec{k} = dS(\epsilon)\cdot(d\vec{k}\cdot\hat{n})$

$$\hat{n}=\frac{\vec{\nabla}_k\,\epsilon_n(\vec{k})}{|\vec{\nabla}_k\,\epsilon_n(\vec{k})|}$$



$\epsilon_n(\vec{k}+d\vec{k}) = \epsilon_n(\vec{k}) + d\vec{k}\cdot\nabla_k\epsilon_n(\vec{k})$ $\therefore\ d\vec{k}\cdot\nabla_k\epsilon_n(\vec{k})=d\epsilon$

$$\therefore\ d\vec{k}\cdot\hat{n} = \frac{d\epsilon}{|\nabla_k\epsilon_n(k)|}$$

$$\int d\epsilon\,\delta(\epsilon-\epsilon_n(\vec{k}))=1$$

$$\therefore\ g_n(\epsilon)=\frac{2}{(2\pi)^d}\int\frac{dS}{|\nabla_k\epsilon_n(\vec{k})|}\bigg|_{\epsilon_k=\epsilon} \quad \text{---} ⑫$$

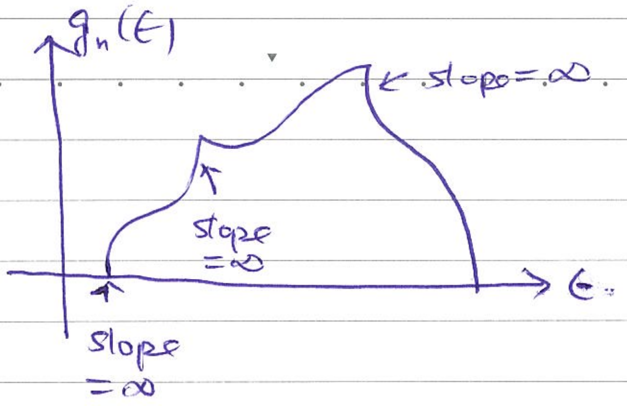
$\because$ $\epsilon_n(\vec{k})$ is continuous, periodic $\vec{k}$ & bounded, there must be points at which $|\nabla_k\epsilon_n(\vec{k})|=0$

max, min, saddle points!

$\therefore$ Integrand diverges in ⑫

In 3D, these divergences are integrable (see HW Ex 8-2), $g_n(\epsilon)$ is finite but slopes are infinite;

example

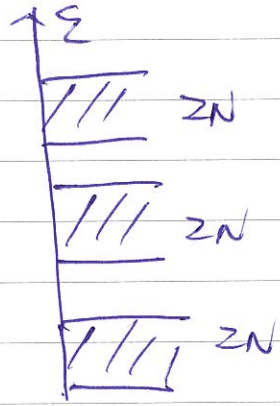


For 2D, $g_n(\epsilon) \sim \ln\left|\frac{\epsilon}{\epsilon_0} - 1\right|$ or $\Theta(\pm\epsilon)$

1D, $g_n(\epsilon) \sim \frac{1}{\sqrt{\epsilon}}$

Fermi energy, metals & insulators

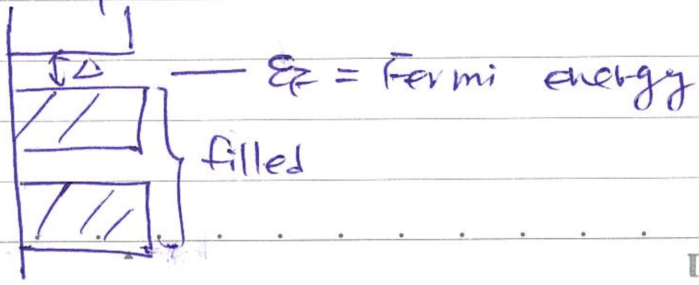
As we have counted, # of k in a Brioullin zone = # of lattice points.



Therefore, including spin ↑ & ↓, each band can hold 2N electrons!

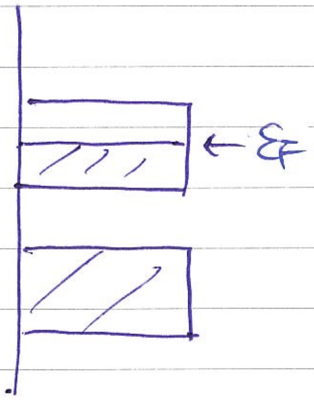
Therefore, the most important aspect of lattice is the emergent properties of metals & insulators (band)

(i) # of electrons in a primitive cell = even



In this case, to excite the electron, one needs an energy of Δ. The system is gapped and is a band insulator. The Electric field can't excite the electron across the gap.

(ii) # of electrons in a primitive cell = odd



The energy band that ε_F cuts through is half-filled. Therefore, there is no energy gap to excite an electron. The system is a metal.

Mean velocity of electrons in periodic potential

Classically, an electron constantly collides with ions. Quantum mechanically, this is no longer true.

In fact, we find that the average velocity (momentum) for the Bloch state is

$$\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_k \varepsilon_n(\vec{k})$$

$$= \frac{1}{m}\int d^3\vec{r}\, \psi^*_{n,k}\, \frac{\hbar}{i}\vec{\nabla}\, \psi_{n,k}$$

To show it, we note that

$$\varepsilon_n(k+q) = \varepsilon_n(k) + \vec{q}\cdot\vec{\nabla}_k \varepsilon_n(\vec{k}) + O(q^2)$$

$$H_{k+q} = \underbrace{H_k}_{\frac{\hbar^2}{2m}\left(\frac{1}{i}\vec{\nabla}+\vec{k}\right)^2 + U(\vec{r})} + \frac{\hbar^2}{m}\vec{q}\cdot\left(\frac{1}{i}\nabla+\vec{k}\right) + \frac{\hbar^2 q^2}{2m}$$

$$\updownarrow$$

$$\left[\frac{\hbar^2}{2m}\left(\frac{1}{i}\vec{\nabla}+k+q\right)^2 + U(r)\right]u_{k+q}(\vec{r}) = \varepsilon_{k+q}u_{k+q}(\vec{r})$$

∴ The $\overset{\text{linear}}{\vee}$ perturbation is $\hat{U} = \frac{\hbar^2}{m}\vec{q}\cdot\left(\frac{\hbar}{i}\nabla+\vec{k}\right)$

Hence, $\vec{q}\cdot\vec{\nabla}_k \varepsilon_n(\vec{k}) = \int d^3\vec{r}\, u^*_{nk}\, \hat{V}\, u_{nk}$

$$= \frac{\hbar^2}{m}\vec{q}\cdot\int d^3\vec{r}\, u^*_{nk}\left(\frac{1}{i}\vec{\nabla}+\vec{k}\right)u_{nk}$$

$$\therefore \vec{\nabla}_k \varepsilon_n(\vec{k}) = \frac{\hbar^2}{m}\int d^3\vec{r}\, u^*_{nk}\left(\frac{\hbar}{i}\vec{\nabla}+\vec{k}\right)u_{nk}$$

$$\because \psi_{nk} = e^{i\vec{k}\cdot\vec{r}}u_{nk} \quad \therefore \left(\frac{1}{i}\vec{\nabla}+\vec{k}\right)u_{nk} = e^{-i\vec{k}\cdot\vec{r}}\frac{1}{i}\vec{\nabla}\psi_{nk}$$

$$\therefore \vec{\nabla}_k \varepsilon_n(\vec{k}) = \hbar\frac{1}{m}\int d^3\vec{r}\, \psi^*_{nk}\frac{\hbar}{i}\nabla\psi_{nk} = \hbar\frac{\langle\hat{p}\rangle}{m}$$

$$= \hbar\vec{v}_n(\vec{k})$$

$$\therefore \vec{v}_n(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_k \varepsilon_n(\vec{k})$$

This relation clearly implies that for ideal lattices, electrons can propagate with definite velocity. There force, $l=\infty$ which explains why l can be larger than the lattice spacing.

Symmetries of Schrödinger equation on a lattice

In addition to translational invariance, crystals also have discrete rotational symmetries (G) and etc summarize in the point group.

The translational invariance, summarized in the Bloch theorem, enables us to reduce the computational effort to a unit cell.

Do we have similar advantage in using point group symmetries?

* Symmetry points

First, the point group also acts on k so that there are special points in the k space.

Rotation on real space = inverse rotation on k point:

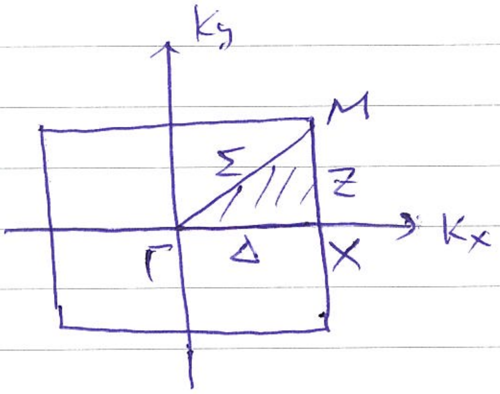
$$\vec{k}\cdot R\vec{r} = k^T \overleftrightarrow{R}\, r = (R^T k)^T\cdot r$$
$$= (R^{-1}\vec{k})\cdot\vec{r}$$

Therefore, under the group operation, the label k of the Bloch election becomes $\underline{R^{-1}\vec{k}}$!

There are special points that are invariant (up to a reciprocal lattice vector) under point group operations. For instance $\vec{k}=0$.

$R^{-1}0 = 0$. This is usually denoted by Γ point.

Take the square lattice as an example.



The point group is 4mm

$$G = \{E, \overset{R_1}{\overset{\|}{R_{\pi/2}}}, \overset{R_3}{\overset{\|}{R_{-\pi/2}}}, \overset{R_2}{\overset{\|}{R_{\pi}}}, m_x, m_y, \underbrace{m_+, m_-}\}$$

mirror w.r.t. x±y axes

The 1st Brillauin zone is shown in the above.

Γ is invariant under $G_\Gamma = G$

M is also invariant (up to a reciprocal lattice vector) $G_M = G_\Gamma = G$

$G_X = \{E, R_2, m_x, m_y\}$

$\overline{\Gamma X} \equiv \Delta$. $G_\Delta = \{E, m_x\}$

$\overline{\Gamma M} \equiv \Sigma$. $G_\Sigma = \{E, M_+\}$

$\overline{XM} = Z$

$G_Z = \{E, m_y\}$

* $\Delta \Gamma X M$

To characterize (e.g. $\varepsilon_n(k)$) the 1st Brillouin zone, it is sufficient to characterize the region bounded by $\Gamma - X - M$.

$$\because \quad H\psi_k = \varepsilon_k \psi_k$$

$$\Rightarrow \quad g H g^{-1} g \psi_k = \varepsilon_k g \psi_k \qquad g \in G$$

Now, H is invariant under g

$$\therefore \quad H g \psi_k = \varepsilon_k g \psi_k \qquad --- ⑬$$

In other words, ψ_k, $g\psi_k$ possess the same ε_k. As already shown, $g\psi_k = \psi_{g^{-1}k}(\vec{r})$

$$\therefore \quad g\psi_k = \psi_{k'}, \qquad k' = g^{-1}k$$

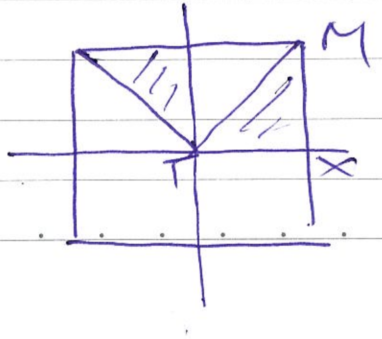
$$\because \quad H\psi_{k'} = \varepsilon_{k'}\psi_{k'} \qquad -- ⑭$$

$$\therefore \quad \varepsilon_{k'} = \varepsilon_k, \qquad \text{i.e.} \quad \varepsilon_{g^{-1}k} = \varepsilon_k$$

Example: 4mm (square lattice)

$$g = R_3, \qquad g^{-1} = R_1, \qquad g^{-1}\vec{k} = (-k_y, k_x)$$

$$\therefore \quad \varepsilon(k_x, k_y) = \varepsilon(-k_y, k_x)$$



(see left figure)

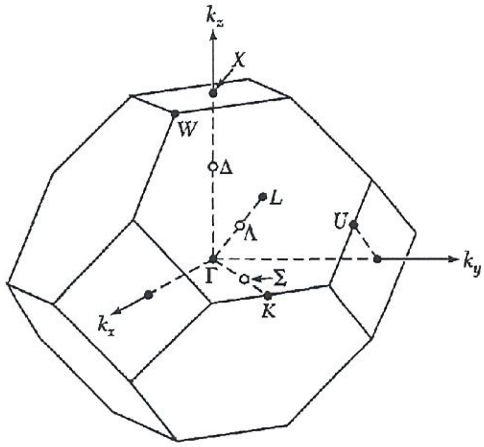
i.e. two triangles are related to each other.

It's suffice to know ε_k in $\Delta\Gamma X M$

One can convince himself that all other regions are related to $\Delta\Gamma XM$ by symmetries!

Therefore, it's suffice to know ε_k in $\Delta\Gamma XM$.

Similar constructions apply to other crystals. The followings are a couple of examples.



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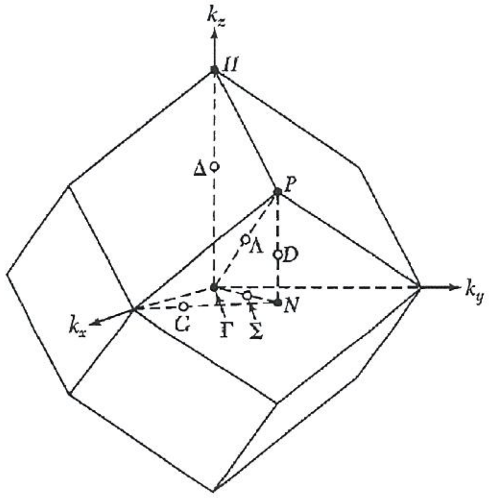

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* Degeneracies at symmetry points

There is a tendency for $\varepsilon(k)$ to be degenerate at symmetry points such as Γ, M & X. The reason is that crystals possess both point group symmetry & translational symmetry.

For instance, Γ doesn't just represent $k=0$.

but it also represent $\vec{k} = \vec{G}, 2\vec{G}, -\vec{G}, \cdots$

Example: square lattice

$$\overbrace{\left(\frac{2\pi}{a}, 0\right)}^{G_1}, \overbrace{\left(-\frac{2\pi}{a}, 0\right)}^{G_2}, \overbrace{\left(0, \frac{2\pi}{a}\right)}^{G_3}, \overbrace{\left(0, \frac{-2\pi}{a}\right)}^{G_4}$$

map into each other under $\underbrace{\text{4mm point}}_{\text{operations of}}$ group.

$\because$ if $g \in G_{4mm}$ $\quad gHg^{-1} = H$

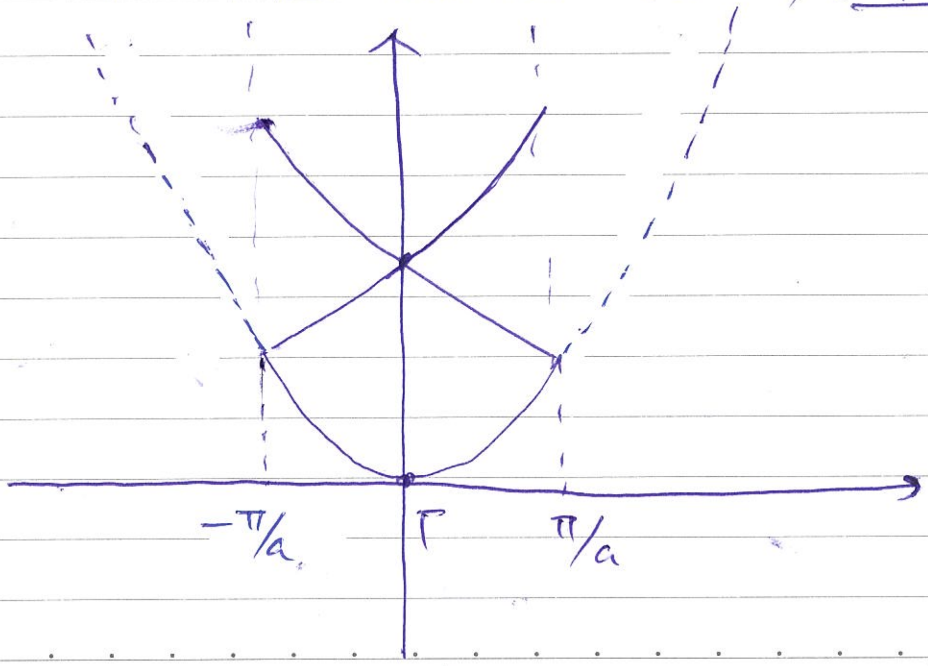
$$\therefore gHg^{-1}(g\psi_{G_i}) = \varepsilon(g\psi_{G_i})$$

$$\therefore H(g\psi_{G_i}) = \varepsilon(g\psi_{G_i})$$

$g\psi_{G_i} = \psi_{g^{-1}G_i}$ are degenerate with ψ_{G_i}

Since they are all labelled by $k=0$, $k=0$ is highly degenerate in ε!

Example: 1D Simple lattice $(U=0)$ (empty lattice)



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Example: Empty lattice bands for 2D square lattice

$$E_{n,m} = \frac{\hbar^2}{2m}(\vec{k}+\vec{G}_{nm})^2 ,$$

$$\vec{G}_{nm} = \frac{2\pi}{a}(n\hat{x}+m\hat{y}) , \quad \vec{k} \equiv \frac{2\pi}{a}(x,y)$$

$$-\tfrac{1}{2} \le x,y \le \tfrac{1}{2}$$

$$\psi_{nm}(\vec{k},\vec{r}) = e^{i(\vec{k}+\vec{G}_{nm})\cdot\vec{r}}$$

$$E_{n,m} = \frac{\hbar^2}{2ma^2}\left[(x+n)^2+(y+m)^2\right]$$

At Γ ($k=0$) : $E_{0,0} = 0$ $\quad E_{1,\pm1} = \frac{\hbar^2}{2ma^2}\times 2$

$E(0,\pm1) = E(\pm1,0) = \frac{\hbar^2}{2ma^2}$ $\quad E_{-1,\pm1} = \frac{\hbar^2}{2ma^2}\times 2$

At X ($\vec{k}=(1,0)$) $\quad E_{0,0} = \frac{\hbar^2}{2ma^2}\times\left(\frac{1}{2}\right)^2 = \frac{1}{4}\frac{\hbar^2}{2ma^2}$

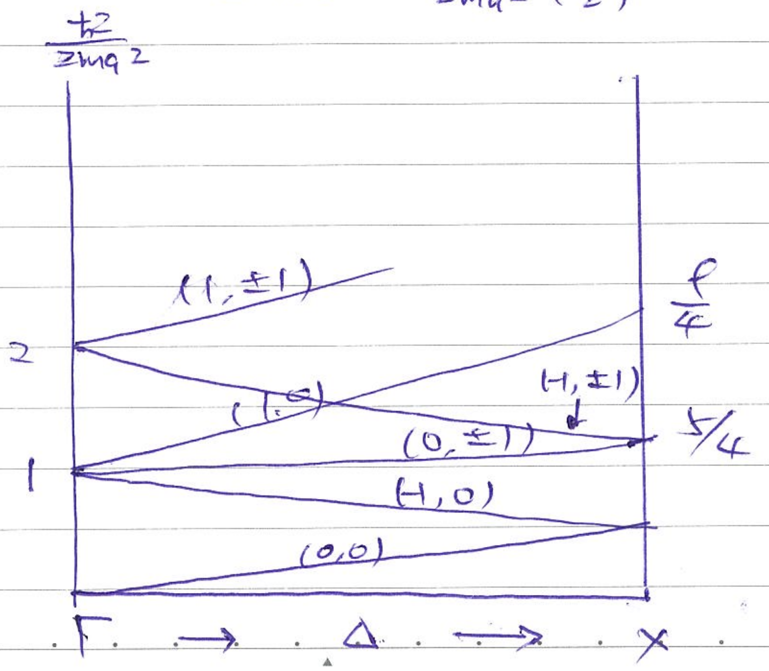
$E_{-1,0} = \frac{\hbar^2}{2ma^2}\times\left(-\frac{1}{2}\right)^2 = \frac{1}{4}$ 〃

$E_{0,\pm1} = \frac{\hbar^2}{2ma^2}\left[\left(\frac{1}{2}\right)^2+1^2\right] = \frac{5}{4}$ 〃

$E_{-1,\pm1} = \frac{\hbar^2}{2ma^2}\left[\left(-\frac{1}{2}\right)^2+1^2\right) = 5/4$ 〃

$E_{1,0} = \frac{\hbar^2}{2ma^2}\left(\frac{3}{2}\right)^2$

We find



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* Irreducible represenations & reduction of computational effort

It is well known that in quantum mechanics, if one finds another operator (observable $\hat{O}$) that is commute with $\hat{H}$, one can save the computational effort by restricting us to the simultaneous eigenvalue spaces.

For instance, $\underline{[H, L^2] = 0}$, $\underline{[H, L_z] = 0}$

L_z = z component of angular momentum

L^2 = square of angular momentum

Hence, L_z, L^2 & H can be diagonalized simultaneously. Since the eigenfunctions to L_z & L^2 is $Y_l^m(\theta, \phi)$, if we use these eigenfunctions as basis in (θ, ϕ) to expand H, H is block diagonalized :

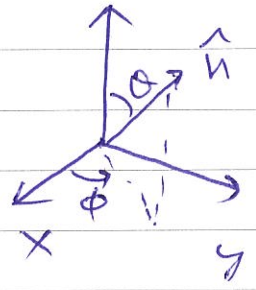
$$\begin{pmatrix} \boxed{l=1} & 0 & 0 & 0 \\ 0 & \boxed{l=2} & \overset{2l+1}{0} & 0 \\ 0 & \overset{2l+1}{0} & \boxed{l=3} & 0 \\ 0 & 0 & 0 & \ddots \end{pmatrix}$$

In other words, $\langle l | H | l' \rangle \propto \delta_{ll'}$, different matrix elements of $l = 0$! Hence rotational symmetries reduce the computational effort to each block of a $(2l+1)(2l+1)$ matrix !

Similar reduction also exists for point groups.

In this case, one needs to find representations of group elements first. In the case of continuous rotations, the group element is

$$R(\theta, \phi) = e^{\frac{i}{\hbar} \vec{J} \cdot \hat{n}}$$



where $\hat{n}$ is the axis of rotation.

$\vec{J} = \vec{L}$ if there is no spin.

Using $Y_l^m(\theta, \phi)$, $R = \begin{pmatrix} \boxed{l=1} & 0 & 0 \\ 0 & \boxed{l=2} & 0 \\ 0 & 0 & \boxed{l=3} \end{pmatrix}$

is also block diagonalized !

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Therefore, we have to represent elements of the point group in terms of matrices. This is terms as <u>representation of the group</u>.

Irreducible representation of point groups

A representation is reducible if the corresponding matrices can be brought into the block diagonal by choosing appropriate basis. Otherwise, it is irreducible. For rotational groups, the $(2\ell+1)\times(2\ell+1)$ blocks in $R(\theta,\phi)$ can't be reduced further, they are irreducible.

Two useful theorems:

(i) # of irreducible representations (IRs) = # of conjugate classes

<u>a class</u> = subset of a group in which $R' = ARA^{-1}$. $A, R, R' \in$ the same subset.

Example: 4mm.

$$\left.\begin{array}{l} 5 \text{ classes } ① E \quad ② R_{\pi/2}, R_{-\pi/2} \quad ③ R_{\pi} \\ \qquad ④ m_x, m_y \quad ⑤ m_+, m_- \end{array}\right\} \therefore \# \text{ of IRs} = 5. \ \Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4, \Gamma_5$$

(ii) For ith IRs, l_i = dimension (of the matrix), $\sum_i l_i^2$ = # of group elements

example : 4mm ⇒ l_1, l_2, l_3, l_4, l_5.

$$l_1^2+l_2^2+l_3^2+l_4^2+l_5^2 = 8$$

∴ only $1^2+1^2+1^2+1^2+2^2 = 8$ is possible

∴ 4 IRs ⇒ 1 dimension

1 IRs ⇒ 2×2 matrix.

Basis functions

To represent point groups by matrices, one needs to choose basis functions.

Usually, one chooses polynomials of x, y, z as basis functions.

example : 4mm

In 4mm, x always ⟶ ±x, or ±y

	E	R_π	$R_{\pi/2}$	$R_{-\pi/2}$	m_x	m_y	m_+	m_-
x	x	$-x$	y	$-y$	x	$-x$	y	$-y$
y	y	$-y$	$-x$	x	$-y$	y	x	$-x$

IR. Γ_1 $\quad \psi_0 = x^2+y^2$

$$D(E) = D(R_\pi) = D(R_{\pi/2}) = D(R_{-\pi/2}) = D(R_{mx})$$
$$= D(R_{my}) = D(R_+) = D(R_-) = 1$$

IR Γ_4 $\quad \psi_4 = xy$

$$D(E) = D(R_\pi) = D(m_+) = D(m_-) = 1$$
$$D(R_{\pi/2}) = D(R_{-\pi/2}) = D(m_x) = D(m_y) = -1$$

These are usually summarized in the group table:

	$\psi_0 = x^2+y^2$	$\psi_2 = xy(x^2-y^2)$	$\psi_3 = x^2-y^2$	$\psi_4 = xy$	$\psi_5 = \begin{pmatrix} x \\ y \end{pmatrix}$
	D_{Γ_1}	D_{Γ_2}	D_{Γ_3}	D_{Γ_4}	D_{Γ_5}
E	1	1	1	1	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
R_π	1	1	1	1	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$
$R_{\pi/2}$	1	1	-1	-1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
$R_{-\pi/2}$	1	1	-1	-1	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
m_x	1	-1	1	-1	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
m_y	1	-1	1	-1	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$
m_+	1	-1	-1	1	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
m_-	1	-1	-1	1	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$
	$l_1 = 1$	$l_2 = 1$	$l_3 = 1$	$l_4 = 1$	$l_5 = 2$

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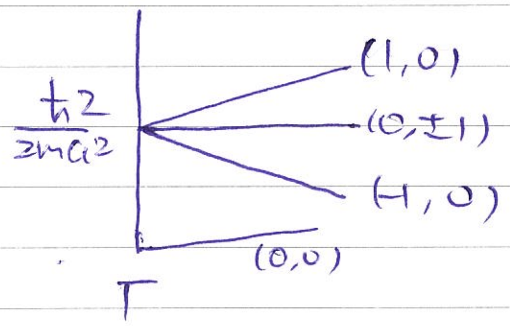
The basis functions are convenient choices by one's construction. They are not unique, hence IRs are not unique. Using these basis functions, one can rewrite $\hat{H}$. $\hat{H}$ will be block diagonalized. However; to apply this to energy bands, one needs to combine the point group with the translational operations, summarized by $\vec{k}$!

As we have seen, not all of $\vec{k}$'s are invariant (up to reciprocal lattice vectors) under operations of point group. Hence, using point group to reduce the computational effort only restrict to symmetry points (such as Γ, X, M, ..) In this case, basis functions are also choosen differently by taking $\vec{k}$ into considerations!

As an example, we shall consider the T point of the square lattice.

As we have seen, when $U=0$,



$$\psi = e^{i\vec{G}_{nm}\cdot\vec{r}}$$

$$\vec{G}_{nm} = \frac{2\pi}{a}(n,m)$$

$\therefore\ \bar{\psi}_{00}(T)=1$ is a choose of basis functions.

$\Rightarrow$ This is IR Γ_1, all elements $\Rightarrow$ I

For $\varepsilon = \frac{\hbar^2}{2ma^2}$, one has

$$\bar{\psi}_{\pm1,0} = e^{\pm\frac{2\pi i}{a}x}$$

$$\bar{\psi}_{0,\pm1} = e^{\pm\frac{2\pi i}{a}y}$$

Hence, to analyze ~~effects~~ due to small $U\neq0$, it's convenient to use $\bar{\psi}_{\pm1,0}$ & $\bar{\psi}_{0,\pm1}$ to construct basis functions.

$\because$ under 4mm, $x \to \pm x$, or $\pm y$
$y \to \pm x$ or $\pm y$

Clearly, from combinations of $\bar{\psi}_{\pm1,0}$, $\bar{\psi}_{0,\pm1}$, one has

IR Γ_1 : $\psi_0 = x^2 \pm y^2 \Leftrightarrow \psi(\Gamma_1) = \cos\frac{2\pi x}{a} + \cos\frac{2\pi y}{a}$

$$\propto \bar{\psi}_{1,0} + \bar{\psi}_{-1,0} + \bar{\psi}_{0,1} + \bar{\psi}_{0,-1}$$

$$\psi(T_3) = \cos\frac{2\pi x}{a} - \cos\frac{2\pi y}{a} \propto \psi_{1,0} + \psi_{-1,0} - \psi_{0,1} - \psi_{0,-1}$$

$$\psi(T_5) = \begin{pmatrix} \sin\frac{2\pi x}{a} \\ \sin\frac{2\pi y}{a} \end{pmatrix} \propto \begin{pmatrix} \psi_{10} - \psi_{-1,0} \\ \psi_{0,1} - \psi_{0,-1} \end{pmatrix}$$

There fore, to investigate effect of U at $\varepsilon \simeq \frac{\hbar^2}{2ma^2}$, $k=0$, one only needs to consider. $\psi(T_1)$, $\psi(T_3)$ & $\psi(T_5)$

$\downarrow$
$|1, T_1\rangle$

& $\psi_{00}(T_1)$ $(=1)$

$\downarrow$
$|0\, T_1\rangle$

Using these basis functions, computational effort is reduced as one can see in below:

To solve $\hat{H}|\psi\rangle = \varepsilon|\psi\rangle$ --- ⑮

One expand $|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle$

$\langle n|$ ⑮

$$\sum_n \underbrace{\langle n|\hat{H}|m\rangle}_{H_{nm}} \underbrace{\langle m|\psi\rangle}_{\psi_m} = \varepsilon\langle n|\psi\rangle$$

$$\underbrace{\begin{pmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & \cdots & \\ H_{31} & H_{32} & & \\ \vdots & \vdots & & \end{pmatrix}}_{\hat{H}} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \vdots \end{pmatrix} = \varepsilon \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \vdots \end{pmatrix}$$

At $k=0$, we use $\begin{pmatrix} \psi_0(\Gamma_1) \\ \psi_1(\Gamma_1) \\ \psi_1(\Gamma_3) \\ \psi_1(\Gamma_5^-) \\ \vdots \\ \vdots \end{pmatrix}$; $\hat{H} = \frac{p^2}{2m} + U$

$$\hat{H} = \begin{pmatrix} \varepsilon_0(\Gamma_1) & \langle 0\Gamma_1|U|1\Gamma_1\rangle & \langle 0\Gamma_1|U|1\Gamma_3\rangle & \langle 0\Gamma_1|U|1\Gamma_5^-\rangle & \cdots \\ \langle 1\Gamma_1|U|0\Gamma_1\rangle & \varepsilon_1(\Gamma_1) & \langle 1\Gamma_1|U|1\Gamma_3\rangle & \langle 1\Gamma_1|U|1\Gamma_5^-\rangle & \cdots \\ \langle 1\Gamma_3|U|0\Gamma_1\rangle & \langle 1\Gamma_3|U|1\Gamma_1\rangle & \varepsilon_1(\Gamma_3) & \langle 1\Gamma_3|U|1\Gamma_5^-\rangle & \cdots \\ \langle 1\Gamma_5^-|U|0\Gamma_1\rangle & \langle 1\Gamma_5^-|U|1\Gamma_1\rangle & \langle 1\Gamma_5^-|U|1\Gamma_3\rangle & \varepsilon_1(\Gamma_5^-) & \cdots \\ - & - & - & & \end{pmatrix}$$

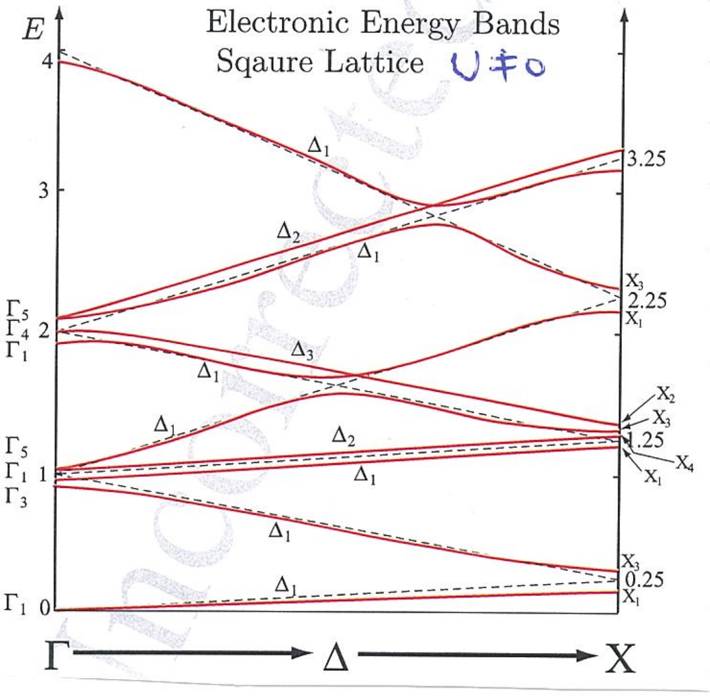
$\Downarrow$ reduces to $\varepsilon_0(\Gamma_1) = 0$, $\varepsilon_1(\Gamma_1) = \frac{\hbar^2}{2ma^2}$

$$\hat{H} = \begin{pmatrix} \varepsilon_0(\Gamma_1) & \langle 0\Gamma_1|U|1\Gamma_1\rangle & 0 & 0 & \cdots \\ \langle 0\Gamma_1|U|1\Gamma_1\rangle & \varepsilon(\Gamma_1) & 0 & 0 & \cdots \\ 0 & 0 & \varepsilon(\Gamma_3) & 0 & \\ 0 & 0 & 0 & \varepsilon(\Gamma_5^-) & \\ \cdots & & & & \ddots \end{pmatrix}$$

elements between different representation $= 0$!

Hence at symmetry points, different IRs of point groups are block diagonalized.

Solving the corresponding determinant, one finds



Clearly, we have seen that translational invariance & point group symmetry have strong effects on electronic states. This, of course, does not restrict to electronic states. E.M. waves & sound waves are also subjected to the same effects.