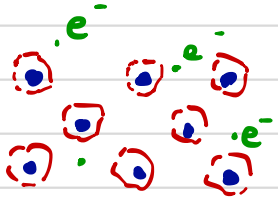
Crystal Structure and Band Theory

P715

Band theory and crystal structure

solids: atoms arrange themselves in crystalline structure



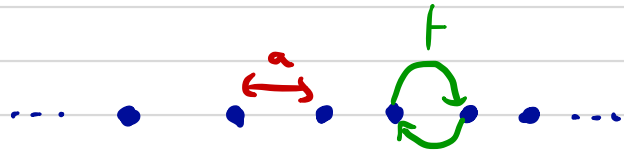
Recall Drude picture: valence e^- scatter off lattice sites (ions)

We'll see that this picture is not correct. Electrons move mostly freely in periodic lattices.

But $E = \frac{p^2}{2m}$ modified by lattice (p not conserved!)

(I) Electrons moving in one dimension

(a) Tight-binding model in 1d



N lattice sites

("tight binding approximation": later). Electrons live on lattice sites.

- Consider a single electron: $|j\rangle$: e^- on site j.

$$\langle i|j\rangle = \delta_{ij}$$

- local onsite energy: E_0, local hopping term: "t" $\neq$ time!

$$H = E_0 \sum_j |j\rangle\langle j| - t \sum_j \left(|j\rangle\langle j+1| + |j+1\rangle\langle j| \right)$$

Use periodic boundary conditions: $|N+1\rangle \equiv |1\rangle$

Solution: $|\psi\rangle = \sum_j \psi_j |j\rangle$

$j \to j-1$

$$H|\psi\rangle = E|\psi\rangle \Rightarrow E_0 \sum_j \psi_j |j\rangle - t\left(\sum_j \psi_{j+1}|j\rangle + \psi_j |j+1\rangle \right)$$

$$= E \sum_j \psi_j |j\rangle$$

$$\Rightarrow E_0 \psi_j - t(\psi_{j+1} + \psi_{j-1}) = E\psi_j$$

lattice second derivative

Solve by lattice Fourier (plane waves) modes:

$$\psi_j = \frac{1}{\sqrt{N}} e^{iKja}$$

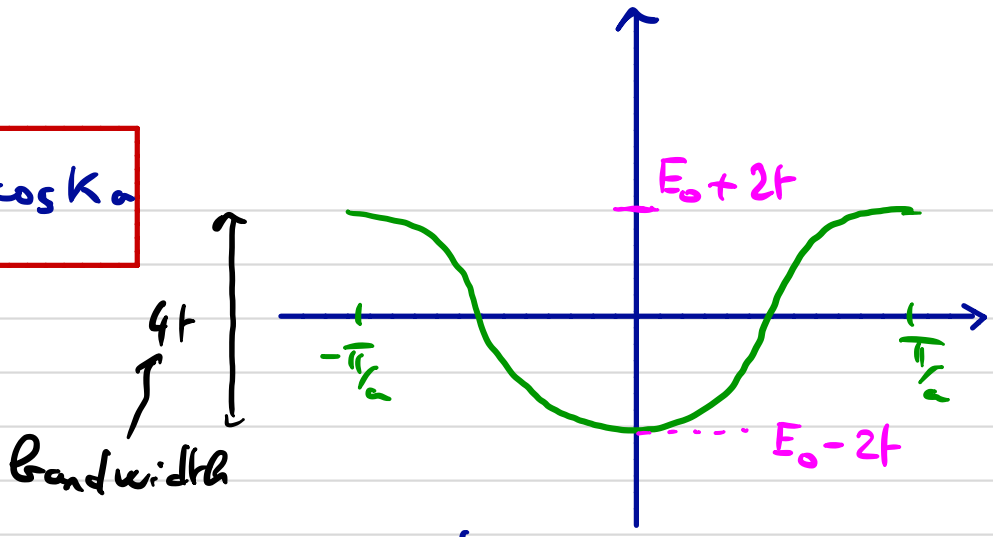
K = wavenumber

$p = \hbar K$ ~ momentum

$$|\psi_K\rangle = \sum_j \frac{1}{\sqrt{N}} e^{iKja} |j\rangle$$

- $K \to K + 2\pi/a$. We can take $K \in \left[-\pi/a, \pi/a\right]$ Brillouin zone
- $\psi_{N+1} = \psi_1$: $e^{iKNa} = 1 \Rightarrow K = \frac{2\pi}{aN} n$, n integer
- $\langle \psi_K | \psi_{K'} \rangle = \frac{1}{N} \sum_j e^{i(K'-K)ja} = \delta_{K,K'}$
- Now we have $\psi_{j\pm1} = e^{\pm iKa} \psi_j$

$$\Rightarrow \boxed{E_k = E_0 - 2t\cos ka}$$



$v_k = \frac{dE}{dk}$ $\quad k>0$: right moves

Note:

- Space discrete $\longleftrightarrow$ k periodic
  Space periodic $\longleftrightarrow$ k discrete
  (property of Fourier transforms)
- Electron wave functions are completely delocalized!
  (even if t is very small)
- single e^-: low k: $E_k \simeq E_0 - 2t + \underbrace{\frac{tk^2a^2}{\hbar k^2}}_{2m_{eff}}$

$m_{eff} = \frac{\hbar^2}{2ta^2}$ inherited from lattice

Many electrons: ignore interactions.

Each lattice site contributes Z e^-.

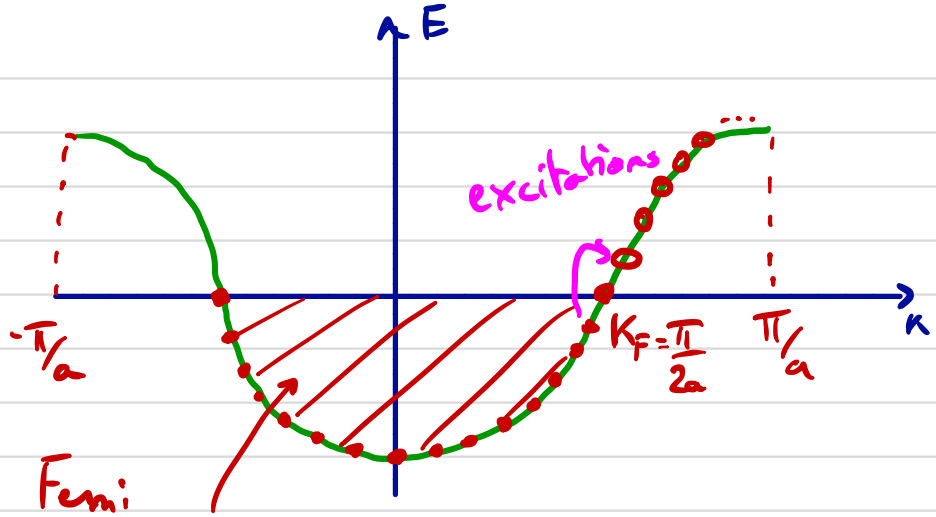
ZN free e^- total; $2N$ states (spin)

(our model only makes for $Z \leq 2$, $Z = 1$ or 2 here)

$Z=1$: "Half-filling"

First fill $k = 0$ (2 states), then $k = \pm\frac{2\pi}{Na}$ etc

(Pauli exclusion principle)



As many e^- with $k>0$ and $k<0$ in groundstate (no current)

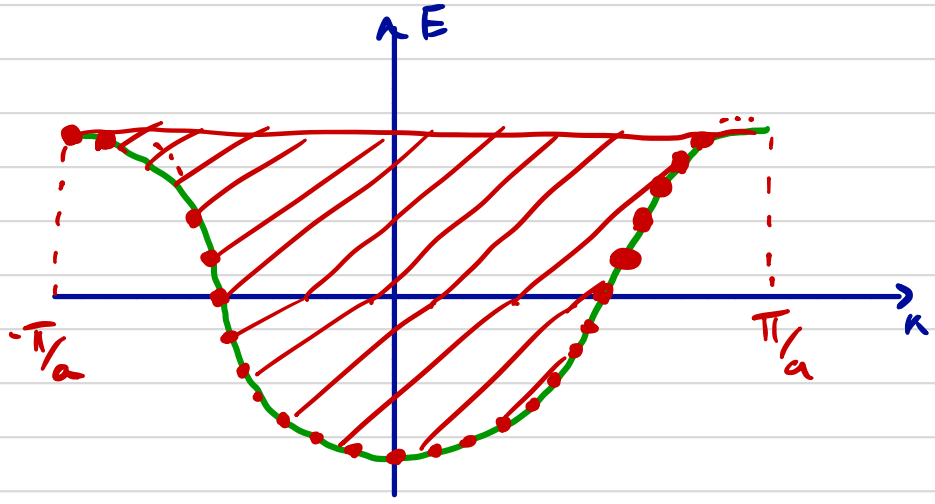
Linearize near $k = k_F$: $E = E_0 - 2t \cos(\pi/2 + \delta k a)$ ($-\sin \delta k a$)

$\simeq E_0 + 2t a\, \delta k$

- Linear (relativistic in Bank!) dispersion!
- With E field : Deplete FS on the left, more on the right (later), more $k>0$: current!

Conductor

$Z=2$: Fully filled Band



Band insulator

(some insulators due to interactions) disorder etc...

(b) Nearly free electrons

Tight Binding: tightly bound e^- with tunneling.

Let's consider the opposite limit: Almost free e^- with weak periodic potential.

$$H = \underbrace{\frac{p^2}{2m}}_{H_0} + V(x) \qquad p = -i\hbar \frac{d}{dx} \quad \text{(continuum model)}$$

$V(x+a) = V(x)$ and periodic system of size L

$L = Na$ with N integer (# atoms)

H_0: $\psi_k(x) = \langle x|k\rangle = \frac{1}{\sqrt{L}} e^{ikx}$ and $\langle k|k'\rangle = \frac{1}{L}\int_0^L dx\, e^{i(k'-k)x} = \delta_{k,k'}$

eigenstates $|k\rangle$ labelled by $p = \hbar k$, k is quantized in units of $2\pi/L$ since $\psi(x+L) = \psi(x)$

$$H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \qquad E_k = \frac{\hbar^2 k^2}{2m}$$

Perturbation theory: $E_k = E_{-k}$ degenerate perturbation theory needed?

Depends on matrix elements: $\langle k'|V|k\rangle$

$$V(x) = \sum_{n\in\mathbb{Z}} V_n e^{2\pi i n x/a} \qquad V_n = V_{-n}^*$$

with Fourier coefficients: $V_n = \frac{1}{a}\int_0^a dx\, V(x)\, e^{-2\pi i n x/a}$

$$\langle k|V|k'\rangle = \frac{1}{L}\int_0^L dx \sum_{n\in\mathbb{Z}} V_n\, e^{i(k'-k+2\pi n/a)x}$$

$$= \sum_{n\in\mathbb{Z}} V_n\, \delta_{k-k',\,2\pi n/a}$$

Perturbation can only mix: $\boxed{k = k' + \frac{2\pi n}{a}}$ with $n \in \mathbb{Z}$

Mixing between $k' = -k$ and k : $k = \frac{\pi n}{a}$

(edge of Brillouin zone for $n=1$).

Low momentum (non degenerate perturbation theory)

$\frac{\pi n}{a} \ll k \ll \frac{\pi(n+1)}{a}$ (far from special points where mixing occurs)

$$E_k = \frac{\hbar^2 k^2}{2m} + \underbrace{\langle k|V|k\rangle}_{V_0 = \text{constant}} + \sum_{k'\neq k} \frac{|\langle k|V|k'\rangle|^2}{E_k^0 - E_{k'}^0} + \dots$$

No mixing to 1st order

$k' = k + 2\pi n/a$, $n \in \mathbb{Z}$

Small changes... Mostly unaffected by potential in this regime.

However: if $k = \frac{\pi n}{a}$ and $k' = -k$: denominator $= 0$!
$\langle k|V|-k\rangle \neq 0$

$\Rightarrow$ need degenerate perturbation theory.

Edge of BZ (Brillouin zone) $\quad k = n\pi/a$

$$\begin{pmatrix} \langle k|H|k\rangle & \langle k|H|-k\rangle \\ \langle -k|H|k\rangle & \langle -k|H|-k\rangle \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$\Leftrightarrow \quad \begin{pmatrix} \frac{\hbar^2 n^2\pi^2}{2ma^2} + V_0 & V_n \\ V_n^* & \frac{\hbar^2 n^2\pi^2}{2ma^2} + V_0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Eigenvalues: $\left(\frac{\hbar^2}{2m} \frac{n^2\pi^2}{a^2} + V_0 - E \right)^2 - |V_n|^2 = 0$

$$\Rightarrow \quad E_\pm = \frac{\hbar^2}{2m} \frac{n^2\pi^2}{a^2} + V_0 \pm |V_n|$$

$2|V_n|$ opens up at $k = \pm \frac{n\pi}{a}$

Take: $V(x) = 2V_1 \cos \frac{2\pi x}{a}$ $\quad (n = 1$ only; $k = \pm \pi/a)$

Eigenstates: $|k\rangle \pm |-k\rangle$ $\quad (k = \pi/a) \quad \rightarrow \quad \psi_\pm(x) \sim \begin{cases} \cos \frac{\pi x}{a} \\ \sin \frac{\pi x}{a} \end{cases}$

$|\psi_-|^2$ mostly near minima of $V \Rightarrow$ lower energy

Let's repeat this exercise for $k = \frac{n\pi}{a} + \delta$, $k' = -\frac{n\pi}{a} + \delta$ } almost same energy if δ is small

$$\Rightarrow \underbrace{\left(\frac{\hbar^2}{2m}\left(\frac{n\pi}{a}+\delta\right)^2 + V_0 - E\right)\left(\frac{\hbar^2}{2m}\left(\frac{n\pi}{a}-\delta\right)^2 + V_0 - E\right)} = |V_n|^2$$

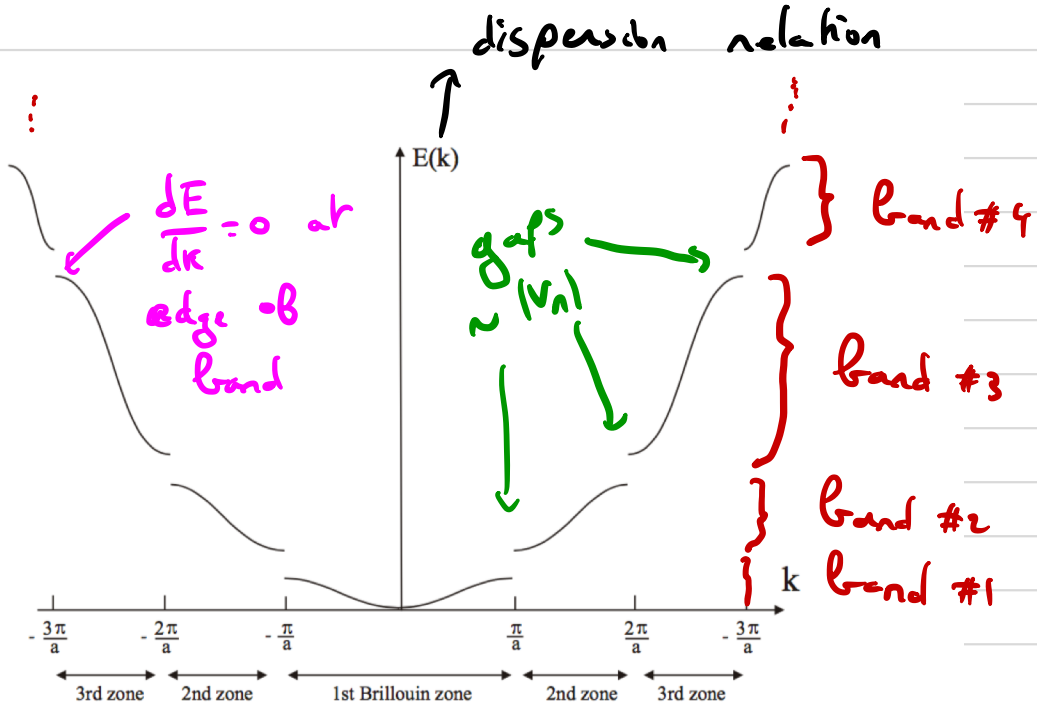
$$\left(\frac{\hbar^2}{2m}\left(\frac{n^2\pi^2}{a^2}+\delta^2\right) + V_0 - E\right)^2 - \left(\frac{\hbar^2}{2m}\frac{2n\pi\delta}{a}\right)^2 = |V_n|^2$$

If δ is large, coincides with 2nd order non degenerate perturbation theory.

Small δ:

$$E_\pm \simeq \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2} + V_0 \pm |V_n| + \frac{\hbar^2}{2m}\left(1 \pm \frac{1}{|V_n|}\frac{n^2\pi^2\hbar^2}{m a^2}\right)\delta^2 + \dots$$

quadratic correction



© Bloch's Theorem in 1d.

Free particles with translation invariance $\xrightarrow{\text{Noether}}$ $[\hat{H}, \hat{p}] = 0$

$\hat{p}$: momentum labels states

In our case: $x \to x + a$ discrete translation invariance.

Let's show that this is enough to label states with "k"

Translation operator: $\hat{T}_\rho \psi(x) = \psi(x+\rho)$

- $\langle \phi | \hat{T}_\rho \psi \rangle = \int dx\, \phi^*(x) \psi(x+\rho) = \int dx\, \phi^*(x-\rho) \psi(x)$

$$= \int dx \left[\hat{T}_{-\rho}\, \phi(x)\right]^* \psi(x) = \langle \hat{T}_{-\rho}\, \phi | \psi \rangle$$

$$\Rightarrow \hat{T}_\rho^\dagger = \hat{T}_{-\rho} = \hat{T}_\rho^{-1} \Rightarrow \hat{T}_\rho \text{ unitary}$$

- $\hat{T}_{\rho_1} \hat{T}_{\rho_2} = \hat{T}_{\rho_1+\rho_2}$ (Abelian group, $[\hat{T}_{\rho_1}, \hat{T}_{\rho_2}] = 0$)

- $\hat{T}_\rho$ can be expressed in terms of $\hat{p} = -i\hbar \frac{d}{dx}$

as $\boxed{\hat{T}_\rho = e^{i\rho\hat{p}/\hbar}}$

Proof: $\hat{T}_\ell \psi(x) = \left(1 + \frac{i\ell\hat{p}}{\hbar} + \frac{1}{2!}\left(\frac{i\ell\hat{p}}{\hbar}\right)^2 + \dots\right)\psi(x)$

$= \left(1 + \ell\frac{d}{dx} + \frac{\ell^2}{2!}\frac{d^2}{dx^2} + \dots\right)\psi(x) = \sum_{n=0}^{\infty} \frac{\ell^n}{n!}\frac{d^n}{dx^n}\psi(x)$

$= \psi(x+\ell)$

$\hat{p}$ is the generator of the translation group

- A system is translation invariant iff $[\hat{H}, \hat{T}_\ell] = 0 \quad \forall \ell$

  $\Rightarrow [\hat{H}, \hat{p}] = 0$ as expected.

- Now iff $[\hat{H}, \hat{T}_a] = 0$, energy eigenstates can be labbeled by the eigenvalues of $\hat{T}_a$: phases $e^{i\theta_a}$

  Eigenvalues of $\hat{T}_\ell = e^{i\ell k}$ so that $e^{i\theta_{\ell_1}} e^{i\theta_{\ell_2}} = e^{i\theta_{\ell_1+\ell_2}}$

  $\hat{T}_a \psi_k(x) = \psi_k(x+a) = e^{ika}\psi_k(x)$ on an eigenvector of H

  Now ψ_k and $\psi_{k+2\pi/a}$ have the same eigenvalue under $\hat{T}_a$: take $k \in [-\pi/a, \pi/a]$ 1st Brillouin Zone

$\Rightarrow$ we can still label eigenstates by k, but $k \in [-\frac{\pi}{a}, \frac{\pi}{a}]$

Bloch's theorem (in 1d): Periodic potential $V(x+a) = V(x)$

Eigenstates can be written as: $\boxed{\psi_k(x) = e^{ikx} u_k(x)}$

$k \in [-\pi/a, \pi/a]$; $u_k(x+a) = u_k(x)$

→ "Mild" modification of plane waves!

Proof: $\psi_k(x+a) = e^{ika}\psi_k(x)$ since we can take ψ_k to be an eigenstate of $\hat{T}_a$. $u_k(x) \equiv e^{-ikx}\psi_k(x)$

$$u_k(x+a) = e^{-ikx} e^{-ika} \psi_k(x+a) = e^{-ikx}\psi_k(x) = u_k(x)$$

Crystal momentum: $\hat{p} = \hbar\hat{k}$ ($\neq$ mass × velocity)

conserved modulo $2\pi/a$ (lattice can "absorb" $\Delta p = \frac{2\pi}{a} n$)

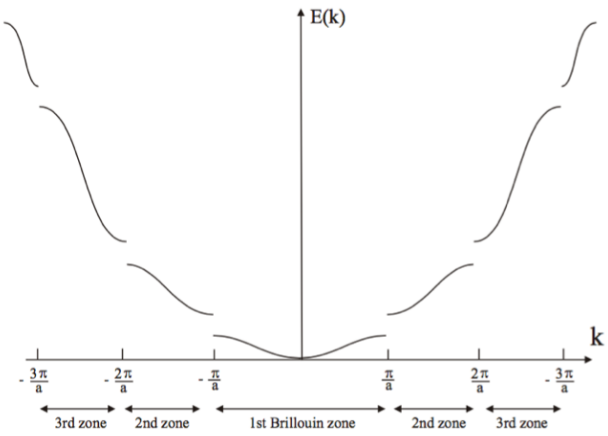


Figure 19: The extended zone scheme.

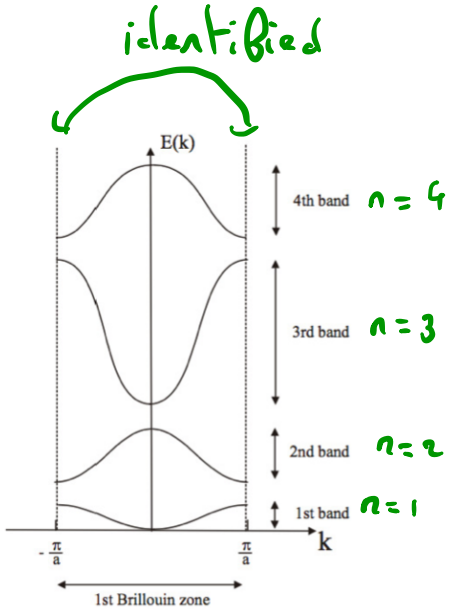


Figure 20: The reduced zone scheme.

II Lattices and Crystal structure

In 2d and 3d, we have to deal with more complicated lattices!

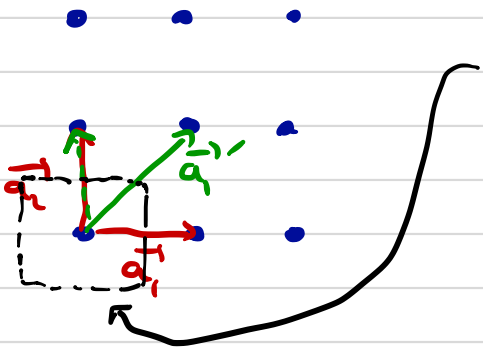
a Bravais lattice (a.k.a. a lattice in math!)

all points have the same environment

2d: $\Lambda = \{ \vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 \; ; \; (n_1, n_2) \in \mathbb{Z}^2 \}$

3d: $\Lambda = \{ \vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3, \; (n_1, n_2, n_3) \in \mathbb{Z}^3 \}$

$\vec{a}_i$: primitive lattice vectors (not unique!)



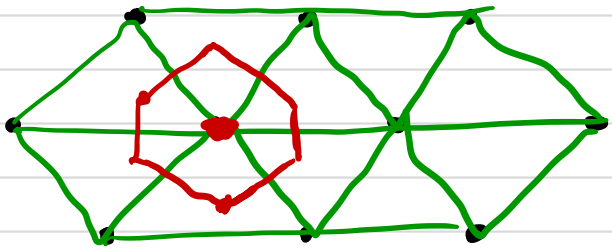
Primitive cell: region of space which tessellates the space when translated by $\vec{a}_i$'s. (Not unique!)

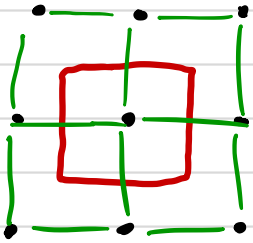
$V = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)| = 1/n$ $\quad$ n: density of lattice points

- $\exists$ unique primitive cell which respects the symmetry of the lattice: Wigner-Seitz (Voronoi) cell:

Region of space such that origin is the closest lattice point

↑ reference site





- Bravais lattices can be classified (Bravais lattices are considered equivalent if they share the same symmetry group)

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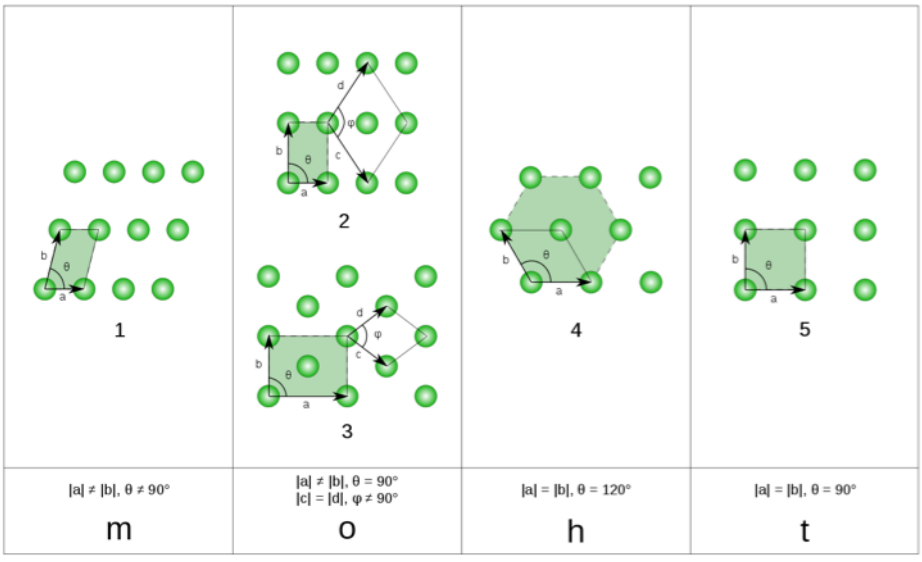
In 2 dimensions

Further information: Lattice (group)

Note: In the following diagrams the lattice points are depicted using green circles and the unit cells are depicted using parallelograms (which may be squares or rectangles) outlined in black. Although each of the four corners of each parallelogram connects to a lattice point, only one of the four lattice points technically belongs to a given unit cell and each of the other three lattice points belongs to one of the adjacent unit cells. This can be seen by imagining moving the unit cell parallelogram slightly left and slightly down while leaving all the green circles of the lattice points fixed.

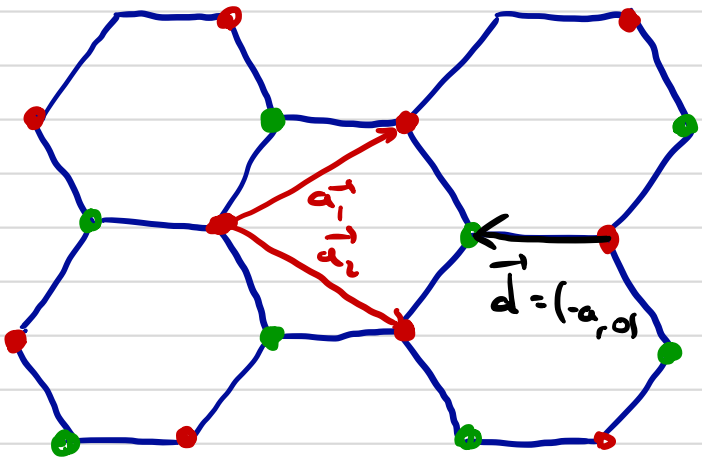


1 – oblique (monoclinic), 2 – rectangular (orthorhombic), 3 – centered rectangular (orthorhombic), 4 – hexagonal, and 5 – square (tetragonal).

In two-dimensional space, there are 5 Bravais lattices,[4] grouped into four crystal families.

Crystal family	Point group (Schönflies notation)	5 Bravais lattices	
		Primitive	Centered
Monoclinic	C_2	Oblique	
Orthorhombic	D_2	Rectangular	Centered rectangular
Hexagonal	D_6	Hexagonal	
Tetragonal	D_4	Square	

- **Non-Bravais lattices**: Honeycomb lattice (see graphene later)



Not all points are equivalent!

BUT:

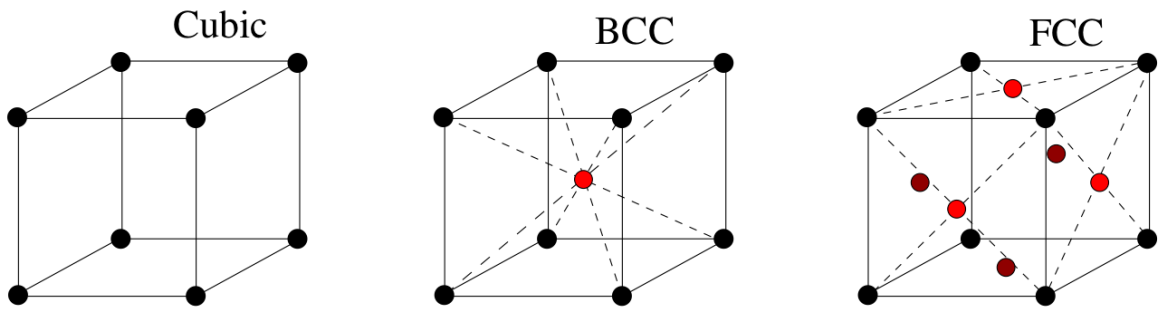
+ underlying triangular Bravais lattice

Red points live on Bravais lattice + translation by $\vec{d}_i$ vectors (Basis). Here $\vec{d}_1 = \vec{d} = (-a, 0)$ to get green points

- **Important 3D examples:**

Cubic: $\vec{a}_1 = a\vec{e}_x$, $\vec{a}_2 = a\vec{e}_y$, $\vec{a}_3 = a\vec{e}_z$

$V = a^3$, Wigner-Seitz cell = cube



Body-Centered Cubic (BCC):

$\vec{a}_1 = a\,\vec{e}_x \qquad \vec{a}_2 = a\,\vec{e}_y \qquad \vec{a}_3 = \frac{a}{2}(\vec{e}_x + \vec{e}_y + \vec{e}_z)$

$V = a^3/2$

Face Centered cubic (FCC):

$\vec{a}_1 = \frac{a}{2}(\vec{e}_y + \vec{e}_z) \qquad \vec{a}_2 = \frac{a}{2}(\vec{e}_x + \vec{e}_z) \qquad \vec{a}_3 = \frac{a}{2}(\vec{e}_x + \vec{e}_y)$

$V = a^3/4$

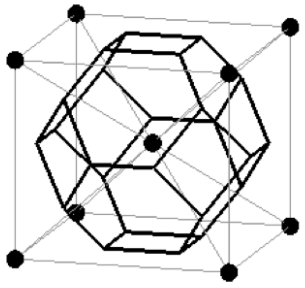


Figure 25: Wigner-Seitz cell for BCC

Non Bravais

FCC lattice + 2 atom Basis

$\vec{d} = \frac{a}{2}(\vec{e}_x + \vec{e}_y + \vec{e}_z)$

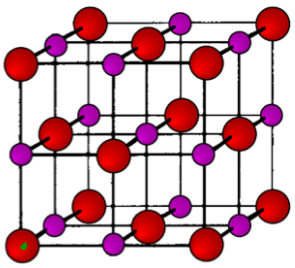


Figure 26: Salt. NaCl

⑫ Reciprocal lattice

$$\Lambda^* = \left\{ \vec{k} = \sum_{i=1}^{d} n_i \vec{e}_i^{\,*}, \quad n_i \in \mathbb{Z} \right\}$$

with $\boxed{\vec{a}_i \cdot \vec{e}_j^{\,*} = 2\pi \delta_{ij}}$

in 3d: $\boxed{\vec{b}_i = \frac{2\pi}{V} \frac{1}{2} \varepsilon_{ijk} \vec{a}_j \times \vec{a}_k}$ (Check this!)

$(\Lambda^*)^* = \Lambda$ with: $\vec{a}_i = \frac{2\pi}{V^*} \frac{1}{2} \varepsilon_{ijk} \vec{b}_j \times \vec{b}_k$

$V^* = |\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)| = (2\pi)^3 / V$

We have: $\boxed{e^{i\vec{K}\cdot\vec{\pi}} = 1}$ $\forall \vec{\pi} \in \Lambda, \vec{K} \in \Lambda^*$

Ex: Cubic lattice $\vec{a}_1 = \begin{vmatrix} a \\ 0 \\ 0 \end{vmatrix}$ $\vec{a}_2 = \begin{vmatrix} 0 \\ a \\ 0 \end{vmatrix}$ $\vec{a}_3 = \begin{vmatrix} 0 \\ 0 \\ a \end{vmatrix}$

$\vec{b}_1 = \frac{2\pi}{a} \begin{vmatrix} 1 \\ 0 \\ 0 \end{vmatrix}$ $\vec{b}_2 = \frac{2\pi}{a} \begin{vmatrix} 0 \\ 1 \\ 0 \end{vmatrix}$ $\vec{b}_3 = \frac{2\pi}{a} \begin{vmatrix} 0 \\ 0 \\ 1 \end{vmatrix}$

BCC: $\vec{a}_1 = \begin{vmatrix} -a/2 \\ a/2 \\ a/2 \end{vmatrix}$ $\vec{a}_2 = \begin{vmatrix} a/2 \\ -a/2 \\ a/2 \end{vmatrix}$ $\vec{a}_3 = \begin{vmatrix} a/2 \\ a/2 \\ -a/2 \end{vmatrix}$

$\vec{b}_1 = \frac{2\pi}{a^3/2} \vec{a}_2 \times \vec{a}_3 = \frac{2\pi}{a} \begin{vmatrix} 0 \\ 1 \\ 1 \end{vmatrix}$ $\vec{b}_2 = \frac{2\pi}{a} \begin{vmatrix} 1 \\ 0 \\ 1 \end{vmatrix}$ $\vec{b}_3 = \frac{2\pi}{a} \begin{vmatrix} 1 \\ 1 \\ 0 \end{vmatrix}$

→ reciprocal lattice = FCC.

Fourier space: $[\vec{b}_i] = 1/\text{length}$: "Momentum space"

Take a periodic function $f(\vec{x} + \vec{\pi}) = f(\vec{x})$

$\forall \vec{\pi} \in \Lambda$

$$\hat{\rho}(\vec{k}) = \int d^3x\, e^{-i\vec{k}\cdot\vec{x}}\, \rho(\vec{x}) = \sum_{\vec{\pi}\in\Lambda} \int_{\Gamma} d^3\vec{x}\, e^{-i\vec{k}(\vec{x}+\vec{\pi})}\, \rho(\vec{x}+\vec{\pi})$$

Γ ← Wigner-Seitz cell

$$= \underbrace{\sum_{\vec{\pi}\in\Lambda} e^{-i\vec{k}\cdot\vec{\pi}}}_{\Delta(\vec{k})} \underbrace{\int_{\Gamma} d^3\vec{x}\, e^{-i\vec{k}\cdot\vec{x}}\, \rho(\vec{x})}_{S(k):\ \text{Fourier coefficients}}$$

"Structure factor"

- We have $\Delta(\vec{k}) = 0$ unless $\vec{k} \in \Lambda^*$.

Proof: $\Delta(\vec{k}) = \sum_{\vec{\pi}\in\Lambda} e^{-i\vec{k}\cdot(\vec{\pi}-\vec{\pi}_0)} = e^{i\vec{k}\cdot\vec{\pi}_0}\,\Delta(\vec{k})$

($\vec{\pi}_0 \in \Lambda$ arbitrary)

$$\Rightarrow \Delta(\vec{k}) = 0 \quad \text{or} \quad e^{i\vec{k}\cdot\vec{\pi}_0} = 1 \ \forall \vec{\pi}_0 \iff \vec{k} \in \Lambda^*$$

- Take $\vec{k} = \sum_{i=1}^{3} k_i \vec{b}_i^*$ $\qquad \vec{\pi} = \sum_{i=1}^{3} n_i \vec{b}_i \in \Lambda$

$k_i \in \mathbb{R}$ have $\qquad n_i \in \mathbb{Z}$

(k_i integers $\Leftrightarrow \vec{k} \in \Lambda^*$)

$$\Delta(\vec{k}) = \sum_{n_1,n_2,n_3} e^{-i2\pi(k_1 n_1 + k_2 n_2 + k_3 n_3)}$$

$$= \sigma(k_1)\,\sigma(k_2)\,\sigma(k_3)$$

Fourier decomposition of Dirac Comb

$$\sigma(k) = \sum_{n \in \mathbb{Z}} e^{-2\pi i k n} \overset{!}{=} \sum_{n \in \mathbb{Z}} \delta(k-n)$$

Because $k_i \in \mathbb{Z}$

$$\Delta(\vec{k}) = \sum_{\vec{n} \in \mathbb{Z}^3} \delta(k_1 - n_1)\, \delta(k_2 - n_2)\, \delta(k_3 - n_3)$$

$$= V^* \sum_{\vec{q} \in \Lambda^*} \delta(\vec{k} - \vec{q})$$

in 1d: $\Delta(k) = \sum_{\vec{n} \in \Lambda} e^{-i \vec{k} \cdot \vec{n}} = \sum_n e^{-2\pi i k n} = \sum_n \delta(k-n)$

$\vec{k} = k \vec{e}$, $\vec{n} = n \vec{a}$, $\vec{a} \cdot \vec{e} = 2\pi$

$= |\vec{e}| \sum_n \hat{\delta}(k\vec{e} - n\vec{e})$

$= V^* \sum_{\vec{q} \in \Lambda^*} \hat{\delta}(\vec{k} - \vec{q})$

- Inverse FT: $\beta(\vec{x}) = \int \frac{d^3\vec{k}}{(2\pi)^3} e^{i \vec{k} \cdot \vec{x}} \underbrace{\hat{\beta}(\vec{k})}_{\Delta(\vec{k}) S(\vec{k})}$

$$\Rightarrow \boxed{\beta(\vec{x}) = \frac{V^*}{(2\pi)^3} \sum_{\vec{q} \in \Lambda^*} e^{i \vec{q} \cdot \vec{x}} S(\vec{q})}$$

Generalized Fourier Series