PHY 530
STEEM Refresher course 4
Introduction to solid state physics

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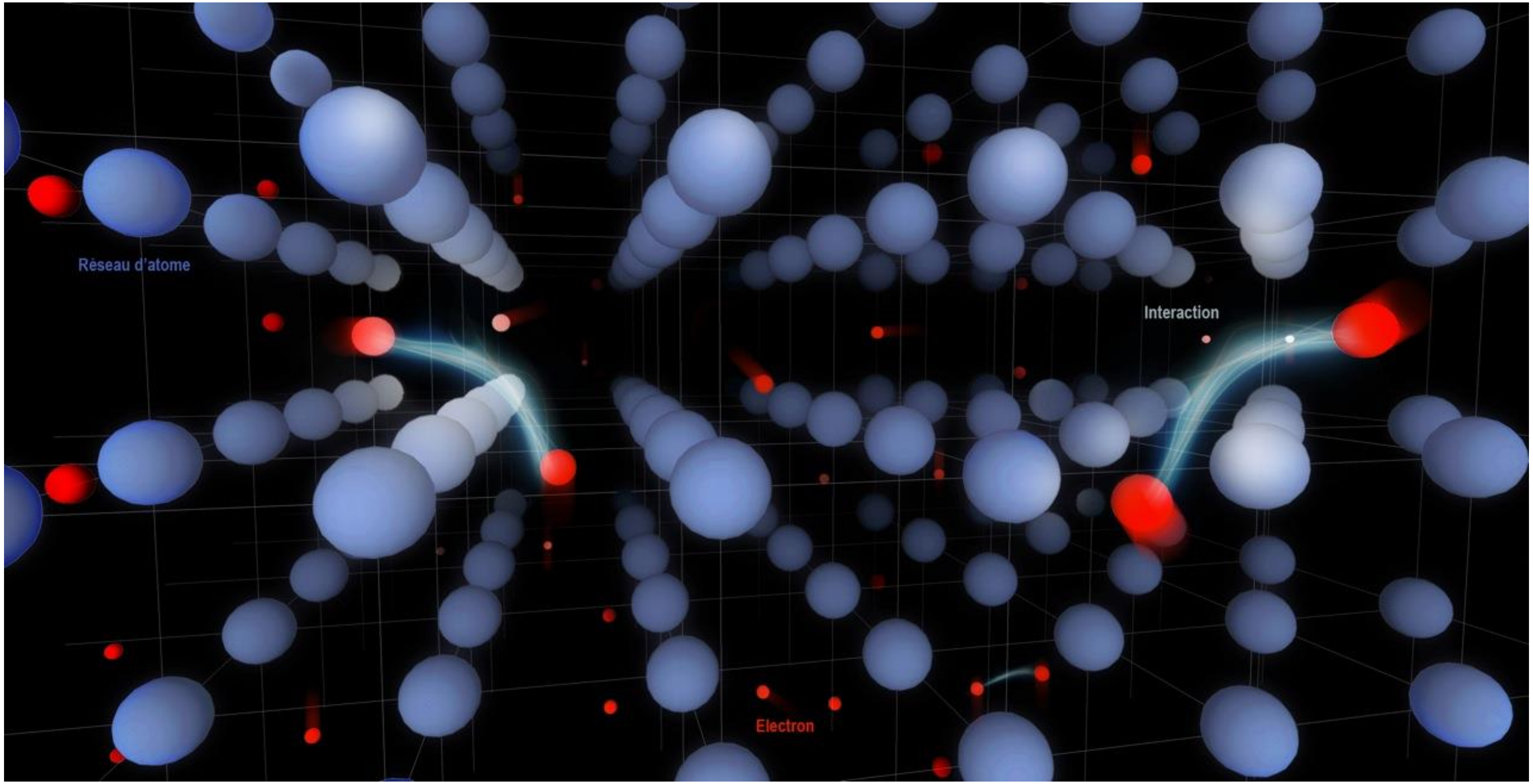
UMR 9006

Introduction to lecture 4



$$H = \sum_{\text{atoms}} \frac{1}{2M}\mathbf{P}_i^2 + \sum_{\text{electrons}} \frac{1}{2m}\mathbf{p}_i^2 + \frac{Z^2}{2}\sum_{\text{at.-at.}} V_c\left(\mathbf{R}_i - \mathbf{R}_j\right) + Z\sum_{\text{at.-el.}} V_c\left(\mathbf{r}_i - \mathbf{R}_j\right) + \frac{1}{2}\sum_{\text{el.-el.}} V_c\left(\mathbf{r}_i - \mathbf{r}_j\right)$$

Way too difficult !

Reminder on lecture 1, 2 & 3

Confinement → discrete energy levels

Coupling → degeneracy lift

Free particles → planewaves

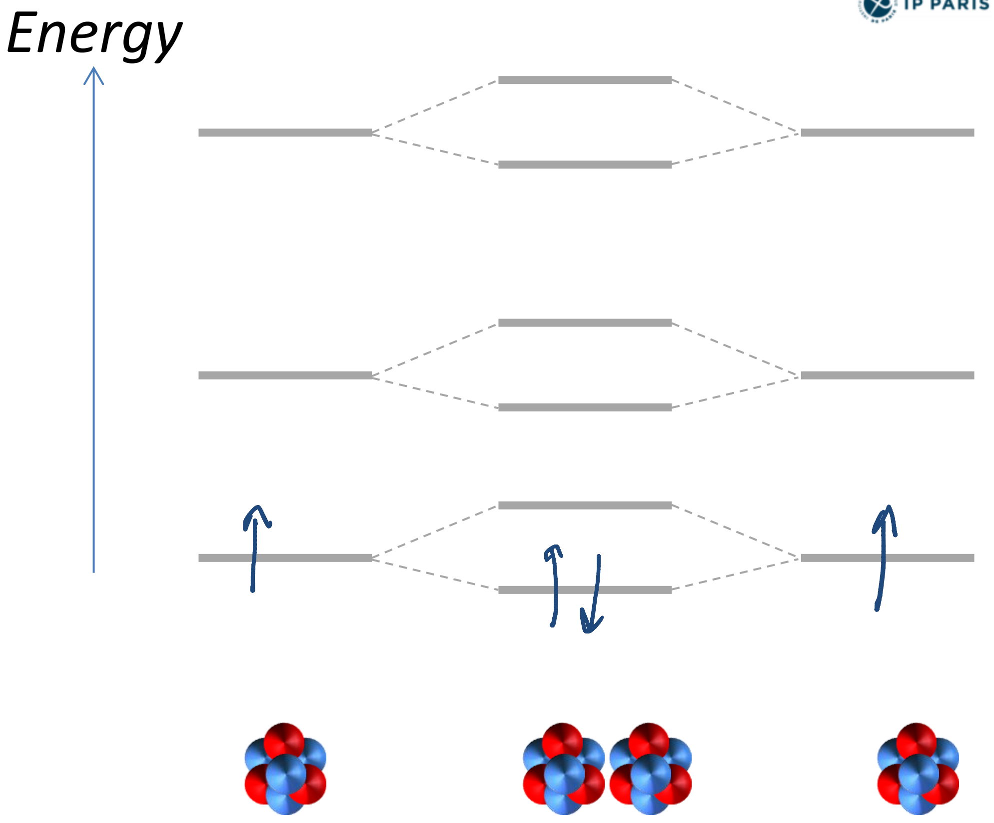
Momentum $\underbrace{\hbar k}_{p}$, *energy* $\frac{\hbar^2 k^2}{2m} \sim \frac{p^2}{2m}$

How many states with energy around E ?

Density of state $D(E)dE$

How are particles distributed among these states ?

Occupation factor (Fermi Dirac for electrons)



STEEM Refresher 4

1. (Tutorial) Tight binding model
2. From the 1D lattice to the crystal structure
3. From the tight binding bands to band diagrams
4. Populating energy bands: metals, insulator and semi-conductors
5. Focus on semi-conductors: the come-back of free particles
6. Focus on semi-conductors: Fermi levels
7. Take home message

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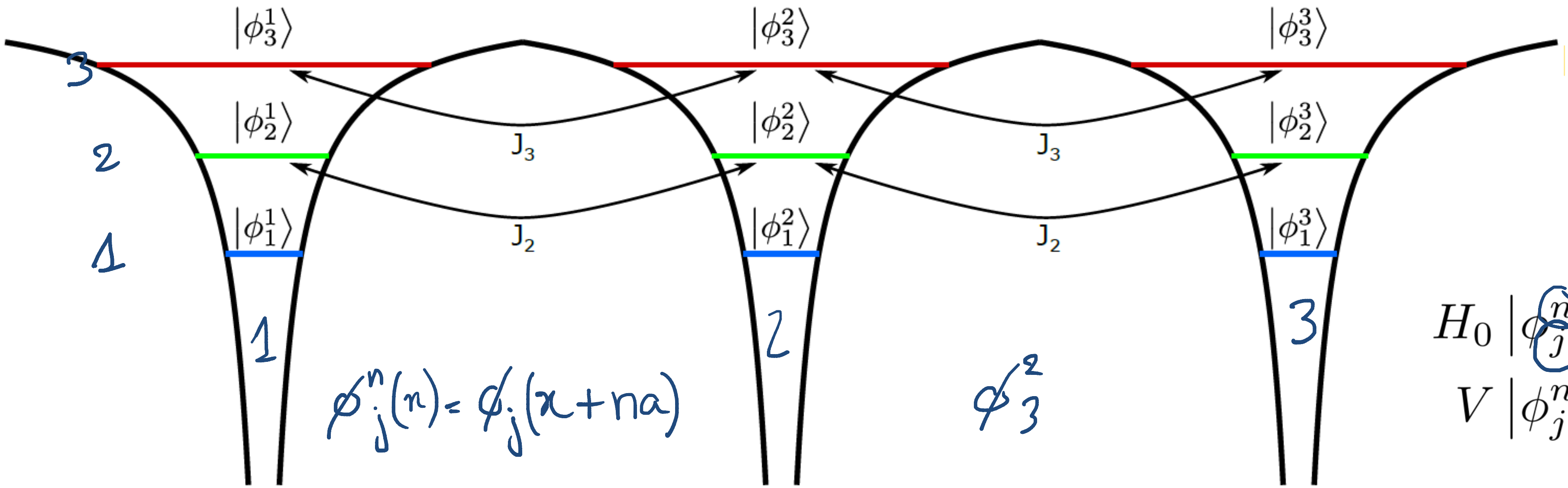
Question 1



$$H\Psi = E\Psi$$

$$H = H_0 + V$$

$$H_0 |\phi_j^n\rangle = E_j |\phi_j^n\rangle$$

$$V |\phi_j^n\rangle = -J_j \left(|\phi_j^{n-1}\rangle + |\phi_j^{n+1}\rangle\right)$$

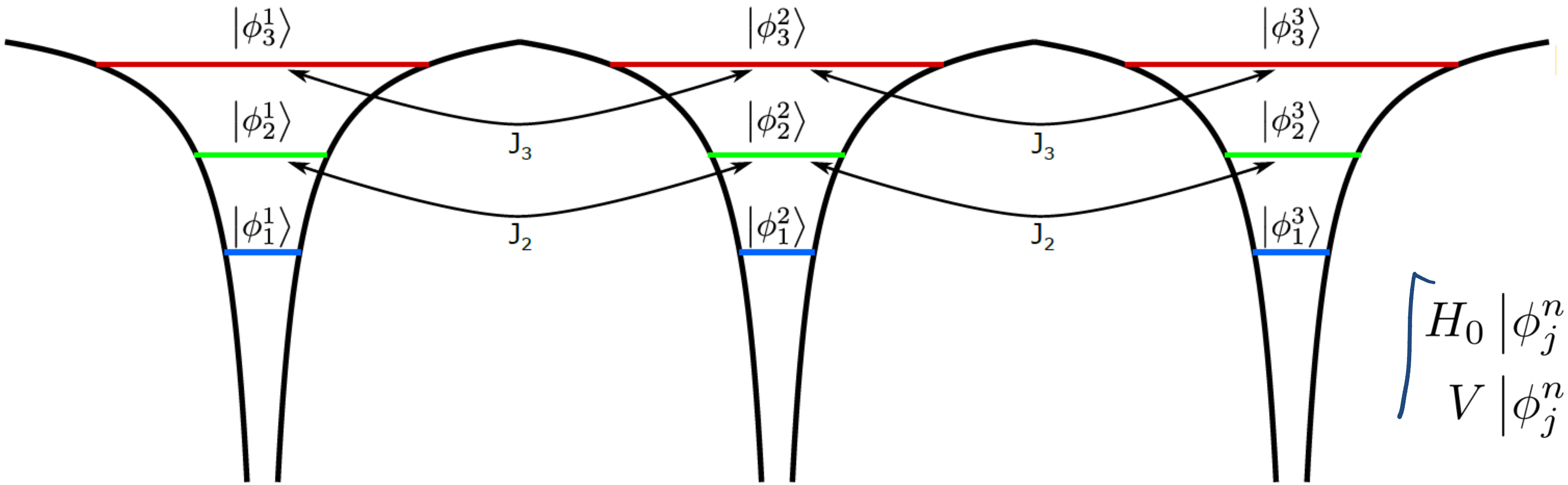
The eigenstates of H_0 (ie ϕ_j^n) are not eigenstates of H, $H\phi_j^n \neq E\phi_j^n$
but they are still a basis for wavefunctions

$$|\psi\rangle = \sum_{n,j} c_j^n |\phi_j^n\rangle$$

States from a given energy level j are not coupled to other levels $i \neq j$
we restrict the linear combination to the j-sub space.

$$|\psi_j\rangle = \sum_{n} c_j^n |\phi_j^n\rangle$$

Question 2



$$H = H_0 + V$$

$$\begin{cases} H_0 |\phi_j^n\rangle = E_j |\phi_j^n\rangle \\ V |\phi_j^n\rangle = -J_j \left(|\phi_j^{n-1}\rangle + |\phi_j^{n+1}\rangle\right) \end{cases}$$

We are looking for eigenstates of H with the form $|\psi_j\rangle = \sum_n c_j^n |\phi_j^n\rangle$

$\hat{H}\Psi = E\Psi$

$$\sum_n (\hat{H}_0 + \hat{V}) c_j^n |\phi_j^n\rangle = \sum_n \left[E_j c_j^n |\phi_j^n\rangle - J_i c_j^n \left(|\phi_j^{n-1}\rangle + |\phi_j^{n+1}\rangle \right) \right]$$

$$= \sum_n \left[\underline{c_j^n E_j - J_i \left(c_j^{n+1} + c_j^{n-1} \right)} \right] |\phi_j^n\rangle = \sum_n \underline{E c_j^n} |\phi_j^n\rangle$$

$$\left[E c_j^n = E_j c_j^n - J_j \left(c_j^{n+1} + c_j^{n-1} \right) \right.$$

Question 3

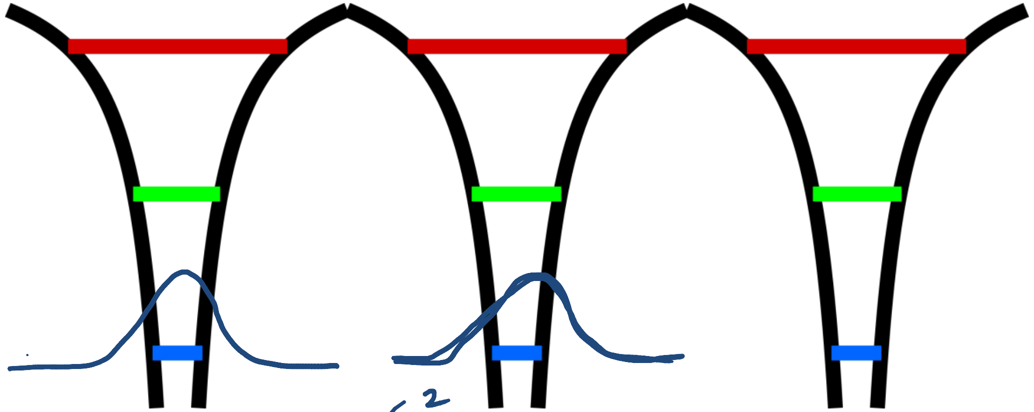
We admit Bloch theorem, leading to

$$\psi_j(x+a) = e^{ika}\psi_j(x)$$

$$\psi(x+a) = \sum_n c_j^n \underbrace{\phi_j^n(x+a)}_{=\phi_j^{n+1}(x)} = \sum_n c_j^{n+1} \phi_j^n(x)$$

$$e^{ika}\psi_j(x) = \sum e^{ika} c_j^n \phi_j^n(x)$$

$$c_j^{n+1} = e^{ika} c_j^n \Rightarrow \boxed{c_j^n = e^{ikna} c_j^0}$$



Question 4

The coefficients of $|\psi_j\rangle = \sum_n c_j^n \, |\phi_j^n\rangle$ have to obey $E\, c_j^n = E_j\, c_j^n - J_j\, \left(c_j^{n-1} + c_j^{n+1}\right)$

with $c_j^n = c_j^0 \exp\left(i\, n\, k\, a\right)$

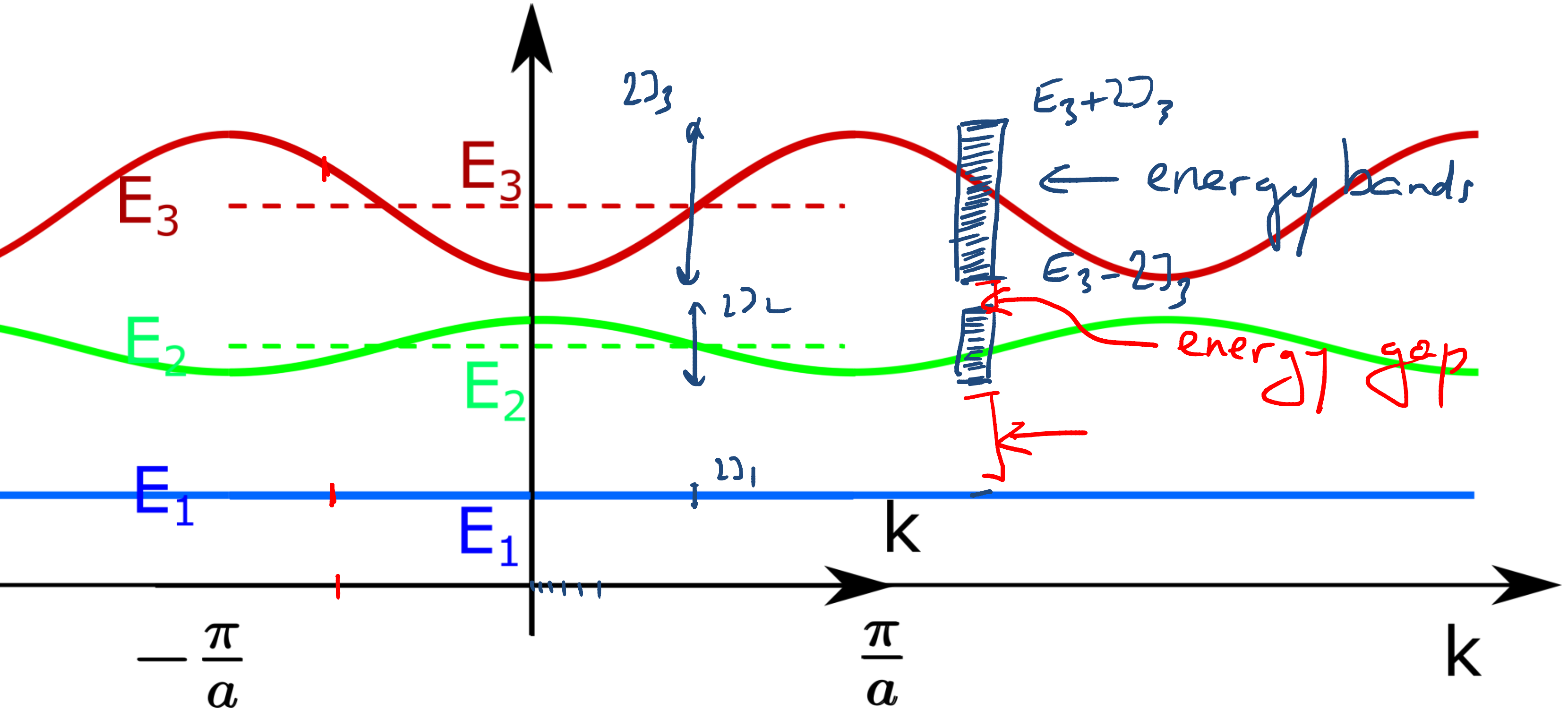
$$E \cancel{c_j^0} e^{ik\cancel{n}a} = E_j \cancel{c_j^0} e^{ik\cancel{n}a} - J_j \Big(\underbrace{\cancel{c_j^0} e^{ik(\cancel{n}+1)a} + \cancel{c_j^0} e^{ik(\cancel{n}-1)a}}_{2\cos ka} \Big)$$

$$\boxed{E = E_j - 2J_j \cos(ka)}$$

Question 4

Eigen states of H $|\psi_{j,k}\rangle = c_0 \sum_n e^{i\,n\,k\,a} \, |\phi_j^n\rangle$ have energies $E = E_i - 2J_i \cos(ka)$

with $k = \dfrac{2p\pi}{N\,a}$ almost continuous



states

↓

discrete index j

+

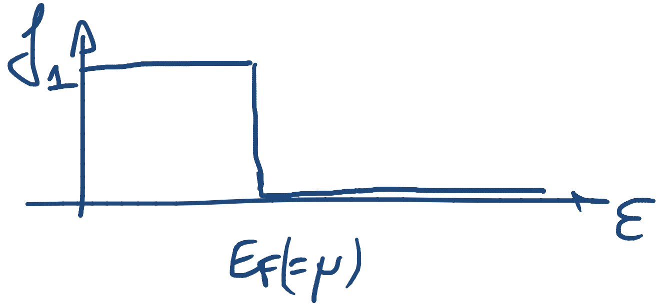
quasi momentum k

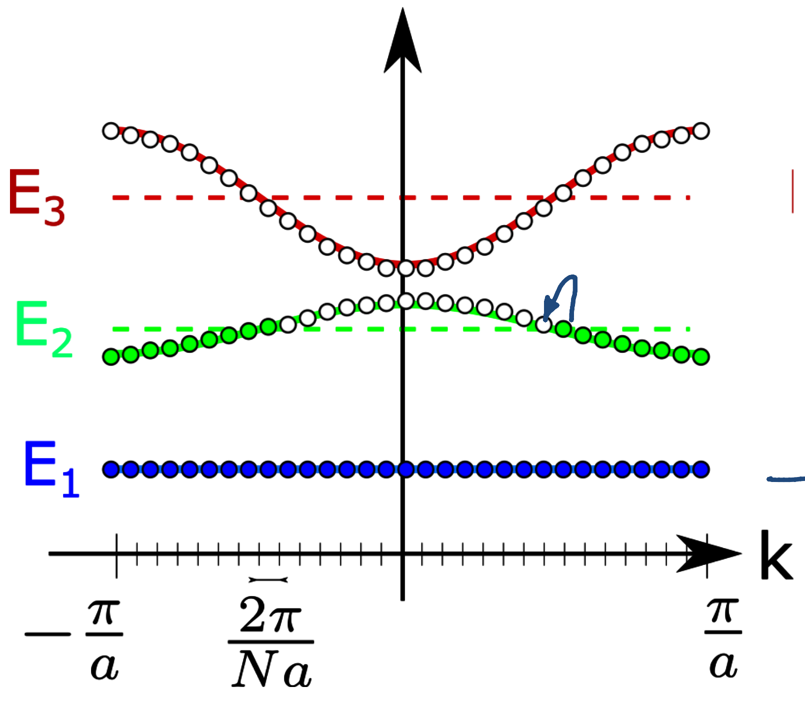
Question 5

How to accomodate fermions inside these energy levels ?

e^- → Fermions → Fermi Dirac distribution

@ 0K ↳





3 e^- per atom → 3N electrons

Fermi level
|| $E_F = E_2$

→ N states and 2 spins → 2N electrons

Fermi level within the band ⇒ can carry energy
(conductor)

3N fermions

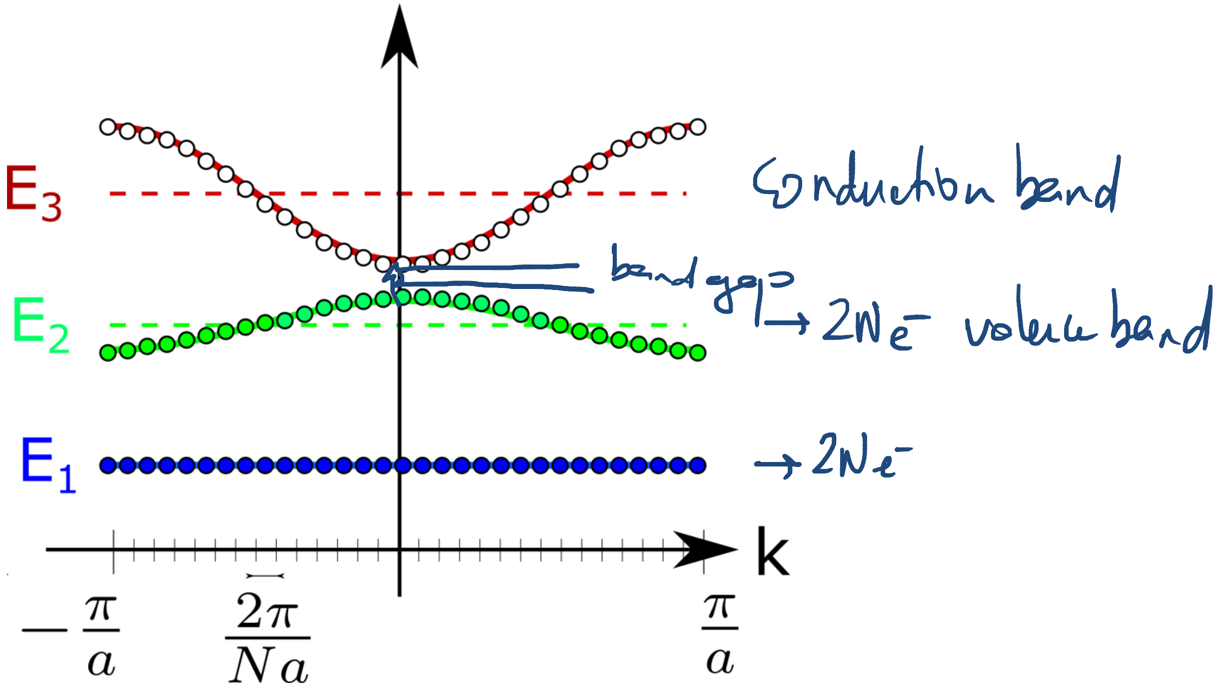
Question 6

How to accomodate fermions inside these energy levels ?

Fermi level lies somewhere within the band gap

↳ insulators

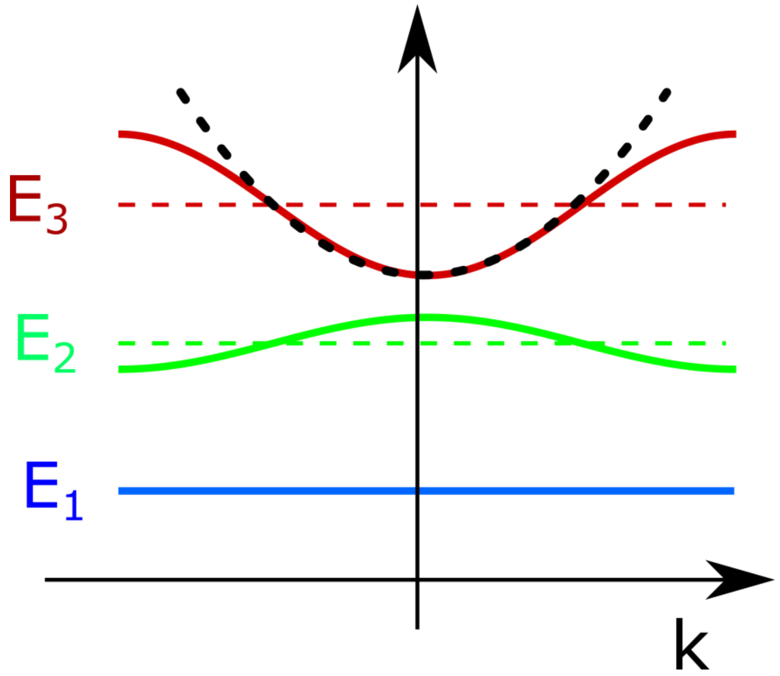
semi conductor



4N fermions

Question 6-b – effective mass

Eigen states of H have energies $$E = E_i - 2J_i \cos(ka)$$



Taylor expansion around $k=0$

$$E \simeq E_i - 2J_i\left(1 - \frac{k^2a^2}{2}\right)$$

$$= (E_i - 2J_i) + J_i a^2 k^2$$

effective mass =

$$\frac{\hbar^2}{2m} = J_i a^2 \rightarrow \boxed{m_{eff} = \frac{\hbar^2}{2J_i a^2}}$$

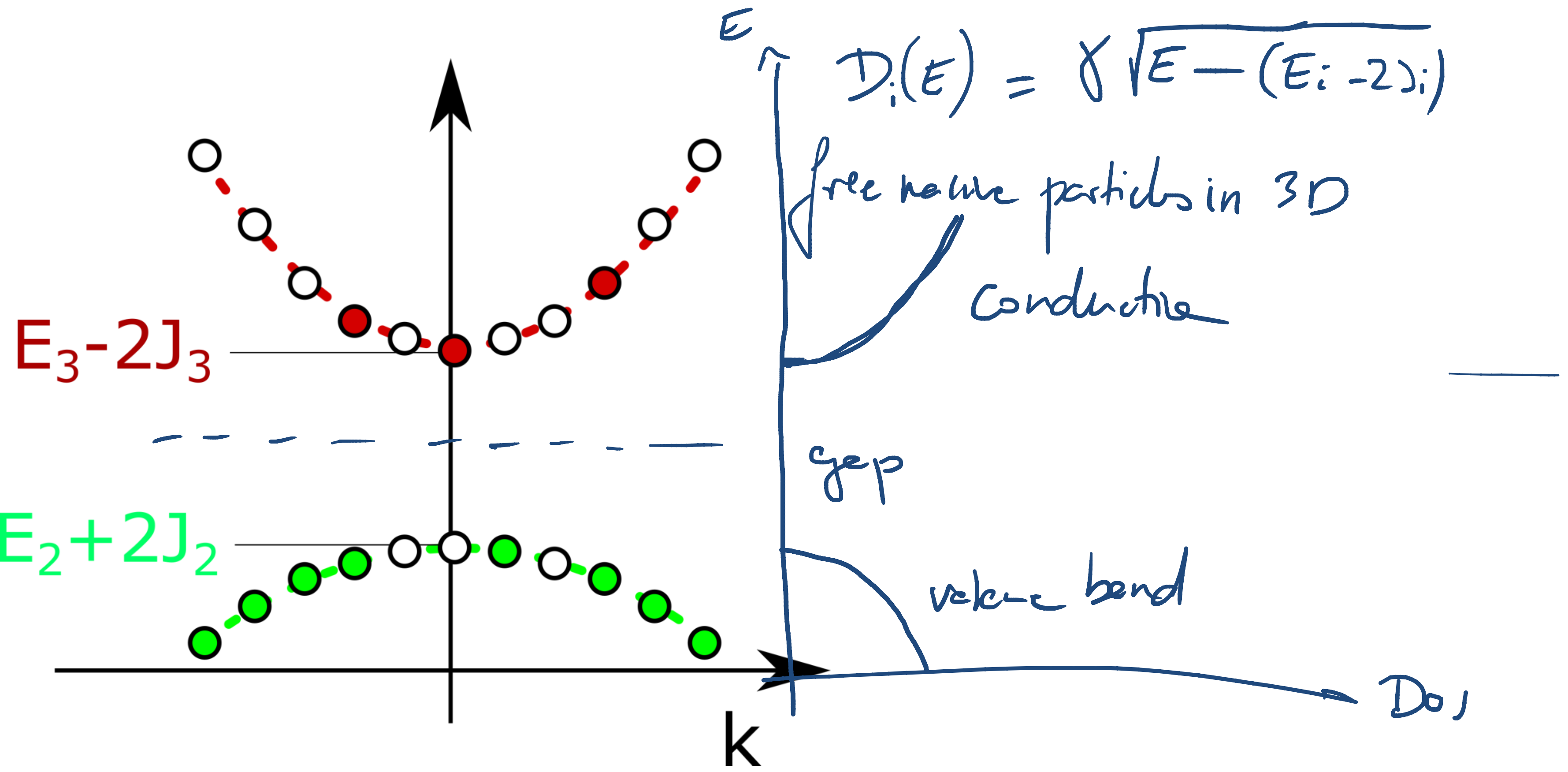
Free particles

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

Question 6-b – effective density of state

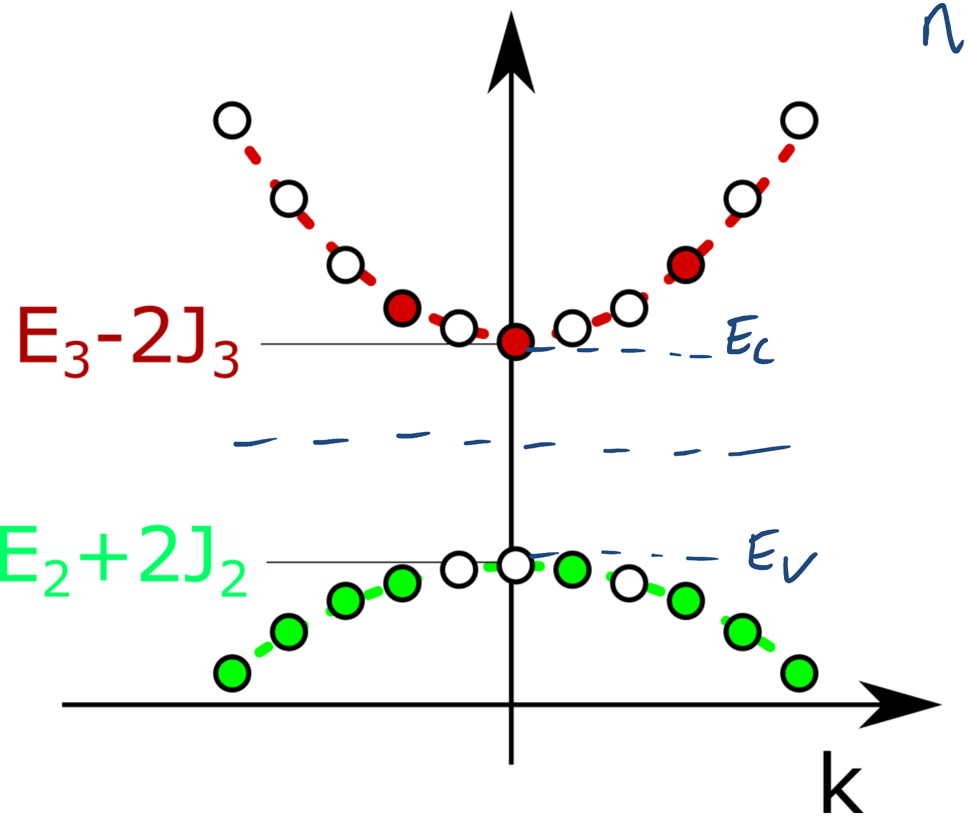
Close to the bottom of the band, $E_i(k) \simeq (E_i - 2J_i) + \dfrac{\hbar^2 k^2}{2m^*}$ with $m^* = 2\hbar^2/Ja^2$

$D_i(E) = \gamma \sqrt{E - (E_i - 2J_i)}$



Question 6-c – electrons in the conduction band

DoS close to the bottom of the conduction band : $D_C(\epsilon) = \left(\frac{1}{2\pi\hbar}\right)^3 4\pi\sqrt{2m_{\text{eff},\,CB}^3}\sqrt{\epsilon - E_C}$



$$n = \int_{CB} D_c(\varepsilon)\, f_{FD}(\varepsilon)\, d\varepsilon$$

$$f_{FD}(\varepsilon) \to \frac{1}{e^{\frac{\varepsilon - E_F}{kT}} + 1} \simeq e^{\frac{E_F - \varepsilon}{kT}}$$

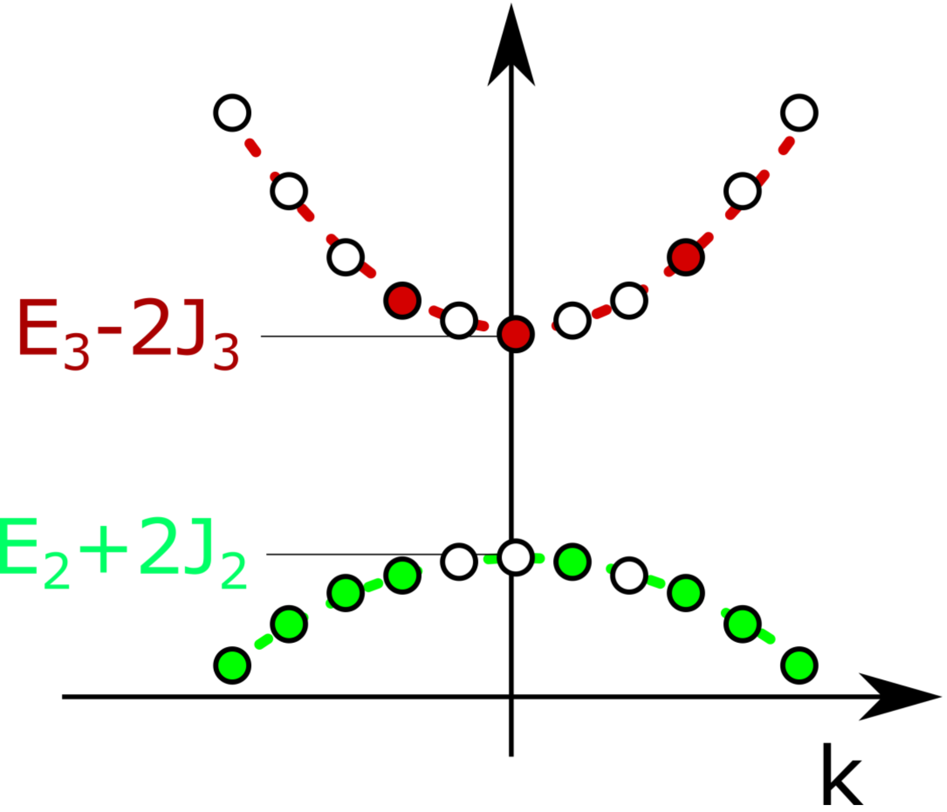
$$= e^{E_F/kT} \int_{\varepsilon > E_c} \gamma \sqrt{\varepsilon - E_c}\, e^{-\varepsilon/kT}\, d\varepsilon$$

$$\boxed{n = N_c\, e^{\frac{E_F - E_c}{kT}}} \qquad N_c = \int_{\varepsilon > 0} \gamma \sqrt{\varepsilon}\, e^{-\varepsilon/kT}\, d\varepsilon$$

Question 6-c – holes in the valence band

DoS close to the top of the valence band :

$$D_V(\epsilon) = \left(\frac{1}{2\pi\hbar}\right)^3 4\pi\sqrt{2m^3_{\mathrm{eff},\,VB}}\sqrt{E_V - \epsilon}$$



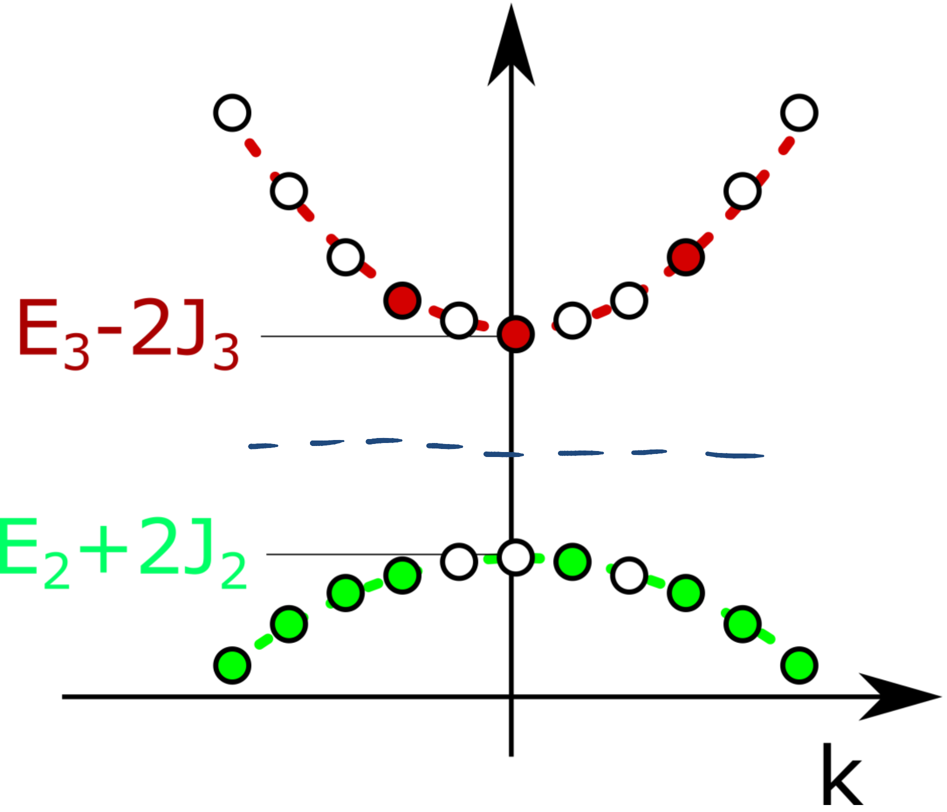
$$p = \int D_V(\varepsilon)\left(1 - f_{FO}(\varepsilon)\right) d\varepsilon$$

$$= N_V \times \exp\left[\frac{E_V - E_F}{kT}\right]$$

$$\int K_v\sqrt{\varepsilon}\, e^{-\varepsilon/kT} d\varepsilon$$

$$n \times p = N_C N_V \underbrace{e^{\frac{\cancel{E_F} - E_C + E_V - \cancel{E_F}}{kT}}}_{N_C N_V e^{-E_g/kT}}$$

Question 6-d – where is the Fermi level?



$$np = N_c N_v e^{-E_g/kT}$$

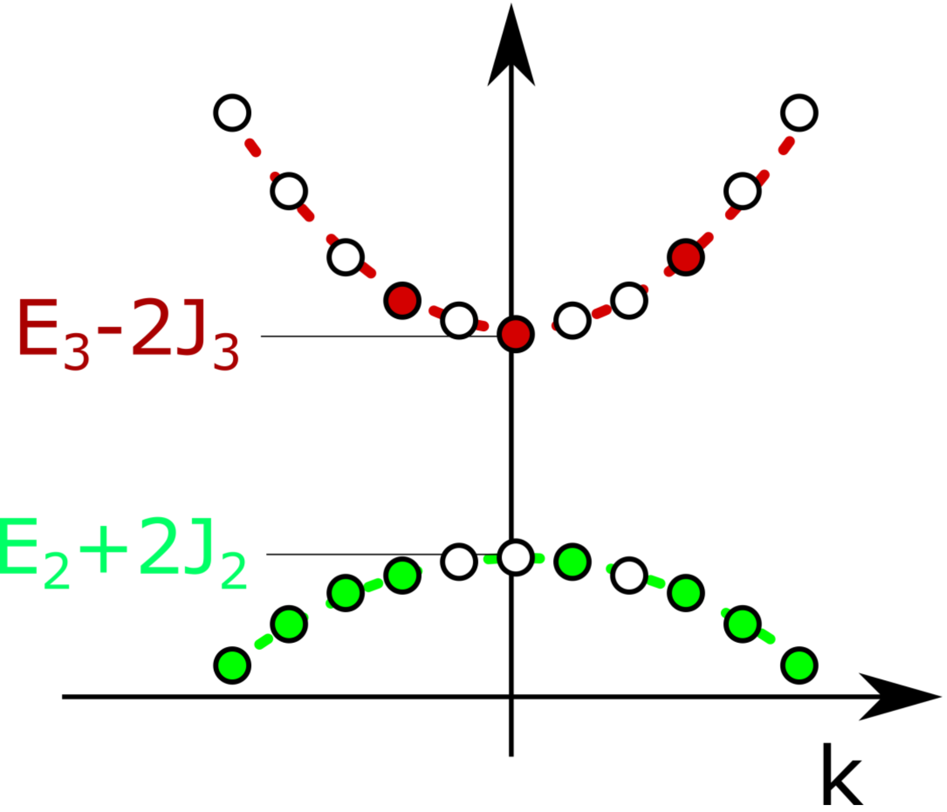
intrinsic $n = p$

$$n^2 = N_c N_v e^{-E_g/kT} = \left[N_c e^{\frac{E_F - E_c}{kT}}\right]^2 \quad N_v e^{-E_g/kT} = N_c e^{2\frac{E_F - E_c}{kT}}$$

for $m_{eff\,CB} = m_{eff\,VB} \rightarrow N_c = N_v$

$$E_F = \frac{E_c - E_v}{2}.$$

Question 6-e – semiconductor & insulators



$$np = N_c N_v e^{-\frac{E_g}{kT}}$$

$$n = p$$

$$n = \sqrt{N_c N_v}\, e^{-\frac{E_g}{2kT}}$$

@ $T = 300\,K$, $kT \simeq 30\,meV$

$\rightarrow E_g \gg 1\,eV$

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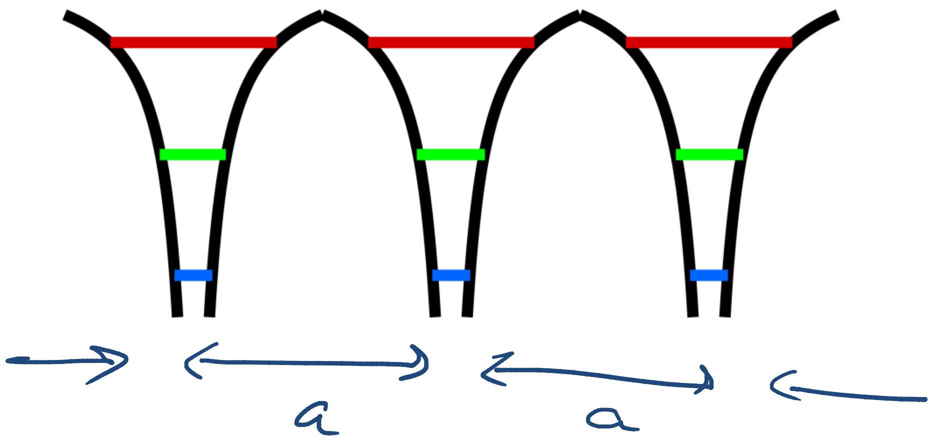
Crystal = motif + lattice

In the tutorial

Atoms equally spaced with distance a in 1D

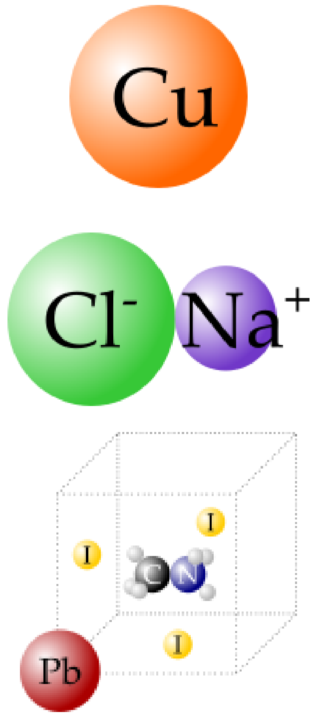


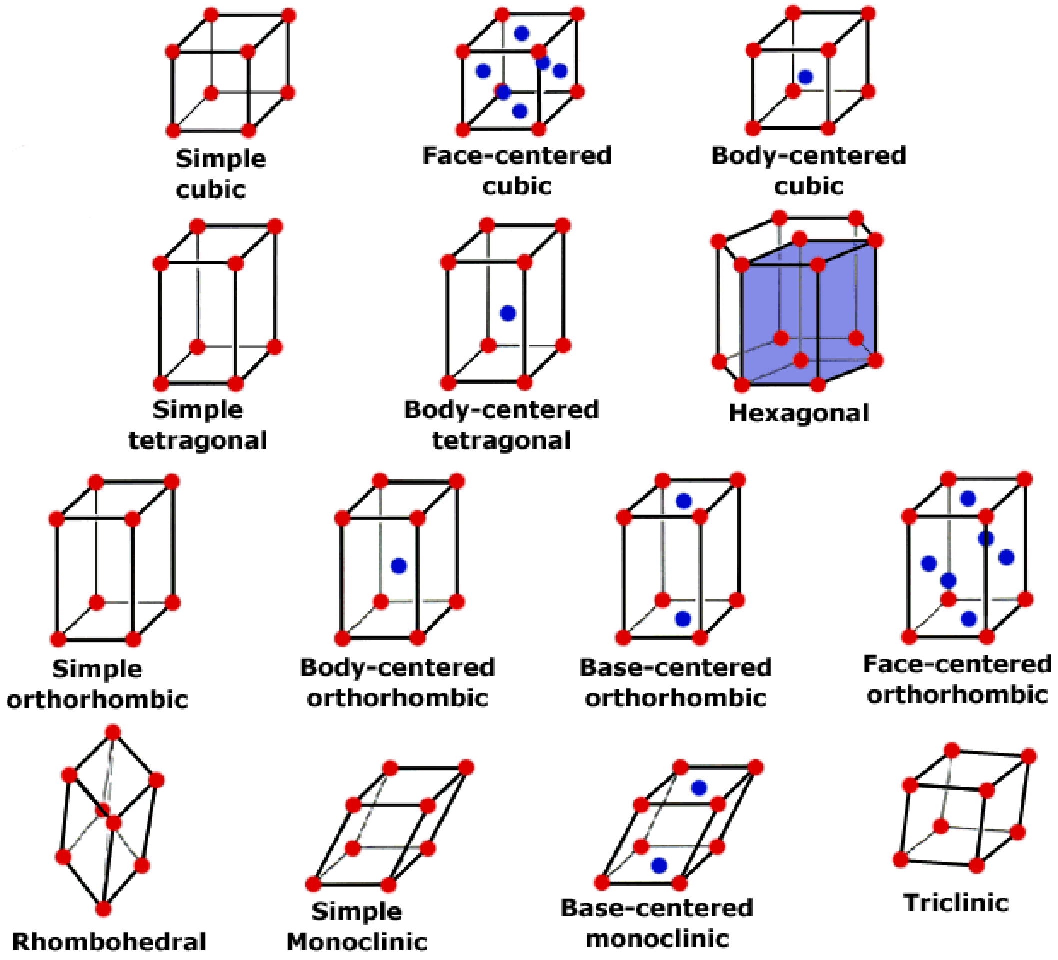
In general

Motives regularly spaced according to a *lattice* in 3D

Crystal = motif + lattice

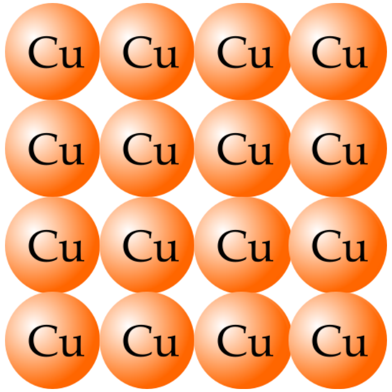
In general: crystal structure = Motives regularly spaced according to a *lattice* in 3D



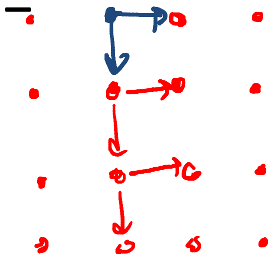


Crystal = motif + lattice

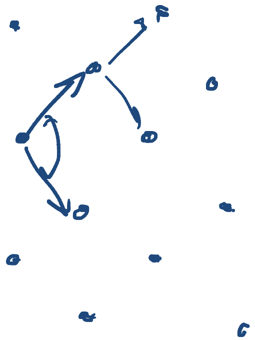
In general: crystal structure = Motives regularly spaced according to a *lattice* in 3D

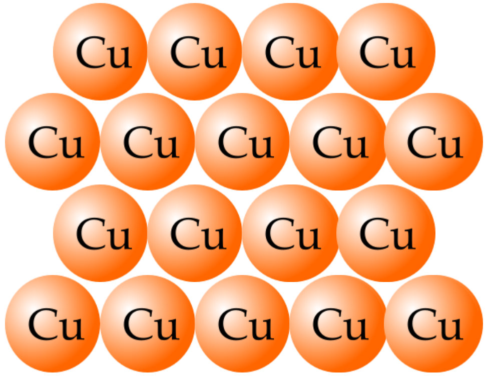


Motif = 

Lattice = 

Same motif
Different lattice





Same lattice
Different motif

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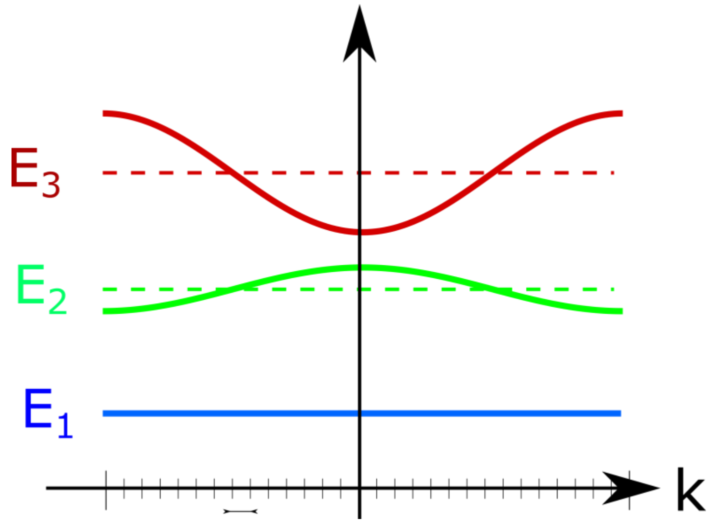
Brillouin zone

In the tutorial

An energy state is labelled by
a discrete index n
and a continuous index k

$$|\psi_{j,k}\rangle = c_0 \sum_n e^{i\,n\,k\,a}\,|\phi_j^n\rangle$$



n tells us to which band the state belongs
k is the quasi-momentum

In general

An energy state is labelled by
discrete indexes
and a continuous index k

$$|\psi_{n,\mathbf{k}}\rangle = e^{i\mathbf{k}.\mathbf{r}} \times u_{n,\,\mathbf{k}}(\mathbf{r})$$

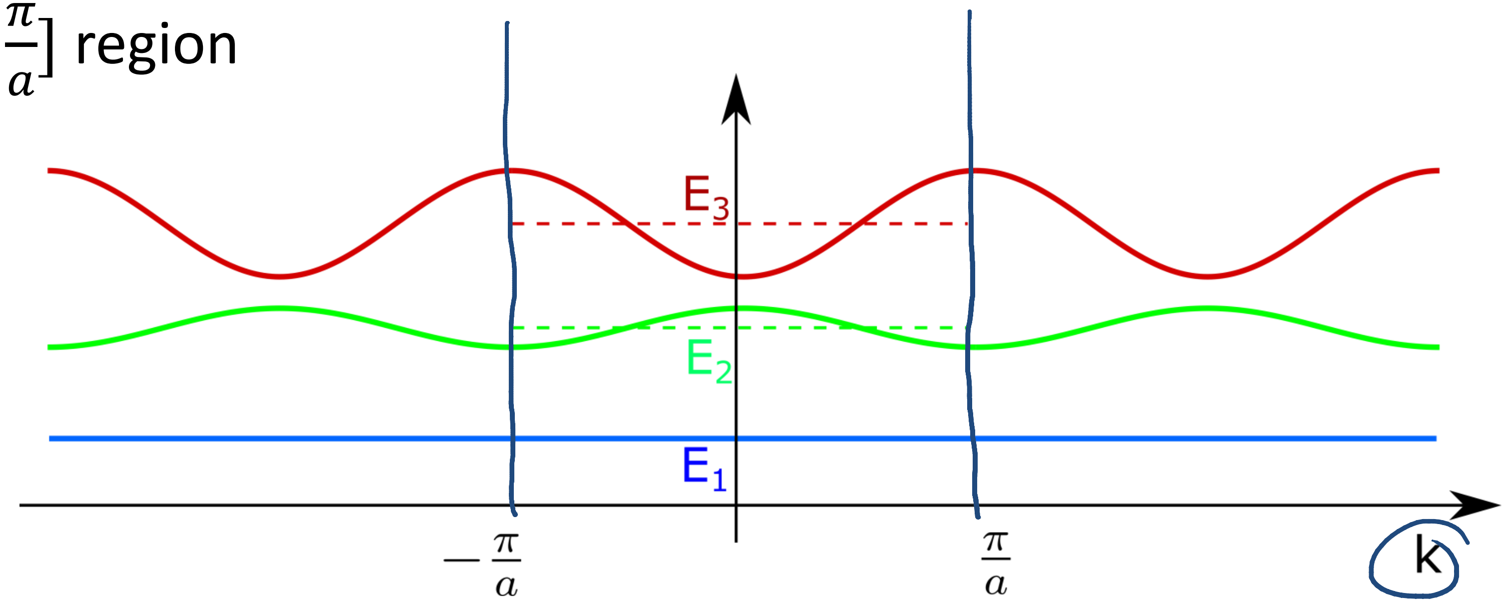
Discrete indexes indicates the band
k is the quasi-momentum

Brillouin zone

In the tutorial

$E(j,k) = E_j - 2J_j \cos(ka)$

All information about the dispersion relation lies in the $k \in [-\frac{\pi}{a}, +\frac{\pi}{a}]$ region

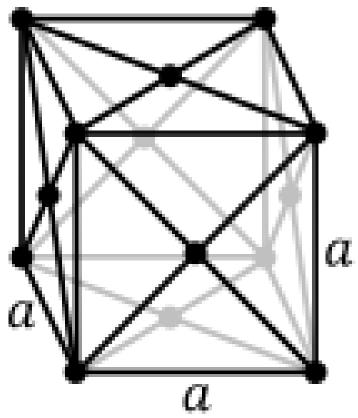
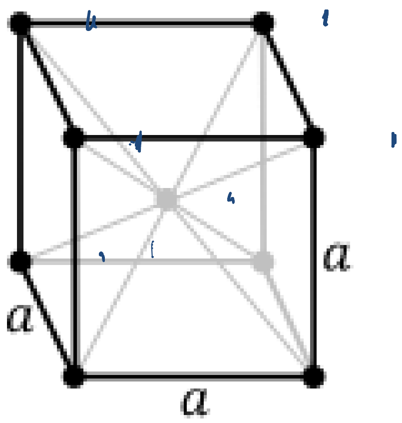
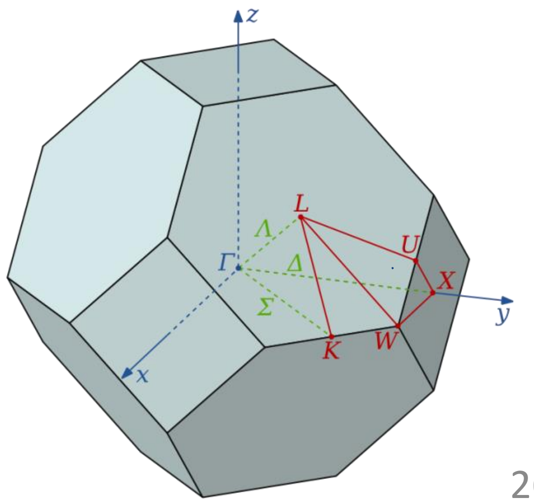


In general

All information about the dispersion relation lies in a limited region associated to the lattice = Brillouin zone

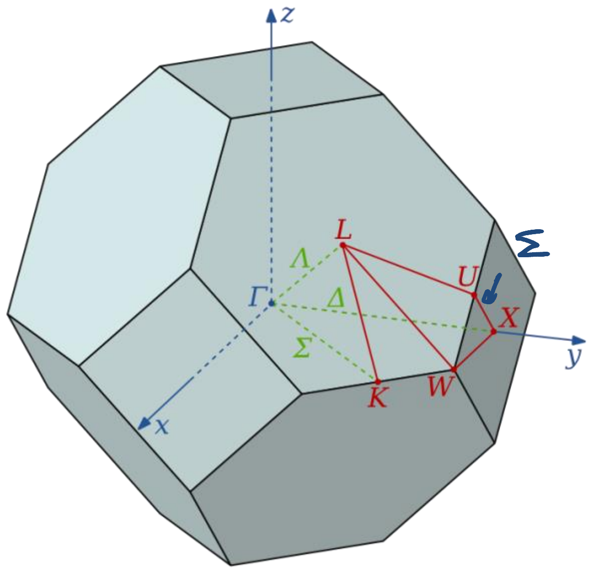
Brillouin zone: example

In general All information about the dispersion relation lies within the *Brillouin zone*

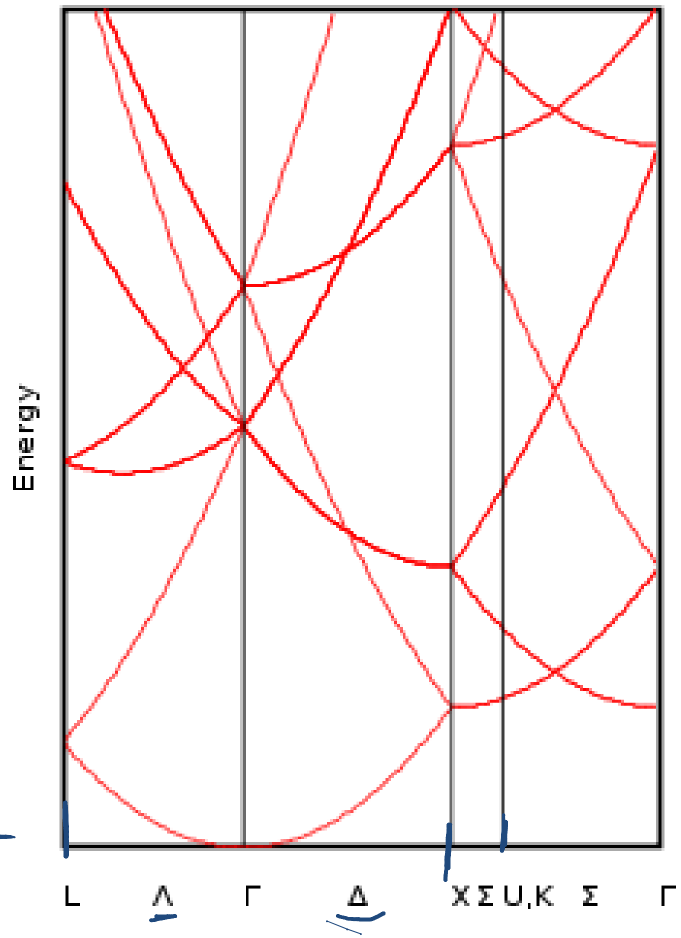
Lattice	Reciprocical lattice *= Fourier transform of the direct lattice*	Brillouin zone
		
a	$\frac{2\pi}{Na}$	$-\frac{\pi}{a}$ $\frac{\pi}{a}$
		

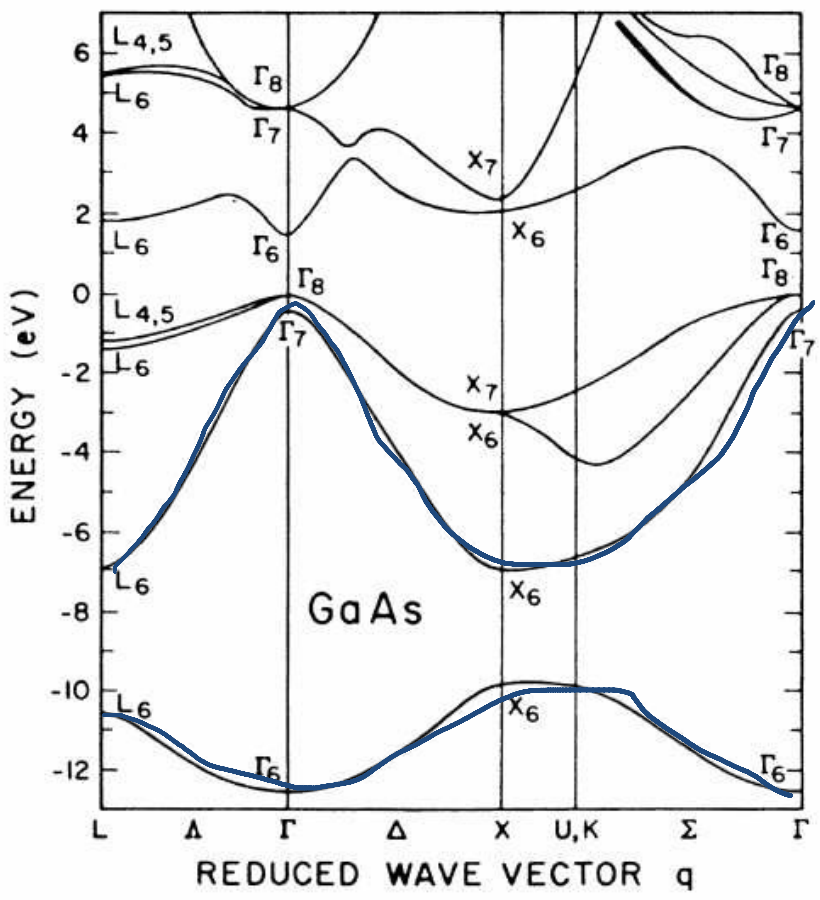
Brillouin zone and band diagrams

In general All information about the dispersion relation lies within the Brillouin zone



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





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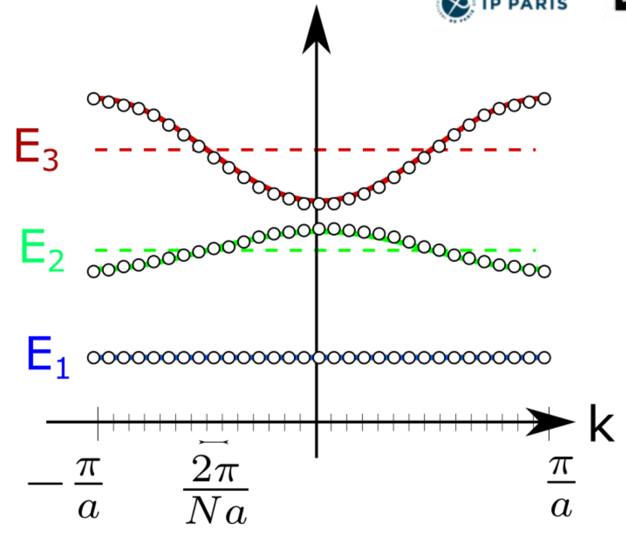
Filling up the bands

In the tutorial

N = number of atoms

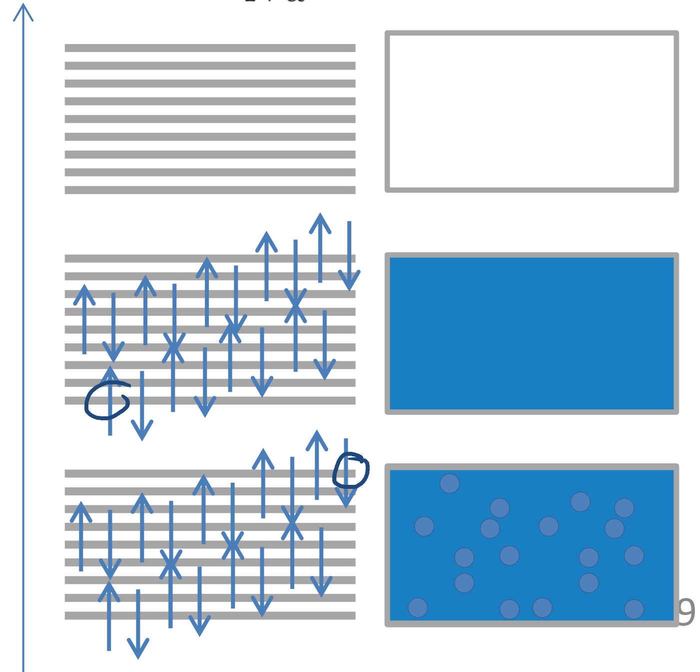
Each band can accomodate 2N particles.
At ''low'' temperature, bands are are filled from bottom to top, until all particles are accomodated



In general

Each band can accomodate 2N particles

2N



Metal, insulator & semi-conductor

In the tutorial

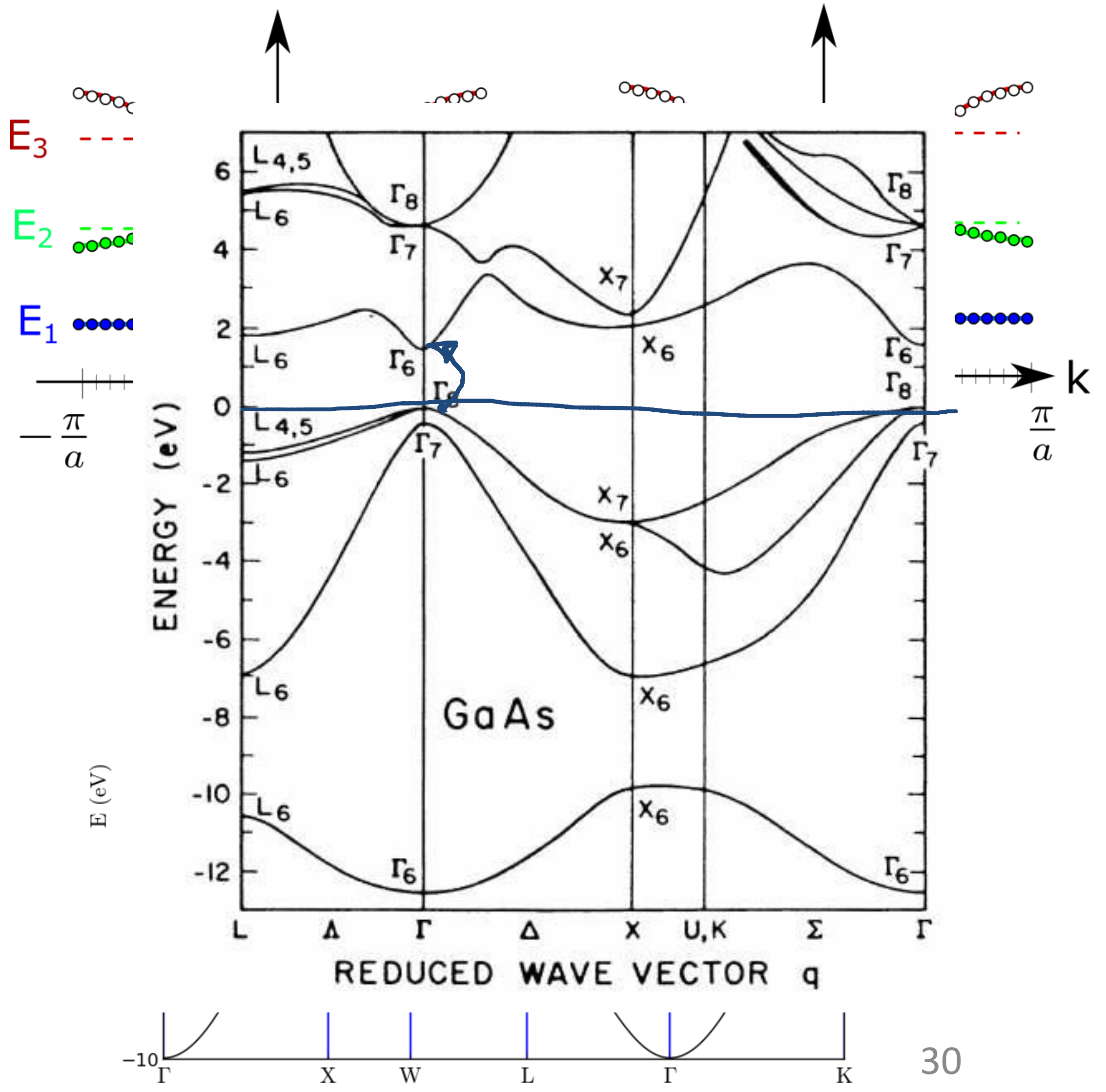
Fermi level within the band → conductor

Fermi level within a large gap → insulator

Fermi level within a small gap → semi conductor

Electrons per atoms ↔ Fermi level position

In general Idem !



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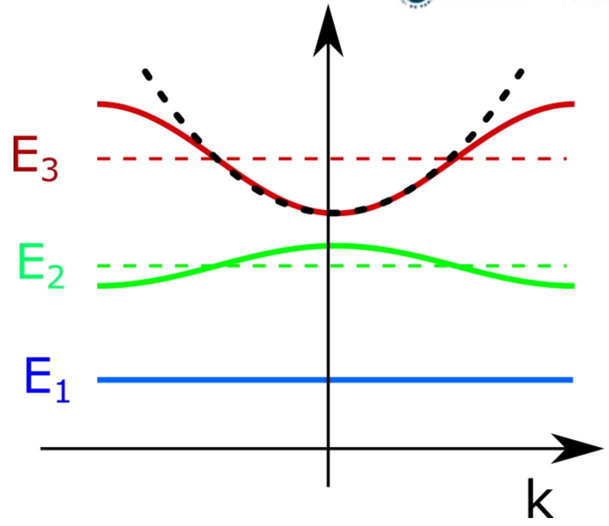
Effective masses

In the tutorial

$$E_{free}(k) = \frac{\hbar^2 k^2}{2m}$$

Close to band edges, particles behave as if free

$$E_i(k) \simeq (E_i - 2J_i) + \frac{\hbar^2 k^2}{2m^*} \quad \text{with} \quad m^* = \hbar^2/2Ja^2$$

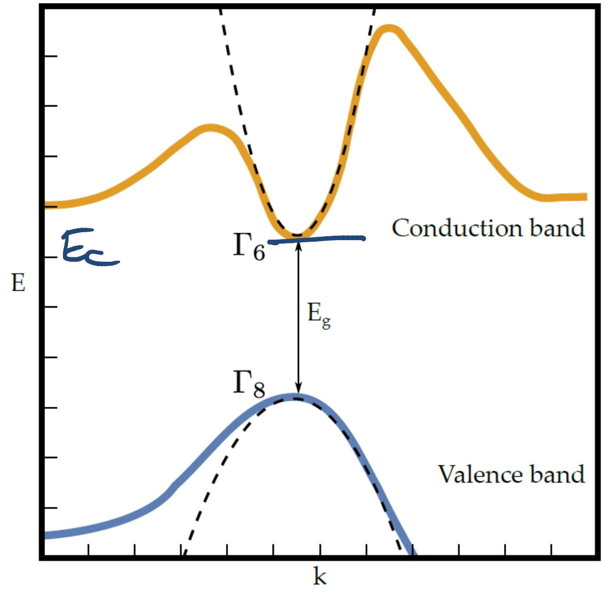


In general

All details of the potential,
All interactions,
Everything
is included in the effective mass

$$E_c(k) \simeq E_c + \frac{\hbar^2 (k-k_0)^2}{2m_c^*}$$

$$E_v(k) \simeq E_v - \frac{\hbar^2 (k-k_0)^2}{2m_v^*}$$



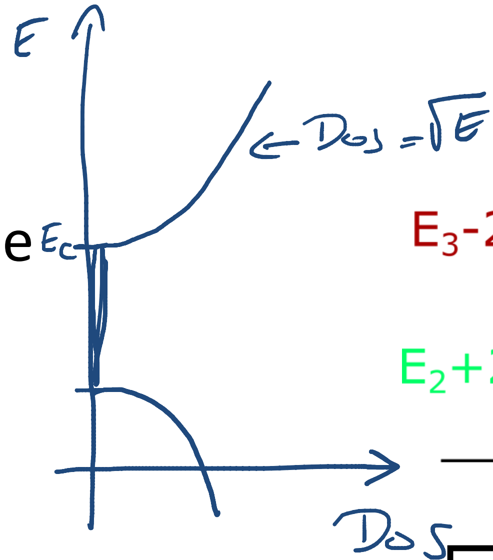
Effective density of state

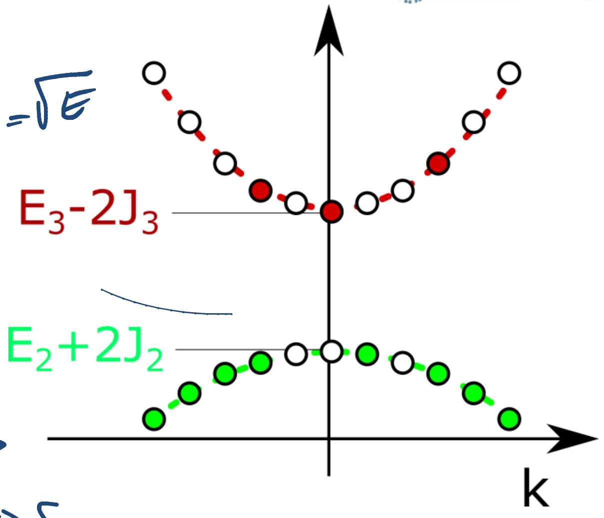
In the tutorial

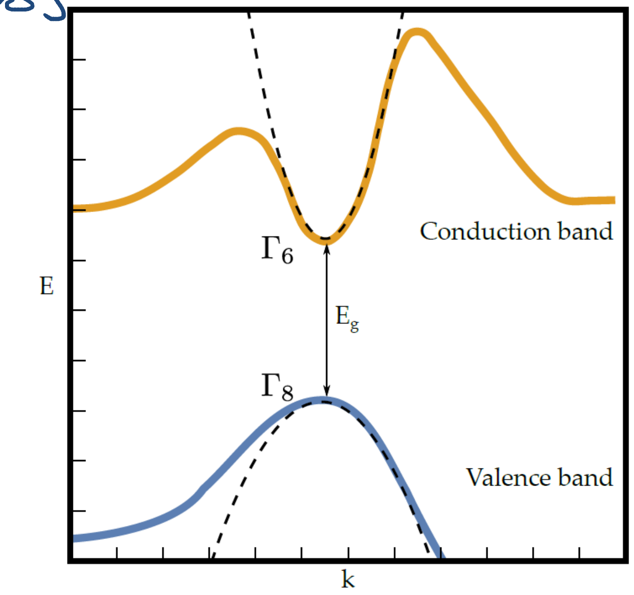
Close to band edges, particles behave as if free

$$D_C(\epsilon) = \left(\frac{1}{2\pi\hbar}\right)^3 4\pi\sqrt{2m^3_{\text{eff},\,CB}}\sqrt{\epsilon - E_C}$$

$$D_V(\epsilon) = \left(\frac{1}{2\pi\hbar}\right)^3 4\pi\sqrt{2m^3_{\text{eff},\,VB}}\sqrt{E_V - \epsilon}$$







In general Idem

Electrons and holes

In the tutorial

Density of electrons in the conduction band

$$n = \int D_c(\epsilon) f_{FD}(\epsilon) d\epsilon \simeq N_C \exp\left(\frac{\mu - E_C}{k_B T}\right)$$

Density of electrons missing from the valence band

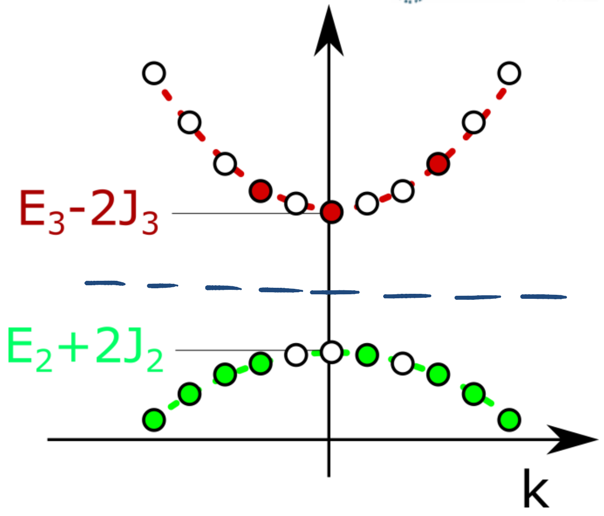
$$p = \int D_V(\epsilon)\left(1 - f_{FD}(\epsilon)\right) d\epsilon \simeq N_V \exp\left(\frac{E_V - \mu}{k_B T}\right)$$

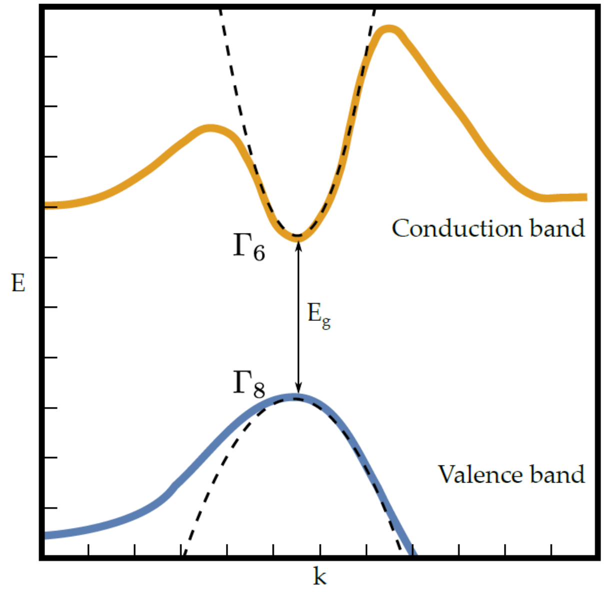
Law of mass action

$$n \times p = N_C N_V \exp\left(-\frac{E_{gap}}{k_B T}\right)$$

In general

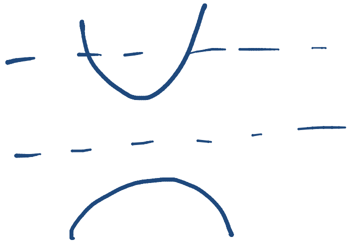
Idem



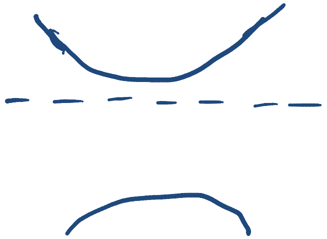


The many purposes of Fermi levels

Insulator or conductor?
Fermi level position



Doping
Fermi level position



Defects
Fermi level pinning

Light absorption
Fermi level splitting

Fermi level

Contact quality
Fermi level uniformity

Electrical current
Fermi level gradient

$J \propto \nabla E_F$

Device built in potential
Fermi level uniformity

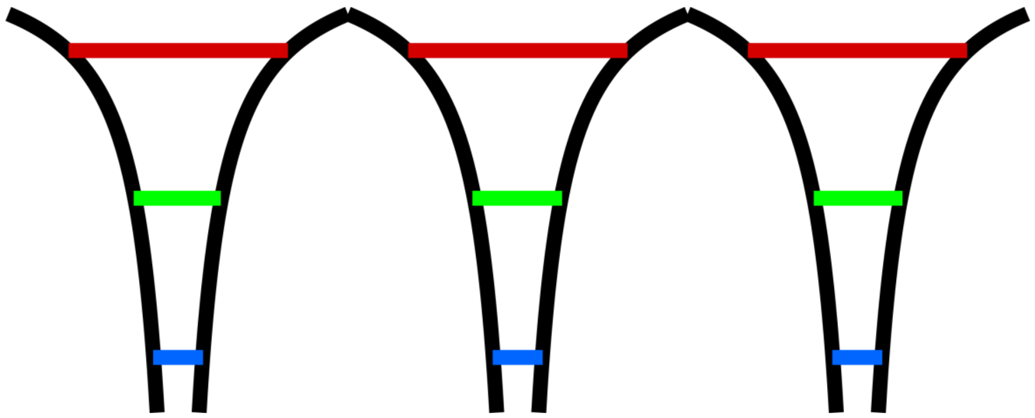
$qV = \Delta E_F$

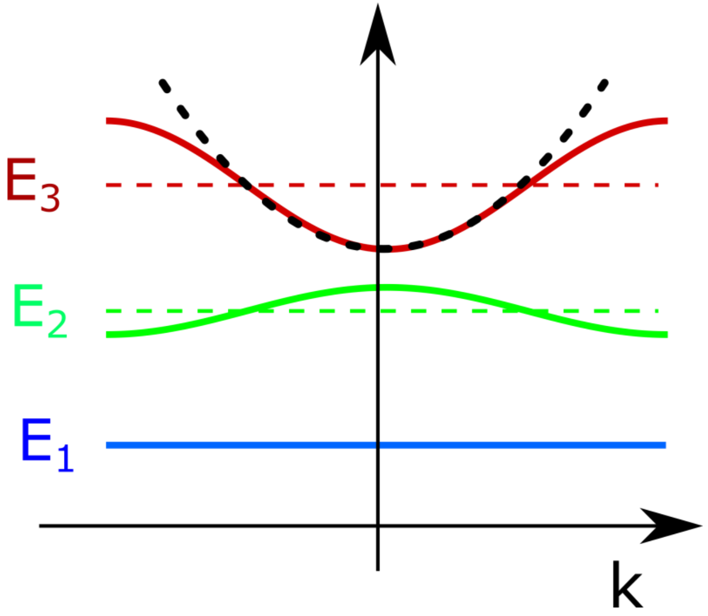
Voltage in a device
Fermi level difference

STEEM Refresher 4

1. (Tutorial) Tight binding model
2. From the 1D lattice to the crystal structure
3. From the tight binding bands to band diagrams
4. Populating energy bands: metals, insulator and semi-conductors
5. Focus on semi-conductors: the come-back of free particles
6. Focus on semi-conductors: Fermi levels
7. **Take home message**

Take-home message





Electrons in a solid :

- ➢ Discrete index *n* for the band
- ➢ Continuous quasi-momentum ***k***

All info. about dispersion relation in Brillouin zone

Electrons per atom → band filling

Completly full band → no conduction

Last band not completly full → conductor

Last band completly full → insulator or semi cond.

Close to band edges, ~ free particles
with an effective mass.