

Digression: Estimate atom density of a solid

Exercise

How many Si atoms (both types A & B) are in the conventional unit cell?

What is the atom density of Si (in atoms/cm³)?

Solution 1: Use lattice parameter $a = 0.543$ nm to calculate the volume of the conventional unit cell. Count how many Si atoms there are in the conventional unit cell. Divide this number by the volume. Convert to atoms /cm³.

Solution 2: There are $\sim 6 \times 10^{23}$ atoms in 1 mole of Si (Avogadro constant).

Si is the # 14 element \rightarrow the atomic mass is ~ 28 g/mol.

The density of water is ~ 1 g/cm³ = 1 kg/l = 1 ton/m³. Typical solids are on the same order of magnitude or one order of magnitude denser.

Let the density of Si be ρ . The volume of 1 mol (i.e. 28 g) of Si is

$$\frac{28 \text{ g}}{\frac{\rho}{\text{g/cm}^3} \text{ g/cm}^3} = \frac{28}{\frac{\rho}{\text{g/cm}^3}} \text{ cm}^3.$$

The denominator is on the order of 10^0 but > 1 . For a rough estimate, let's say this volume is ~ 10 cm³. Therefore, the atom density is $\sim 6 \times 10^{23}$ atoms / 10 cm³ = 6×10^{22} atoms/cm³.

To be more accurate, we can use $\rho = 2.3$ g/cm³ to calculate the volume of 1 mol Si:

$$\frac{28}{\frac{\rho}{\text{g/cm}^3}} \text{ cm}^3 = \frac{28}{2.3} \text{ cm}^3 \approx 12 \text{ cm}^3.$$

Thus, the Si atom density is 6×10^{23} atoms / 12 cm³ = 5×10^{22} atoms/cm³.

Atom densities of semiconductors

	Si	Ge	GaAs
Atomic number	14	32	31 for Ga, 33 for As
Atomic mass (g/mol)	28.1	72.6	69.7 for Ga, 74.9 for As
Density (g/cm ³)	2.3	5.3	5.3
Atom density (10 ²² /cm ³)	5.0	4.4	4.4 (Ga and As total)
Lattice constant (nm)	0.543	0.565	0.565

Semiconductor Physics Review/Overview

Reciprocal lattice

Crystal structure (real space) recap

A crystal is a **periodic** structure.

A period of the crystal structure is a **unit cell**, having an internal structure.

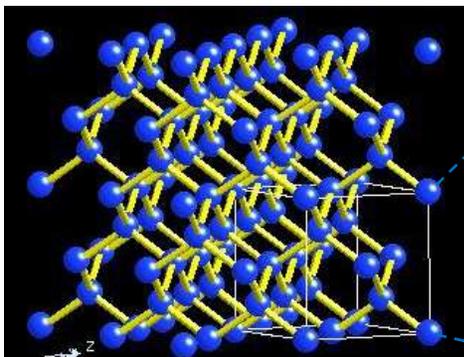
An integer multiple of a period is also a period.

The smallest possible period is called a **primitive unit cell**.

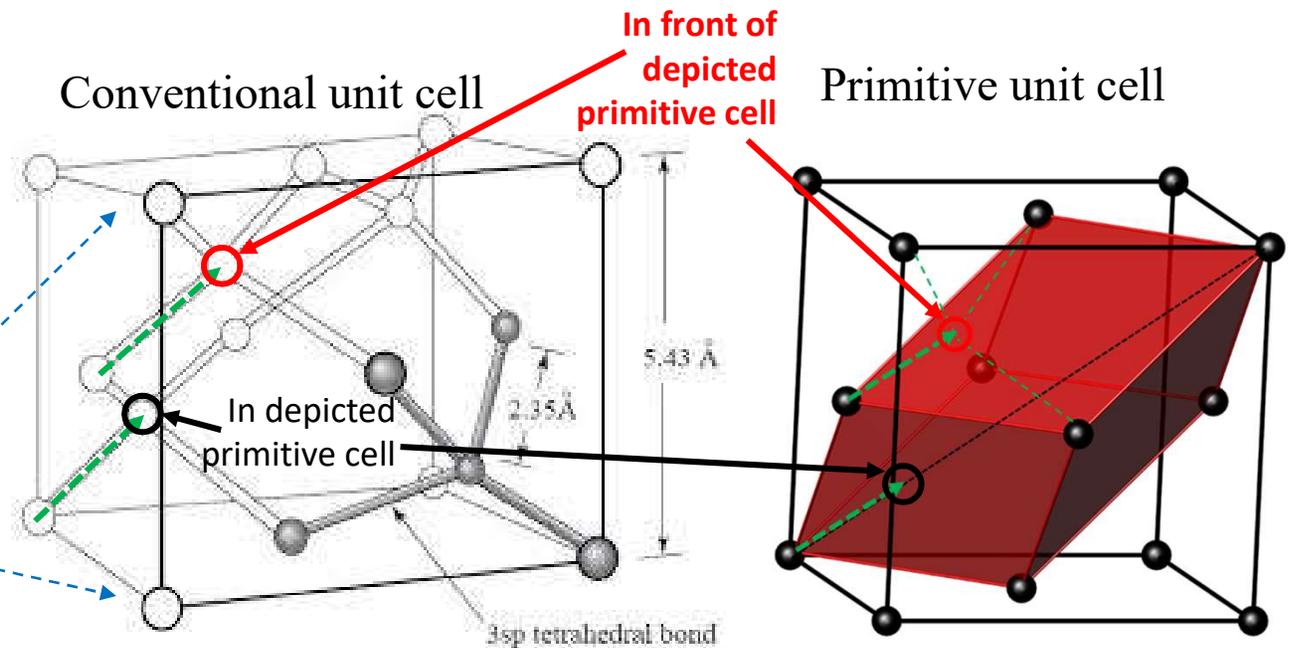
A **conventional unit cell** is often used to better visualize features of a crystal structure.

The underlying periodic lattice of a crystal structure without unit cell internal structure is the **Bravais lattice**.

Si crystal structure



http://www.webelements.com/silicon/crystal_structure.html

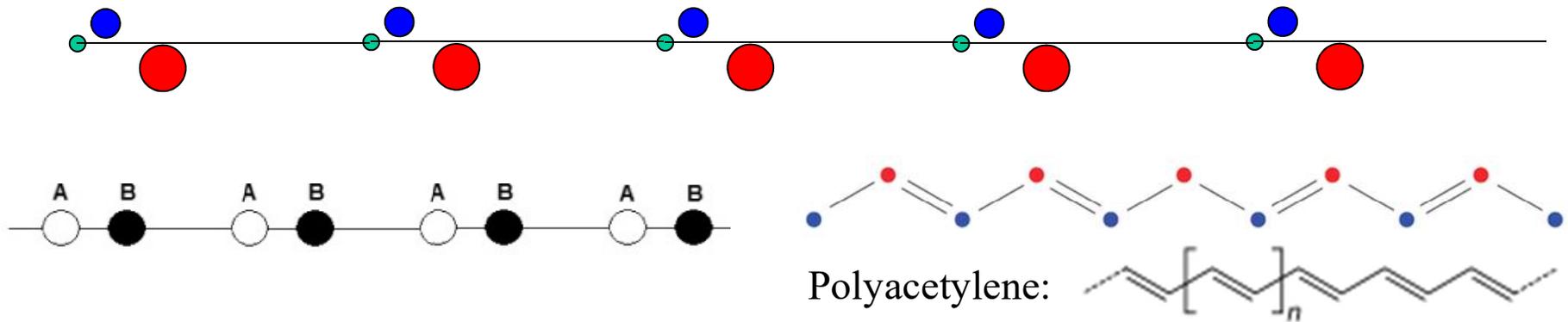


<http://onlineheavytheory.net/silicon.html>

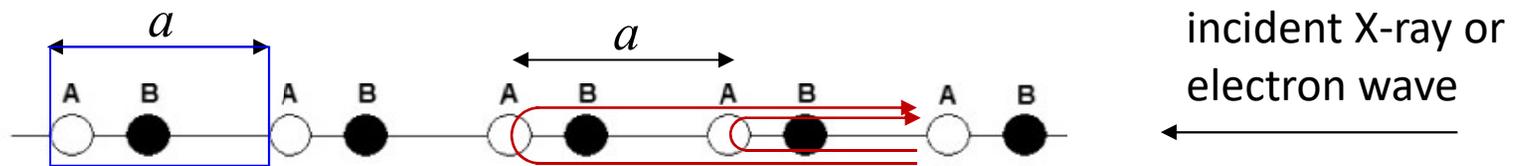
<https://physics.stackexchange.com/questions/210963/primitive-unit-cell-of-fcc>

Electrons viewed as plane waves **diffracted** by the crystal structure as a 3D lattice/grating.

1D example: the unit cell can have an internal structure

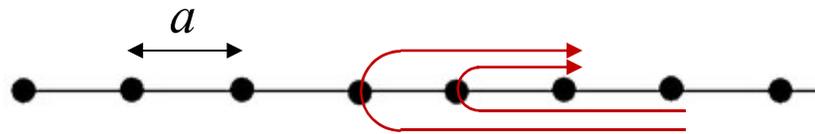


Diffraction is Nature's way of doing Fourier transform:



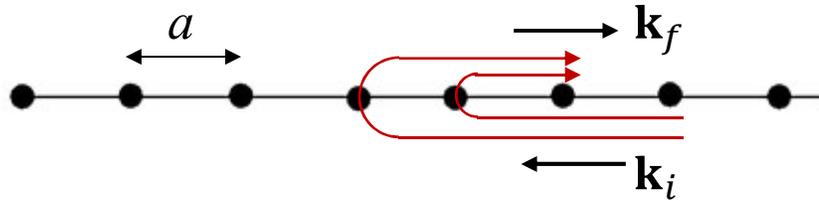
To have constructive interference between reflections by the **same atoms** (e.g. A) of all unit cells: consider the periodicity of the **Bravais lattice**

$$a = \frac{\lambda}{2} n$$



We stopped here on Tue 9/7/2021.

Diffraction is Nature's way of doing Fourier transform.

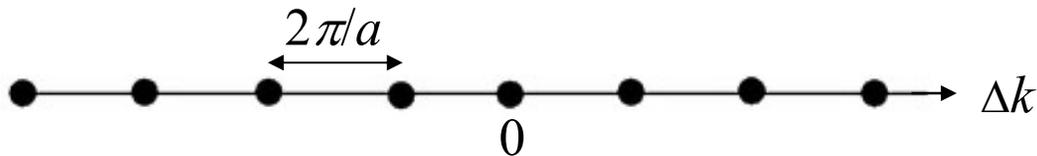


Bragg condition for constructive interference:

$$a = \frac{\lambda}{2} n \quad \text{or} \quad \frac{2\pi}{k} = \lambda = \frac{2a}{n} \quad \Rightarrow \quad k = n \frac{2\pi}{2a}$$

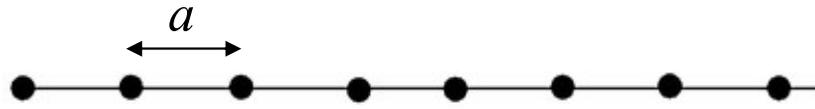
The change in \mathbf{k} (wave vector) upon reflection is

$$|\Delta \mathbf{k}| = |\mathbf{k}_f - \mathbf{k}_i| = 2 \left(n \frac{2\pi}{2a} \right) = n \frac{2\pi}{a}$$



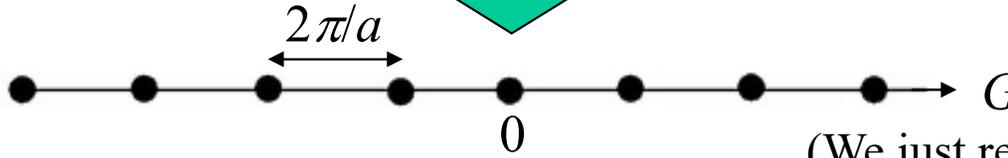
You see, the Fourier transform is just a “spectrum” of $\Delta \mathbf{k}$.

Real space



Fourier transformation

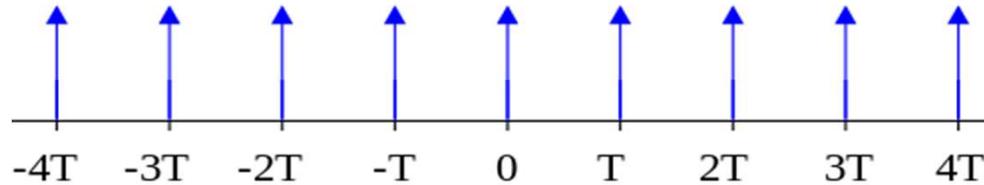
Reciprocal space



(We just renamed Δk as G)

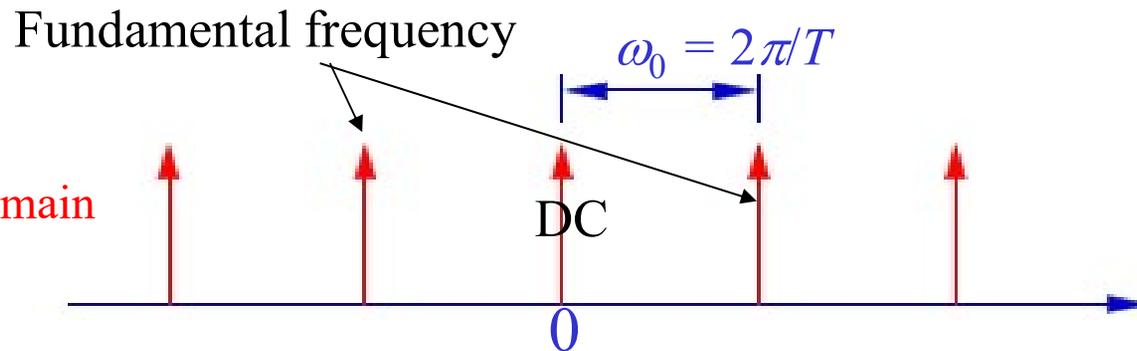
This is just like the Fourier transformation of time domain signals:

Time domain



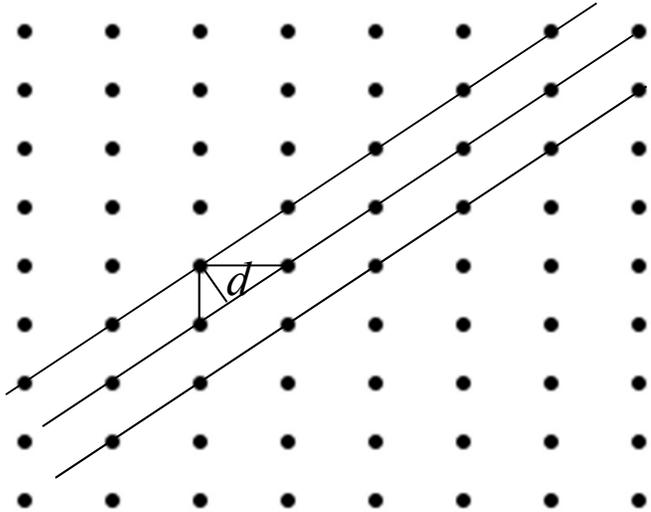
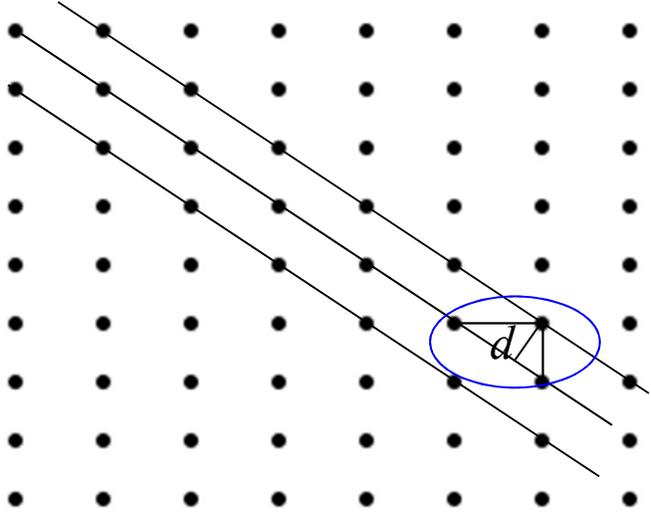
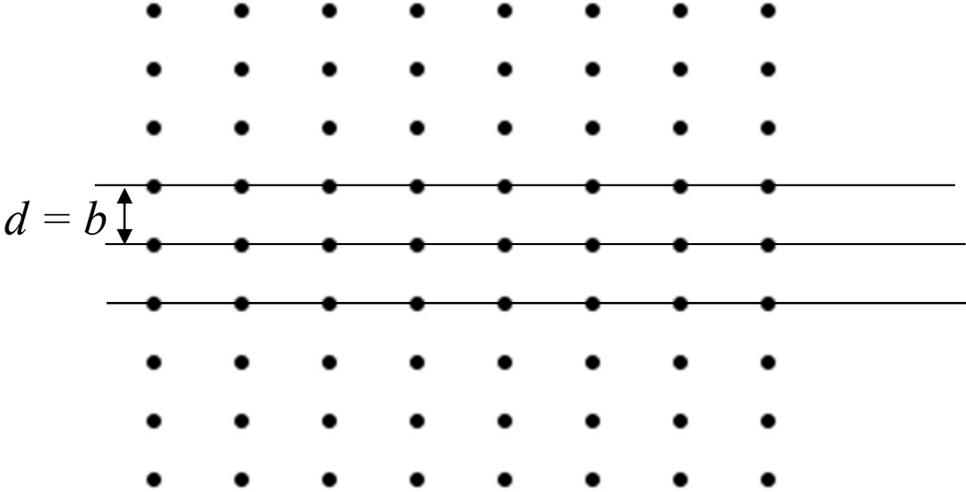
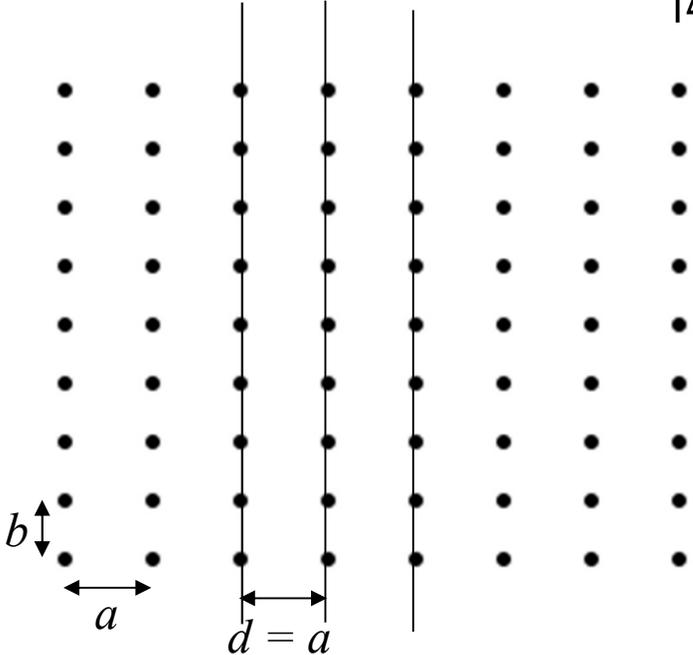
Fourier transformation

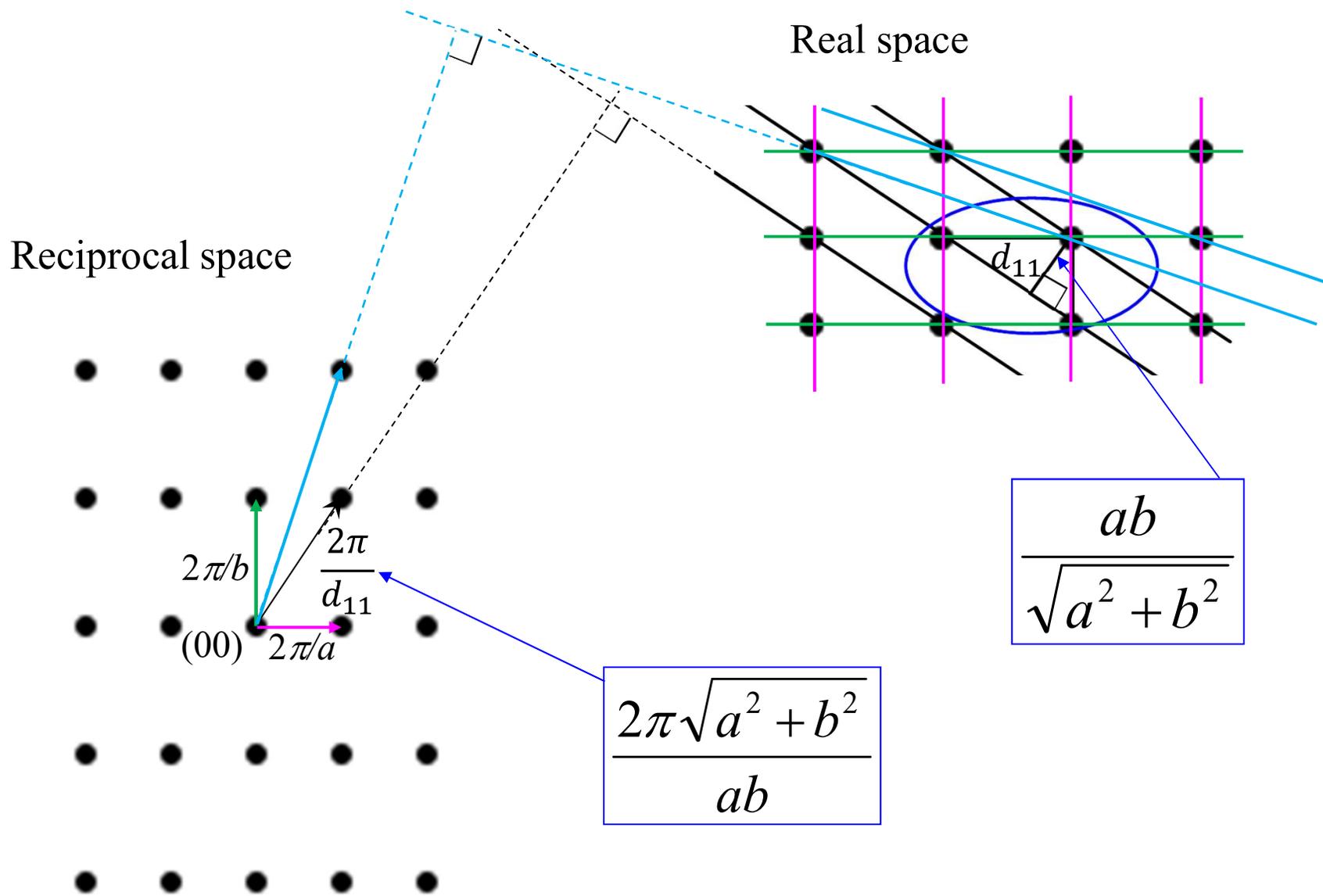
Frequency domain



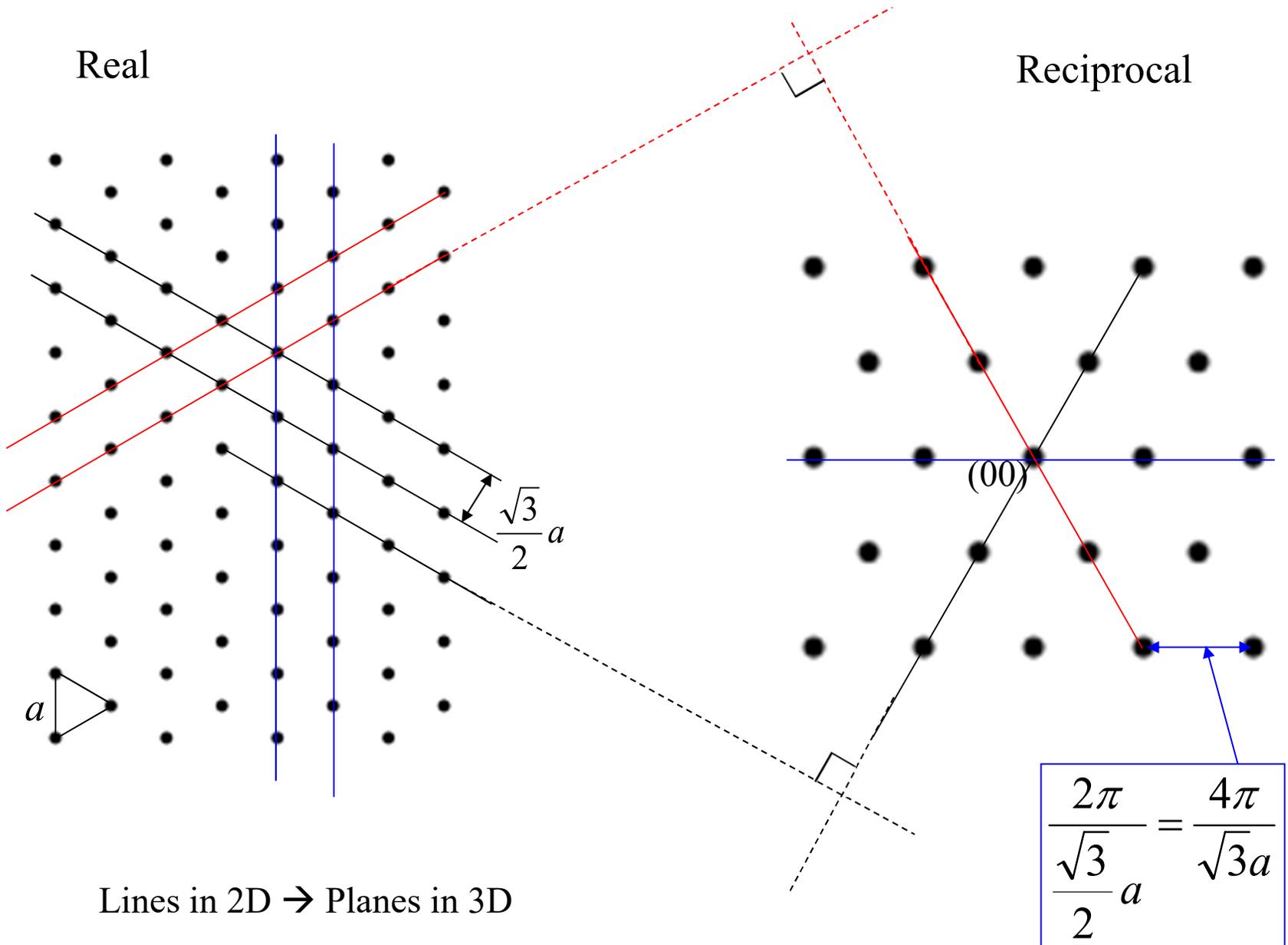
Fourier transform in 2D: Each family of lines has a corresponding Bragg condition

$$|\Delta \mathbf{k}| = n \frac{2\pi}{d}$$





Each reciprocal lattice vector (point) and its integer multiples correspond to one family of parallel **lines** of real lattice points.



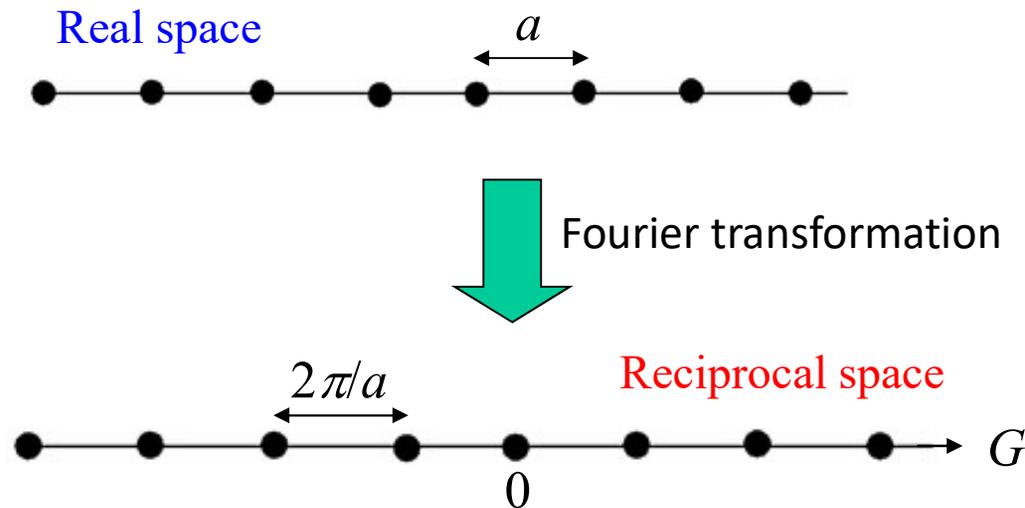
In 3D, each reciprocal lattice vector (point) and its integer multiples correspond to one family of parallel **planes** of real lattice points.

Mathematical formalism of Bravais lattices and the reciprocal space

1D: Each lattice point is represented by a “vector” $R = na$, where n is an integer. The lattice remains the same upon **translation** by R .

The reciprocal lattice vectors are $G = mb$, where m is an integer and $b = 2\pi/a$.

$$GR = 2\pi(mn)$$



Alternative notations/conventions: $a^* \rightarrow b, K \rightarrow G$

2D: Each lattice point is represented by a vector $\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2$, where n_1 and n_2 are integers. The lattice remains unchanged upon **translation** by \mathbf{R} .

The reciprocal lattice vectors are $\mathbf{G} = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2$, where m_1 and m_2 are integers.

$$\left. \begin{aligned} \mathbf{b}_1 &= \frac{2\pi \mathbf{a}_2 \times \hat{\mathbf{n}}}{|\mathbf{a}_1 \times \mathbf{a}_2|} \\ \mathbf{b}_2 &= \frac{2\pi \hat{\mathbf{n}} \times \mathbf{a}_1}{|\mathbf{a}_1 \times \mathbf{a}_2|} \end{aligned} \right\} \Rightarrow \left. \begin{aligned} \mathbf{a}_1 \cdot \mathbf{b}_1 &= 2\pi \\ \mathbf{a}_2 \cdot \mathbf{b}_2 &= 2\pi \end{aligned} \right\} \Rightarrow \mathbf{G} \cdot \mathbf{R} = 2\pi(m_1 n_1 + m_2 n_2)$$

integer

⊙ $\hat{\mathbf{n}}$: normal unit vector of 2D lattice

Area of the real-space lattice **primitive unit cell** is $|\mathbf{a}_1 \times \mathbf{a}_2|$. Area of reciprocal lattice unit cell is $4\pi^2/|\mathbf{a}_1 \times \mathbf{a}_2|$.

Notice that $\mathbf{b}_1 \perp \mathbf{a}_2$ and $\mathbf{b}_2 \perp \mathbf{a}_1$, but the following are **not always true**:

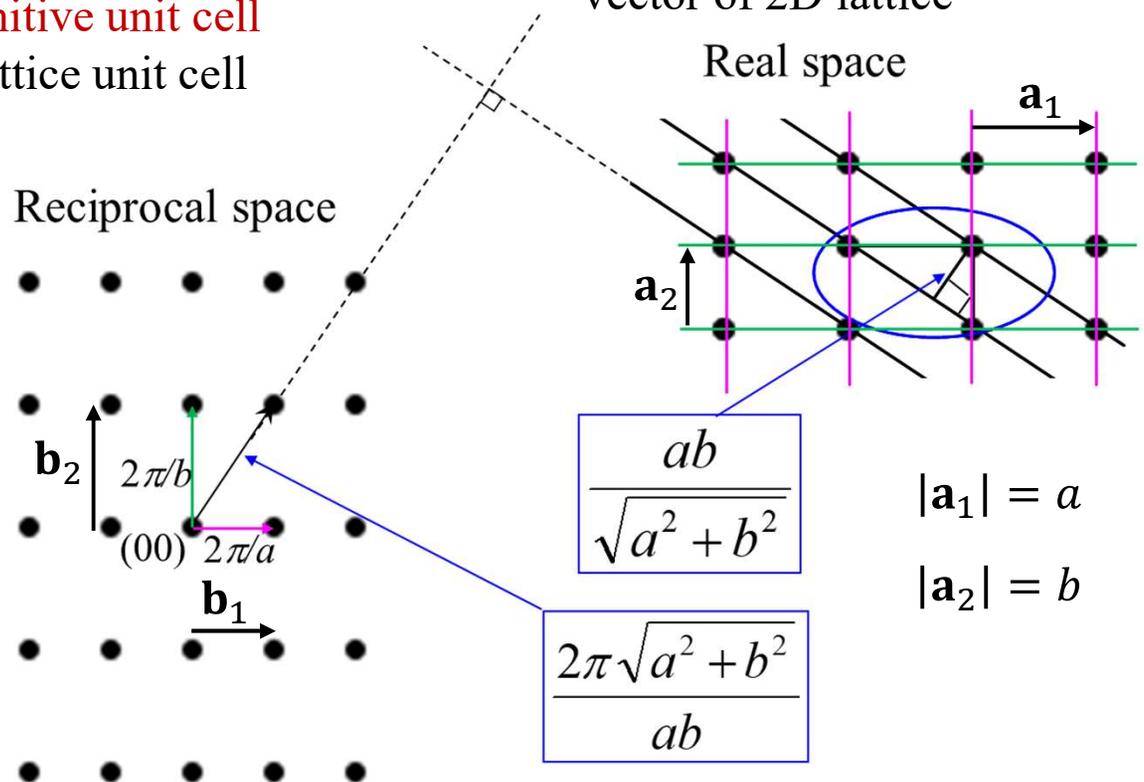
$$\mathbf{b}_1 \parallel \mathbf{a}_1, \mathbf{b}_2 \parallel \mathbf{a}_2$$

Alternative notations/conventions:

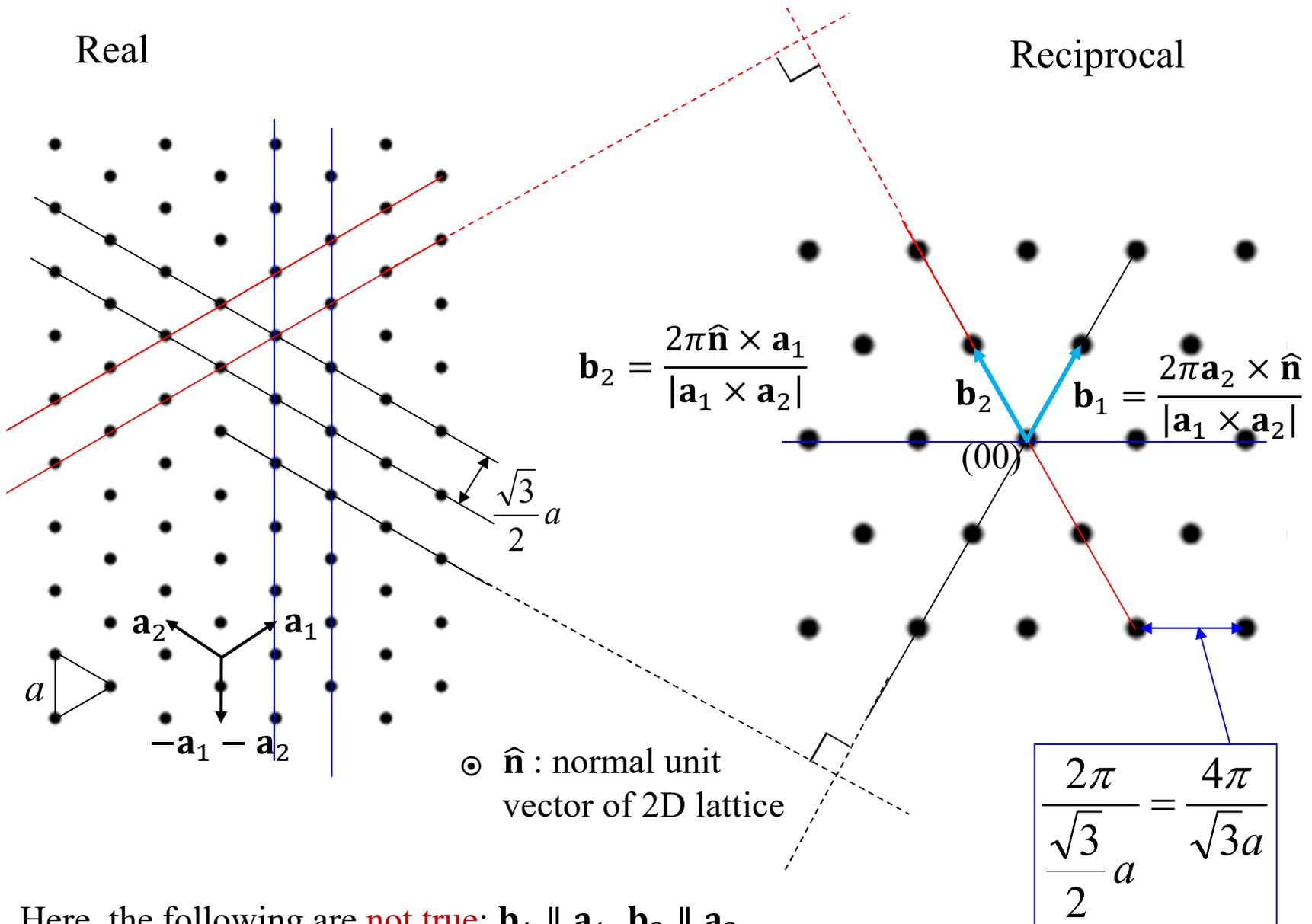
$$\mathbf{a} \rightarrow \mathbf{a}_1, \mathbf{b} \rightarrow \mathbf{a}_2;$$

$$\mathbf{a}^* \rightarrow \mathbf{b}_1, \mathbf{b}^* \rightarrow \mathbf{b}_2;$$

$$\mathbf{K} \rightarrow \mathbf{G}$$



One more example: the 2D triangular lattice



Here, the following are **not true**: $\mathbf{b}_1 \parallel \mathbf{a}_1$, $\mathbf{b}_2 \parallel \mathbf{a}_2$

3D: Each lattice point is represented by a vector $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, where n_1 , n_2 , and n_3 are integers. The lattice remains unchanged upon **translation** by \mathbf{R} .

The reciprocal lattice vectors are $\mathbf{G} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3$, where m_1 , m_2 , and m_3 are integers.

$$\left. \begin{aligned} \mathbf{b}_1 &= \frac{2\pi\mathbf{a}_2 \times \mathbf{a}_3}{(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3} \\ \mathbf{b}_2 &= \frac{2\pi\mathbf{a}_3 \times \mathbf{a}_1}{(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3} \\ \mathbf{b}_3 &= \frac{2\pi\mathbf{a}_1 \times \mathbf{a}_2}{(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3} \end{aligned} \right\} \Rightarrow \left. \begin{aligned} \mathbf{a}_1 \cdot \mathbf{b}_1 &= 2\pi \\ \mathbf{a}_2 \cdot \mathbf{b}_2 &= 2\pi \\ \mathbf{a}_3 \cdot \mathbf{b}_3 &= 2\pi \end{aligned} \right\} \Rightarrow \mathbf{G} \cdot \mathbf{R} = 2\pi(m_1n_1 + m_2n_2 + m_3n_3)$$

integer

Volume of the real-space lattice primitive unit cell is $V_p = (\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3$.

Volume of reciprocal lattice unit cell is $8\pi^3/V_p$.

Notice that $\mathbf{b}_1 \perp \mathbf{a}_2$ and $\mathbf{b}_2 \perp \mathbf{a}_1$, but the following are **not always true**:

$$\mathbf{b}_1 \parallel \mathbf{a}_1, \mathbf{b}_2 \parallel \mathbf{a}_2$$

Alternative notations/conventions:

$$\mathbf{a} \rightarrow \mathbf{a}_1, \mathbf{b} \rightarrow \mathbf{a}_2, \mathbf{c} \rightarrow \mathbf{a}_3; \mathbf{a}^* \rightarrow \mathbf{b}_1, \mathbf{b}^* \rightarrow \mathbf{b}_2, \mathbf{c}^* \rightarrow \mathbf{b}_3; \mathbf{K} \rightarrow \mathbf{G}$$

Alternative notations/conventions

In solid-state physics, we use \mathbf{G} or \mathbf{K} as “spatial (**angular**) frequency” of the real-space lattice; they are the spatial equivalent of **angular frequency** ω .

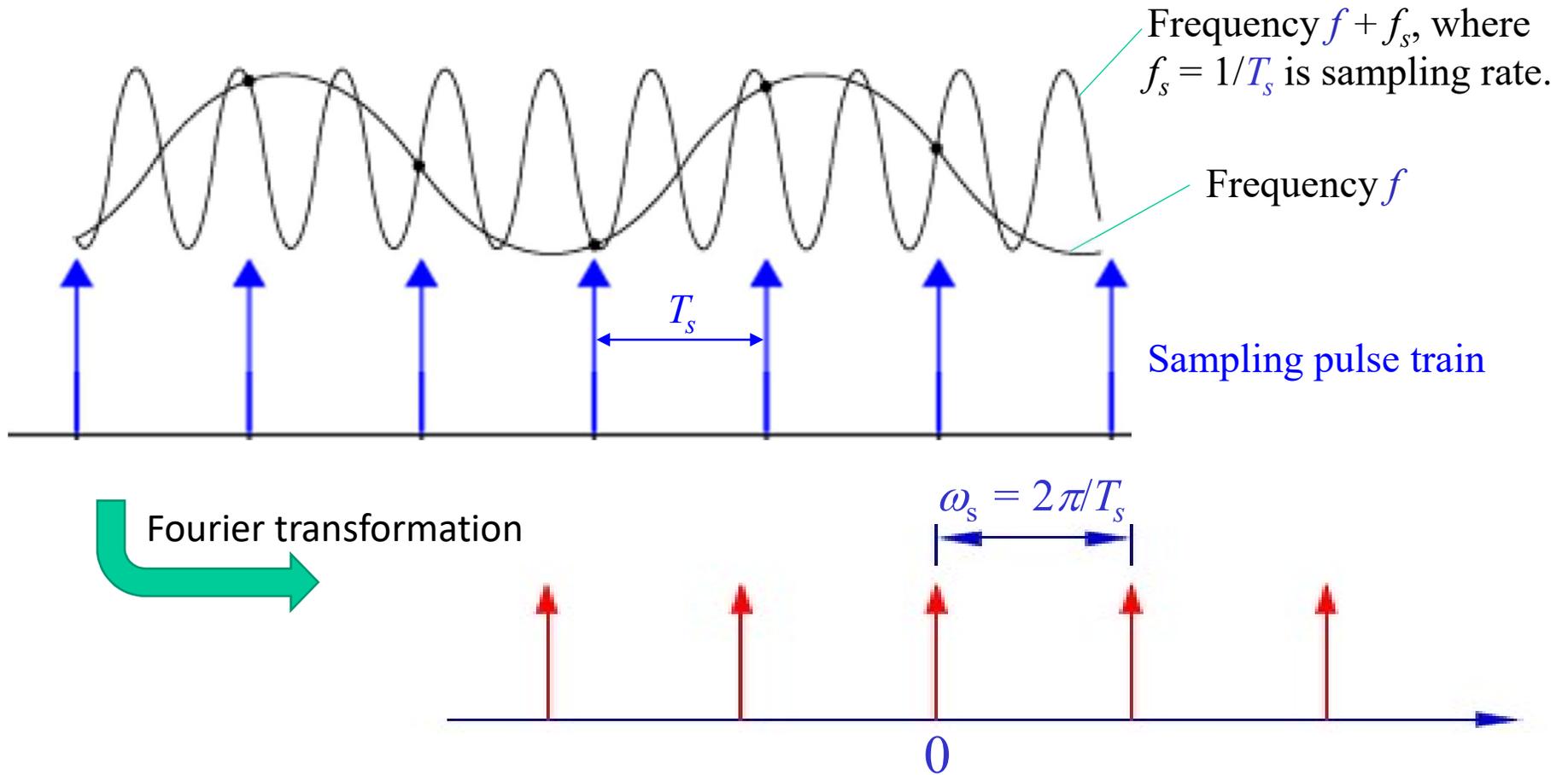
Many research tools (instruments e.g. TEM, image processing software e.g. FFT) instead use the “spatial frequency”, i.e., the spatial equivalent of **frequency** f .

The two differ by a factor 2π .

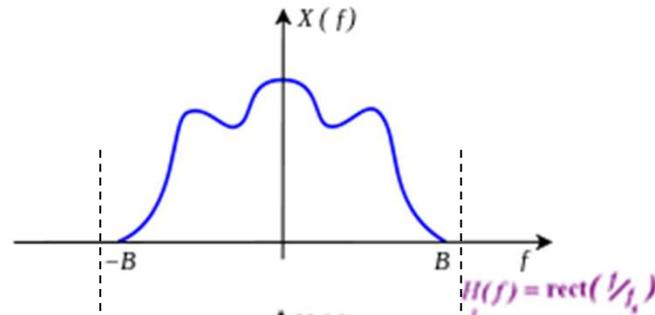
We will use “aliasing” as **analogy** to explain electron waves in crystals.

This is not rigorous, but heuristic. (“No analogy is complete.”)

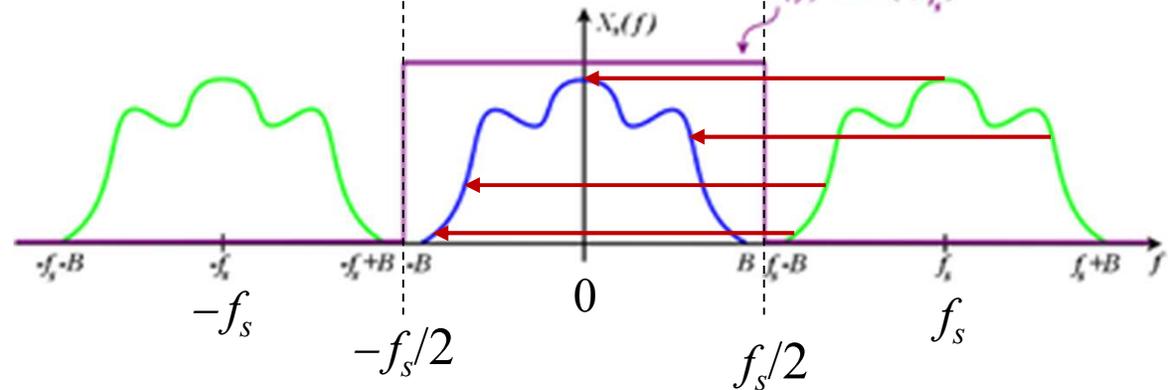
“Aliasing” in signals and systems



Spectrum of original signal



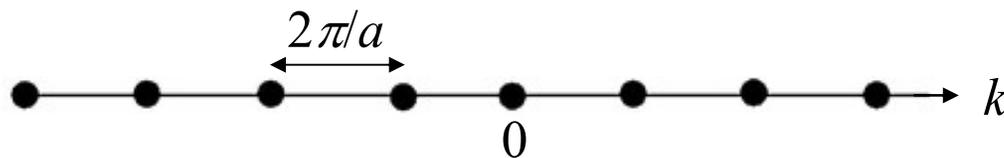
Spectrum of sampled signal



Signals of frequencies $f + nf_s$ are **not distinguishable**. Therefore, we only need to keep one of the replica, usually the one **from $-f_s/2$ to $f_s/2$** .

Similarly, electron waves of wave vectors k and $k + K$ (where $K = n(2\pi/a)$ are **reciprocal lattice vectors**) are **indistinguishable** in a periodic crystal structure.

In this course, we state this point as a conclusion without proof; it is the consequence of Bloch theorem. The electronic states in a periodic crystal structure are called **Bloch states**.



Signals of frequencies $f + nf_s$ are **indistinguishable**.

Therefore, we only need to keep one of the replica in any spectral range that is f_s wide. Usually, we filter out all other replicas and keep the one from $-f_s/2$ to $f_s/2$.

Similarly, electron waves of wave vectors k and $k + K$ (where $K = n(2\pi/a)$ are **reciprocal lattice vectors**) are **indistinguishable** in a periodic crystal structure.

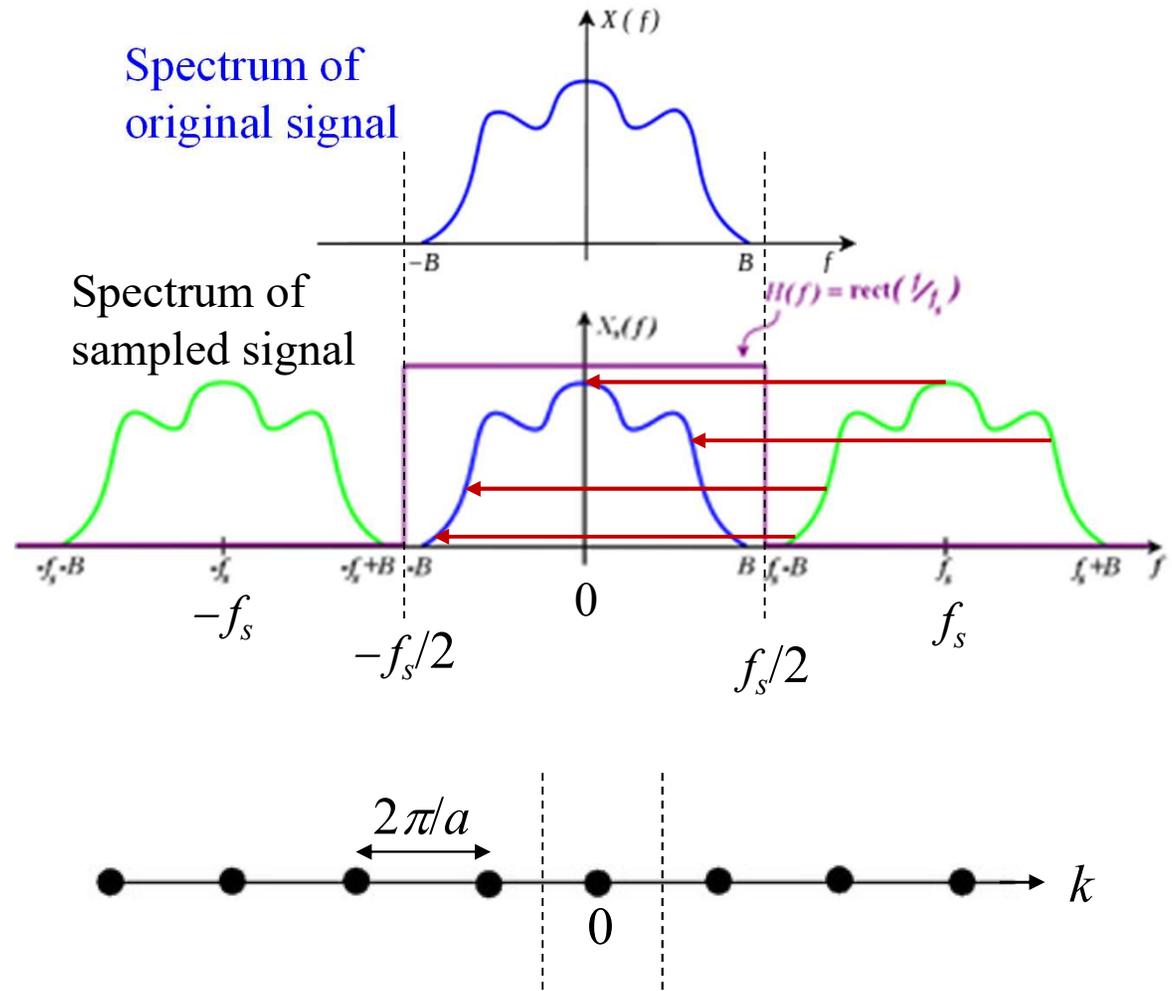
Block states in any range of k that is $2\pi/a$ wide are complete.

Therefore, we can describe electrons with Bloch states in any one of such ranges.

Such a $2\pi/a$ wide region in the reciprocal space is called a **Brillouin zone** (BZ).

A **Brillouin zone** is a primitive unit cell of the reciprocal space.

The Brillouin zone from $-2\pi/a$ to $2\pi/a$ is called the **first Brillouin zone** (1st BZ) or simply BZ.



Energy bands and gaps

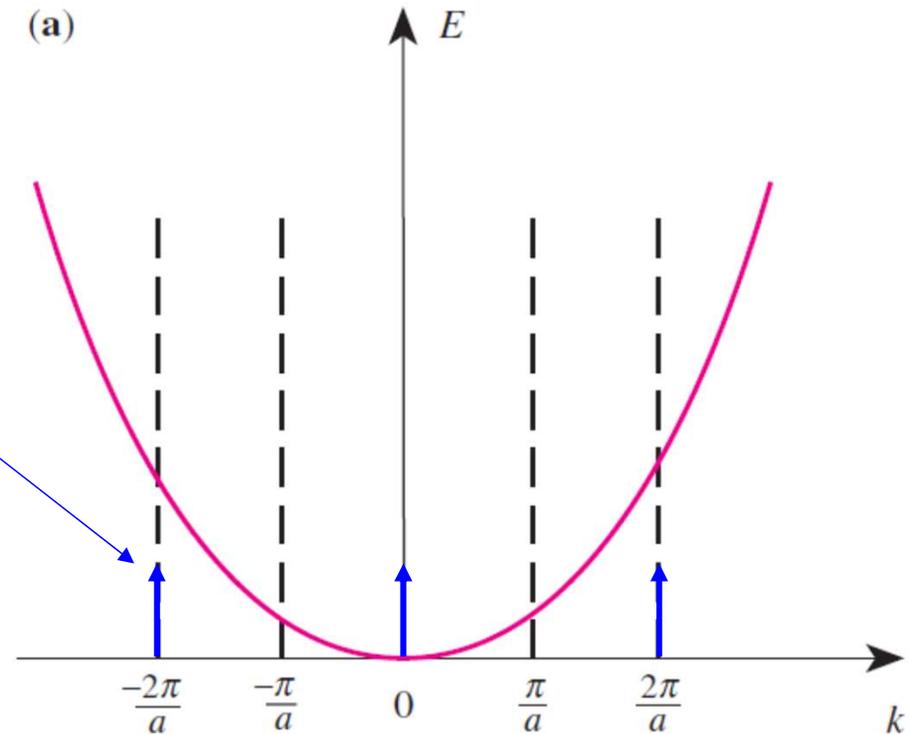
First, we consider **free electrons** (potential energy = 0; all energy is kinetic).
Recall that $p = h/\lambda = hk/(2\pi) = \hbar k$ and $E = p^2/2m$

$$\Rightarrow E = \hbar^2 k^2 / 2m$$

← mass

The **free electrons** are scattered (or diffracted) by a grating represented by “spatial (angular) frequencies” K .

Electron waves of wave vectors k and $k + K$ are indistinguishable due to the interaction, as if the lattice can impart momenta K to the electron without causing any change.



Yu & Cardona, Section 2.2, p. 21.

Bloch states labeled wave by vector k and wave vector $k + K$ are indistinguishable. Thus, we can shift segments of the $E(k)$ dispersion curve outside the 1st BZ into it.

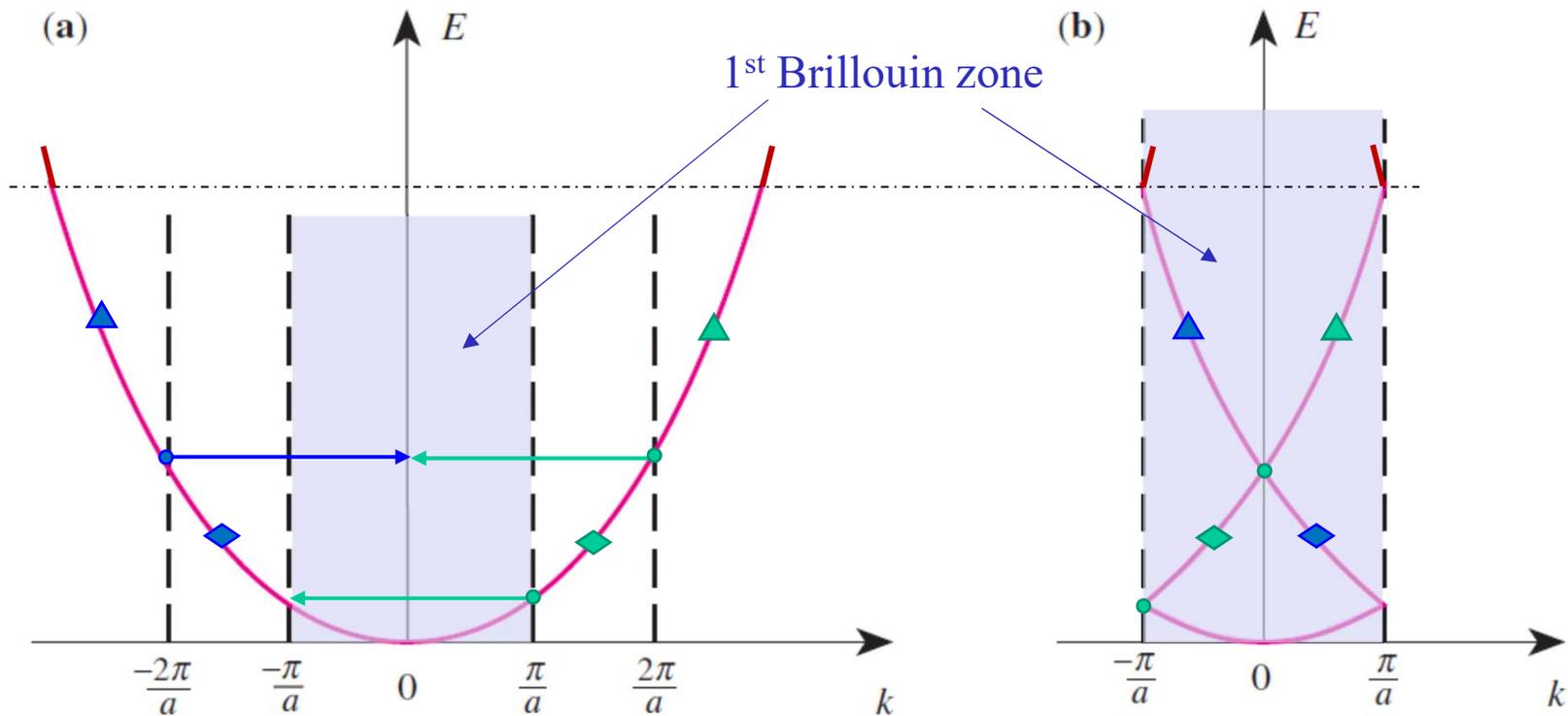
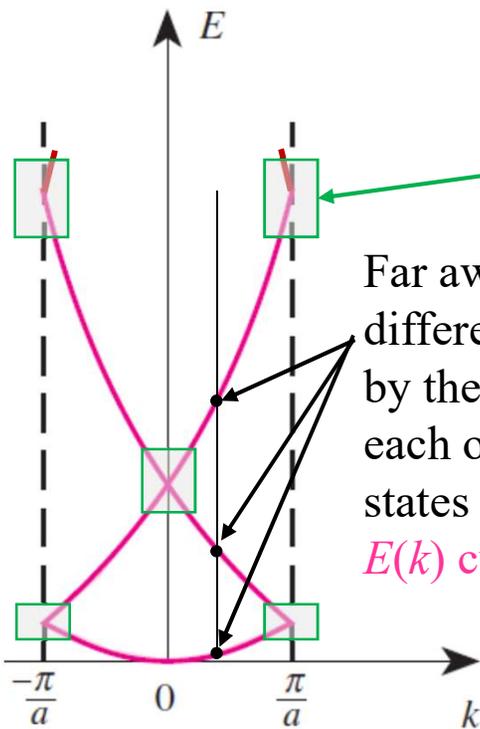


Fig. 2.1. The band structure of a free particle shown in (a) the extended zone scheme and (b) the reduced zone scheme

Yu & Cardona, Section 2.2, p. 21.

Shift segments of $E(k)$ dispersion curve into the 1st Brillouin zone, i.e., $(-\pi/a, \pi/a]$.

Points $k = \pm\pi/a$ in reciprocal space are called **zone boundaries**.

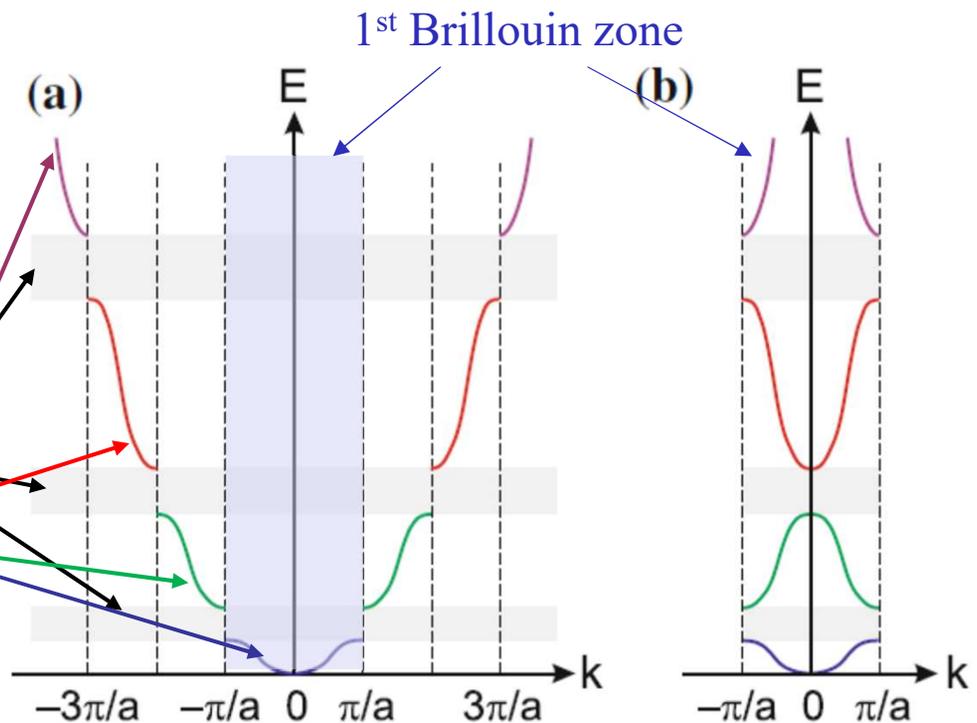


Far away from **zone boundaries**, different Bloch states specified by the same k are far away from each other in energy, i.e., the states are **far from resonance**. $E(k)$ curve similar to free e.

Around **zone boundaries** and **zone center** ($k = 0$), states of similar k (i.e. similar λ) are close to each other in energy, therefore they **interfere** with each other, giving rise to **standing waves**. In other words, they are **resonant**.

Due to standing waves, a wave similar to free e cannot propagate. Energies corresponding to free e at those k are not allowed.

The prohibited energy ranges are **gaps**, and the allowed ranges are **bands**.



Motion of Bloch electrons

An electron is a wave packet.

A wave packet is the superposition of plane waves in a small range of k .

The narrower the wave packet, the wider its k range (just as the narrower a pulse the broader its spectrum), and vice versa: $\Delta x \Delta k \sim 1$.

Since momentum $p = \hbar k$, $\Delta x \Delta p \sim \hbar$. This is the famous **principle of uncertainty**.



The velocity of the electron is the **group velocity** of the wave packet.

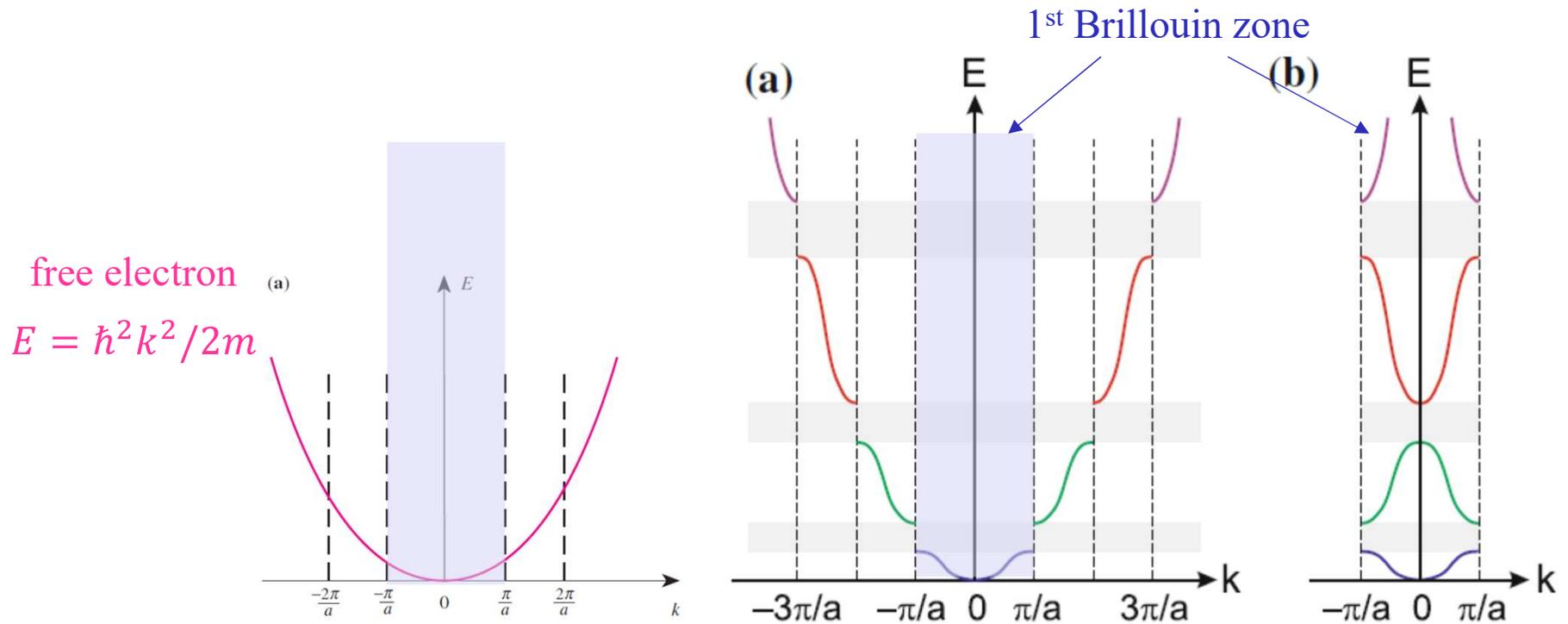
As for any wave, a wave packet (the envelope) moves at the **group velocity**

$$\left. \begin{array}{l} \frac{d\omega}{dk} \equiv v_g \\ E = \hbar\omega \end{array} \right\} \Rightarrow v_g = \frac{d\omega}{dk} = \frac{1}{\hbar} \frac{dE}{dk}$$

First, we consider the free electron. $E = \hbar^2 k^2 / 2m$

$$\begin{array}{c} \downarrow \\ v_g = \frac{1}{\hbar} \frac{dE}{dk} = \frac{\hbar k}{m} = \frac{p}{m} = v \end{array}$$

Next, we use the free e analogy to build a **semi-classical theory for Bloch electrons**.



In our “nearly free electron” model, $E = \hbar^2 k^2 / 2m$ at the bottom of lowest band.

Bottom of each of other bands can be expressed as $E \propto k^2$ (Taylor expansion).
 Therefore, we can write

$$E = \frac{\hbar^2 k^2}{2m^*} \leftarrow \text{Effective mass}$$

Next, we show that the **effective mass** can be defined more generally.

We finished this slide on Thu 9/9/2021.

At the bottom of a band,

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

It appears that we can describe the Bloch e as a **classical** e with a modified mass, m^* .

Let's give it a try. Let's try to make the Bloch e follow Newton's 2nd law:

Externally applied force,
not due to ion cores or
other electrons in crystal

$$F = m^* a = m^* \frac{dv}{dt} = \frac{dp}{dt}$$

$$v = \frac{1}{\hbar} \frac{dE}{dk}$$

$$\Rightarrow \frac{1}{m^*} = \frac{dv}{dp} = \frac{1}{\hbar} \frac{dv}{dk} = \frac{1}{\hbar^2} \frac{d^2E}{dk^2}$$

So, the **effective mass** is just (proportional to) the reciprocal of the **second derivative** (or "curvature") of the $E(k)$ **dispersion curve**.

Summary of the **1D** semi-classical model

Electron moves at the group velocity.

$$v = \frac{1}{\hbar} \frac{dE}{dk}$$

Electron behaves as a classical e with mass m^* .

$$\frac{1}{m^*} = \frac{dv}{dp} = \frac{1}{\hbar} \frac{dv}{dk} = \frac{1}{\hbar^2} \frac{d^2E}{dk^2}$$

In general, m^* is a function of k .

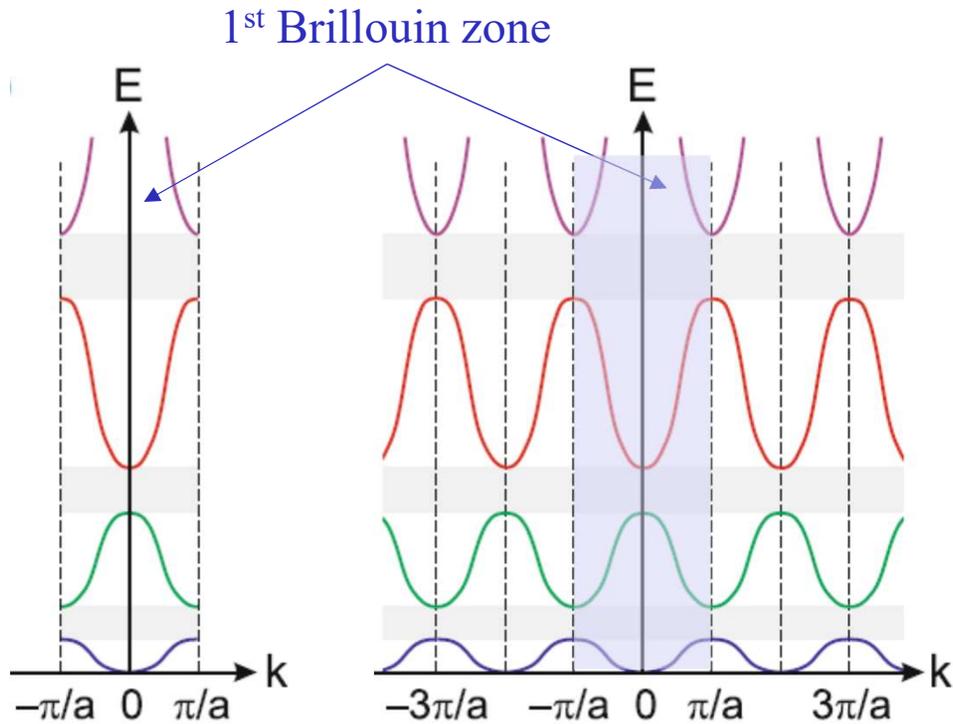
With this, electron follows Newton's laws.

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

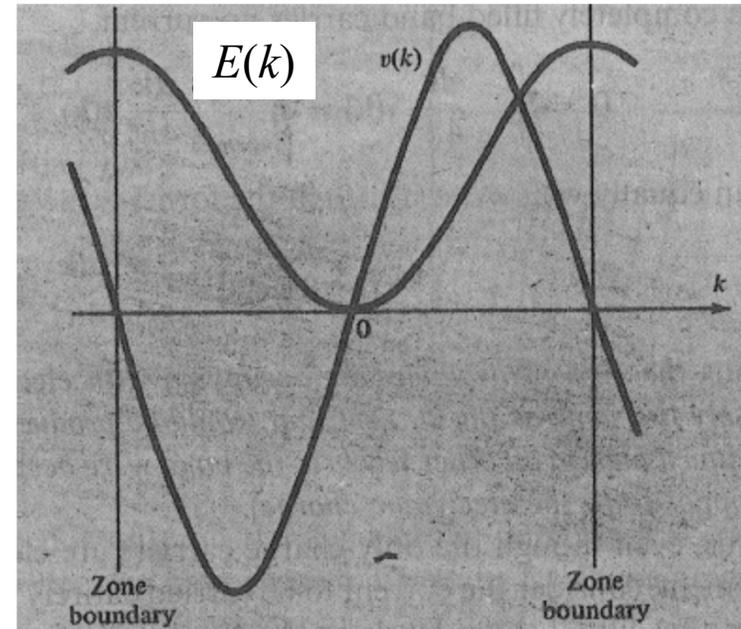
The forces by the ion cores and other electrons are accounted for by the modified mass. **Only applied forces** enter Newton's 2nd law.

$$F = m^* \frac{dv}{dt} = \frac{dp}{dt} = \hbar \frac{dk}{dt}$$

Bloch oscillation: Bloch electrons under DC electric field in perfect crystals



$$F = \frac{dp}{dt} = \hbar \frac{dk}{dt}$$



$$v = \frac{1}{\hbar} \frac{dE}{dk}$$

Bloch oscillation has **never** been observed in natural, bulk solids.

Because one cycle is much longer than scattering (collision) time.

Relaxation time approximation

Bloch e suffers a collision (scattering) in time τ **on average**.

Under electric field \mathcal{E} , each e gains a momentum $\hbar\Delta k = F\tau = -q\mathcal{E}\tau$ **on average**, where q is elementary charge.

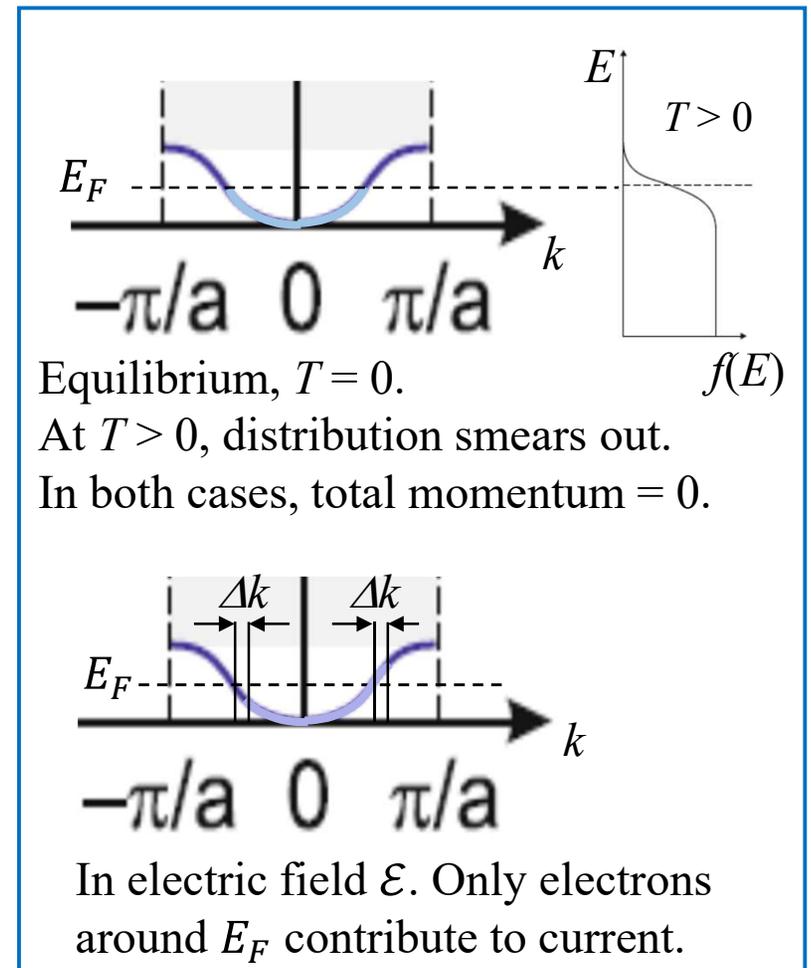
After collision/scattering, the e “forgets” the gained momentum, i.e., **relaxes** to the **average, net** momentum 0.

Collisions/scattering are due to defects (including impurities), surfaces/interfaces, and lattice vibration (a.k.a. **phonons**). These are deviations from perfect periodicity of crystal structure.

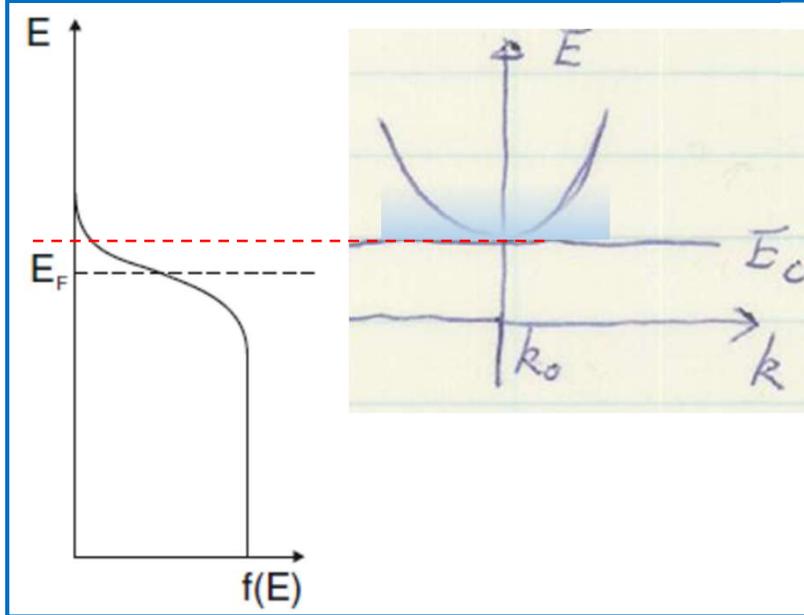
The effects of perfect periodic crystal structure already accounted for by $E(k)$.

For a metal, 

- electron density changes little with temperature;
- only electrons around E_F contribute to current;
- τ decreases thus conductivity decreases with increasing T ;
- m^* is generally depends on k ;



Relaxation time approximation for semiconductors: the concept of mobility



☞ For a semiconductor,

- electron density n changes drastically with temperature;
- τ decreases with increasing T ,
- but n increases more significantly, thus **conductivity increases** with increasing T ;
- there is a need to disentangle the contributions to conductivity by n and τ .
- m^* is largely constant at the bottom of conduction band, where the electrons are.

With a **constant** m^* , we can write $m^* v_d = \hbar \Delta k$, where v_d is the **drift velocity** gained by each conduction electron **on average**.

$$m^* v_d = \hbar \Delta k = F \tau = -q \mathcal{E} \tau \Rightarrow v_d = -\frac{q \mathcal{E} \tau}{m^*}$$

Define **mobility** $\mu = -\frac{q \tau}{m^*} \Rightarrow v_d = \mu \mathcal{E}$

In formal definition, electron mobility is negative. **Conventionally**, we consider v_d a speed (scalar) and μ positive, just keeping in mind that electrons move against field \mathcal{E} .

Due to the lack of need and the inconvenience of varying m^* , mobility is not a useful concept for metals.

Conduction due to conduction-band electrons

$$\text{Current density } J = -nqv_d = -nq\mu\mathcal{E} = \frac{q^2n\tau}{m^*}\mathcal{E}$$
$$\uparrow$$
$$v_d = \mu\mathcal{E} = -\frac{q\mathcal{E}\tau}{m^*}$$

Since the two **negative signs** cancel, the **convention** (positive μ) is okay and convenient:

$$J = nq\mu\mathcal{E} = \frac{q^2n\tau}{m^*}\mathcal{E}$$
$$\uparrow$$
$$J = \sigma\mathcal{E} \quad (\text{Ohm's law})$$

$$\Rightarrow \frac{1}{\rho} = \sigma = qn\mu = \frac{q^2n\tau}{m^*}$$

resistivity conductivity

The concept of the hole

Consider the topmost filled band (**valence band**), $\sum_k v(k) = 0$

A full band of electrons do not conduct (due to symmetry in reciprocal space).

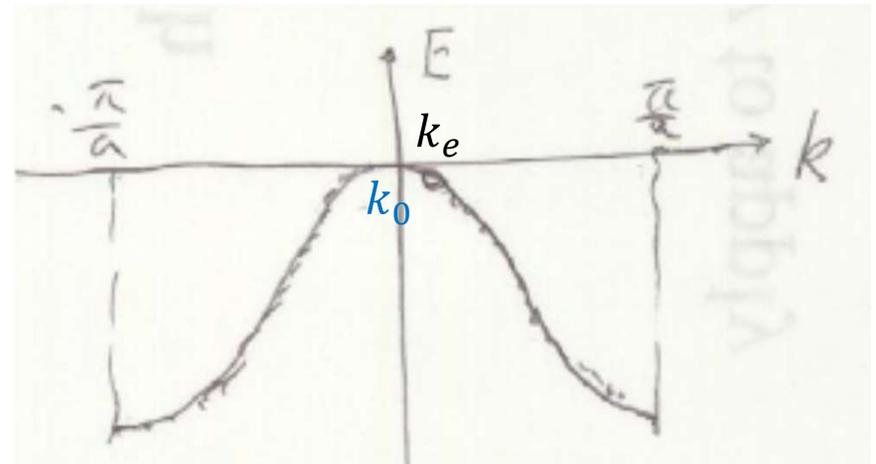
Somehow one electron at k_e is removed.

$$\sum_k v(k) = \sum_{k \neq k_e} v(k) + v_e(k_e) = 0$$

$$\Rightarrow \sum_{k \neq k_e} v(k) = -v_e(k_e)$$

$$\text{Current } I = -q \sum_{k \neq k_e} v(k) = qv_e(k_e)$$

The current due to all remaining valence-band electrons can be represented by a fictitious particle with positive charge q and velocity $v_e(k_e)$.



Note: For the particular vacancy in the figure at k_e , $v_e(k_e)$ is negative. (**Why?**)

Under field \mathcal{E} , each electron is shifted by Δk , so is the **vacancy**, from **equilibrium** (say, VBM k_0).

$v_e(k_e)$ is for the particular vacancy in this figure \leftarrow is positive.

$\hbar\Delta k = -q\mathcal{E}\tau$ does not depend on the sign of m^* .

Electrons move against electric field.

m^* is negative around VBM ($k = k_0$, not necessarily 0):

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2} \Bigg|_{k=k_0}$$

The most convenient definition of the **hole** is for it to, along with **positive charge q** , have **positive effective mass m_h^*** , and to move **along** field \mathcal{E} in k -space. Thus,

$$k_h - k_0 = k_0 - k_e \Rightarrow k_h = 2k_0 - k_e \quad (1)$$

$$\frac{1}{m_h^*} = - \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2} \Bigg|_{k=k_0} = \frac{1}{\hbar^2} \frac{\partial^2}{\partial k^2} (-E) \Bigg|_{k=k_0} \quad (2)$$

In device physics, we rarely need to consider the k of a particular hole, thus (1) not important.

(2) can be simply taken as “**hole energy is positive when measured downward.**”

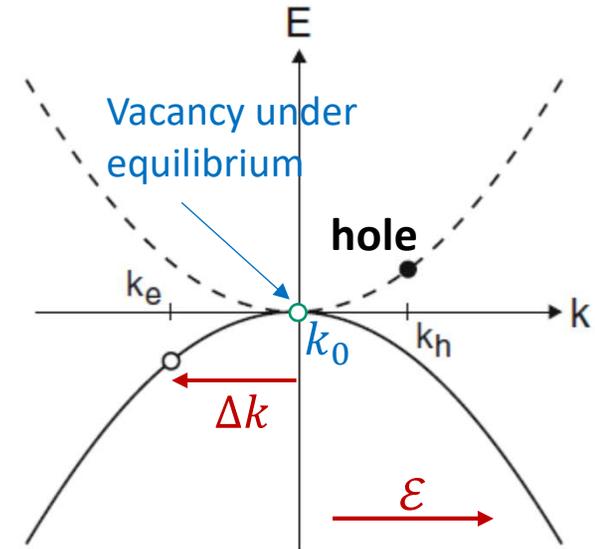


Fig. 6.32 Hole dispersion (dashed line) in relation to the electron dispersion in the valence band (solid line)

Grundmann, *The Physics of Semiconductors*, p. 183.

Conduction in presence of both electrons & holes

Electron current density $J_e = -nq\mu_e\mathcal{E} = \frac{q^2n\tau_e}{m_e^*}\mathcal{E}$ (with μ_e defined to be negative)

or, **conventionally**, $J_e = nq\mu_e\mathcal{E} = \frac{q^2n\tau_e}{m_e^*}\mathcal{E}$ (with μ_e defined to be positive)

Hole current density $J_h = pq\mu_h\mathcal{E} = \frac{q^2p\tau_h}{m_h^*}\mathcal{E}$

Total current density $J = J_e + J_h = nq\mu_e\mathcal{E} + pq\mu_h\mathcal{E}$

\uparrow
 $J = \sigma\mathcal{E}$ (Ohm's law)

\Rightarrow

$$\frac{1}{\rho} = \sigma = q(n\mu_e + p\mu_h)$$

resistivity

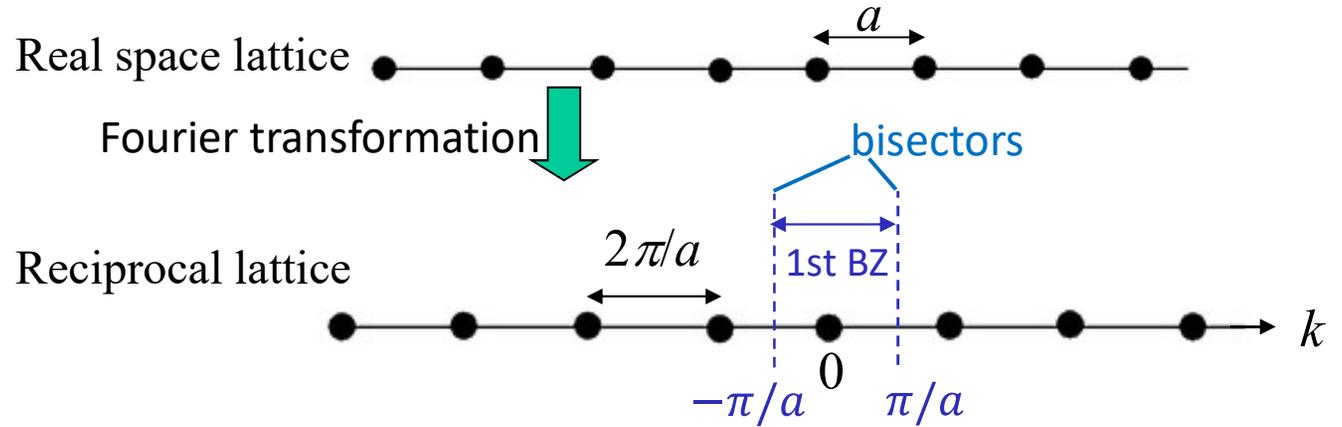
conductivity

Alternative notations: $J_p \rightarrow J_h, \mu_p \rightarrow \mu_h$.

$m_e \rightarrow m_e^*, m_h$ or $m_p \rightarrow m_h^*$ (subscripts e & h or p already imply effective mass thus * not needed; m_0 or simply m for free e mass)

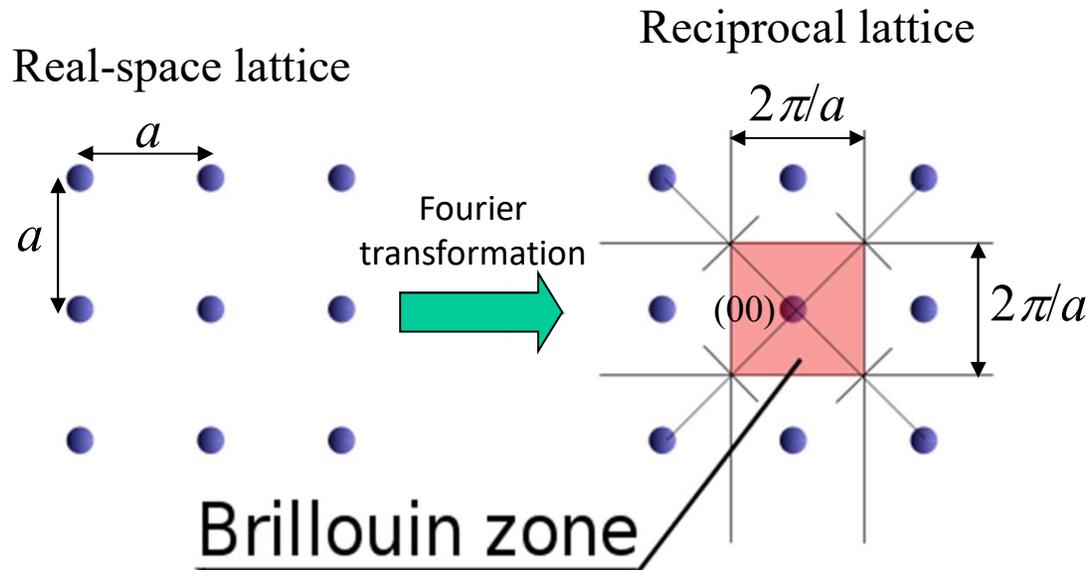
Expand the concepts from 1D to higher dimensionalities

The 1st BZ in 1D



The 1st BZ in 2D

Example: square lattice

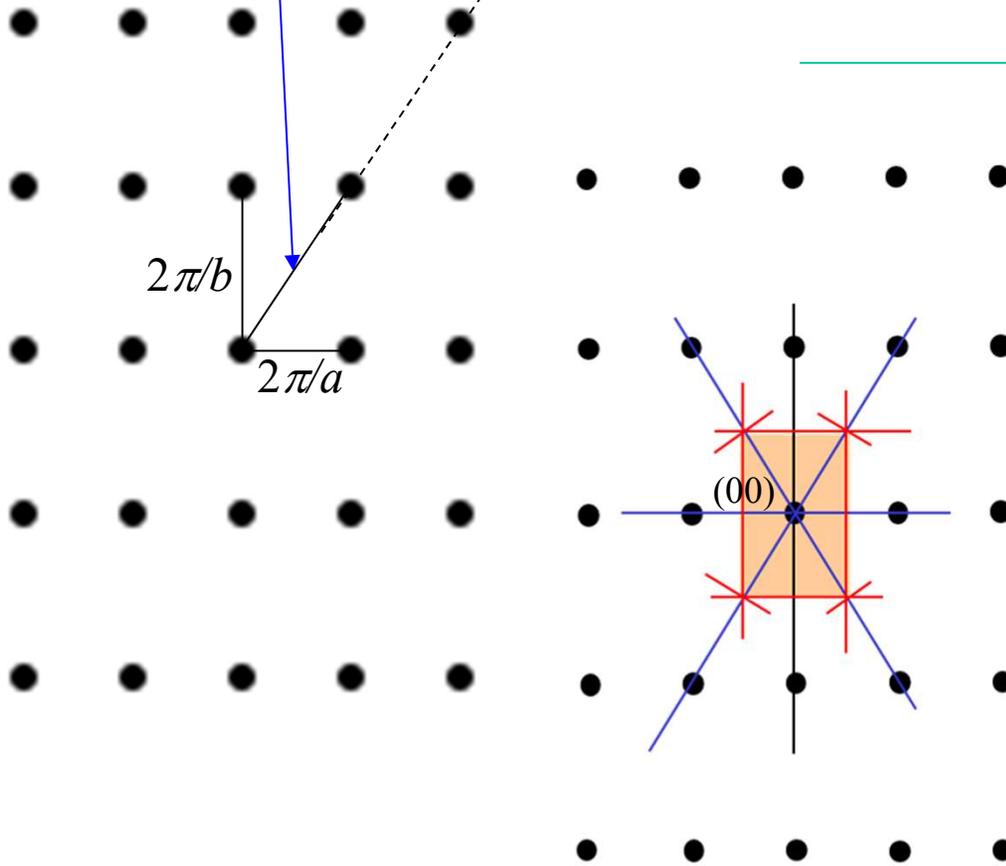


Construct the 1st BZ:
Connect point (00) to nearest neighbors.
Draw bisectors.
Area enclosed by all bisectors is the **1st BZ**.

Example: rectangular lattice

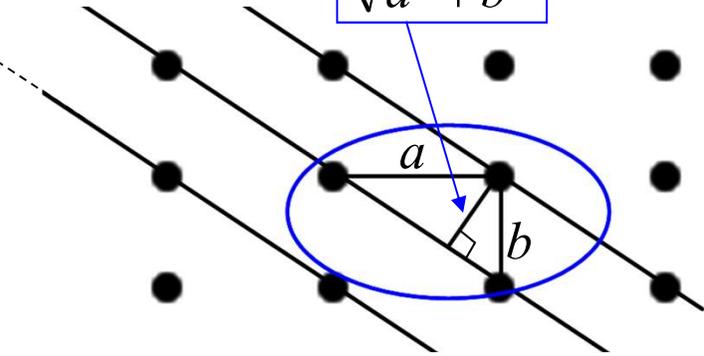
Reciprocal

$$\frac{2\pi\sqrt{a^2 + b^2}}{ab}$$

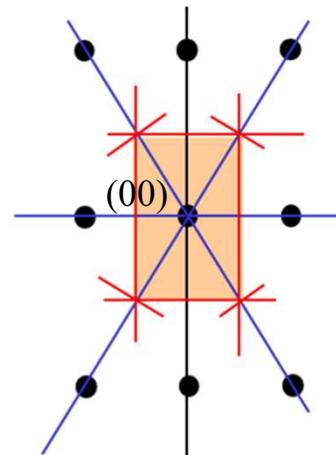


Real

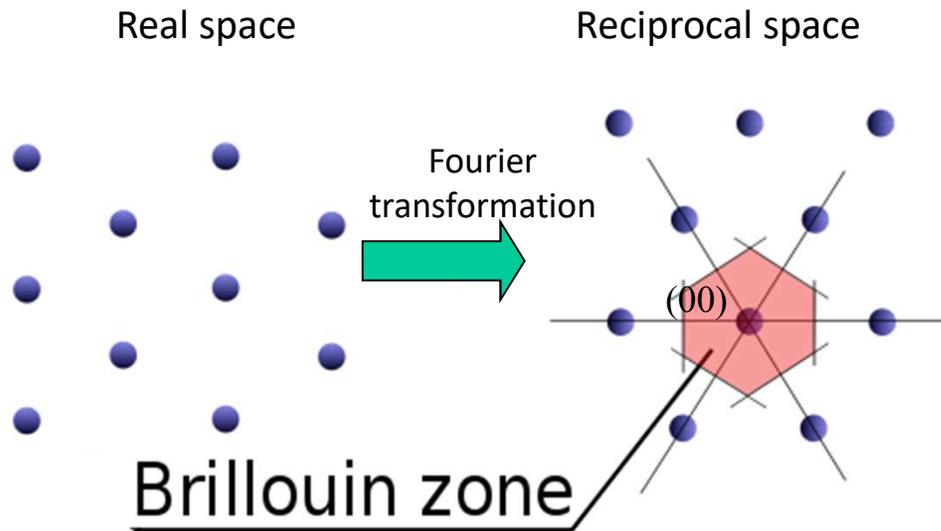
$$\frac{ab}{\sqrt{a^2 + b^2}}$$



Construct the 1st BZ:
 Connect point (00) to nearest neighbors.
 Draw **bisectors**.
 Area enclosed by all bisectors is the 1st BZ.



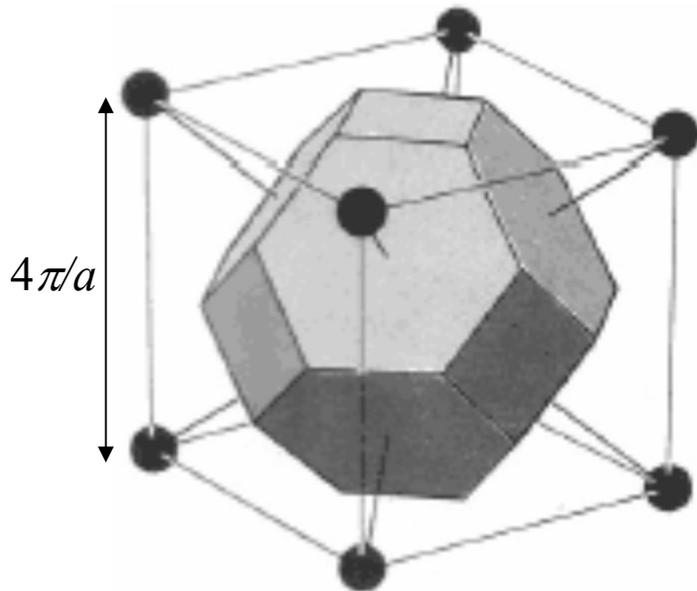
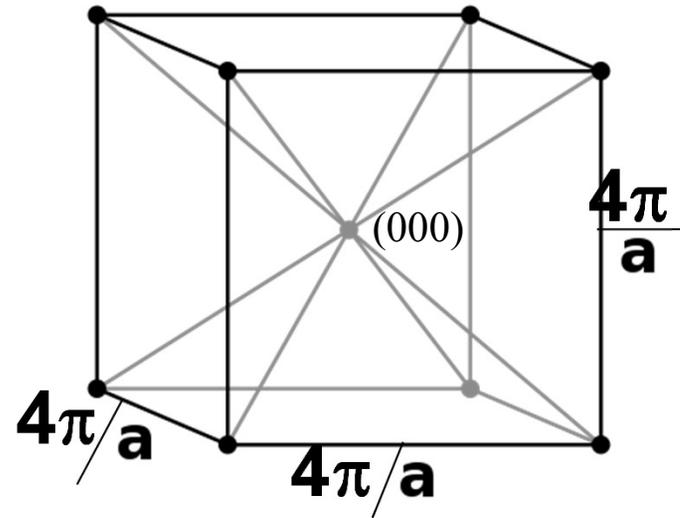
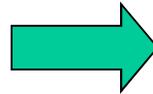
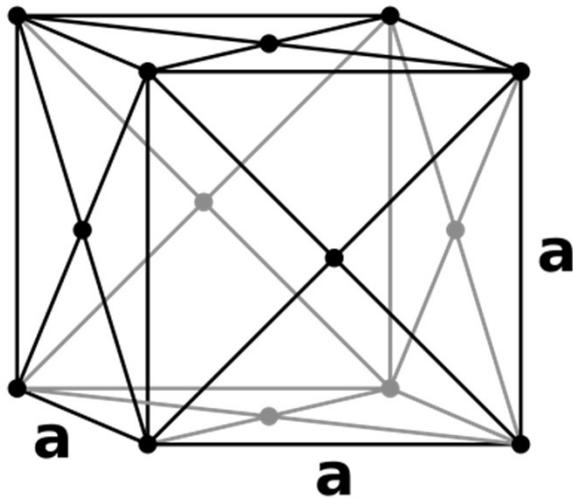
Example: triangular lattice



Construct the 1st BZ:
Connect point (00) to nearest neighbors.
Draw bisectors.
Area enclosed by all bisectors is the 1st BZ.

The 1st BZ in 3D

Example: the underlying Bravais lattice of Si is FCC



Construct the 1st BZ:

Connect point (00) to nearest neighbors.

Draw bisectors. In 3D, bisectors are **planes**.

Volume enclosed by all bisectors is the 1st BZ.

Band structures in 1D

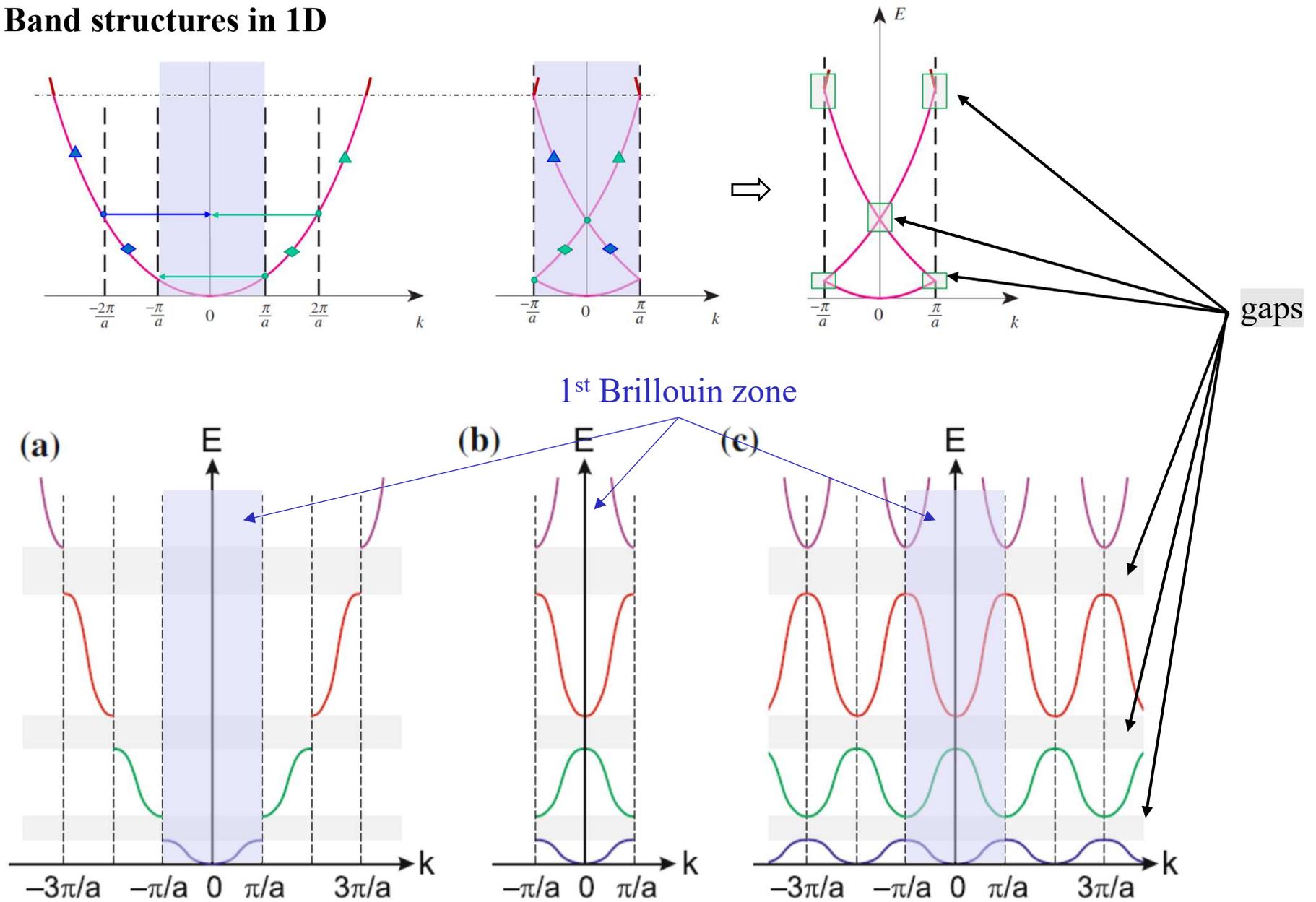
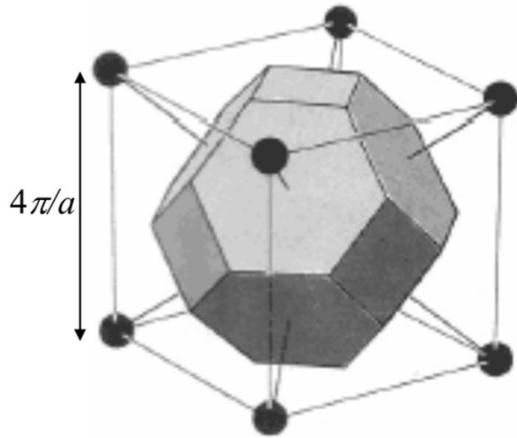


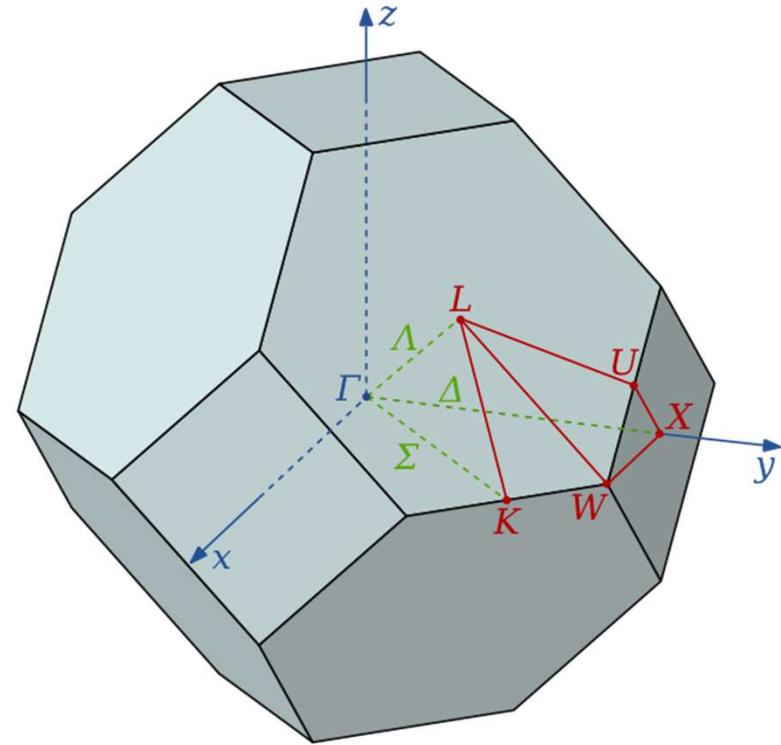
Fig. 6.1 Zone schemes for a band structure: (a) extended, (b) reduced and (c) repetitive zone scheme

Grundmann, *The Physics of Semiconductors*

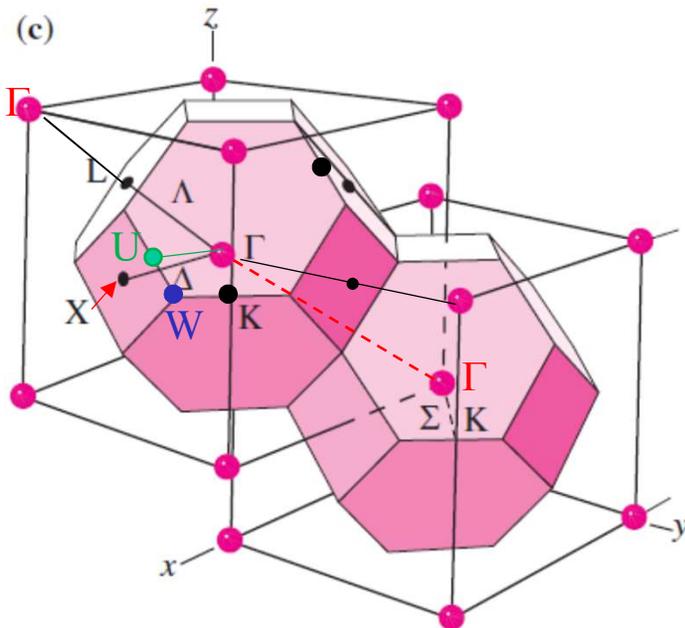
Band structures in 3D



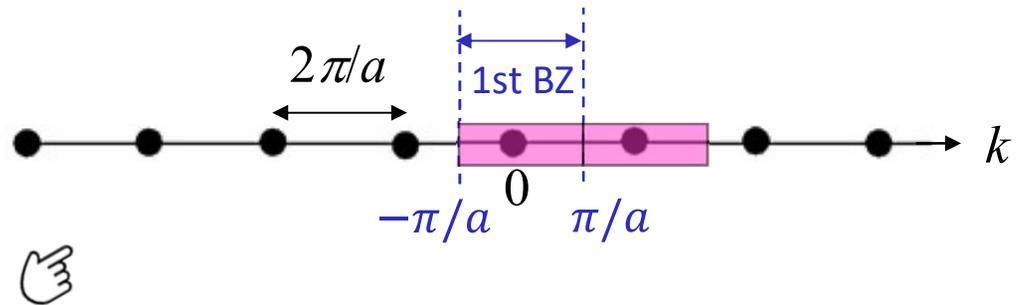
1st BZ of Si (or any FCC lattice)

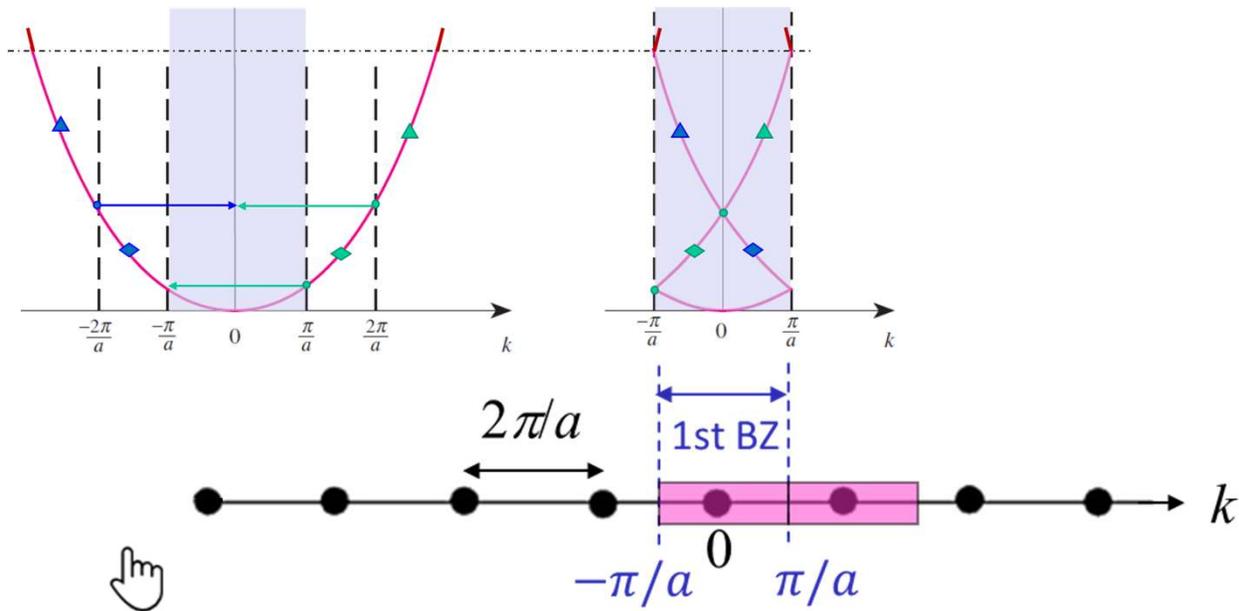


We give names to special points and lines in 1st BZ.

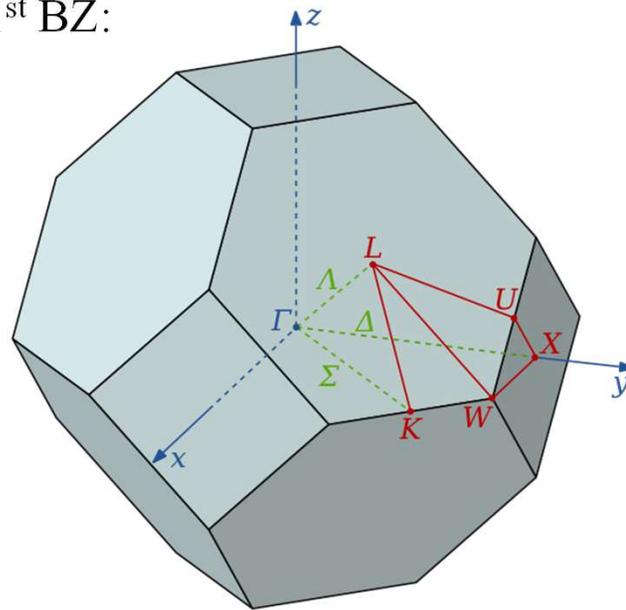
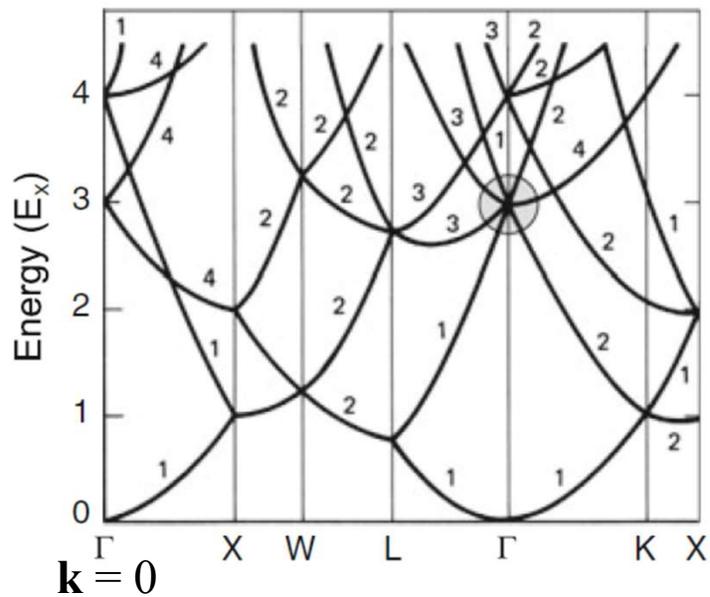


BZs fill entire reciprocal space, as in 1D.

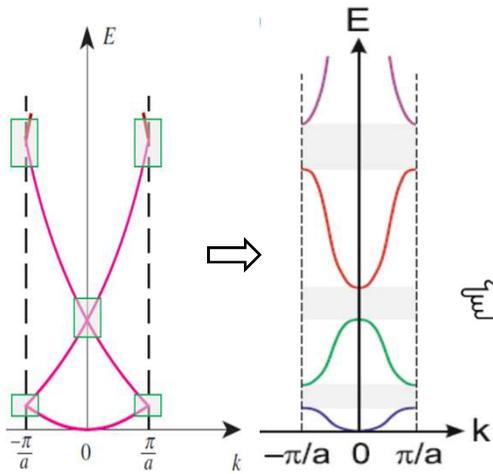




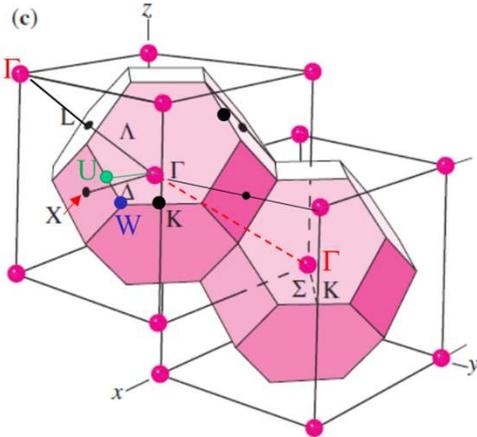
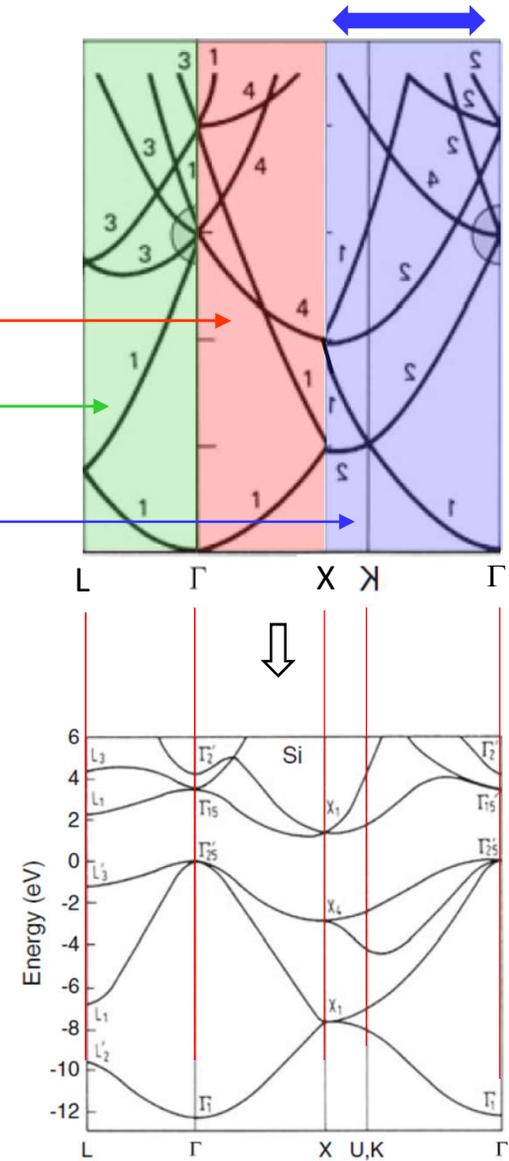
As in 1D, shift/fold the free-e $E(\mathbf{k})$ into 1st BZ:



Hard to visualize 3D function $E(\mathbf{k})$, so we only plot along certain special lines.

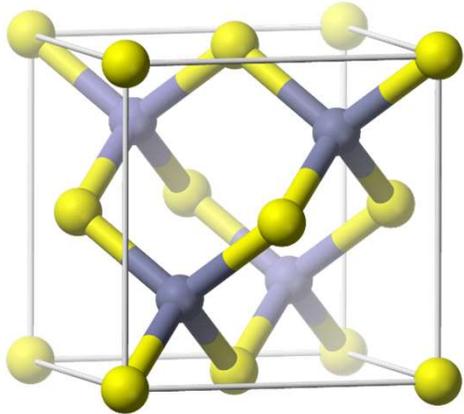


Consider resonance around zone boundaries and other points where free-e bands cross each other, as in 1D.

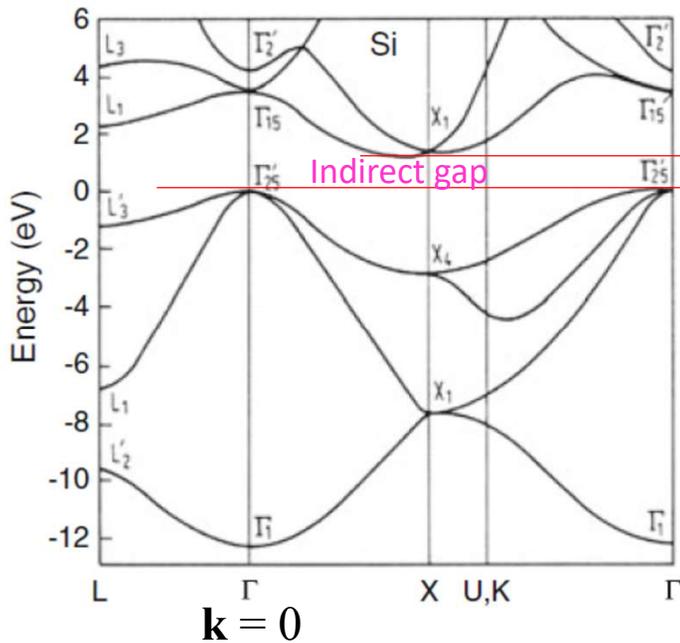
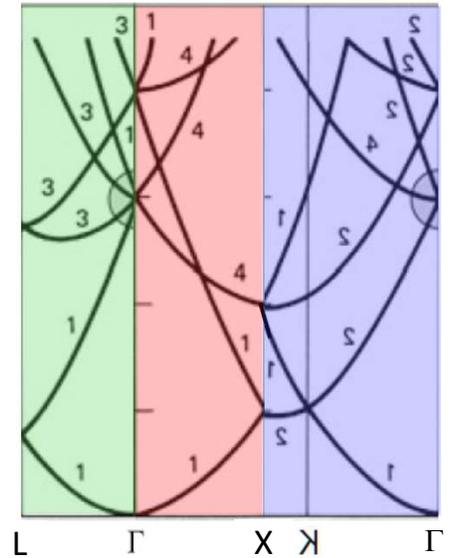
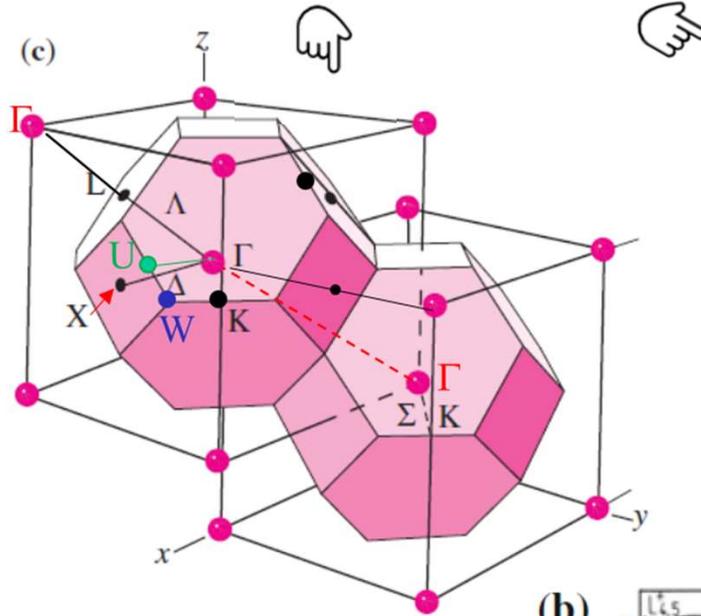


There are many different ways to present $E(\mathbf{k})$.

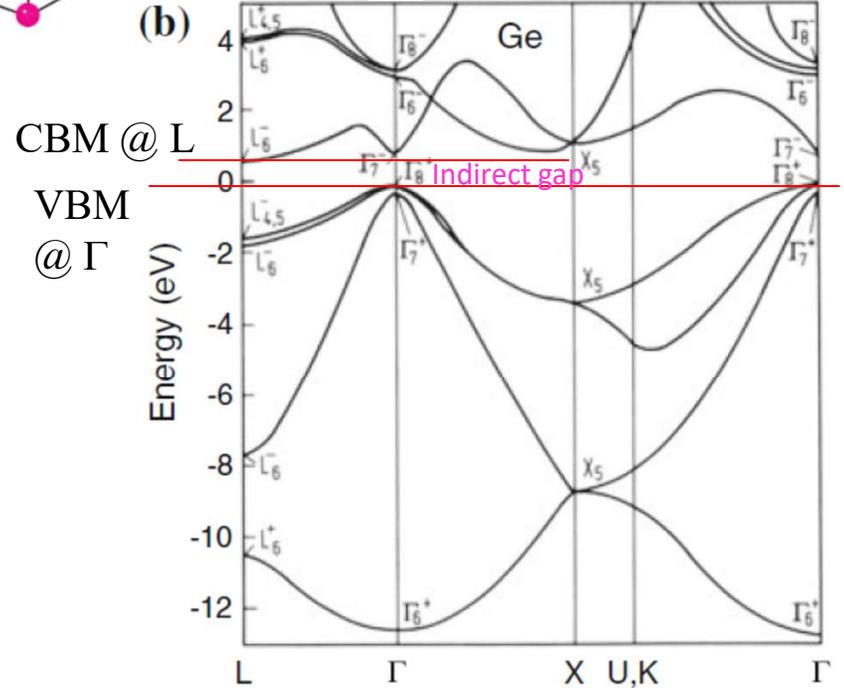
Recall that group VI (Si, Ge) and III-V (GaAs) have similar structures.
 Same underlying FCC Bravais lattice \Rightarrow same BZs \Rightarrow same free-e bands



Diamond (Si, Ge) or zincblende (many III-V) crystal structure

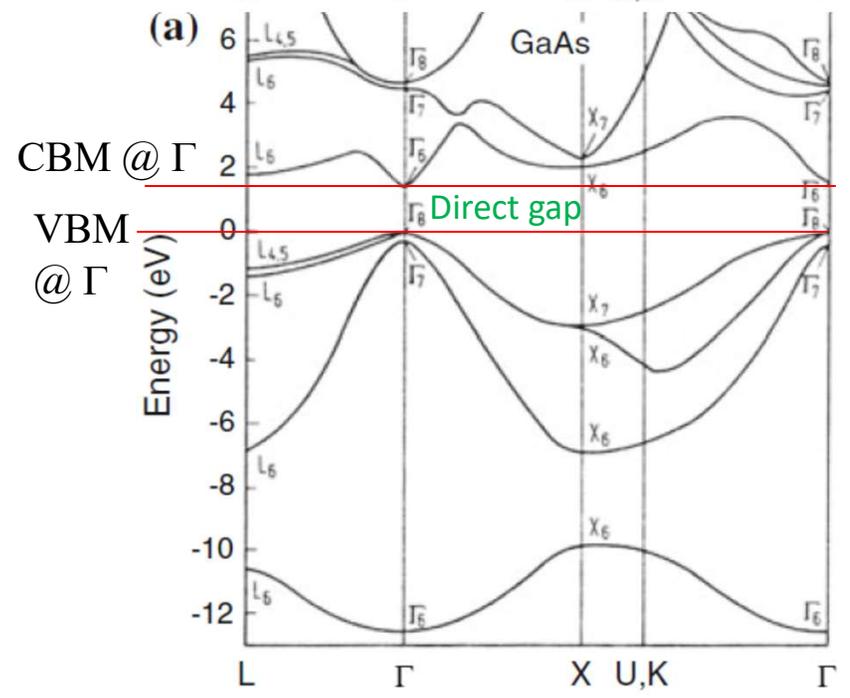
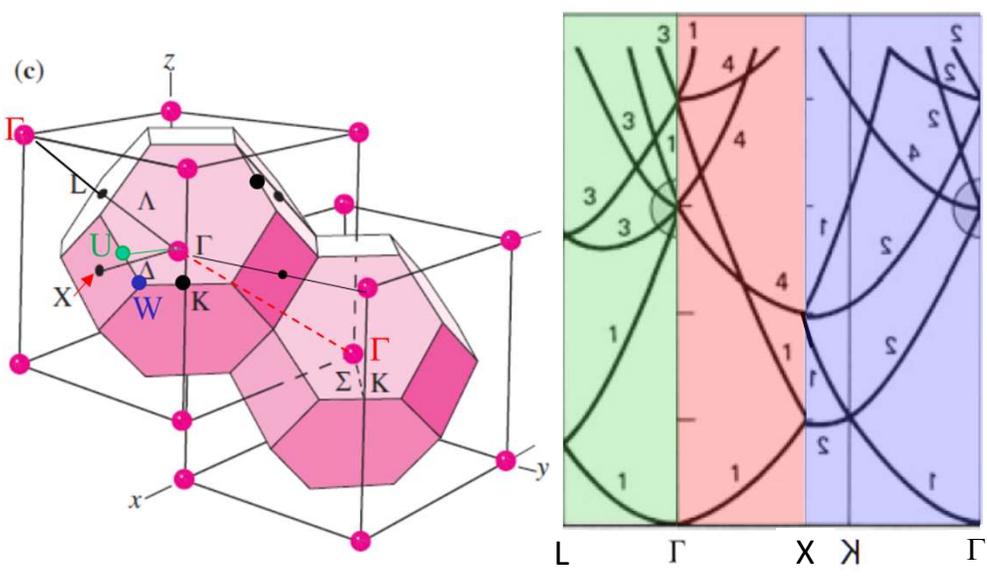
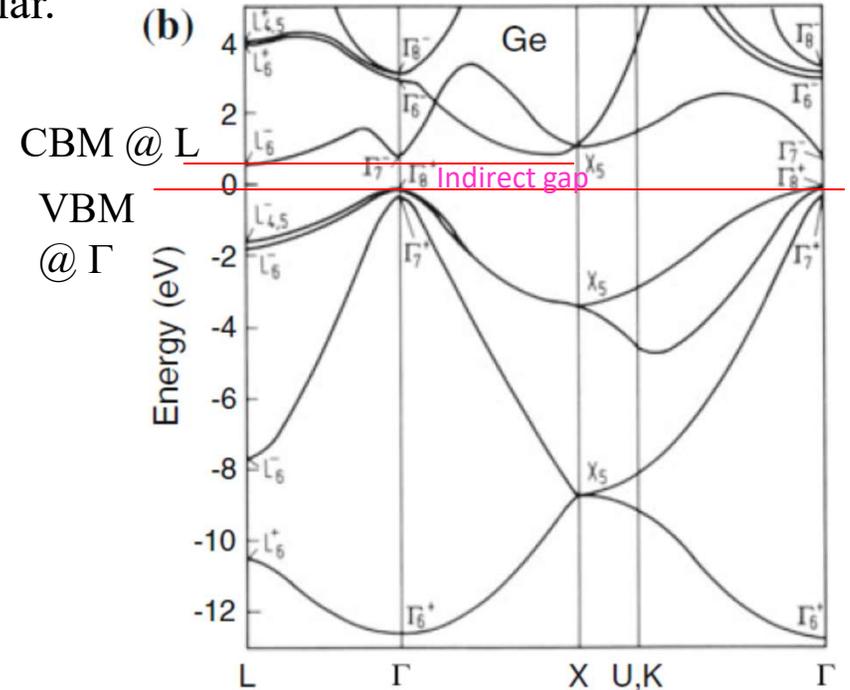
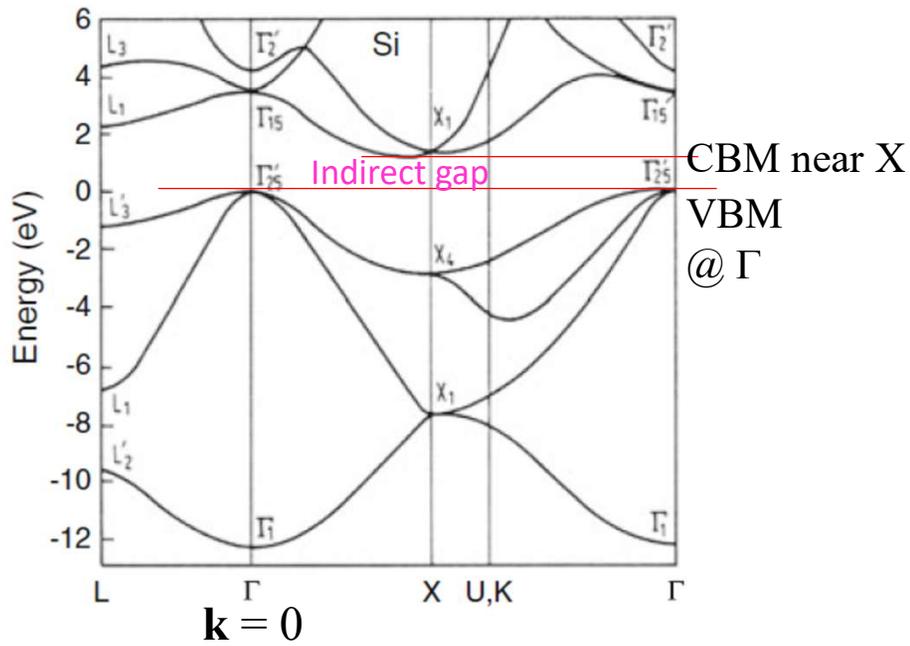


CBM near X
 VBM @ Γ



CBM @ L
 VBM @ Γ

Group VI (Si, Ge) and III-V (GaAs) structurally similar.
 Same BZs \Rightarrow same free-e bands

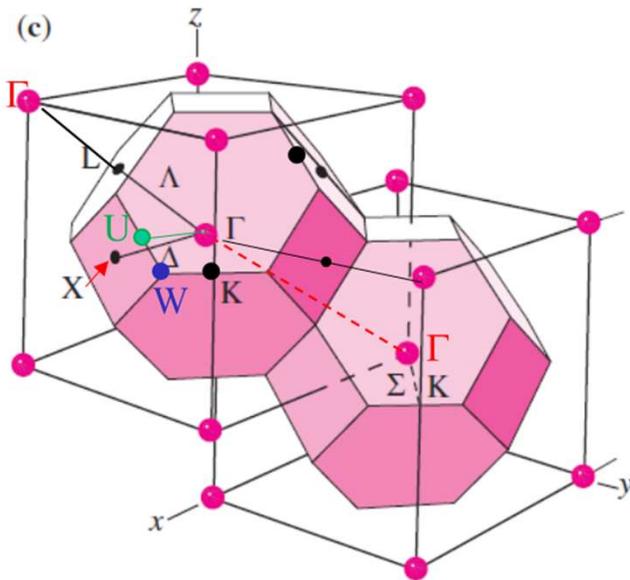


Semi-classical model in 3D

$$\mathbf{v} = \frac{1}{\hbar} \nabla_{\mathbf{k}} E = \frac{1}{\hbar} \left(\hat{\mathbf{x}} \frac{\partial E}{\partial k_x} + \hat{\mathbf{y}} \frac{\partial E}{\partial k_y} + \hat{\mathbf{z}} \frac{\partial E}{\partial k_z} \right)$$

Gradient in k -space (reciprocal space)

Generally, $(m^*)^{-1}$ is a tensor, due to anisotropy.



$$[(m^*)^{-1}]_{ij} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j}$$

i or $j = 1, 2, 3$ are the axes of iso-energy ellipsoid at band extremum.
For Si, the 3 axes are x, y, z .

In device physics, it usually suffices to use an average scalar $(m^*)^{-1}$ for non-degenerate band extremum:

$$(m^*)^{-1} = \frac{[(m^*)^{-1}]_{11} + [(m^*)^{-1}]_{22} + [(m^*)^{-1}]_{33}}{3}$$

Here, this arithmetic average is for the purpose of calculating conductivity. Its reciprocal, $m_{ce} = 1/[(m^*)^{-1}]$ is called the “conductivity effective mass.”

A geometric average of $[(m^*)^{-1}]_{ii}$ is used for a different purpose.

1D analogy

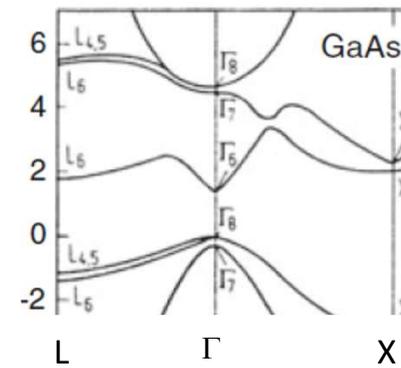
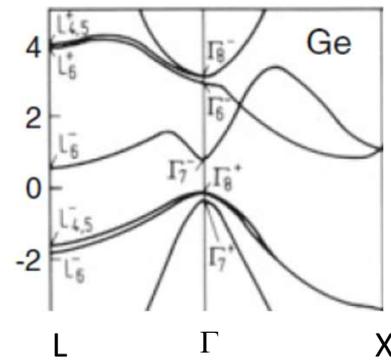
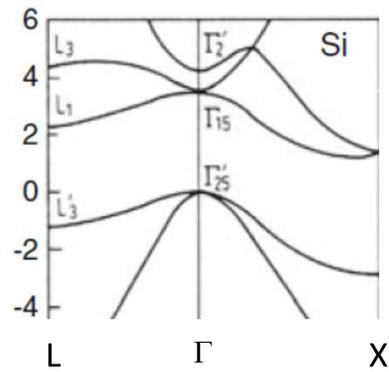
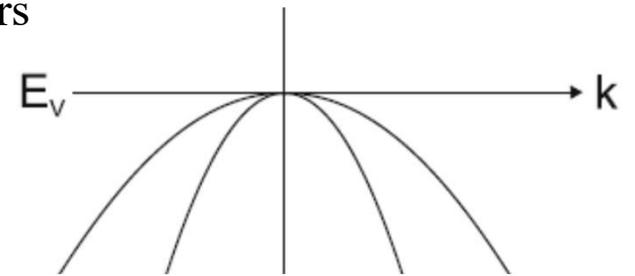
$$v = \frac{1}{\hbar} \frac{dE}{dk}$$

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{d^2 E}{dk^2}$$

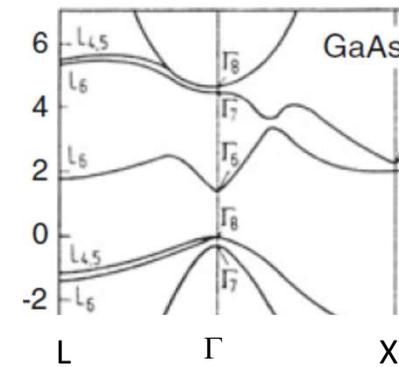
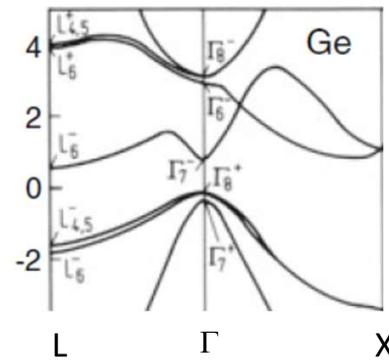
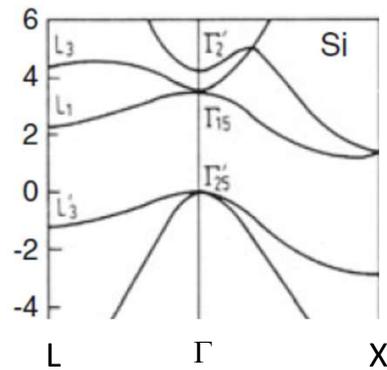
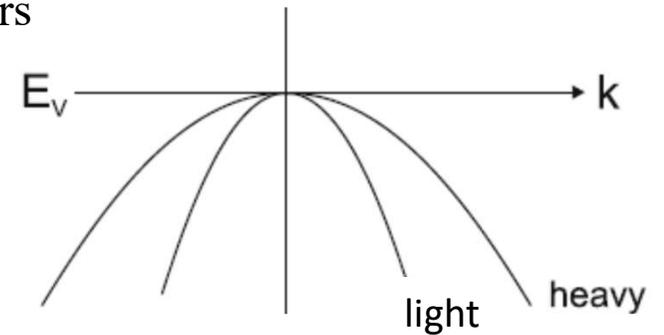
We stopped here on Tue 9/14/2021.

Hole bands are degenerate at VBM for common semiconductors

Question: Which one is the heavy/light hole band?



Hole bands are degenerate at VBM for common semiconductors



There is an average for the **conductive effective mass** for holes.

Another average is used for a different purpose.

Finally, we have learned enough to understand most of **Sections 1.3, 1.4, and 1.5.1** in **Chapter 1 Physics and Properties of Semiconductor – a Resume** of Sze, *Physics of Semiconductor Devices* (2nd Ed.), and are now ready to discuss devices in a serious way.