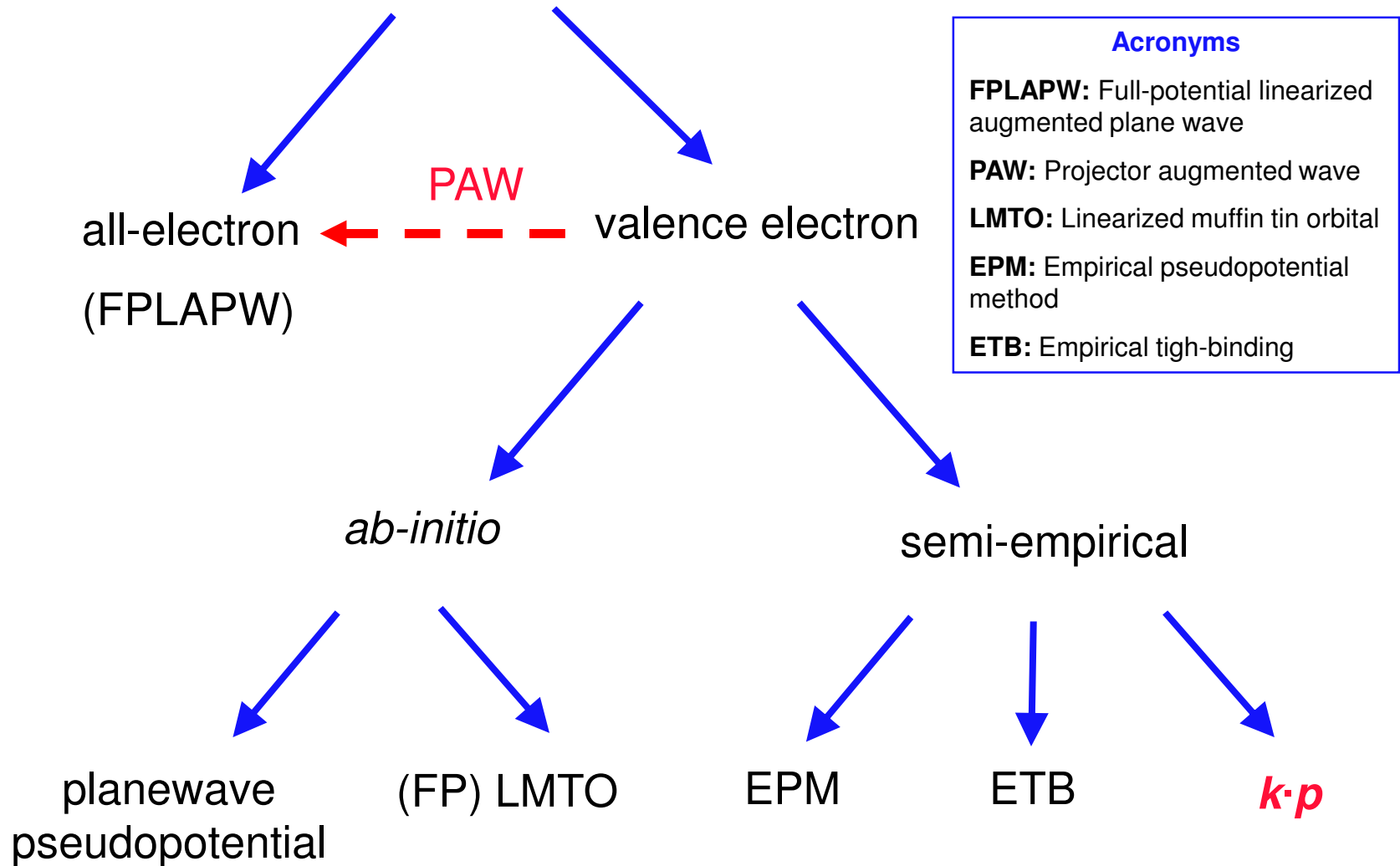


In This Lecture:

- **Electronic Bandstructure: General Info**

Electronic Bandstructure



Perfect Crystal Hamiltonian (cgs units)

$$H = \underbrace{\sum_j \frac{p_j^2}{2m_j} + \frac{1}{2} \sum_{j,j'}' \frac{e^2}{|\vec{r}_j - \vec{r}_{j'}|}}_{\text{over all } e\text{'s}} + \underbrace{\sum_i \frac{P_i^2}{2M_i} + \frac{1}{2} \sum_{i,i'}' \frac{e^2 Z_i Z_{i'}}{|\vec{R}_i - \vec{R}_{i'}|}}_{\text{over all nuclei}} - \underbrace{\sum_{i,j} \frac{e^2 Z_i}{|\vec{r}_j - \vec{R}_i|}}_{\text{e-nuclei}}$$

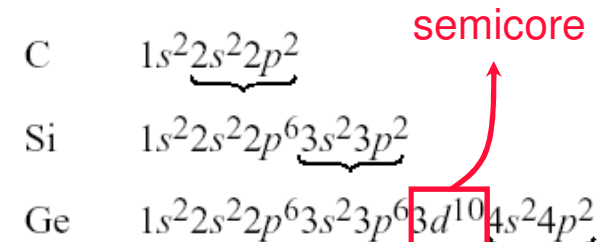
➤ **1st Approximation: core vs. valence e's**

Still Eq. Above Applies with:

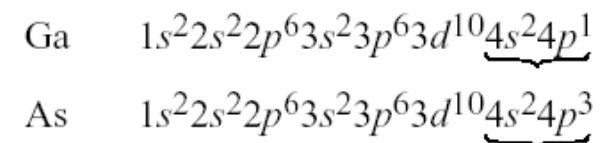
core e's+nucleus → ion core

e's → valence e's

IV Semiconductors



III-V Semiconductors



➤ **2nd Approximation: Born-Oppenheimer or adiabatic approx.**

- ✓ ions are much heavier (> 1000 times) than e 's

So,

for e 's: ions are essentially stationary (at eql. lattice sites $\{R_{j0}\}$)

for ions: only a time-averaged adiabatic electronic potential is seen

In other words,

using the adiabatic approximation, we **separate** the (in principle non-separable) perfect crystal Hamiltonian

Under adiabatic approximation...

$$H = H_{ion}(\vec{R}_i) + H_e(\vec{r}_j, \vec{R}_{i0}) + H_{e-ion}(\vec{r}_j, \delta\vec{R}_i)$$

phonon spectrum

electronic
band structure

e-phonon interaction
(resistance, superconductivity...)

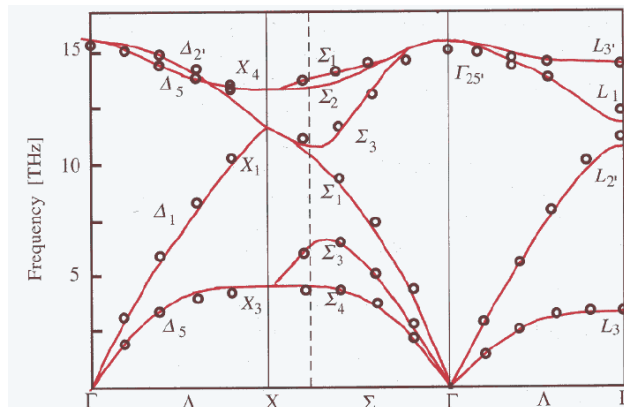
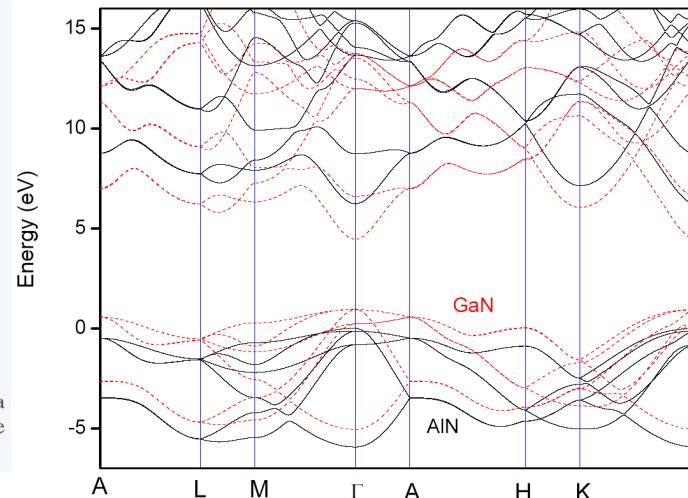


Fig. 3.1. Phonon dispersion curves in Si along high-symmetry axes. The circles are data points from [3.3]. The continuous curves are calculated with the adiabatic bond charge model of Weber [3.4]



Ref: Yu-Cardona

Electronic Hamiltonian

$$H_e = \sum_j \frac{p_j^2}{2m_j} + \underbrace{\frac{1}{2} \sum_{j,j'} \frac{e^2}{|\vec{r}_j - \vec{r}_{j'}|}}_{\text{over all valence } e\text{'s } > 10^{23} \text{ cm}^{-3}} - \sum_{i,j} \frac{e^2 Z_i}{|\vec{r}_j - \vec{R}_{i0}|}$$

over all valence e 's $> 10^{23} \text{ cm}^{-3}$

➤ 3rd Approximation: Mean-field Approximation

$$H_{1e} = \frac{p^2}{2m} + V(\vec{r}); \quad V(\vec{r} + \vec{R}) = V(\vec{r})$$

Density Functional
Theory

$$V_H + V_x + V_c$$

A direct lattice
vector

Translational Symmetry & Brillouin Zones

$$T_R f(x) \equiv f(x+R); \quad T_R: \text{Translational Operator}$$

Introduce a function, $\psi_k(x) \equiv e^{ikx} u_k(x)$, where $u_k(x+nR) = u_k(x)$ with $n \in \mathbb{Z}$

$$T_R \psi_k(x) = \psi_k(x+R) = \boxed{e^{ikR}} \psi_k(x)$$

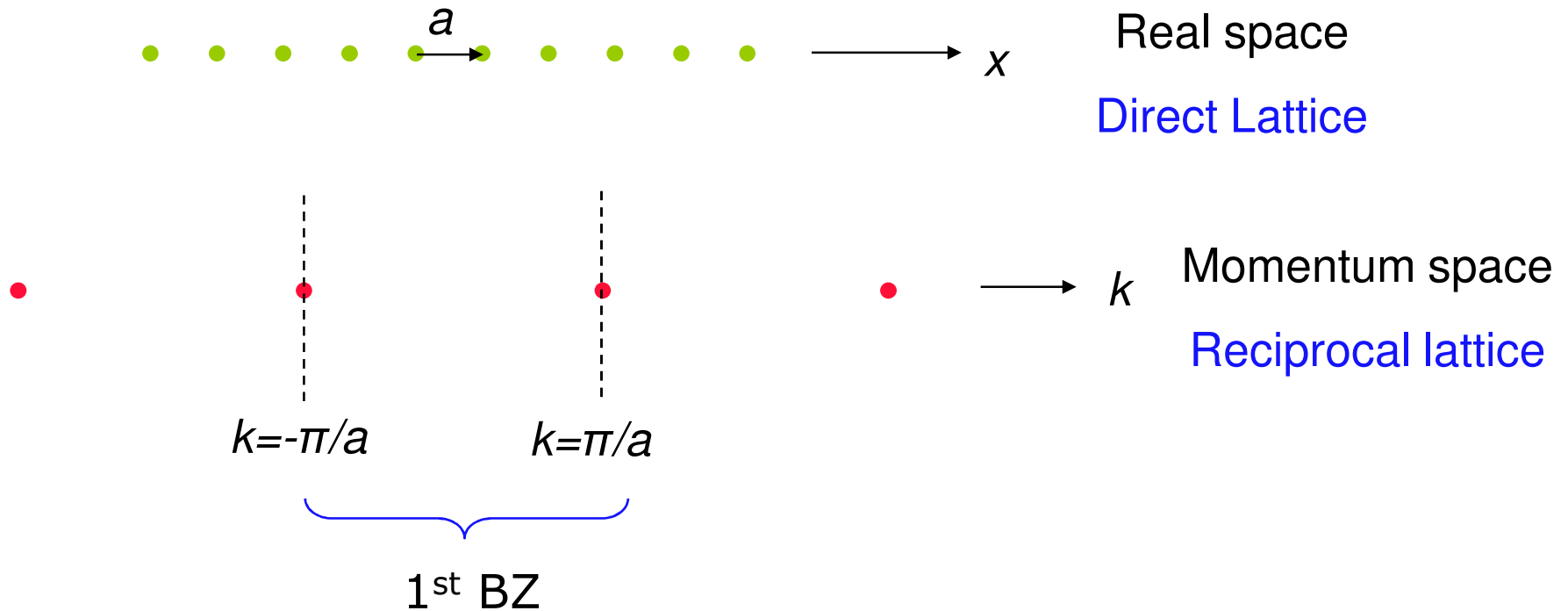
eigenvalues of T_R

$$\text{Since } [H_{1e}, T_R] = 0,$$

Eigenfunctions of H_{1e} can be expressed also as eigenfunctions of T_R

NB: k is only defined modulo $\frac{2\pi}{R}$, i.e., k and $k + \frac{2\pi n}{R}$ are equivalent

One-dimensional Lattice



[Real Space] Primitive lattice vector: a

[Mom. Space] Primitive lattice vector: $2\pi/a$

Three-dimensional Lattice

[Real space] Primitive lattice vectors: $\vec{a}_1, \vec{a}_2, \vec{a}_3$

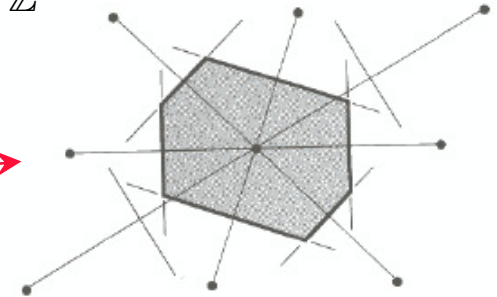
A general direct lattice vector (DLV): $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$; $n_i \in \mathbb{Z}$

[Mom. space] Primitive lattice vectors: $\vec{b}_1, \vec{b}_2, \vec{b}_3$

where, $\vec{b}_i \equiv 2\pi \frac{\vec{a}_j \times \vec{a}_k}{(\vec{a}_1 \times \vec{a}_2) \cdot \vec{a}_3}$ — Volume of the real space primitive cell

A general reciprocal lattice vector (RLV): $\vec{G} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$; $n_i \in \mathbb{Z}$

NB: $\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$



1st Brillouin zone is the Wigner-Seitz cell of the reciprocal lattice

Direct vs. Reciprocal Lattices

➤ SC

Direct Lattice

Primitive
translation
vectors

$$\begin{cases} \vec{a}_1 = a \hat{x} \\ \vec{a}_2 = a \hat{y} \\ \vec{a}_3 = a \hat{z} \end{cases}$$



Reciprocal Lattice

$$\begin{cases} \vec{b}_1 = \frac{2\pi}{a} \hat{x} \\ \vec{b}_2 = \frac{2\pi}{a} \hat{y} \\ \vec{b}_3 = \frac{2\pi}{a} \hat{z} \end{cases} \quad \left. \vphantom{\begin{cases} \vec{b}_1 \\ \vec{b}_2 \\ \vec{b}_3 \end{cases}} \right\} \text{also a SC lattice!}$$

1st BZ of SC lattice is again a cube

➤ BCC

Direct Lattice

$$\bar{a}_1 = \frac{a}{2}(\hat{y} + \hat{z} - \hat{x})$$

$$\bar{a}_2 = \frac{a}{2}(\hat{z} + \hat{x} - \hat{y})$$

$$\bar{a}_3 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$



Reciprocal Lattice

$$\bar{b}_1 = \frac{2\pi}{a}(\hat{y} + \hat{z})$$

$$\bar{b}_2 = \frac{2\pi}{a}(\hat{z} + \hat{x})$$

$$\bar{b}_3 = \frac{2\pi}{a}(\hat{x} + \hat{y})$$

forms an
fcc lattice!

a is the side of the conventional cube

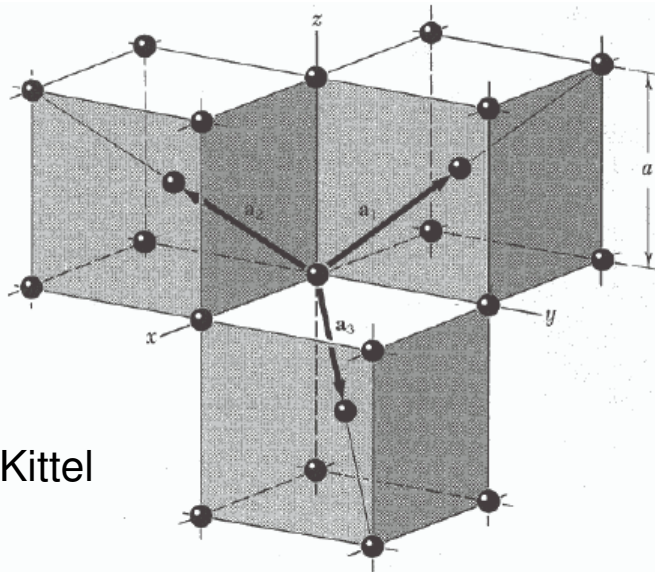


Figure 12 Primitive basis vectors of the body-centered cubic lattice.

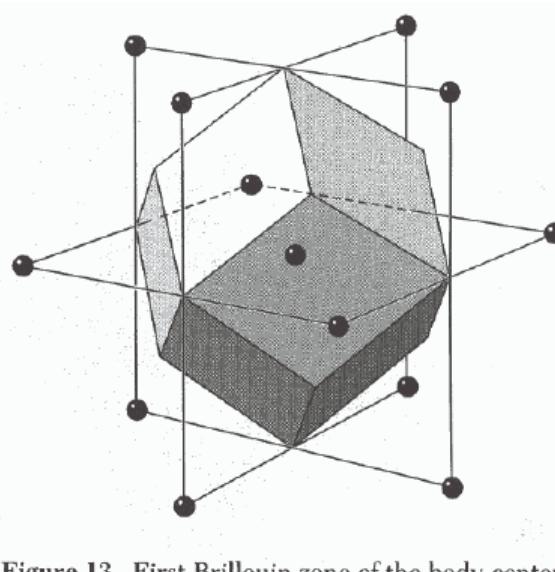


Figure 13 First Brillouin zone of the body-centered cubic lattice. The figure is a regular rhombic dodecahedron.

1st BZ of bcc lattice

Ref: Kittel

➤ FCC

Direct Lattice

$$\bar{a}_1 = \frac{a}{2} (\hat{y} + \hat{z})$$

$$\bar{a}_2 = \frac{a}{2} (\hat{z} + \hat{x})$$

$$\bar{a}_3 = \frac{a}{2} (\hat{x} + \hat{y})$$



Reciprocal Lattice

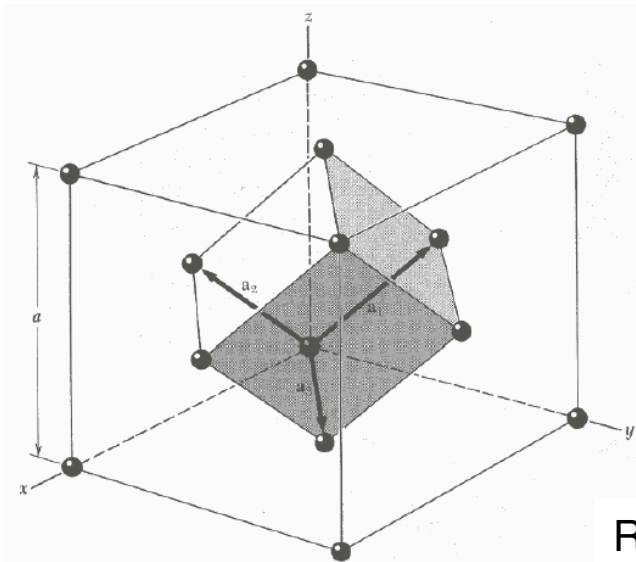
$$\bar{b}_1 = \frac{2\pi}{a} (\hat{y} + \hat{z} - \hat{x})$$

$$\bar{b}_2 = \frac{2\pi}{a} (\hat{z} + \hat{x} - \hat{y})$$

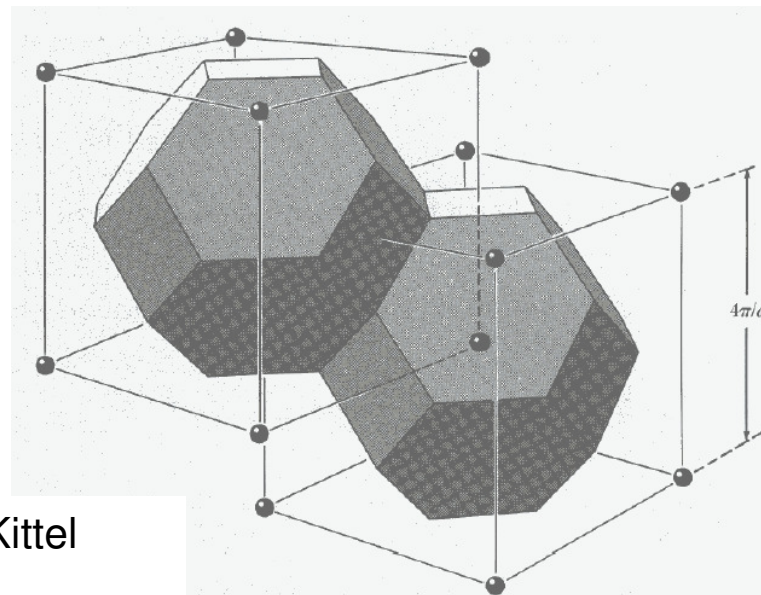
$$\bar{b}_3 = \frac{2\pi}{a} (\hat{x} + \hat{y} - \hat{z})$$

forms an
bcc
lattice!

a is the side of the conventional cube

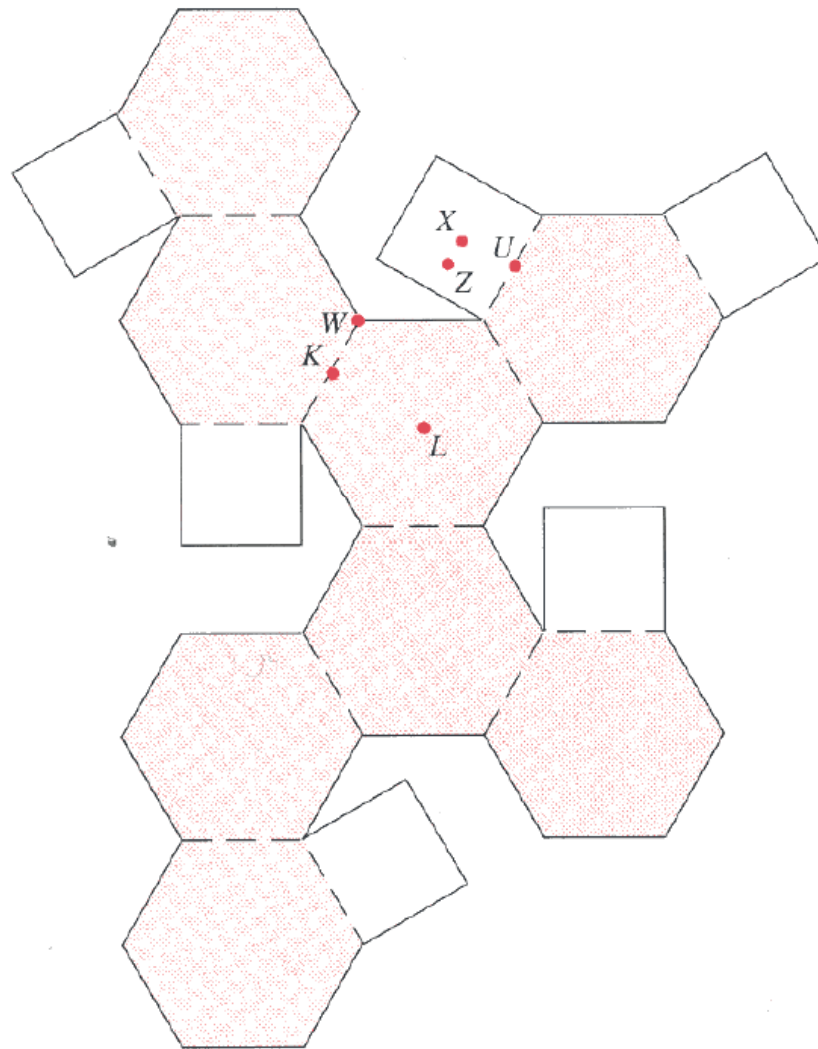


Ref: Kittel

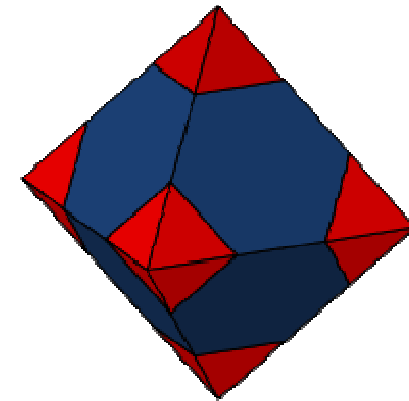


1st BZ of
fcc lattice

fcc 1st BZ Cardboard Model



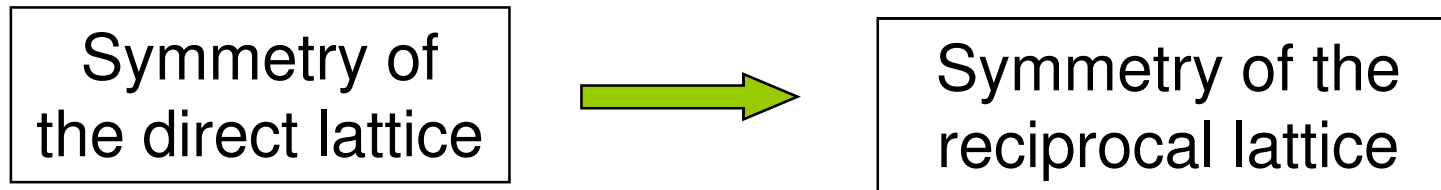
Truncated Octahedron



Ref: Wikipedia

Fig. 2.27. Template for constructing a model of the Brillouin zone of the fcc lattice. Paste this sheet on thin cardboard and cut along *solid lines*. Score along *broken lines* and tape the joints
Ref: Yu-Cardona

More on Symmetry



- **The star of a k -point**

All have the same energy eigenvalues

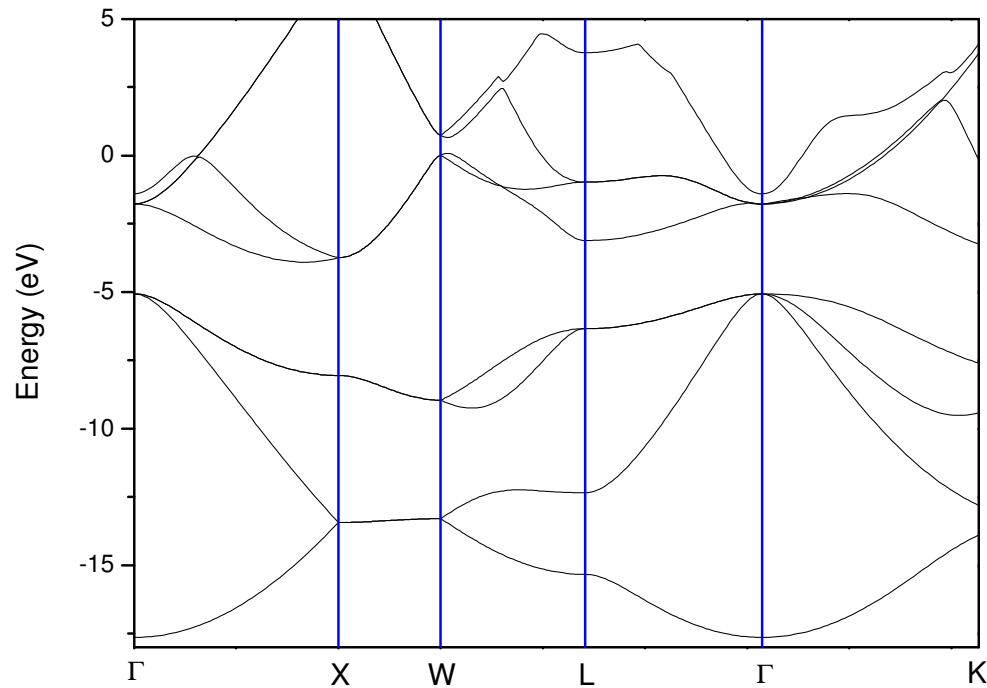
- **Wavefunctions can be expressed in a form such that they have definite transformation properties under symmetry operations of the crystal**

Selection rules: certain matrix elements of certain operators vanish identically...

- **Formal analysis is remedied by the use of Group theory**

Symmetry Points & Plotting the Band Structure

EPM Bandstructure of Si



Bloch Functions vs Wannier Functions

- Felix Bloch provided the important theorem that the solution of the Schrodinger equation for a periodic potential must be of the special form:

Cell-periodic functions

$$\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{n\vec{k}}(\vec{r}), \quad \text{with } u_{n\vec{k}}(\vec{r}) = u_{n\vec{k}}(\vec{r} + \vec{R}),$$

Orthonormality:

$$\int_{\text{all space}} \psi_{n\vec{k}}^*(\vec{r}) \psi_{n'\vec{k}'}(\vec{r}) d\vec{r} = \delta_{nn'} \delta_{\vec{k}\vec{k}'}$$

$\hbar\vec{k}$ is the crystal momentum (more on this later)

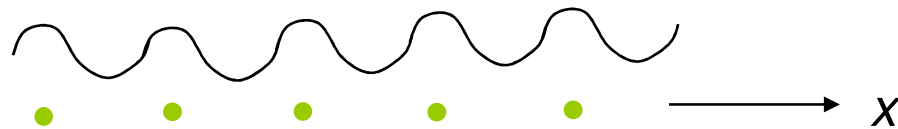
Wannier functions

$$a_n(\vec{r}; \vec{R}_i) = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}_i} \psi_{n\vec{k}}(\vec{r}),$$

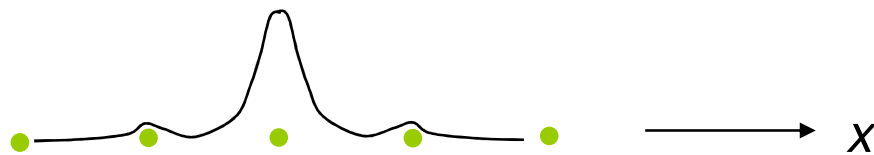
$$\psi_{n\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}_i} e^{i\vec{k}\cdot\vec{R}_i} a_n(\vec{r}; \vec{R}_i)$$

Transformation relations

Bloch vs. Wannier Functions



Bloch functions are extended



Wannier fn's are localized around lattice sites R_i

Wannier form is useful in describing impurities, excitons...

But note that the Wannier functions are not unique!

Crystal Momentum

$$\psi_{n\vec{k}}(\vec{r} + \vec{T}) = e^{i\vec{k} \cdot \vec{r}} \psi_{n\vec{k}}(\vec{r})$$

\vec{k} determines the phase factor by which a BF is multiplied under a translation in real space

\vec{k} labels different eigenstates together with the band index n

\vec{k} is determined up to a reciprocal lattice vector; this arbitrariness can be removed by restricting it to 1st BZ

A typical conservation law in a xtal: $\vec{k} + \vec{q} = \vec{k}' + \vec{G}$

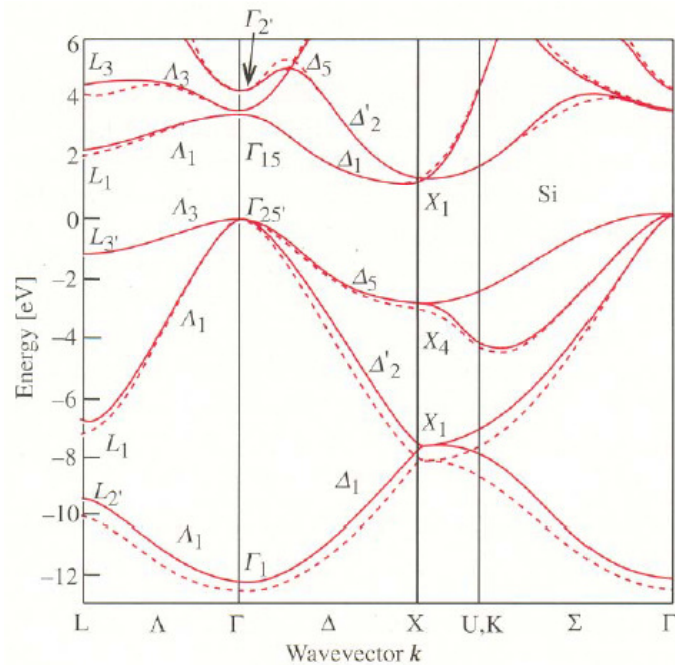
Any arbitrariness in labelling the BFs can be absorbed in these additive RLVs w/o changing the physics of the process

Physically, the lattice supplies necessary recoil momentum so that **linear momentum is exactly conserved**

Be ware of the Complex Bandstructure

$$e^{i\vec{k}\cdot\vec{r}} u_{n\vec{k}}(\vec{r})$$

“Real” bandstructure of Si



What if we allow k to become complex?

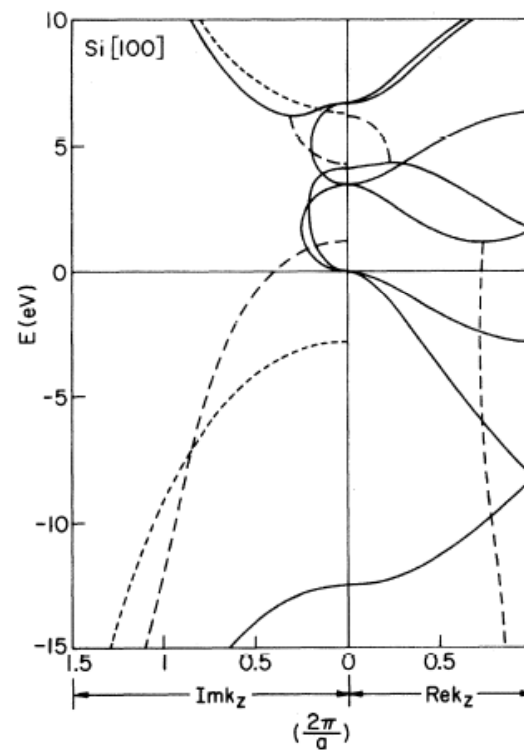


FIG. 2. Complex band structure of Si along [100] direction obtained in the tight-binding scheme. Solid curves denote real bands (right) and imaginary bands (left), short-dashed curves denote complex bands with $\text{Re}k_z$ located at the zone boundary, and long-dashed curves denote complex bands with general values of $\text{Re}k_z$.

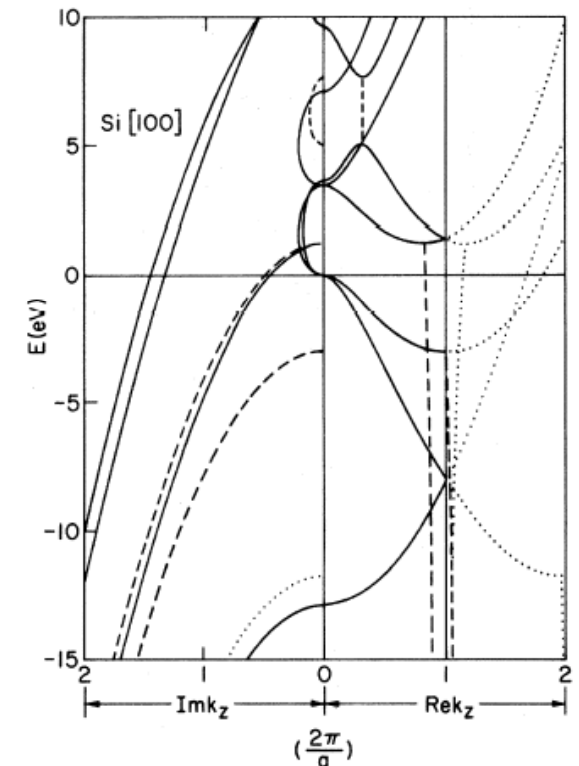


FIG. 5. Complex band structure of Si along [100] direction obtained in the $\vec{k}\cdot\vec{p}$ scheme. Solid curves denote real bands (right) and imaginary bands (left), and dashed curves denote complex bands. Dotted curves denote the repeated solutions, which should be discarded (see text).

Ref: Chang-Schulman PRB 1982

Complex Bandstructure (cont'd)

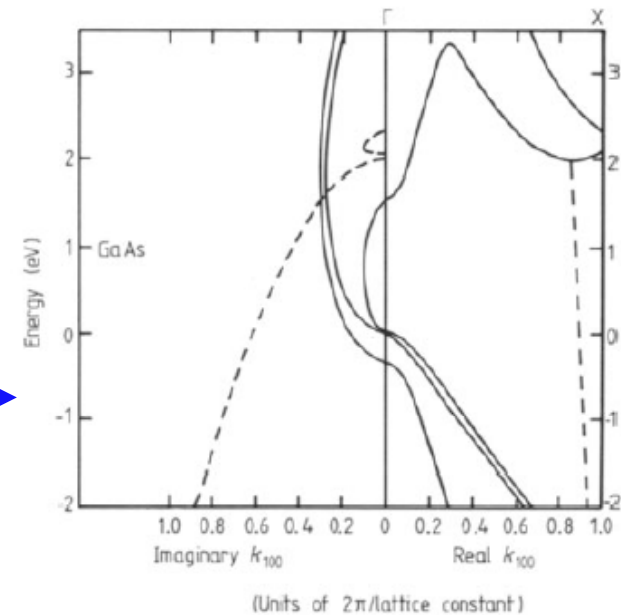
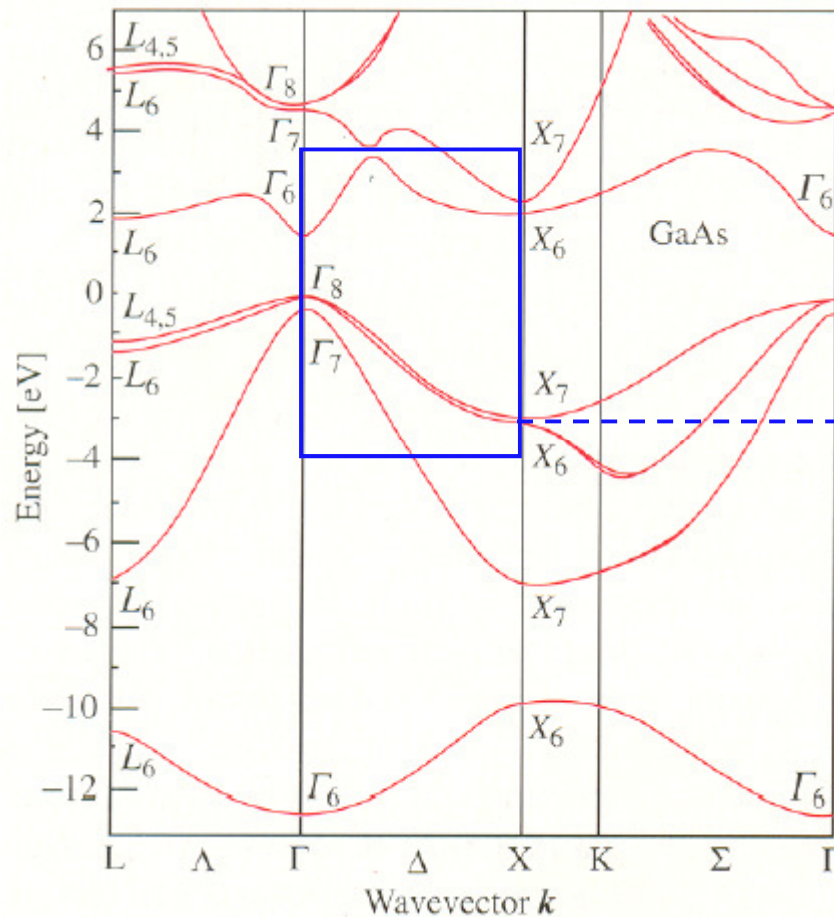


Figure 1. Part of the complex band structure of GaAs in the (100) direction. —, real and imaginary solutions; - - -, general complex solutions.

Ref: Brand *et al* SST 1987

Evanescent modes play an important role in low-dimensional structures
They are required in mode matching at the boundaries etc...