Lattice Structures and Energy Bands

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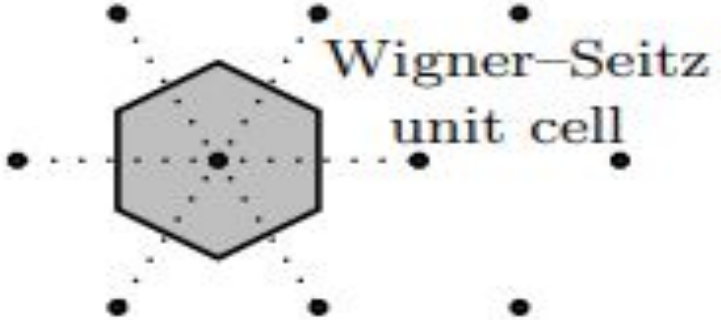
Lattices

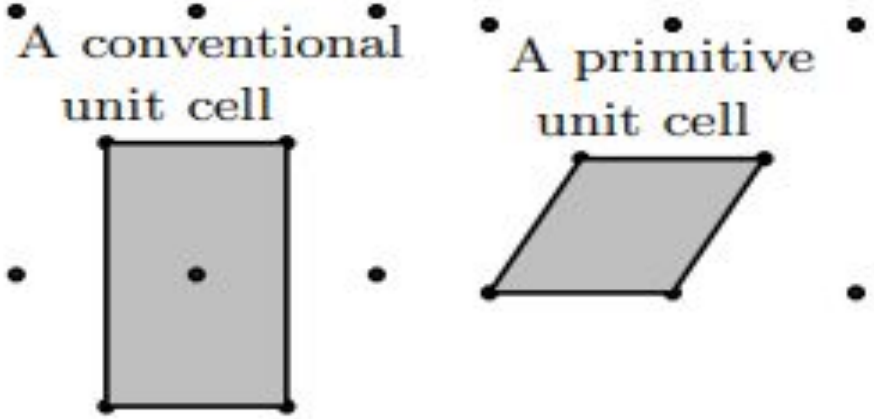
Lattice — infinite set of points, space periodic, equivalent surrounding environment

Unit cell — "generator" – repeating motif

Primitive unit cell — unit cell containing a single lattice point; smallest possible one

Wigner-Seitz unit cell — unit cell closest to a particular lattice point compared to others

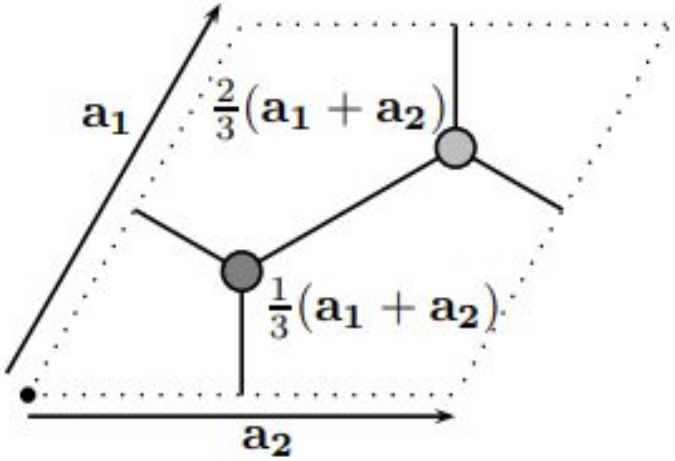


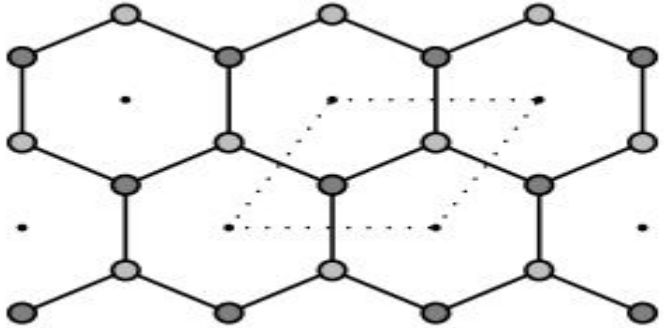


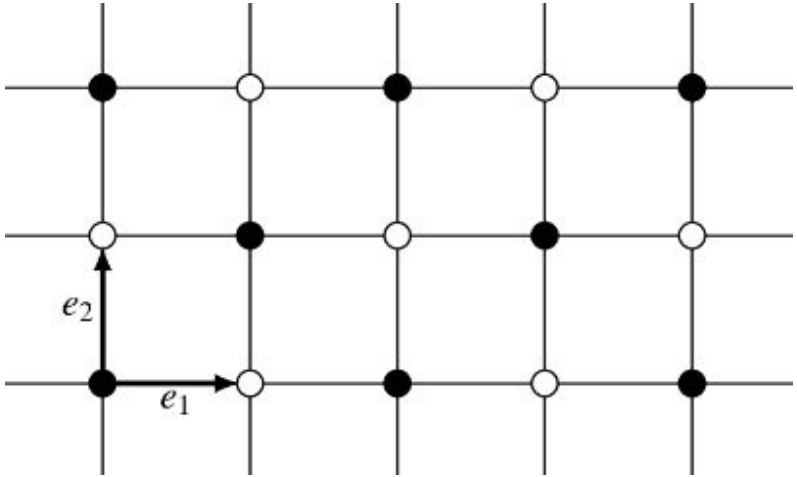
$$R_{nm} = n_1 a_1 + n_2 a_2 + n_m a_m$$

$$n_m \in Z$$

where a denotes primitive lattice vectors and n denotes the specific points of the lattice and m is the index for those points







Basis — where are you with respect to a reference lattice point in the unit cell; used to describe objects in the unit cell

Dual coordinate system defined by basis vectors and lattice vectors

Lattice vectors describe translations

Basis vectors span unit cell

Lattices and Group Structures

Group Axioms

-closure s.t $a, b \in G$ then $a * b, b * a \in G$

-identity s.t $e \in Gs.ta * e = e * a = a \forall a$

-inverse s.t $a \in G \exists a^{-1} \in Gs.ta * a^{-1} = a^{-1} * a = e$

The translations of a lattice are a finitely-generated free* abelian* symmetric group $(G, \circ)$ s.t G = { $\ldots, T^{-1}, I, T, T^2, \ldots$ } isomorphic to Z^n (discrete) (Euclidean space)

The transformations of a lattice constitute a space group (3d bravais)

The transformations excluding translations are a point group

*Abelian except for dislocation *commutative and with basis *generated by basis vectors

Reciprocal Lattice

Reciprocal lattice:

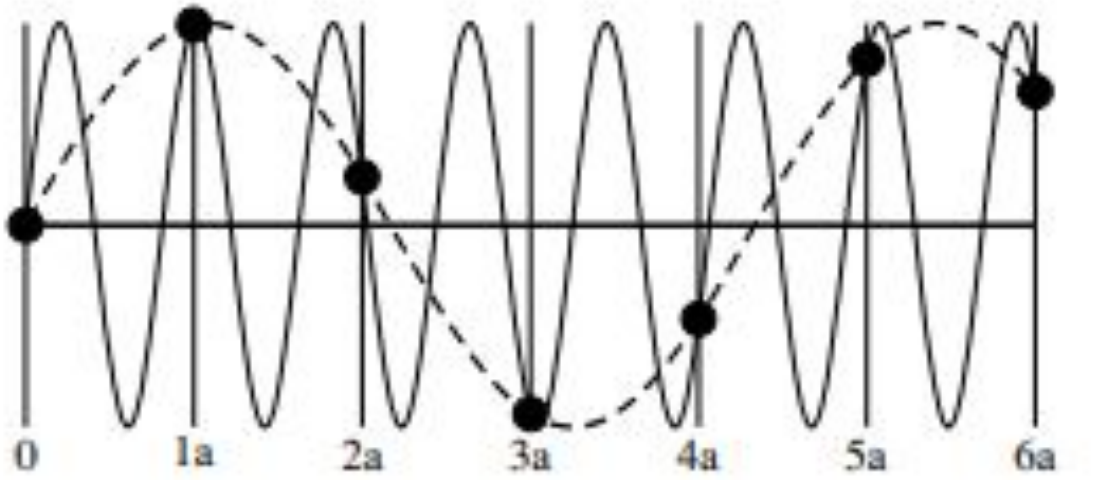
- set of points in k-space physically equivalent to k = 0
- FT of the direct lattice
- for all R in the direct lattice $e^{iG\cdot R} = 1$

system with periodicity Δx = a, then in k-space with periodicity Δk = 2π/a

primitive lattice vectors of the reciprocal lattice (bj) defined by: ai · bj = 2πδij

$$G = m_1 b_1 + m_2 b_2 + \ldots mjbj$$

$$\begin{array}{lllllll} x_n & = & \ldots & -2a, & -a, & 0, \quad a, & 2a, \quad \ldots \\ G_n & = & \ldots & -2\left(\frac{2\pi}{a}\right), & -\frac{2\pi}{a}, & 0, \quad \frac{2\pi}{a}, & 2\left(\frac{2\pi}{a}\right), \quad \ldots \end{array}$$



$G_m = 2\pi m/a$

$K = k + G_m$ (physical equivalence- differ by G_m, element of reciprocal lattice)

Fourier Transform

Density function

$$\rho(r) = \sum_n \delta(r - an)$$

Perform the fourier transform

$$\mathcal{F}[\rho(r)] = \int dr e^{ikr} \rho(r) = \sum_n \int dr e^{ikr} \delta(r - an) = \sum_n e^{ikan}$$
$$= \frac{2\pi}{|a|} \sum_m \delta(k - 2\pi m/a).$$

Generalize the result to higher dimensions

$$\mathcal{F}[\rho(\mathbf{r})] = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} = \frac{(2\pi)^D}{v} \sum_{\mathbf{G}} \delta^D(\mathbf{k} - \mathbf{G})$$

FT any function with a lattice-like periodicity

$$\rho(\mathbf{r}) = \rho(\mathbf{r} + \mathbf{R})$$

Translation invariance

$$\mathcal{F}[\rho(\mathbf{r})] = \int \mathbf{dr}\ e^{i\mathbf{k}\cdot\mathbf{r}} \rho(\mathbf{r}).$$

$$\mathcal{F}[\rho(\mathbf{r})] = \sum_{\mathbf{R}} \int_{unit-cell} \mathbf{dx}\ e^{i\mathbf{k}\cdot(\mathbf{x}+\mathbf{R})} \rho(\mathbf{x} + \mathbf{R})$$
$$= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \int_{unit-cell} \mathbf{dx}\ e^{i\mathbf{k}\cdot\mathbf{x}} \rho(\mathbf{x}).$$

$$\mathcal{F}[\rho(\mathbf{r})] = (2\pi)^D \sum_{\mathbf{G}} \delta^D(\mathbf{k} - \mathbf{G}) S(\mathbf{k})$$

Structure factor

$$S(\mathbf{k}) = \int_{unit-cell} \mathbf{dx}\ e^{i\mathbf{k}\cdot\mathbf{x}} \rho(\mathbf{x})$$

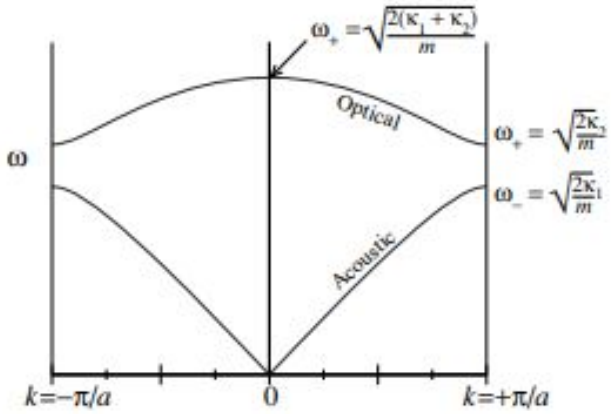
Brillouin Zone

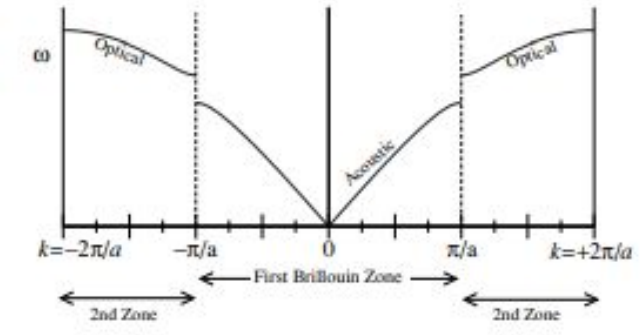
Brillouin Zone — unit cell of reciprocal lattice; “first Brillouin zone” is a Wigner–Seitz unit cell in k-space centered around the point k = 0

Crystal momentum — K = k + Gm where Gm = 2πm/a is a point in the reciprocal lattice; momentum of the reciprocal lattice described within the first Brillouin zone

restrict k to the first Brillouin zone so every Bloch state has unique k

used first BZ to depict all of the Bloch states without redundancy





Bloch's Theorem

Bloch's Theorem: An electron in a periodic potential has eigenstates of the form

$$\Psi^{\alpha}_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u^{\alpha}_{\mathbf{k}}(\mathbf{r})$$

where $u^{\alpha}_{\mathbf{k}}$ is periodic in the unit cell and $\mathbf{k}$ (the crystal momentum) can be chosen within the first Brillouin zone.

Sum over reciprocal lattice vectors because periodic

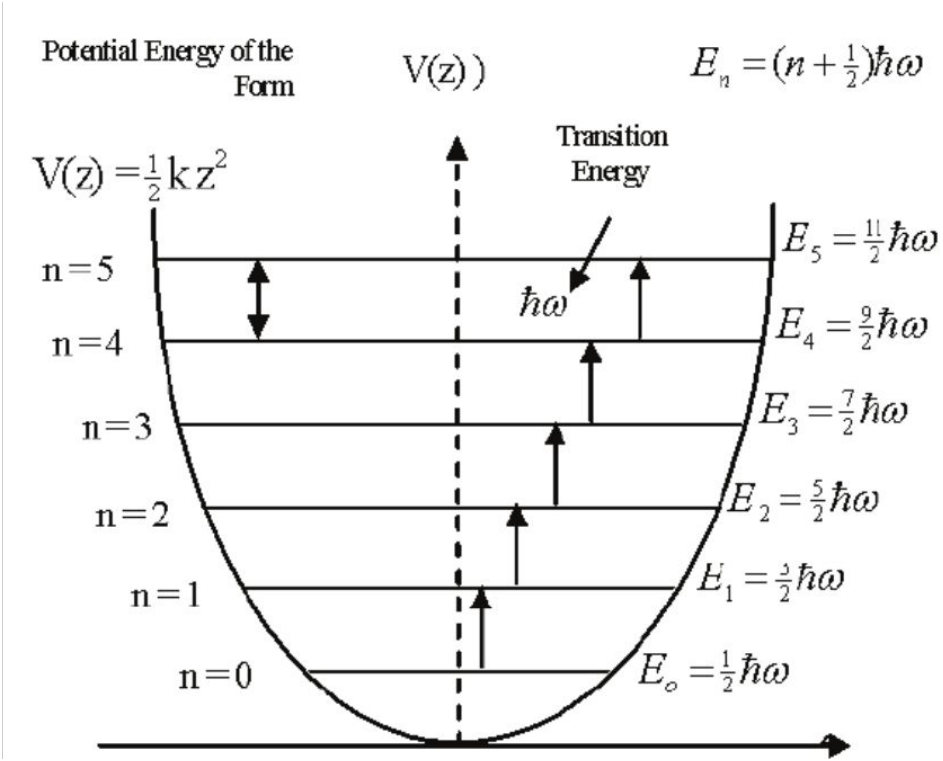
This form guarantees[12] that $u^{\alpha}_{\mathbf{k}}(\mathbf{r}) = u^{\alpha}_{\mathbf{k}}(\mathbf{r}+\mathbf{R})$ for any lattice vector $\mathbf{R}$. Therefore the full wavefunction is expressed as

$$\Psi^{\alpha}_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} \tilde{u}^{\alpha}_{\mathbf{G},\mathbf{k}}\, e^{i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}} \,. \qquad (15.13)$$

- guarantees that all eigenstates are some periodic function * plane wave
- though e- feels strong potential from each atom from, behave otherwise
- almost form plane-wave eigenstates but with the Bloch function and crystal momentum

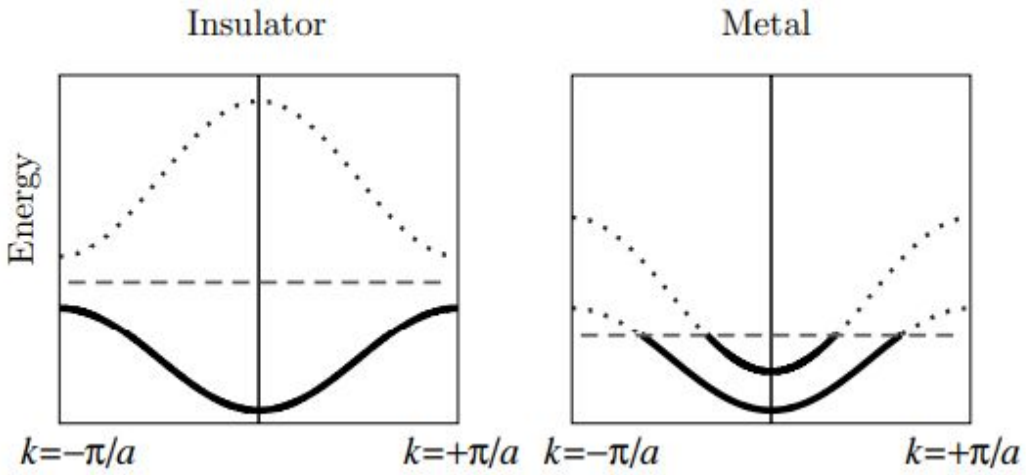
Note: all we're trying to do is represent the wavefunctions of electrons in a crystalline structure

Simple Harmonic Oscillator



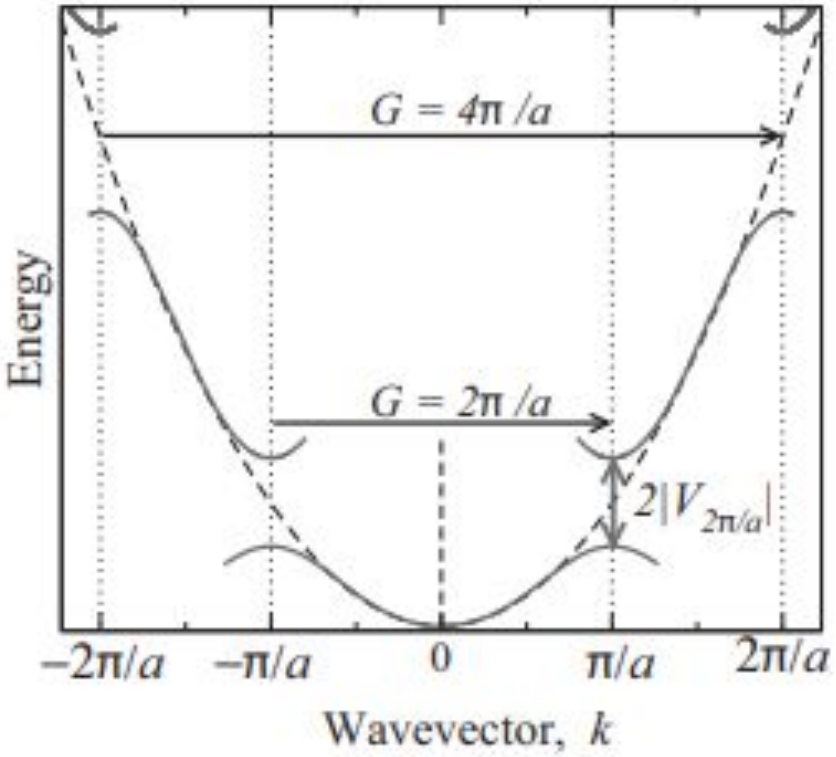
Energy Bands

- Electrons
- Wavefunctions
- Solutions to bloch's function
- Plot energies with respect to k— how energies depend on crystal momentum dispersion
- Bands!!
- Looking at the Brillouin zone and since unit cells are unique we have specific band structures corresponding to different lattices



Nearly Free Electron Model

- applying perturbation theory can allow for more distinct band formations
- electrons are exposed to a periodic potential so gaps form in their dispersion relation at BZ boundary
- electronic spectrum breaks into bands, with forbidden energy gaps between the bands.
- gaps are proportional to the periodic potential |VG| here



A lattice, a structure, so strong and so true,
A mathematical wonder, for physicists to view,
The atoms aligned, in a symmetrical array,

Forming a grid, in a most perfect way.

The groups they create, with bonds so tight,
Have properties unique, to bring to light,
Symmetry operations, to reflect and to glide,

To rotate and invert, with their bonds at their side.

In condensed matter, they play a key role,
From metals to crystals, to semiconducting soul,
Their properties so vast, and so complex,

Give rise to phenomena, that scientists can't reject.

From Bloch's Theorem to Wigner-Seitz,
Their impact on physics, will never cease,
Their group structures, so elegant and grand,

Will always be studied, in the physicist's land. - Chat GPT