PHYSICS 211B : SOLID STATE PHYSICS

Topics :

- Energy bands in solids (ch. 4)
- Boltzmann transport (ch. 5)
- interacting systems:
  - Hartree-Fock and DFT (ch. 8)
  - Fermi liquid theory (ch. 10)
  - Superconductivity (chs. 11-13)
  - Magnetism (ch. 14)

- **Lecture 1 (Jan. 5) : Energy bands in solids**

  - describe energy levels of noninteracting electrons in a periodic potential :

$$H = \frac{\vec{p}^2}{2m} + V(\vec{x})$$

where $V(\vec{x}+\vec{R}) = V(\vec{x})$ for $\vec{R} \in \mathcal{L}$ = Bravais lattice

  - **Bravais lattices** : in d space dimensions, $\mathcal{L}$ is defined by d linearly independent basis vectors $\vec{a}_j$ ($j \in \{1, \dots, d\}$) which span a **unit cell** of volume

$$\Omega = \epsilon_{\mu_1 \cdots \mu_d} a_1^{\mu_1} \cdots a_d^{\mu_d} > 0$$

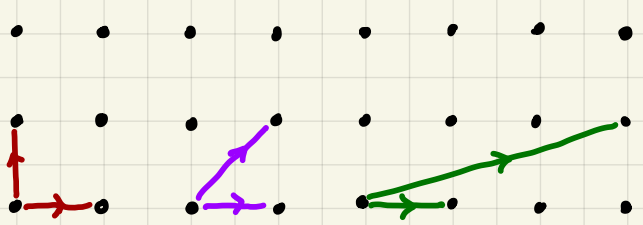
For $d=2$, $\Omega = a_1^x a_2^y - a_1^y a_2^x = \hat{z} \cdot \vec{a}_1 \times \vec{a}_2$

For $d=3$, $\Omega = \epsilon_{\alpha\beta\gamma} a_1^\alpha a_2^\beta a_3^\gamma = \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3$

The **direct lattice** $\mathcal{L}$ is the collection

$$\mathcal{L} = \left\{ \vec{R} = \sum_{j=1}^{d} n_j \vec{a}_j \;\middle|\; n_i \in \mathbb{Z} \;\forall\, i \right\}$$

NB: The set $\{\vec{a}_j\}$ is not unique. For example, on the square lattice,



$\vec{a}_1 = a\hat{x}$, $a_2 = a\hat{y}$

$a_1 = a\hat{x}$, $a_2 = a\hat{x} + a\hat{y}$

$\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = 3a\hat{x} + a\hat{y}$

all three choices generate the same $\mathcal{L}$.

- **Reciprocal lattice** ($\hat{\mathcal{L}}$): define the elementary reciprocal lattice vectors (RLVs),

$$b_k^{\nu} = \frac{2\pi}{\Omega} \epsilon_{\mu_1 \cdots \mu_{k-1} \nu \mu_{k+1} \cdots \mu_d} a_1^{\mu_1} \cdots a_{k-1}^{\mu_{k-1}} a_{k+1}^{\mu_{k+1}} \cdots a_d^{\mu_d}$$

So that $\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$. This also entails

$$\sum_{j=1}^{d} a_j^{\mu} b_j^{\nu} = 2\pi \delta^{\mu\nu}$$

For $d = 2$, $\vec{b}_1 = \frac{2\pi}{\Omega} \vec{a}_2 \times \hat{z}$, $\vec{b}_2 = \frac{2\pi}{\Omega} \hat{z} \times \vec{a}_1$

For $d = 3$,

$$\vec{b}_1 = \frac{2\pi}{\Omega} \vec{a}_2 \times \vec{a}_3 \quad , \quad \vec{b}_2 = \frac{2\pi}{\Omega} \vec{a}_3 \times \vec{a}_1 \quad , \quad \vec{b}_3 = \frac{2\pi}{\Omega} \vec{a}_1 \times \vec{a}_2$$

The reciprocal lattice $\hat{\mathcal{L}} = \left\{ \vec{G} = \sum_{j=1}^{d} m_j \vec{b}_j \;\middle|\; m_i \in \mathbb{Z} \;\forall\, i \right\}$

is also a Bravais lattice. The reciprocal lattice of the reciprocal lattice is the direct lattice: $\hat{\hat{\mathcal{L}}} = \mathcal{L}$.

The unit cell volume of $\hat{\mathcal{L}}$ is

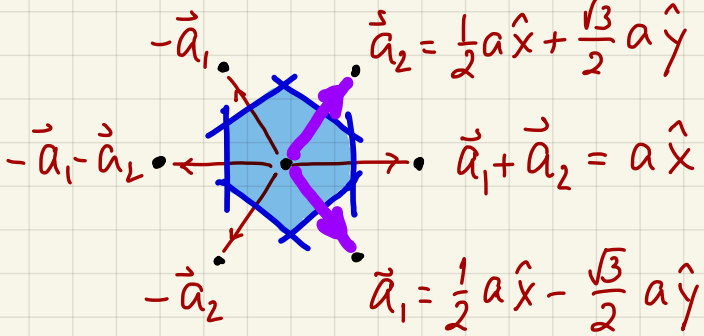
$$\hat{\Omega} = \epsilon_{\mu_1 \cdots \mu_d} b_1^{\mu_1} \cdots b_d^{\mu_d} = \frac{(2\pi)^d}{\Omega}$$

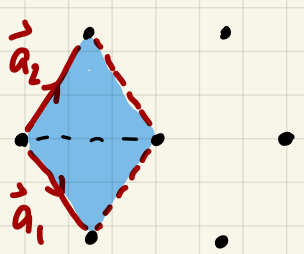
- The collections of points,

$$\vec{x} = \sum_{j=1}^{d} u_j \vec{a}_j \quad , \quad \vec{k} = \sum_{j=1}^{d} v_j \vec{b}_j$$

with each $u_j, v_j \in [0,1]$, constitutes a unit cell for $\mathcal{L}$ and $\hat{\mathcal{L}}$, respectively. The spatial symmetries of the direct and reciprocal lattices are more fully elicited by shifting each such point $\vec{x}$ or $\vec{k}$ by a DLV $\vec{R}$ or a RLV $\vec{G}$ so that it is as close as possible to the origin. Equivalently, sketch all the nonzero shortest DLVs/RLVs emanating from the origin and bisect each such vector with a perpendicular hyperplane. The collection of all such points bounded by these hyperplanes are unit cells of $\mathcal{L}$ and $\hat{\mathcal{L}}$, known as the first **Wigner-Seitz cell** (of $\mathcal{L}$) and the first **Brillouin zone** (of $\hat{\mathcal{L}}$).

Example: triangular lattice





$$\Omega = \frac{\sqrt{3}}{2} a^2$$

- In $d=2$ there are five distinct Bravais lattices, arranged in four families ("lattice systems"):

SQUARE OBLIQUE HEXAGONAL RECTANGULAR (simple, centered)

In $d=3$, there are 14 distinct Bravais lattices, arranged in seven families:

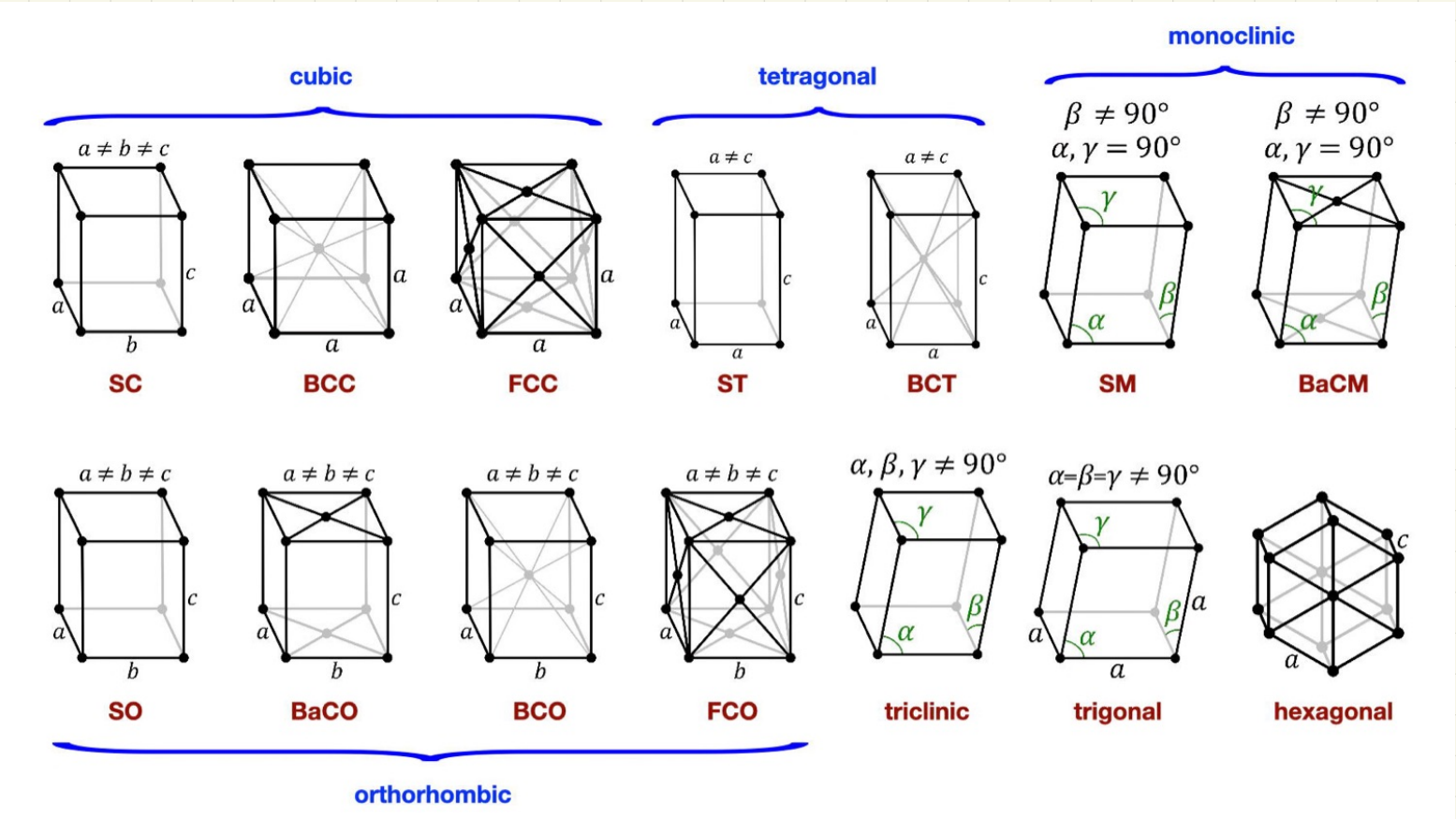
CUBIC (3): simple, body-centered, face-centered

TETRAGONAL (2): simple, body-centered

ORTHORHOMBIC (4): simple, base-centered, body-centered, face-centered

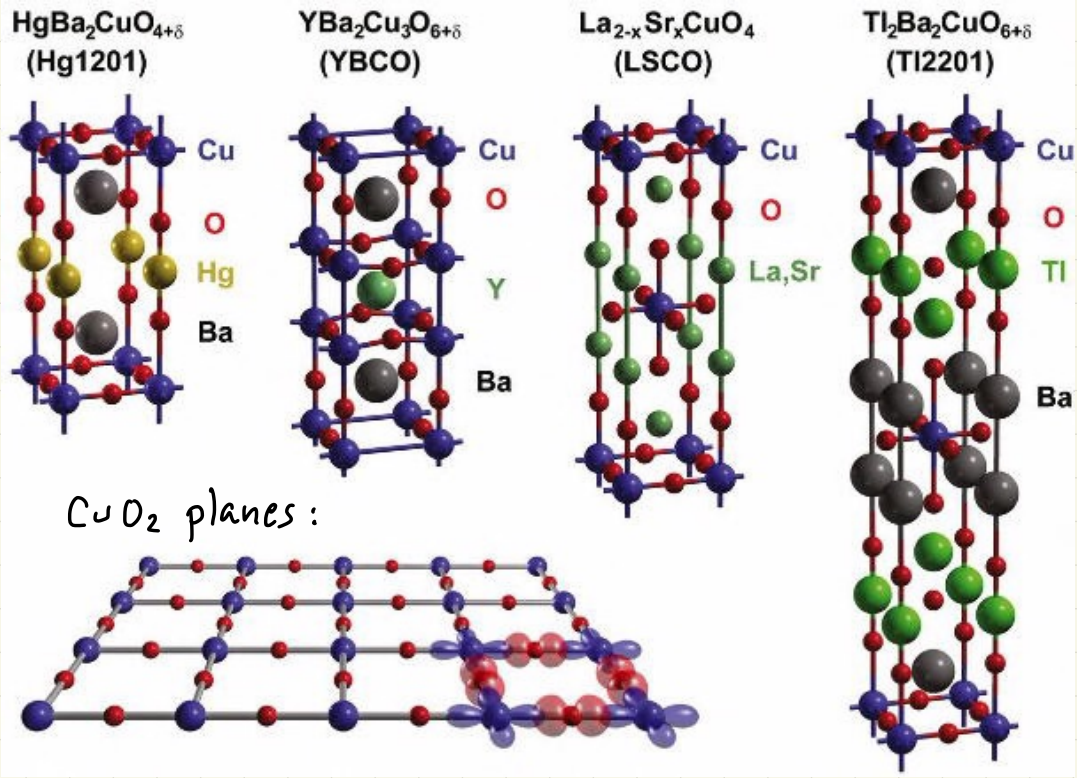
MONOCLINIC (2): simple, base-centered

TRICLINIC (1) TRIGONAL (1) HEXAGONAL (1)



- Crystalline lattices (BL with a **basis** $\{\vec{\delta}_j\}$)

The unit cell of a Bravais lattice is akin to an empty canvas (with special symmetries). A <u>crystalline unit cell</u> consists of r atoms or ions at positions $\vec{\delta}_j$ relative to any DLV $\vec{R}$, with all $\vec{\delta}_j$ ($j \in \{1,\dots,r\}$) lie within a single direct lattice unit cell. Examples: cuprate superconductors. The underlying BL is orthorhombic.



If we model the density of the crystal as

$$\rho(\vec{r}) = \sum_{\vec{R}} \sum_{j=1}^{r} c_j \, \delta(\vec{r} - \vec{R} - \vec{\delta}_j) \qquad (T=0)$$

then the scattering intensity at wavevector $\vec{k}$ is proportional to

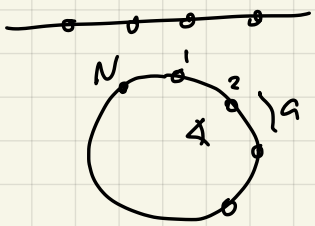
$$I(\vec{k}) \propto \frac{1}{N} \left|\hat{\rho}(\vec{k})\right|^2 = F(\vec{k}) \sum_{\vec{R}} e^{-i\vec{k}\cdot\vec{R}} = \hat{\Omega} \sum_{\vec{G}} F(\vec{G}) \, \delta(\vec{k} - \vec{G})$$

N: # of unit cells

Poisson summation formula

Bragg peak

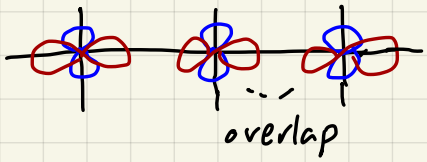
where the unit cell form factor is



$$F(\vec{G}) = \left| \sum_{j=1}^{r} c_j e^{-i\vec{G}\cdot\vec{\delta}_j} \right|^2$$

The form factor modifies the intensity of each Bragg peak and can lead to systematic extinctions of certain RLVs. (Example: problem #2 on HW #1.)

• Tight-binding models



- ingredients: set of orthonormal orbitals $\{|a\vec{R}\rangle\}$ where $\vec{R} \in \mathcal{L}$ and $a \in \{1, \ldots, N_{orb}\}$ where N_{orb} is the total number of <u>orbitals</u> associated with a crystalline unit cell. Each atom/ion can support multiple such orbitals. Note that <u>atomic</u> orbitals, which we denote by $|n\vec{R})$, i.e. with rounded brackets, are not mutually orthogonal, viz.

$$(n\vec{R}\,|\,n'\vec{R}') = \int d^d x\, \varphi_n^*(\vec{r}-\vec{R})\,\varphi_{n'}(\vec{r}-\vec{R}') \equiv S_{nn'}(\vec{R}-\vec{R}')$$

$$\longrightarrow S_{nn'}(0) = \delta_{nn'}$$

the overlap matrix. In principle we can build a basis of orthonormal orbitals $|a\vec{R}\rangle$, for which

$$\langle a\vec{R}\,|\,a'\vec{R}'\rangle = \delta_{\vec{R}\vec{R}'}\,\delta_{aa'}$$

from the various atomic orbitals. Henceforth we will work in this orthonormal basis.

The most general tight-binding Hamiltonian we write as

$$H = \sum_{\vec{R},\vec{R}'} \sum_{a,a'} H_{aa'}(\vec{R}-\vec{R}') \, |a\vec{R}\rangle\langle a'\vec{R}'|$$

where

$$H_{aa'}(\vec{R}-\vec{R}') = H^*_{a'a}(\vec{R}'-\vec{R}) = \langle a\vec{R}|H|a'\vec{R}'\rangle$$

Aside: the orbital label a can also denote spin polarization.

We partially diagonalize by defining the orbitals

$$|a\vec{k}\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{R}} |a\vec{R}\rangle e^{i\vec{k}\cdot\vec{R}}, \qquad |a\vec{R}\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{k}} |a\vec{k}\rangle e^{-i\vec{k}\cdot\vec{R}}$$

($\vec{k} \in \hat{\Omega}$; sum on $\vec{R} \in \mathcal{L}$; sum on $\vec{k} \in \hat{\Omega}$ (1st Brillouin zone))

Then, using the results

$$\frac{1}{N} \sum_{\vec{k}} e^{-i\vec{k}\cdot(\vec{R}-\vec{R}')} = \delta_{\vec{R}\vec{R}'}, \qquad \frac{1}{N} \sum_{\vec{R}} e^{i(\vec{k}-\vec{k}')\cdot\vec{R}} = \delta_{\vec{k}\vec{k}'}$$

we can write the Hamiltonian as

$$H = \sum_{\vec{k}} \sum_{a,a'} \hat{H}_{aa'}(\vec{k}) \, |a\vec{k}\rangle\langle a'\vec{k}|$$

where

$$\hat{H}_{aa'}(\vec{k}) = \sum_{\vec{R}} H_{aa'}(\vec{R}) \, e^{-i\vec{k}\cdot\vec{R}}$$

Thus, for each wavevector $\vec{k}$, we must diagonalize the matrix $\hat{H}_{aa'}(\vec{k})$, which is of size $N_{orb} \times N_{orb}$. Plotting the N_{orb} eigenvalues $E_n(\vec{k})$ versus $\vec{k}$ yields the **band structure**.

The **cell eigenfunctions** $u_{na}(k)$ satisfy

$$\sum_{a'} \hat{H}_{aa'}(k)\, u_{na'}(k) = E_n(k)\, u_{na}(k)$$

where n is the band index. The full Bloch state is then

$$|\psi_{nk}\rangle = |k\rangle \otimes |u_{nk}\rangle$$

($|u_{nk}\rangle$: internal wavefunction within each unit cell; $|k\rangle$: unit cell plane wave envelope)

so that

$$\psi_{nk}(\vec{R}, a) = \left(\langle \vec{R}| \otimes \langle a|\right)\left(|k\rangle \otimes |u_{nk}\rangle\right)$$

$$= \langle \vec{R}|k\rangle \langle a|u_{nk}\rangle = \frac{1}{\sqrt{N}} e^{ik\cdot\vec{R}}\, u_{na}(k)$$

- Second quantized notation:

$$H = \sum_{\vec{R},\vec{R}'} \sum_{a,a'} H_{aa'}(\vec{R}-\vec{R}')\, c^{\dagger}_{a\vec{R}}\, c_{a'\vec{R}'}$$

$$= \sum_{k} \sum_{a,a'} \hat{H}_{aa'}(k)\, c^{\dagger}_{ak}\, c_{a'k}$$

where

$$\{c_{a\vec{R}}, c^{\dagger}_{a'\vec{R}'}\} = \delta_{aa'}\delta_{\vec{R}\vec{R}'} \quad , \quad \{c_{a\vec{R}}, c_{a'\vec{R}'}\} = \{c^{\dagger}_{a\vec{R}}, c^{\dagger}_{a'\vec{R}'}\} = 0$$

$$\{A, B\} = AB + BA = \text{anticommutator}$$

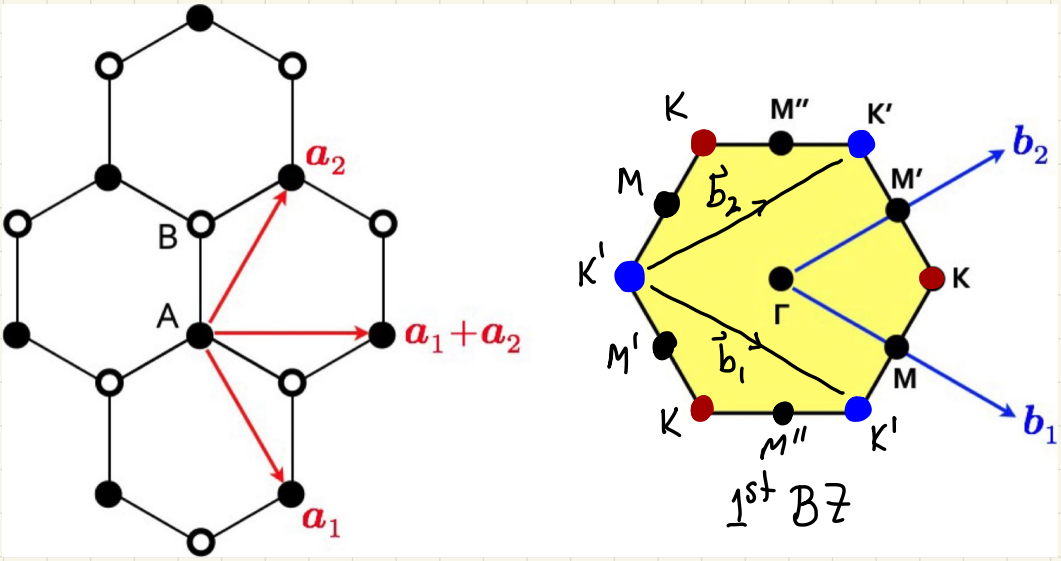
Second quantization becomes essential when we start to consider interacting systems.

– notation : we will write

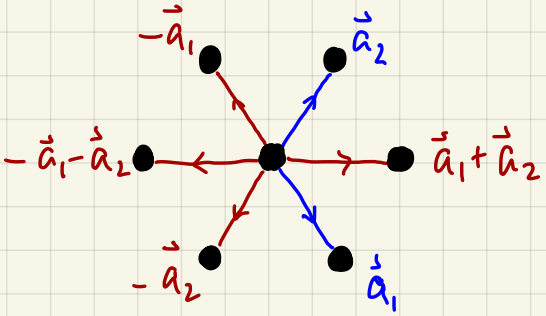
$$\varepsilon_a \equiv H_{aa}(0) \quad , \quad t_{aa'}(\vec{R}) \equiv -H_{aa'}(\vec{R})$$

(on-site energy) (hopping matrix element; either $a \neq a'$ or $\vec{R} \neq 0$)

• **Examples**: triangular and honeycomb lattices



The honeycomb lattice is a triangular Bravais lattice with a two element basis (A and B). The first BZ for the corresponding reciprocal lattice (also triangular) is shown. Let's first consider nearest-neighbor s-orbital hopping on the triangular lattice.



$$\vec{a}_1 = a\left(\tfrac{1}{2}\hat{x} - \tfrac{\sqrt{3}}{2}\hat{y}\right) \quad , \quad \vec{a}_2 = a\left(\tfrac{1}{2}\hat{x} + \tfrac{\sqrt{3}}{2}\hat{y}\right)$$

$$t(\vec{R}) = t\,\delta_{\vec{R},\vec{a}_1} + t\,\delta_{\vec{R},\vec{a}_2} + t\,\delta_{\vec{R},\vec{a}_1+\vec{a}_2} + t\,\delta_{\vec{R},-\vec{a}_1} + t\,\delta_{\vec{R},-\vec{a}_2} + t\,\delta_{\vec{R},-\vec{a}_1-\vec{a}_2}$$

Thus,

$$\hat{t}(\vec{k}) = \sum_{\vec{R}} t(\vec{R})\, e^{-i\vec{k}\cdot\vec{R}}$$

$\vec{a}_3 \equiv \vec{a}_1 + \vec{a}_2$

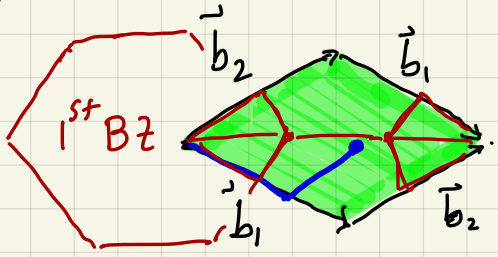
$$= 2t\cos(\vec{k}\cdot\vec{a}_1) + 2t\cos(\vec{k}\cdot\vec{a}_2) + 2t\cos(\vec{k}\cdot\vec{a}_3)$$

$$= 2t\cos\theta_1 + 2t\cos\theta_2 + 2t\cos(\theta_1+\theta_2)$$

There is a single band, with dispersion $E(\vec{k}) = -t(\vec{k})$.

Note we have written

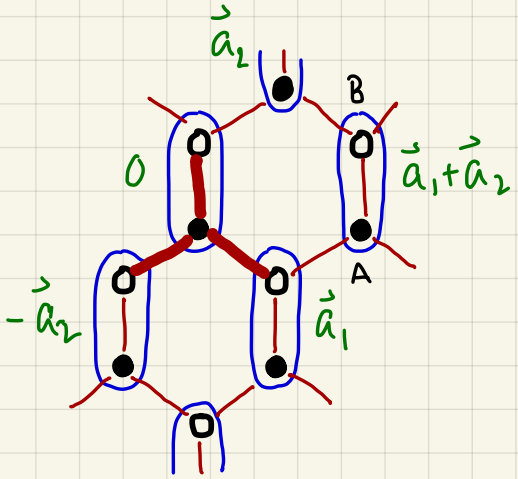
$$\vec{k} = \frac{\theta_1}{2\pi}\vec{b}_1 + \frac{\theta_2}{2\pi}\vec{b}_2 \;\Rightarrow\; \vec{k}\cdot\vec{a}_j = \theta_j$$



One finds $E(\Gamma) = -6t$, $E(K) = 3t$, and $E(M) = 2t$, where

$$\vec{k}_\Gamma = 0 \quad , \quad \vec{k}_K = \tfrac{1}{3}(\vec{b}_1 + \vec{b}_2) \quad , \quad \vec{k}_M = \tfrac{1}{2}\vec{b}_1$$
$$\vec{\theta}_\Gamma = (0,0) \quad , \quad \vec{\theta}_K = \left(\tfrac{2\pi}{3}, \tfrac{2\pi}{3}\right) \quad , \quad \vec{\theta}_M = (\pi, 0)$$

Now, graphene. Assuming nearest-neighbor hopping,



$$t_{AB}(\vec{R}) = t\,\delta_{\vec{R},0} + t\,\delta_{\vec{R},\vec{a}_1} + t\,\delta_{\vec{R},-\vec{a}_2}$$

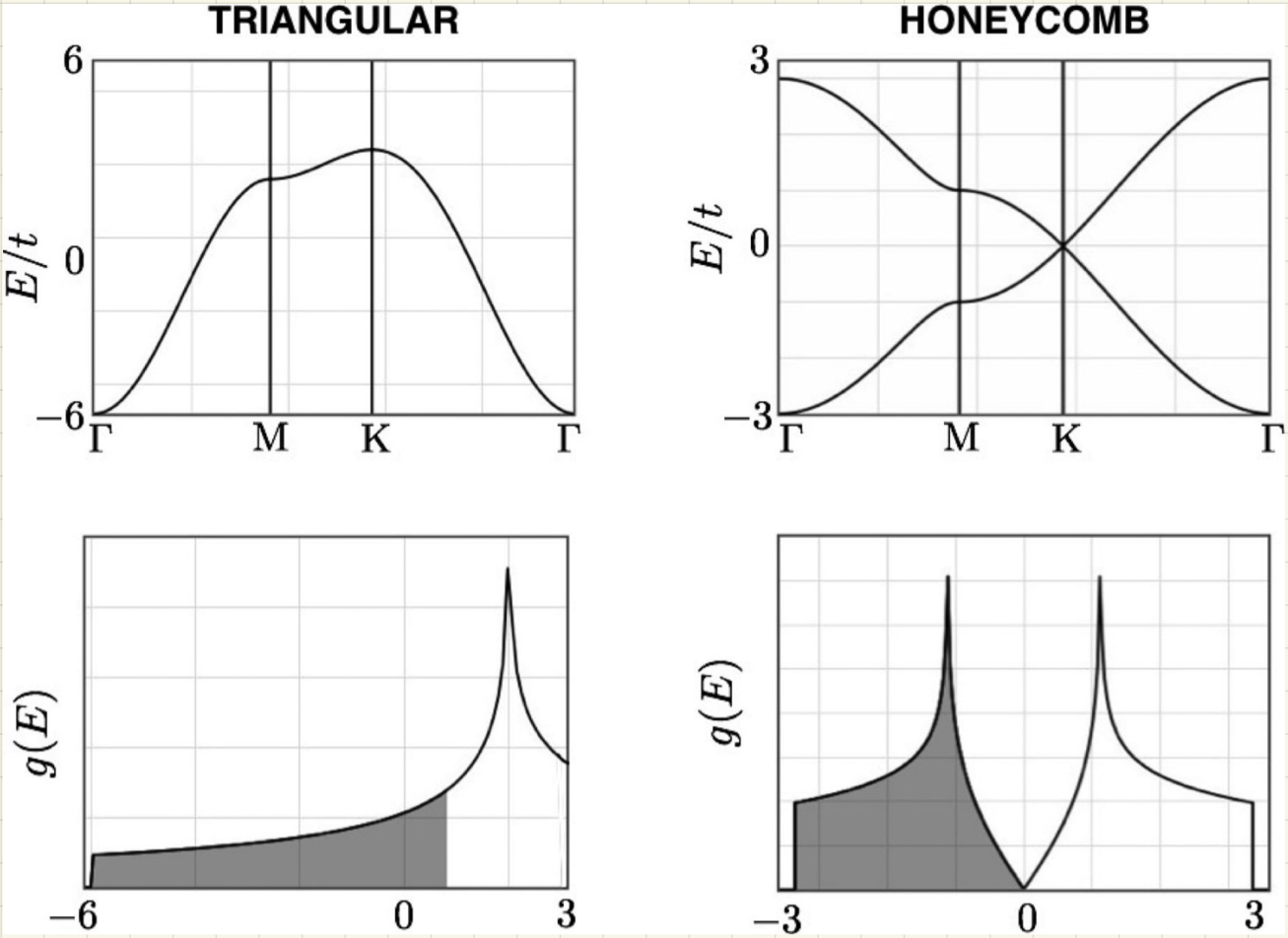
$$\hat{t}_{AB}(\vec{k}) = t\left(1 + e^{-i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2}\right) = \hat{t}^*_{BA}(\vec{k})$$

$$\hat{H}(\vec{k}) = -\begin{pmatrix} 0 & \hat{t}_{AB}(\vec{k}) \\ \hat{t}^*_{AB}(\vec{k}) & 0 \end{pmatrix}$$

eigenvalues: $E_\pm(\vec{k}) = \pm\left|\hat{t}_{AB}(\vec{k})\right|$

$$= \pm t\sqrt{3 + 2\cos\theta_1 + 2\cos\theta_2 + 2\cos(\theta_1+\theta_2)}$$

The triangular and honeycomb lattice tight binding spectra are:



Also shown is the density of states per unit cell,

$$g(E) = \sum_n \Omega \int_{\hat{\Omega}} \frac{d^d k}{(2\pi)^d} \, \delta(E - E_n(\hbar k))$$

The greyed areas show filled states of either spin polarization when there is one electron per site. The highest occupied state defines the Fermi level. For the triangular lattice, there is a logarithmic singularity, known as a **van Hove singularity**, at $E = +2t$. For the honeycomb lattice, the spectrum is symmetric, $g(E) = g(-E)$, and

there are van Hove singularities at $E = \pm t$. Note that for the honeycomb lattice

$$E_\pm(\Gamma) = \pm 3t \quad , \quad E_\pm(K) = 0 \quad , \quad E_\pm(M) = \pm t$$

In the vicinity of either of the two inequivalent zone corners K and K', if we write $\vec{k} = \vec{K} + \vec{q}$ or $\vec{k} = \vec{K}' + \vec{q}$, we have $E = \pm \hbar v_F |\vec{q}|$ with $v_F = \frac{\sqrt{3}}{2} ta/\hbar$. This is a 2D Dirac spectrum, and K and K' are the locations of Dirac points.

Lecture 2 (Jan. 7): How to go flux yourself

Simple model: spinless s-orbitals in a 2D crystal

The Hamiltonian is

$$H = -\sum_{\vec{r}<\vec{r}'} \left(t_{\vec{r}\vec{r}'} c^\dagger_{\vec{r}} c_{\vec{r}'} + t^*_{\vec{r}\vec{r}'} c^\dagger_{\vec{r}'} c_{\vec{r}} \right)$$
$$= -\sum_{\vec{r}<\vec{r}'} \left(t_{\vec{r}\vec{r}'} |\vec{r}\rangle\langle\vec{r}'| + t^*_{\vec{r}\vec{r}'} |\vec{r}'\rangle\langle\vec{r}| \right)$$

The notation $\vec{r} < \vec{r}'$ means that each pair $(\vec{r}, \vec{r}')$ is included only once in the sum. We may write

$$t_{\vec{r}\vec{r}'} = t^*_{\vec{r}'\vec{r}} = |t_{\vec{r}\vec{r}'}| \, e^{iA_{\vec{r}\vec{r}'}} \qquad (A_{\vec{r}\vec{r}'} \text{ defined mod } 2\pi)$$

where $A_{\vec{r}\vec{r}'}$ is a gauge field living on the link $(\vec{r}, \vec{r}')$. Note $A_{\vec{r}'\vec{r}} = -A_{\vec{r}\vec{r}'}$. The tight-binding Hamiltonian exhibits a **gauge invariance**,