SFB 1143

# Solid State Theory (SS2020)

## Lecture 3: Lattice dynamics

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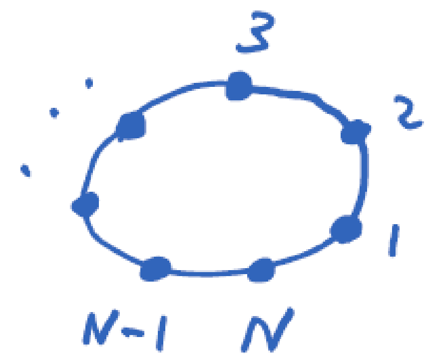
# § 1.2 Quantum monoatomic chain

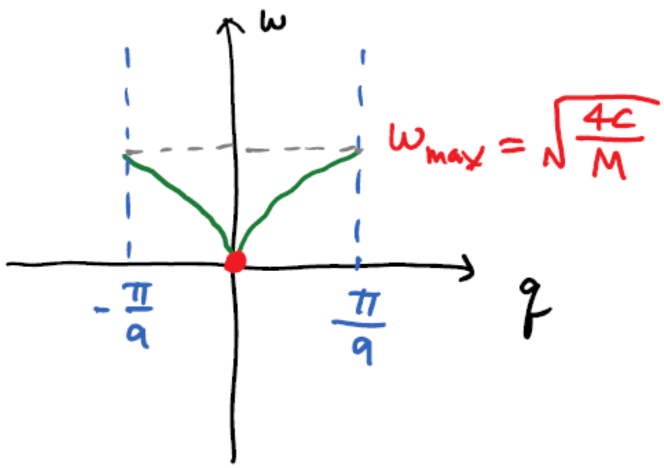
- Last lecture: Quantum theory of a monoatomic chain

$$H = \sum_{j=1}^{N} \frac{P_j^2}{2M} + \frac{1}{2} c \sum_{j=1}^{N} \left( u_{j+1} - u_j \right)^2$$




successive canonical transformations

$$H = \sum_q \hbar \omega_q \left( a_q^\dagger a_q + \frac{1}{2} \right)$$




➢ Collective excitations: phonons

# § 1.2 Quantum monoatomic chain

- Next step: lattice dynamics in higher dimensions (d=2,3 => more realistic).

$$H_{ion} = \sum_i \frac{\vec{p}_i^{\,2}}{2M_i} + \frac{1}{2}\sum_{i \neq j} V(\vec{r}_i - \vec{r}_j)$$

- Before that, we need a better understanding of the lattice structure…

  - Find out common and distinct features!

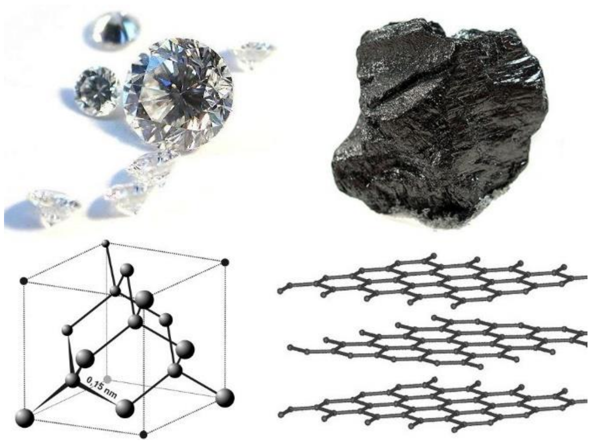


Figure from Wikimedia

# § 1.3 Lattice structure

- Bravais lattice: defined by a set of basis vectors (primitive vectors)

$$\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \, ,$$

$$n_1, n_2, n_3 \in \mathbb{Z} \quad \text{(integers)}$$

$$\vec{a}_1, \vec{a}_2, \vec{a}_3 \, : \quad \text{primitive vectors}$$

Equilibrium positions of atoms!

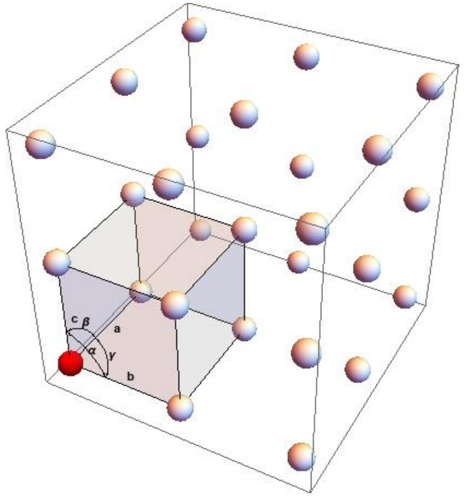
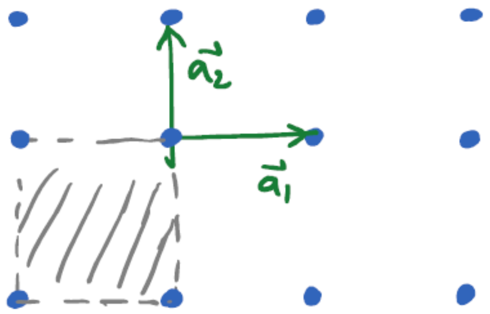



Figure from Wolfram Demonstrations project

- Full classification available (see Wikipedia)
  - 3d: 7 lattice systems, 14 Bravais lattices

# § 1.3 Lattice structure

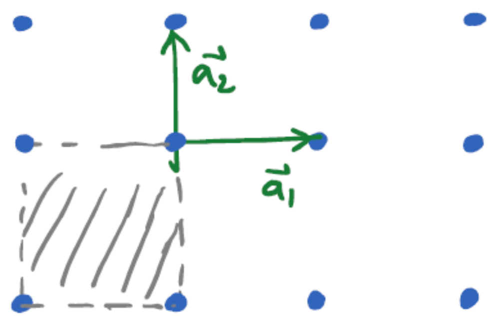
- Unit cell (primitive cell): smallest repeating volume in the crystal




Different choices possible, usually choose the most convenient one.

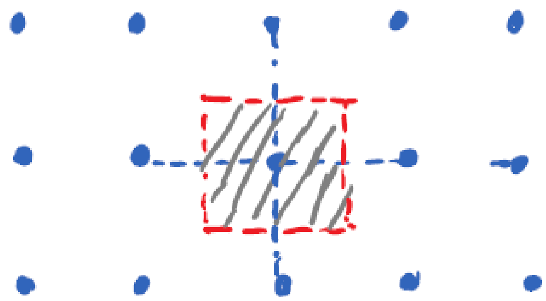
# § 1.3 Lattice structure

- Unit cell (primitive cell): smallest repeating volume in the crystal




Different choices possible, usually choose the most convenient one.

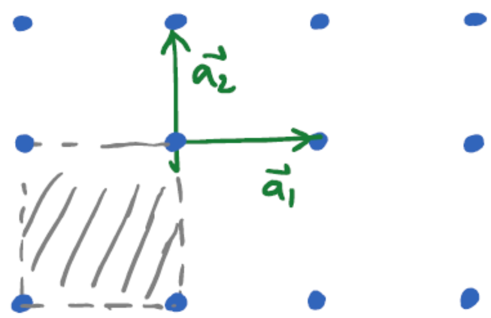
- Wigner-Seitz cell: special choice of unit cell (with atom at the center)



Draw perpendicular lines (planes in 3d) through the center of all lines connecting neighboring sites of the Bravais lattice

# § 1.3 Lattice structure

- Unit cell ([primitive cell]): smallest repeating volume in the crystal

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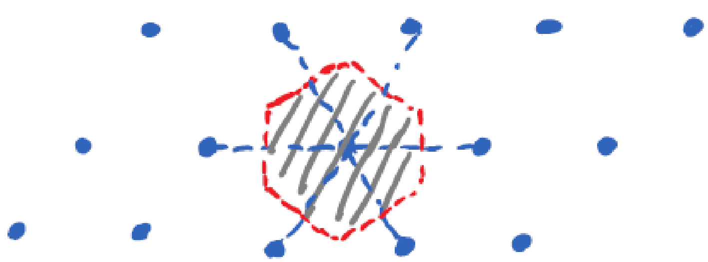


Draw perpendicular lines (planes in 3d) through the center of all lines connecting neighboring sites of the Bravais lattice

# § 1.3 Lattice structure

- Reciprocal lattice

Bravais lattice: $\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

$n \in \mathbb{Z}$

We need to determine all allowed $\vec{G}_m$ satisfying

$$e^{i\vec{G}_m \cdot \vec{R}_n} = 1$$

$$\Rightarrow \quad \vec{G}_m \cdot \vec{R}_n = 0, \pm 2\pi, 4\pi, \ldots$$

➢ $\vec{G}_m$ is called reciprocal vectors and defines the reciprocal lattice.

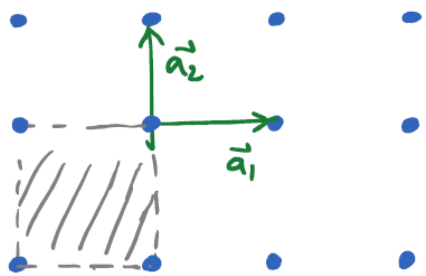
# § 1.3 Lattice structure

- The reciprocal lattice corresponds to the Fourier transform of the Bravais lattices.

Example: periodic potential $V(\vec{r}) = V(\vec{r} + \vec{R}_n)$

$$V(\vec{r}) = \sum_{\vec{G}} V(\vec{G}) e^{i\vec{G}\cdot\vec{r}}$$

$$V(\vec{r} + \vec{R}_n) = \sum_{\vec{G}} V(\vec{G}) e^{i\vec{G}\cdot(\vec{r}+\vec{R}_n)}$$




$\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2$

$$\Rightarrow \quad e^{i\vec{G}\cdot\vec{R}_n} = 1$$

Solutions of $\vec{G}$ are the discrete reciprocal vectors $\vec{G}_m$.

# § 1.3 Lattice structure

- Reciprocal lattice

Example : square lattice

$$\begin{cases} \vec{a}_1 = a\hat{x} \\ \vec{a}_2 = a\hat{y} \end{cases} \qquad \vec{G} = G_x\hat{x} + G_y\hat{y}$$

$$\Rightarrow \begin{cases} e^{i\vec{G}\cdot\vec{a}_1} = e^{iG_x a} = 1 \\ e^{i\vec{G}\cdot\vec{a}_2} = e^{iG_y a} = 1 \end{cases}$$

$$G_x = 0, \pm\frac{2\pi}{a}, \pm\frac{4\pi}{a}, \ldots$$ (same for $G_y$)

# § 1.3 Lattice structure

- Reciprocal lattice

Example : square lattice

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

$$\vec{G} = G_x \hat{x} + G_y \hat{y}$$

Solution for $\vec{G}_m$ :

$$\vec{G}_m = m_1 \frac{2\pi}{a} \hat{x} + m_2 \frac{2\pi}{a} \hat{y} , \qquad m_1 , m_2 \in \mathbb{Z}$$

# § 1.3 Lattice structure

- Reciprocal lattice

General solution in 3D :

$$\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

$$e^{i \vec{G}_m \cdot \vec{R}_n} = 1$$

$$\vec{G}_m = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3$$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij} \qquad i, j = 1, 2, 3$$

$$\Rightarrow \quad \boxed{\vec{b}_i = 2\pi \frac{\vec{a}_j \times \vec{a}_k}{\vec{a}_i \cdot (\vec{a}_j \times \vec{a}_k)}}$$

# § 1.3 Lattice structure

- Reciprocal lattice

2D: (x-y plane) $\vec{G}_m = m_1 \vec{b}_1 + m_2 \vec{b}_2$ and $\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2$

take $\vec{a}_3 = a\hat{z}$ and use the above formula

$\Rightarrow$ $\vec{b}_1, \vec{b}_2$ in x,y plane

$$\vec{b}_3 = \frac{2\pi}{a} \hat{z}$$

1D: $\vec{G}_m = m_1 \vec{b}_1 = m_1 b \hat{x}$ and $\vec{R}_n = n_1 \vec{a}_1 = n_1 a \hat{x}$

$$\Rightarrow \quad b = \frac{2\pi}{a}$$

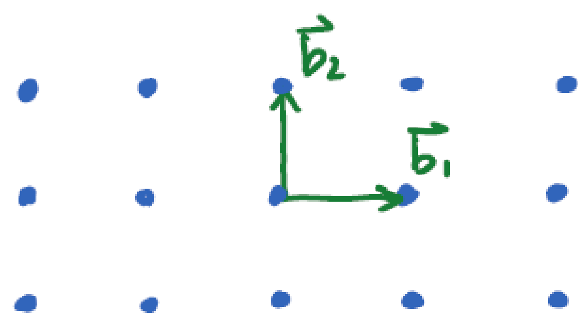
$$\vec{G}_m = m_1 \frac{2\pi}{a} \hat{x}, \quad m_1 \in \mathbb{Z}$$

# § 1.3 Lattice structure

Example : Reciprocal lattice of the square lattice

$$\vec{G}_m = m_1 \vec{b}_1 + m_2 \vec{b}_2 \qquad \vec{R}_n : \begin{cases} \vec{a}_1 = a\hat{x} \\ \vec{a}_2 = a\hat{y} \end{cases}$$

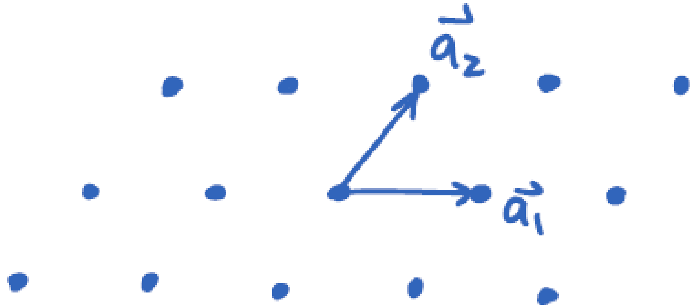
$$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij} \Rightarrow \begin{cases} \vec{b}_1 = \frac{2\pi}{a} \hat{x} \\ \vec{b}_2 = \frac{2\pi}{a} \hat{y} \end{cases}$$




reciprocal lattice : square

# § 1.3 Lattice structure

Example: Reciprocal lattice of the triangular lattice




$$\vec{R}_n : \begin{cases} \vec{a}_1 = a\hat{x} \\ \vec{a}_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y} \end{cases}$$

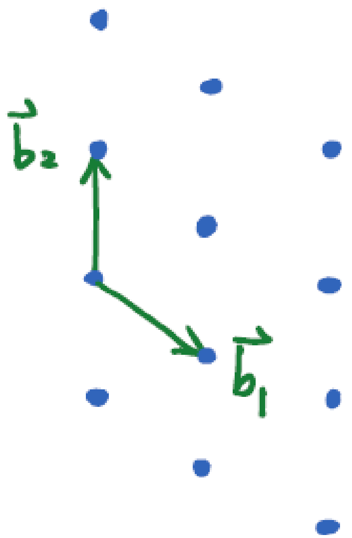
$$\vec{G}_m = m_1\vec{b}_1 + m_2\vec{b}_2$$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij} \implies \begin{cases} \vec{b}_1 = \frac{\pi}{a}\hat{x} - \frac{\pi}{\sqrt{3}a}\hat{y} \\ \vec{b}_2 = \frac{2\pi}{\sqrt{3}a}\hat{y} \end{cases}$$

# § 1.3 Lattice structure

Reciprocal vectors for the triangular lattice:

$$\begin{cases} \vec{b}_1 = \dfrac{\pi}{a}\hat{x} - \dfrac{\pi}{\sqrt{3}a}\hat{y} \\ \vec{b}_2 = \dfrac{2\pi}{\sqrt{3}a}\hat{y} \end{cases}$$




reciprocal lattice: triangular

# § 1.3 Lattice structure

- First Brillouin zone (FBZ):

The Wigner-Seitz primitive cell of the reciprocal lattice is called the FBZ.

# § 1.3 Lattice structure

- First Brillouin zone (FBZ):

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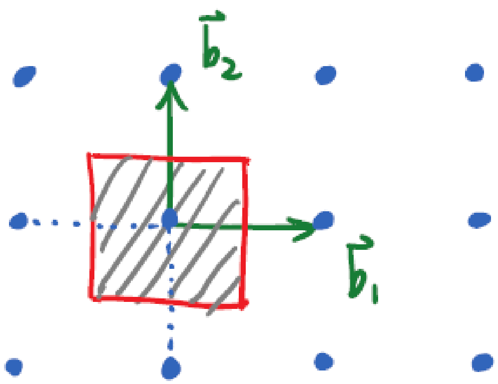
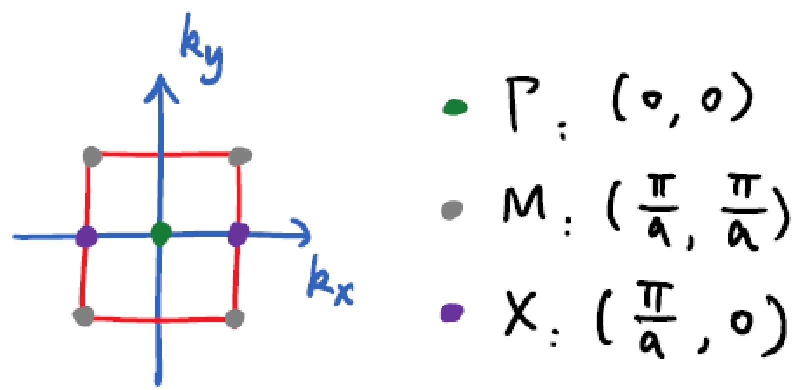
Square :



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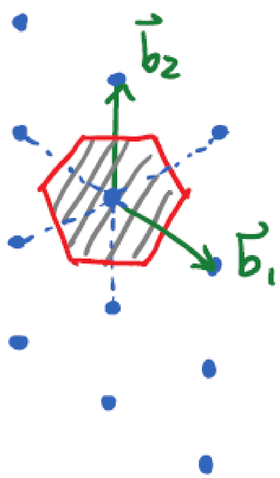
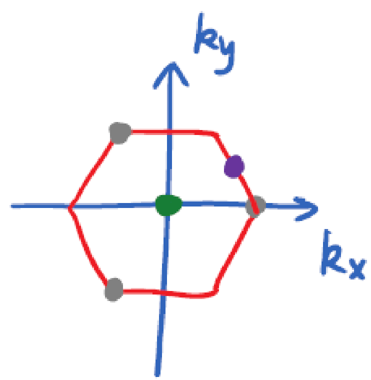
Triangular:




- $\Gamma$: $(0, 0)$
- $K$: $\left(\frac{2\pi}{3a}, 0\right)$
- $M$: $\left(\frac{\pi}{2a}, \frac{\pi}{2\sqrt{3}a}\right)$

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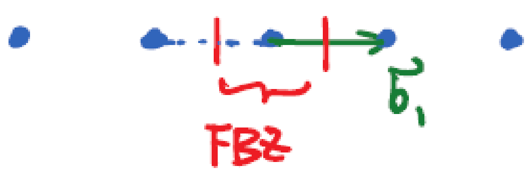
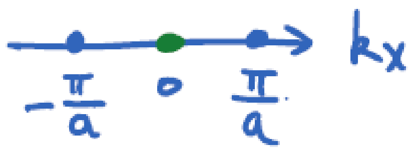
1D:




FBZ: $k_x \in [-\frac{\pi}{a}, \frac{\pi}{a}]$