Physics 410/510 - Solid State Physics
Spring 2015
Wednesday, Week 2:

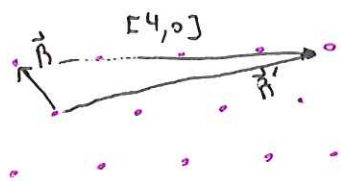
Review:

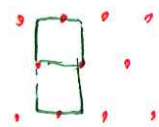
A lattice is a set of points where the environment looks the same at any point:

$$\vec{R}' = \vec{R} + [n_1, n_2, n_3]$$

$$\downarrow$$

$$n_1\vec{a}_1 + \cdots + n_3\vec{a}_3$$



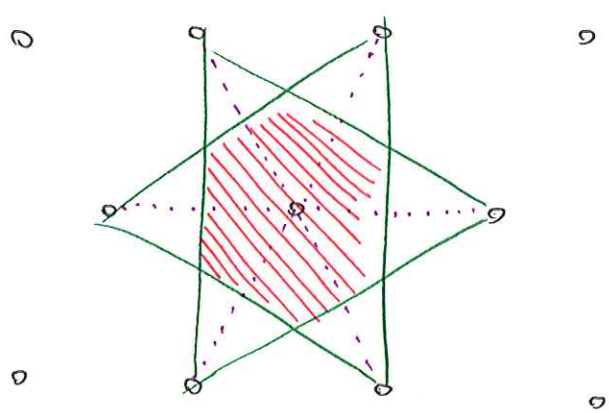


the conventional unit cell is rectangular.

For period structures (not necessarily lattices), the unit cell is the repeated motif & building block that can be tiled or stacked to fill all space.

The points of repeating motif are called the basis.

- Primitive unit cells contain only one lattice point
  - The Wigner-Seitz Cell:



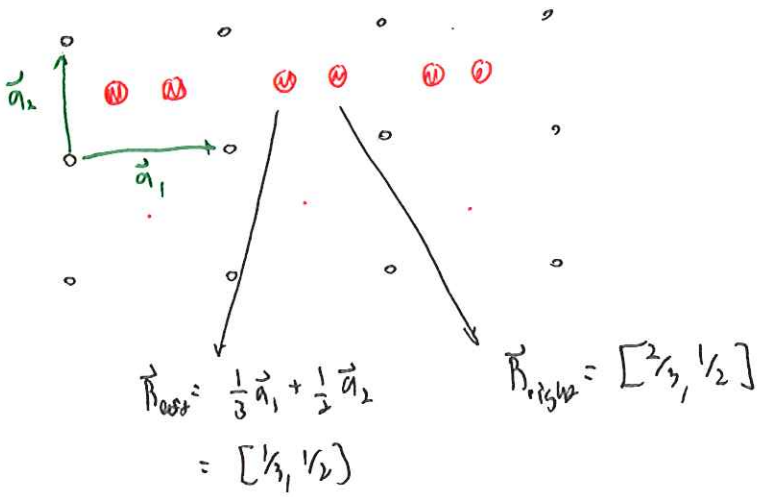
Thus, a periodic structure (such as a crystal) is:

$$\text{Crystal} = \text{Lattice} + \text{Basis}$$

A great example of this is the Honeycomb crystal.

Show PPT of Honeycomb structure

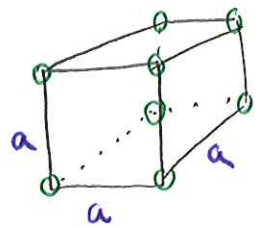
Ex. of Basis in terms of primitive lattice vectors:



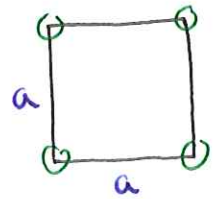
Later, we'll see that a wave gets diffracted by the lattice, but the intensity of the diffraction pattern is determined by the basis.

Lattices in 3D:

The simplest is the cubic: (Simple Cubic)

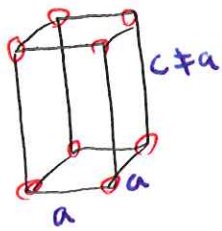


Plan View

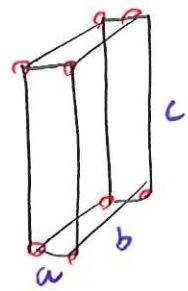


It has $8 \times 1/8 = 1$ atom (lattice point) per unit cell.

other simple lattices:

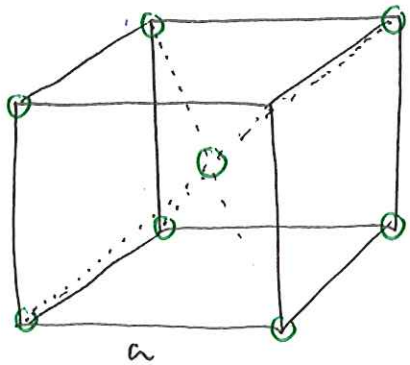


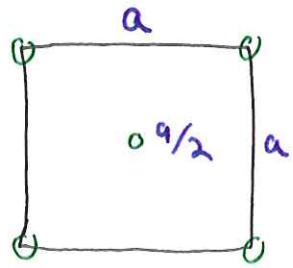
Tetragonal



Orthorhombic

The Body-Centered Cubic:





The conventional cubic cell for the bcc-lattice has $8 \times 1/8 + 1 = 2$ atoms.

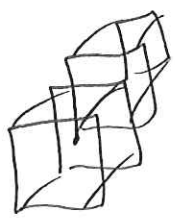
Thus viewing the bcc lattice a 2-atom basis simple cubic crystal, the basis atoms can be written as:

$$\vec{B}_{corner} = [n_1, n_2, n_3]$$

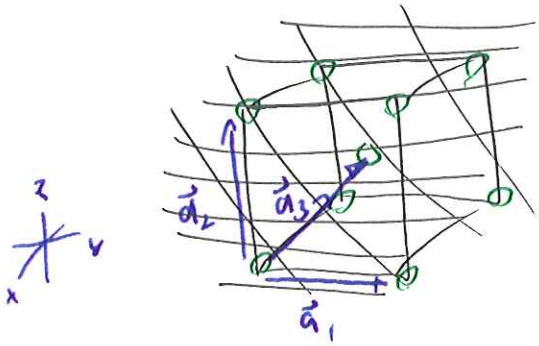
$$\vec{B}_{center} = [n_1, n_2, n_3] + [1/2, 1/2, 1/2]$$

However, the bcc is a lattice, so $\vec{B}_{corner}$ & $\vec{B}_{center}$ are related by a lattice vector of its true lattice vector representation. Here, they appear different because we chose a conventional cubic unit cell.

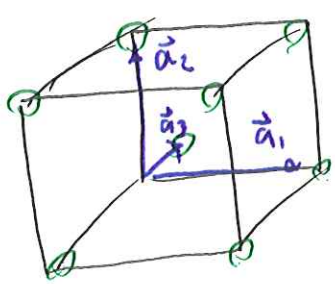
The bcc can be viewed as two interpenetrating sc:



The primitive lattice vectors of the bcc lattice are:



$$\boxed{\begin{aligned} \vec{a}_1 &= [1,0,0] = a\cdot\hat{x} \\ \vec{a}_2 &= [0,1,0] = a\cdot\hat{y} \\ \vec{a}_3 &= [1/2, 1/2, 1/2] = \tfrac{1}{2}a\hat{x} + \cdots + \tfrac{1}{2}a\hat{z} \end{aligned}}$$



- One can check that any point can be written as a integer sum of $\vec{a}_i$'s!!
- Every point has the same environment... bcc is a lattice. Every point has 8 nearest neighbors.

The coordination number or the number of nearest neighbors (Z) for the bcc lattice is :

$$Z = 8$$

Another set of primitive translation vectors is:

$$\vec{a}_1 = \left[\tfrac{1}{2}, \tfrac{1}{2}, -\tfrac{1}{2}\right]$$
$$\vec{a}_2 = \left[\tfrac{1}{2}, -\tfrac{1}{2}, \tfrac{1}{2}\right]$$
$$\vec{a}_3 = \left[-\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\right]$$

Note $\vec{a}_1 + \vec{a}_2 = [1, 0, 0] = \vec{a}_1$ from page 4.

Is the volume the same in each case:

$$|\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$$

I.

$$\vec{a}_2 \times \vec{a}_3 = a^2 \begin{vmatrix} i & j & k \\ 0 & 1 & 0 \\ \tfrac{1}{2} & \tfrac{1}{2} & \tfrac{1}{2} \end{vmatrix} = \begin{pmatrix} \tfrac{1}{2} \\ 0 \\ -\tfrac{1}{2} \end{pmatrix} a^2$$

$$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = a \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} \tfrac{1}{2} \\ 0 \\ -\tfrac{1}{2} \end{pmatrix} a^3 = \tfrac{1}{2} a^3$$

II.

$$\vec{a}_2 \times \vec{a}_3 = \begin{vmatrix} i & j & k \\ \tfrac{1}{2} & -\tfrac{1}{2} & \tfrac{1}{2} \\ -\tfrac{1}{2} & \tfrac{1}{2} & \tfrac{1}{2} \end{vmatrix} a^2 = \begin{pmatrix} -\tfrac{1}{2} \\ -\tfrac{1}{2} \\ 0 \end{pmatrix} a^2$$

$$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \begin{pmatrix} \tfrac{1}{2} \\ \tfrac{1}{2} \\ -\tfrac{1}{2} \end{pmatrix} a \cdot \begin{pmatrix} -\tfrac{1}{2} \\ -\tfrac{1}{2} \\ 0 \end{pmatrix} a^3 = -\tfrac{1}{2} a^3$$

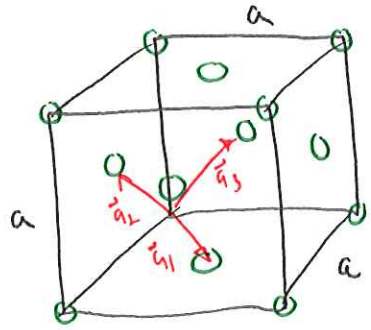
✓

The Wigner-Seitz cell of the bcc lattice is a truncated octahedron.

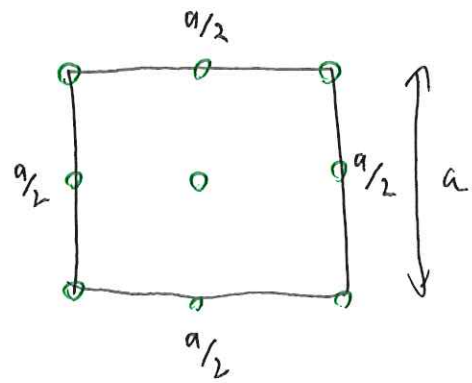
Show PPT of truncated octahedron

N.B. 2 atoms (lattice points) in the conventional unit cell which have volume a^3. So volume per lattice point must be: $\frac{1}{2} a^3$

The face-centered Cubic (fcc) Lattice:



Traditional unit cell



Lattice points per cell?

$$8 \times 1/8 + 6 \times \frac{1}{2} = 4$$

Viewed in the traditional cubic unit cell, the 4-point basis have positions:

$$\vec{R}_{corner} = [n_1, n_2, n_3]$$

$$\vec{R}_{xy\,face} = \quad " \quad + [1/2, 1/2, 0]$$

$$\vec{R}_{xz\,face} = \quad " \quad + [1/2, 0, 1/2]$$

$$\vec{R}_{yz\,face} = \quad " \quad + [0, 1/2, 1/2]$$

The fcc is a lattice, so the primitive lattice vectors are:

$$\boxed{\begin{aligned} \vec{a}_1 &= [1/2, 1/2, 0] = \tfrac{1}{2}a\hat{x} + \tfrac{1}{2}a\hat{y} \\ \vec{a}_2 &= [1/2, 0, 1/2] = \tfrac{1}{2}a\hat{x} + \tfrac{1}{2}a\hat{z} \\ \vec{a}_3 &= [0, 1/2, 1/2] = \tfrac{1}{2}a\hat{y} + \tfrac{1}{2}a\hat{z} \end{aligned}}$$

What is the coordination number for an fcc lattice?

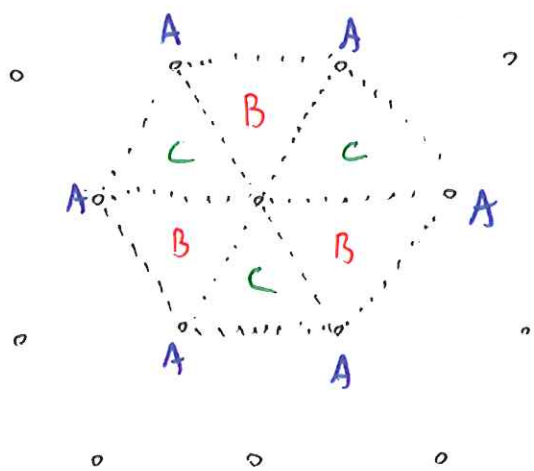
$$z = 12$$

Volume of primitive cell? $\frac{1}{4}a^3$ → # lattice points in conventional cell

The Wigner-Seitz Cell for the fcc lattice is the "rhombic dodecahedron."

☆ PPT of rhombic dodecahedron

The fcc lattice can also be constructed from a certain stacking of the hexagonally close-packed (hcp) structure:



No, but it has two atom basis w/ hexagonal lattice

Is the HCP structure a lattice?

☆ Show PPT of hexagonally close-packed structure.

There are many different polytypes of stacked close-packed layers.

- <u>Sphere Packing:</u>
  - Crystals are rarely found in the SC lattice structure. Why?
    - Atoms will push together by interaction forces to get as close as possible.
    - The most efficient way to push spheres is <u>any</u> hexagonally close packed stacking such as FCC or HCP

☆ Show PPT

      - Proved in 1998! Conjectured in 1601 by Kepler!

- A few real crystals:

* Show PDT

  - Cesium chloride → Two atom basis SC
  - Copper → FCC
  - NaCl → Two-atom basis FCC
  - Diamond → Two-atom basis FCC

    basis [0 0 0] & [1/4, 1/4, 1/4]

* Show PDT

- There are only 14 space lattices → the Bravais lattices.
  - Proof requires group theory.

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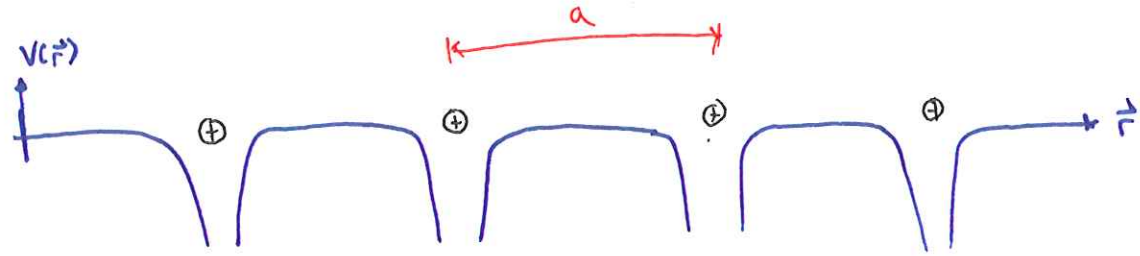
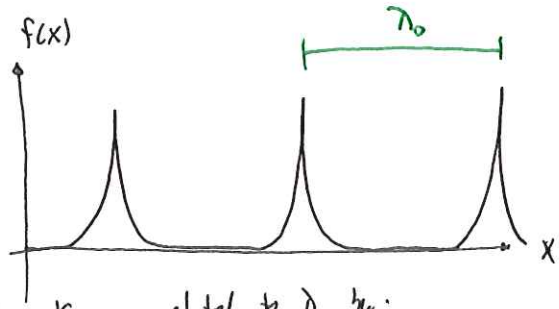
Friday, week 2:

Last time we looked at some crystals (periodic structures) in 3D. The periodicity of the crystal will lead to a periodic electrical potential, electron density, scattering landscape, etc.:



It is useful to rewrite the periodic function in terms of periodic trigonometric functions, in the same way it is useful to write $f(x) = a_0 + a_1 x + a_2 x + \dots$

Assume that a function $f(x)$ is periodic in space w/ "wavelength" λ_0



$$f(x+\lambda_0) = f(x)$$

for a crystal, $\lambda_0 = a$

Then the wavevector K_0 is related to λ_0 by:

$$\boxed{K_0 \cdot \lambda_0 = 2\pi}$$

Now we wish to expand $f(x)$ in terms of functions periodic in λ_0. Some fundamental functions are:

$$\sin(K_0 \cdot n x)$$
$$\cos(K_0 \cdot n x) \qquad \text{where } n \in \mathbb{Z}$$
$$e^{i K_0 n x}$$

since

$$\begin{aligned}
\sin(K_0 \cdot n(x+\lambda_0)) &= \sin(K_0 \lambda_0 n + K_0 n x) \\
&= \sin(2\pi \cdot n + K_0 n x) \\
&= \cos(2\pi \cdot n)\sin(K_0 \cdot n x) + \cos(K_0 \cdot n x)\underbrace{\sin(2\pi \cdot n)}_{0} \\
&= \sin(K_0 \cdot n x)
\end{aligned}$$

So $\sin(k_0 \cdot n(x+\lambda_0)) = \sin(k_0 \cdot n x)$

For $e^{i k_0 \cdot n x}$ it is easier,

$$e^{i k_0 \cdot n (x+\lambda_0)} = e^{i k_0 \cdot \lambda_0 \cdot n} e^{i k_0 \cdot n x}$$
$$= e^{i 2\pi \cdot n} e^{i k_0 n x}$$
$$= e^{i k_0 \cdot n x} \quad \blacksquare$$

So we write,

$$\boxed{f(x) = \sum a_n \cos(k_0 \cdot n x) + \sum b_n \sin(k_0 \cdot n x)}$$

Discrete Fourier series

To obtain a_n's & b_n's :

$$\int_0^{\lambda_0} f(x) \cos(k_0 \cdot m x)\, dx$$

$$= \sum_n \left(\int_0^{\lambda_0} a_n \underbrace{\cos(k_0 \cdot n x) \cos(k_0 \cdot m x)}_{0 \text{ if } m \neq n}\, dx + \int_0^{\lambda_0} b_n \underbrace{\sin(k_0 \cdot n x) \cos(k_0 \cdot m x)}_{0}\, dx \right)$$

$$= a_n \int_0^{\lambda_0} \cos^2(k_0 \cdot n x)\, dx$$

$$= a_n \int_0^{\lambda_0} \frac{1}{2}\left(1 + \underbrace{\cos(2 k_0 \cdot n x)}_{0}\right) dx$$

$$= \frac{a_n \lambda_0}{2}$$

$$\boxed{a_n = \frac{2}{\lambda_0} \int_0^{\lambda_0} f(x) \cos(k_0 \cdot n x)\, dx \qquad b_n = \frac{2}{\lambda_0} \int_0^{\lambda_0} f(x) \sin(k_0 \cdot n x)\, dx}$$

$$\boxed{a_0 = \frac{1}{\lambda_0} \int_0^{\lambda_0} f(x)\, dx} \quad \boxed{b_0 = 0}$$

Complex Exponentials are more convenient...

$$\boxed{f(x) = \sum_{n=-\infty}^{\infty} A_n e^{i k_0 n x}}$$

where $A_{-n} = A_n^*$ (Required to get both sin, cos expansion)

&

$$\int_0^{\lambda_0} f(x) e^{-i k_0 m x} dx = \sum \int A_n e^{i k_0 (n-m) x} dx$$

$$= \sum A_n \frac{1}{i k_0 (n-m)} e^{i k_0 (n-m) x} \Big|_0^{\lambda_0} + A_n \cdot \lambda_0$$

$n \neq m$

$n = m$

$$e^{i k_0 \lambda_0 (n-m)} - 1$$

$$= e^{i 2\pi \cdot (n-m)} - 1$$

$$= 0$$

$$\Rightarrow \boxed{A_n = \frac{1}{\lambda_0} \int_0^{\lambda_0} f(x) e^{-i k_0 n x} dx}$$

Thus, any periodic function $f(x)$ will have a representation in terms of sinusoidal functions with wave vectors given by

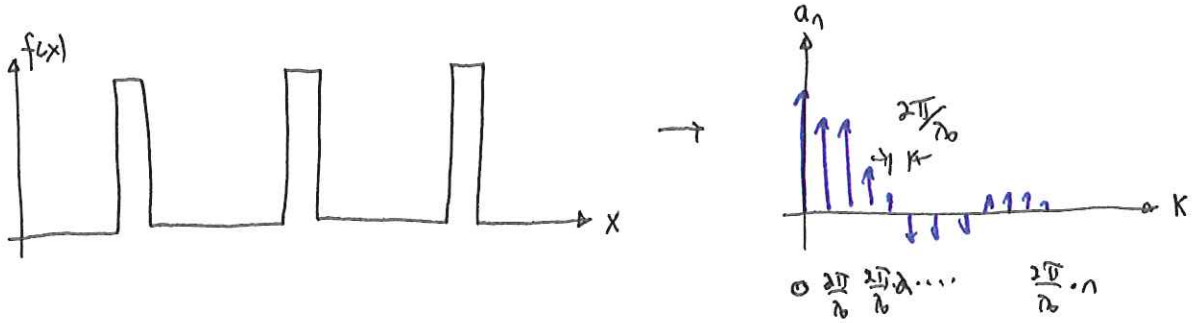
$$K_n = K_0 \cdot n$$

$$= \frac{2\pi}{\lambda_0} \cdot n$$

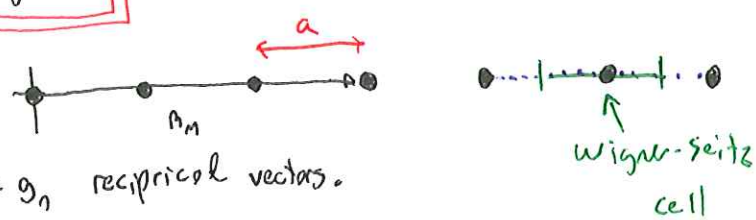
Much like the Taylor Series, the Fourier series lets you focus on just the few important leading terms of $f(x)$. Typically, $|A_n| \propto 1/n^\alpha$ $\alpha \geq 1$. We also say,

$f(x)$ lives in real space A_n live in K-space or reciprocal space.

Ex



For a crystal $\boxed{\lambda_0 = a}$



& we call $K_n = g_n$ reciprocal vectors.

$$\boxed{g_n = \frac{2\pi}{a}\cdot n}$$

[Reciprocal Lattice Vectors in 1D]

For our 1D lattice, primitive lattice vectors are:

$$R_m = a\cdot m$$

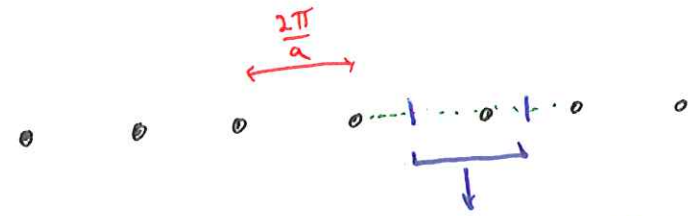
Notice that,

$$e^{g_n R_m} = e^{\frac{2\pi}{a}\cdot n\cdot a\cdot m}$$
$$= e^{2\pi\cdot n\cdot m}$$
$$= 1$$

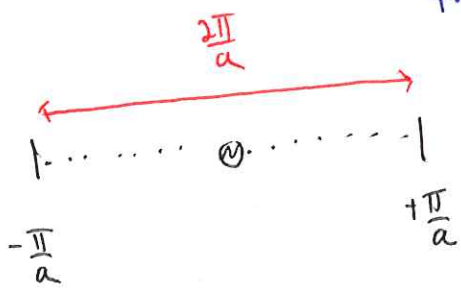
So the periodicity condition of $f(x)$ applies to any g_n & R_n:

$$f(x+R_m) = \sum_{n=-\infty}^{\infty} A_n e^{i g_n (x+R_m)}$$
$$= \sum A_n e^{i g_n x}$$
$$= f(x)$$

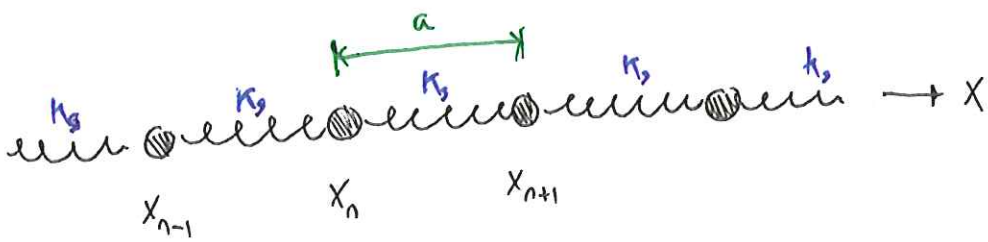
Again, the g_n in reciprocal space for a lattice:



Wigner-Seitz Cell in Reciprocal space is the 1st Brillouin (Bri-yaw(n)) Zone



The significance of the Brillouin Zone is illustrated in the following example:



X_n = motion of nth mass

Look at motion about equilibrium,

$$\delta X_n = X_n - X_n^{eq}$$
$$= X_n - n \cdot a$$

By N.2 (Newton's 2nd Law):

$$m\,\delta\ddot{X}_n = -2k_s\,\delta X_n + k_s(\delta X_{n+1} + \delta X_{n-1}) \qquad (1)$$

which has normal mode solutions:

$$\boxed{\begin{aligned}\delta X_n &= A e^{i(k x_n^{eq} - \omega t)} \\ &= A e^{i(k \cdot n a - \omega t)}\end{aligned}}$$

These solutions are "waves" except we limit the x-values to $x_n^{eq} = a \cdot n$,

since the masses will oscillate about x_n^{eq}'s.

The dispersion relation $\omega(K)$ will be determined by (1); we'll get back to that topic later!!

For now, notice that:

1. pick any K satisfying $\omega(K)$
2. Consider $K + g_m$ where $g_m = \frac{2\pi}{a} \cdot m$ is a reciprocal lattice vector.
3. then,

$$\xi x_n = A e^{i((K+g_m)\cdot na - \omega t)}$$

$$= \underbrace{A e^{i g_m \cdot na}}_{e^{i g_m \cdot R_n} = 1} e^{i(K \cdot na - \omega t)}$$

$$= A e^{i(K \cdot na - \omega t)}$$

Thus, even though K can be anything $K \in [-\infty, \infty]$, we only need to look at K inside the 1st Brillouin Zone since K outside is obtained by adding g_m & this doesn't affect, in this case, ξx_n.

$$\boxed{\therefore \text{ Only look at } K \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]}$$

In order to understand the Brillouin Zone, we need to understand the reciprocal lattice & reciprocal lattice vectors $\vec{G}_n$. In 3D:

$$\boxed{f(\vec{r}) = \sum_{\vec{G}} A_{\vec{G}} \exp(i \vec{G} \cdot \vec{r})}$$

Reciprocal Lattice vector

Lattice vector

where $e^{i \vec{G} \cdot \vec{R}(n_1, n_2, n_3)} = 1$

Given a real-space lattice w/ $\vec{R}(n_1, n_2, n_3)$ lattice points, how do we find $\vec{G}$ such that

$$e^{i\vec{G}\cdot\vec{R}(n_1,n_2,n_3)} = 1 \quad ?$$

<u>Claim</u>:

$$\boxed{\vec{G} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3 \qquad m_i \in \mathbb{Z}}$$

where

$$\boxed{\begin{aligned} \vec{b}_1 &= \frac{2\pi\, \vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \\ \vec{b}_2 &= \frac{2\pi\, \vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \\ \vec{b}_3 &= \frac{2\pi\, \vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \end{aligned}}$$

Notice that

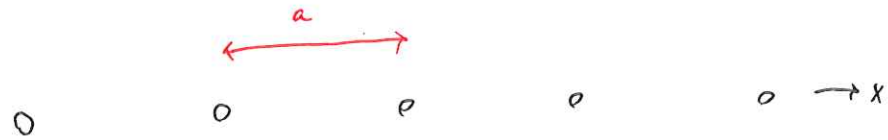
$$\boxed{\vec{a}_i \cdot \vec{b}_j = 2\pi\,\delta_{ij}}$$

Then

$$\begin{aligned} \vec{G}\cdot\vec{R}(n_1,n_2,n_3) &= m_1 n_1\, 2\pi + \cdots + m_3 n_3\, 2\pi \\ &= \underbrace{\left(\sum m_i n_i\right)}_{\in \mathbb{Z}} 2\pi \end{aligned}$$

$$\Rightarrow \quad e^{i\vec{G}\cdot\vec{R}(n_1,n_2,n_3)} = 1 \qquad \blacksquare$$

The reciprocal lattice has further significance. It is the Fourier transform of the real space lattice.



The density of lattice points is:

$$\rho(x) = \sum_n \delta(x - a\cdot n) = \begin{cases} 0 & x \neq a\cdot n \\ \infty & x = a\cdot n \end{cases}$$

Density of points in real space

Then $\rho(x) = \sum A_n e^{i k_n \cdot n x}$

where
$$A_m = \frac{1}{a}\int \rho(x) e^{-i k_m \cdot m x}\, dx$$
$$= \frac{1}{a}\sum_n \int \delta(x - a\cdot n)\, e^{-i k_m \cdot m x}\, dx$$
$$= \frac{1}{a}\sum_n e^{-i k_m \cdot m \cdot a\cdot n}$$
$$= \frac{1}{a}\sum_n e^{-i\left(\frac{2\pi}{a}\cdot m\right)\cdot a\cdot n}$$
$$= \frac{1}{a}\sum_n e^{-i g_m \cdot a\cdot n}$$
$$= \frac{1}{a}\sum_m \delta(k - \underbrace{g_m}_{\frac{2\pi}{a}\cdot m}) = \begin{cases} 0 & k \neq g_m \\ \infty & k = g_m = \frac{2\pi}{a}\cdot m \end{cases}$$

So the reciprocal lattice is the Fourier transform of the real space lattice.