6.730 Physics for Solid State Applications

Lecture 6: Periodic Structures

Tuesday February 17, 2004

<u>Outline</u>

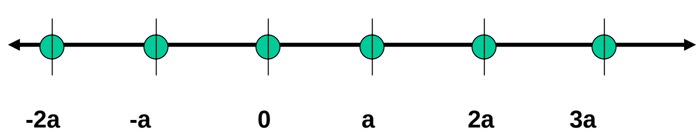
- Point Lattices
- Crystal Structure= Lattice + Basis
- Fourier Transform Review
- 1D Periodic Crystal Structures: Mathematics

Point Lattices: Bravais Lattices

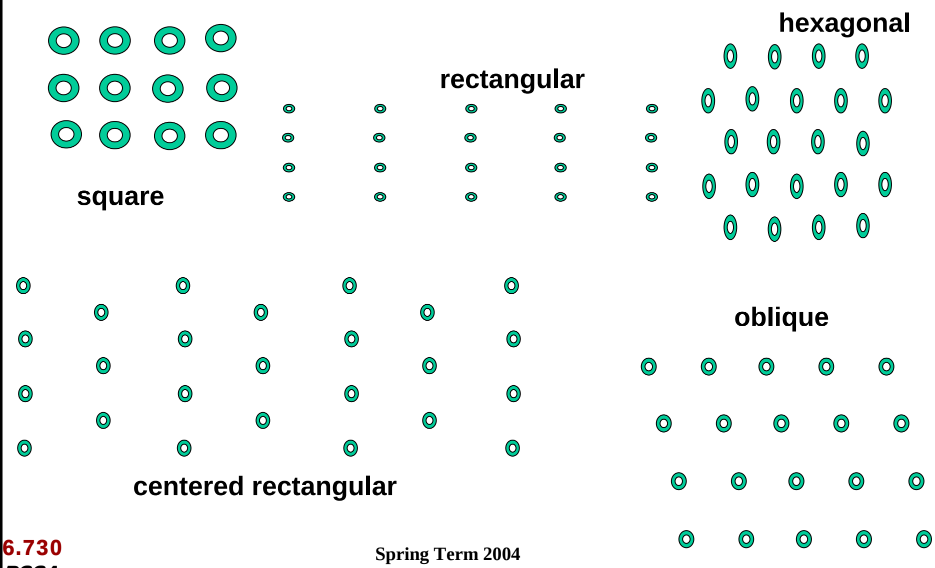
Bravais lattices are point lattices that are classified topologically according to the symmetry properties under rotation and reflection, without regard to the absolute length of the unit vectors.

A more intuitive definition:
At every point in a Bravais lattice the "world" looks the same.

1D: Only one Bravais Lattice



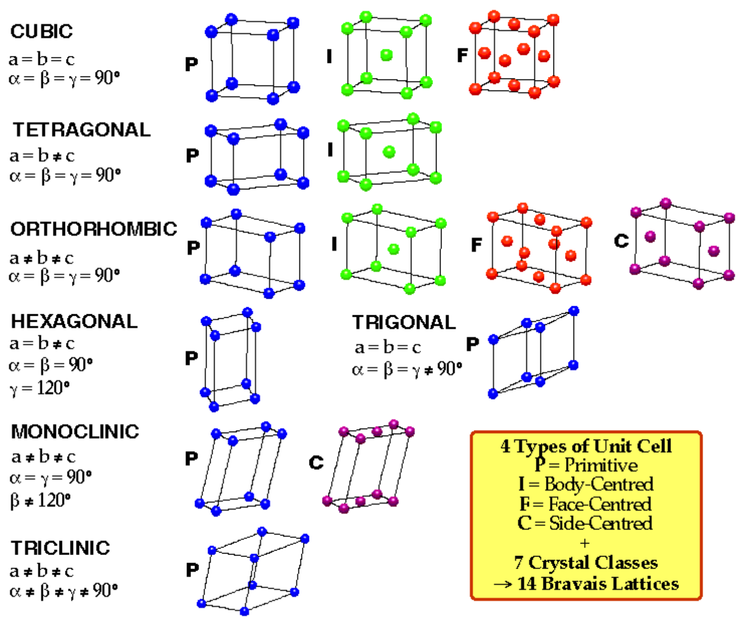
2D Bravais Lattices



6.730
PSSA

Spring Term 2004

3D: 14 Bravais Lattices



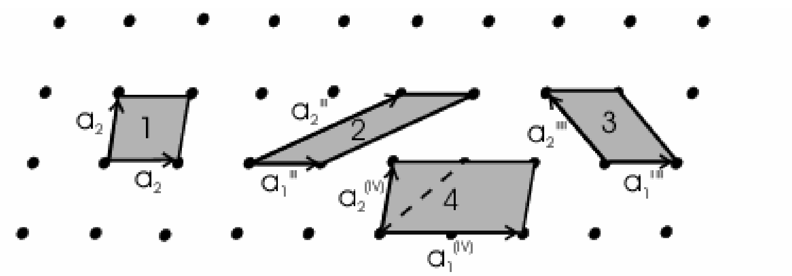
6.730
PSSA

Lattice and Primitive Lattice Vectors

A **Lattice** is a regular array of points {$\mathbf{R}_l$ } in space which must satisfy (in three dimensions)

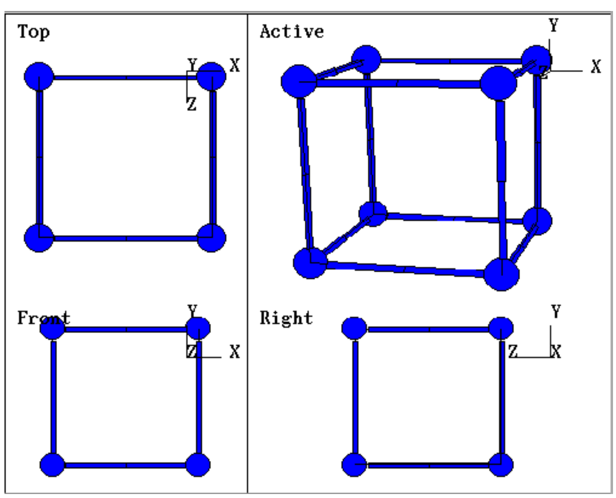
$$\mathbf{R}_\ell = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \qquad \text{for all} \qquad n_i = 0, \pm1, \pm2, \ldots$$

The vectors $\mathbf{a}_i$ are know as the **primitive lattice vectors**.



A two dimensional lattice with different possible choices of primitive lattice vectors.

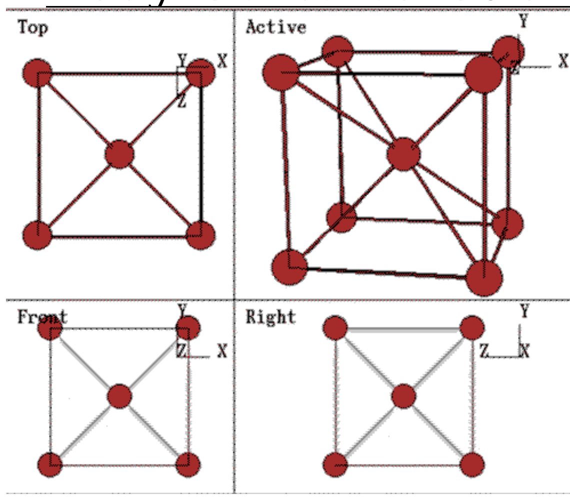
Cubic



$$\mathbf{a}_1 = a\mathbf{i}_x \qquad \mathbf{a}_2 = a\mathbf{i}_y \qquad \mathbf{a}_3 = a\mathbf{i}_z$$

http://cst-www.nrl.navy.mil/lattice/struk.picts/a_h.s.png

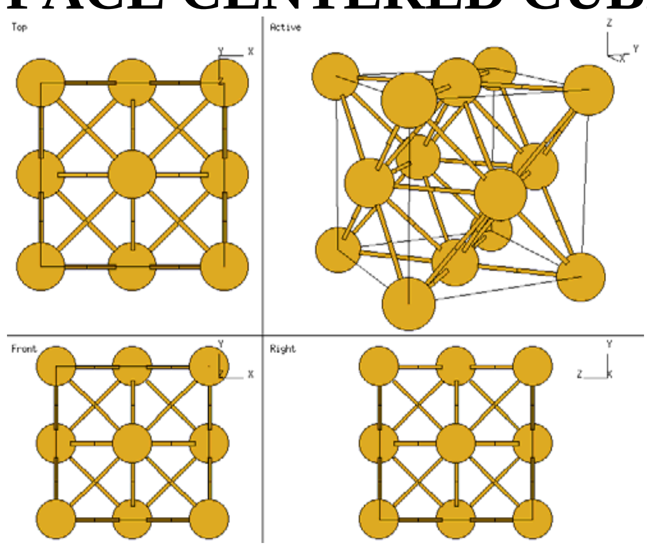
Body Centered Cubic



$$\mathrm{a}_1 = \frac{a}{2}(\mathrm{i}_y + \mathrm{i}_z - \mathrm{i}_x) \qquad \mathrm{a}_2 = \frac{a}{2}(\mathrm{i}_z + \mathrm{i}_x - \mathrm{i}_y) \qquad \mathrm{a}_3 = \frac{a}{2}(\mathrm{i}_x + \mathrm{i}_y - \mathrm{i}_z)$$

http://cst-www.nrl.navy.mil/lattice/struk.picts/a2.s.png

FACE CENTERED CUBIC

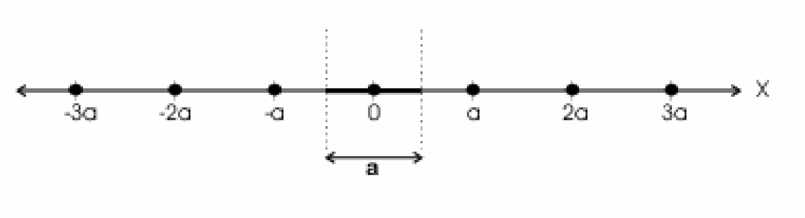


$$\mathrm{a}_1 = \frac{a}{2}(\mathrm{i}_y + \mathrm{i}_z) \qquad \mathrm{a}_2 = \frac{a}{2}(\mathrm{i}_z + \mathrm{i}_x) \qquad \mathrm{a}_3 = \frac{a}{2}(\mathrm{i}_x + \mathrm{i}_y)\ .$$

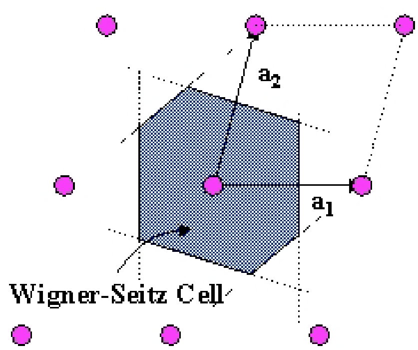
http://cst-www.nrl.navy.mil/lattice/struk.picts/a1.s.png

Wigner-Sietz Cell

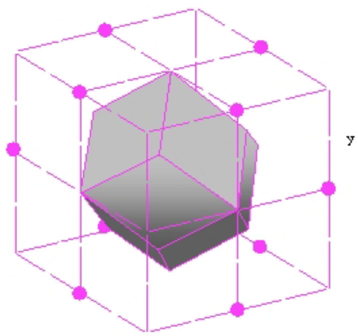
1. Choose one point as the origin and draw lines from the origin to each of the other lattice points.
2. Bisect each of the drawn lines with planes normal to the line.
3. Mark the space about the origin bounded by the first set of planes that are encountered. The bounded space is the Wigner-Sietz unit cell.



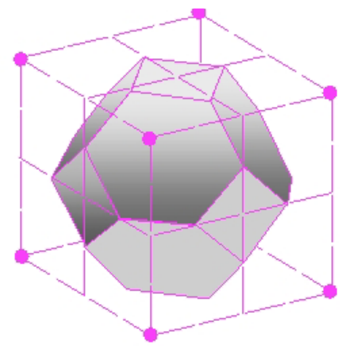
Wigner-Sietz Cell



Wigner-Sietz Cell

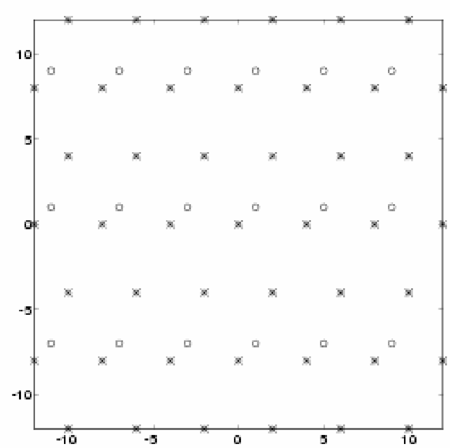


FCC



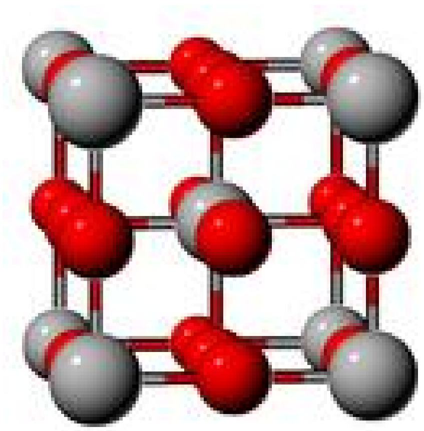
BCC

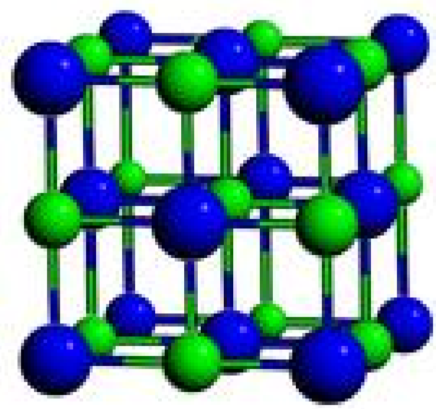
Crystal Structure = Lattice + Basis



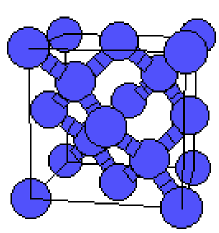
A two dimensional lattice with a basis of three atoms

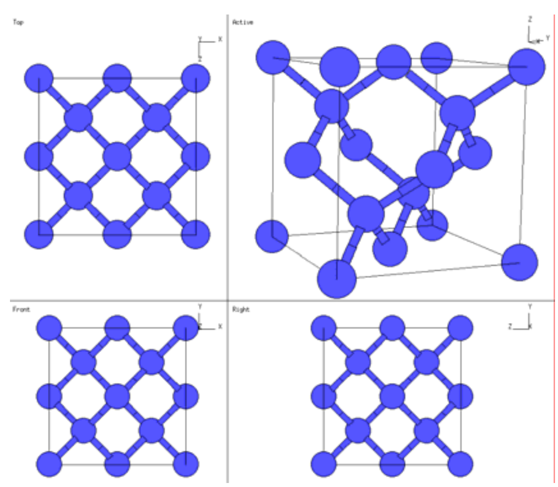
Cubic Structure with atomic basis





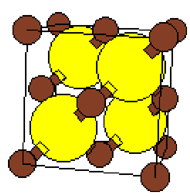
Diamond Crystal Structure

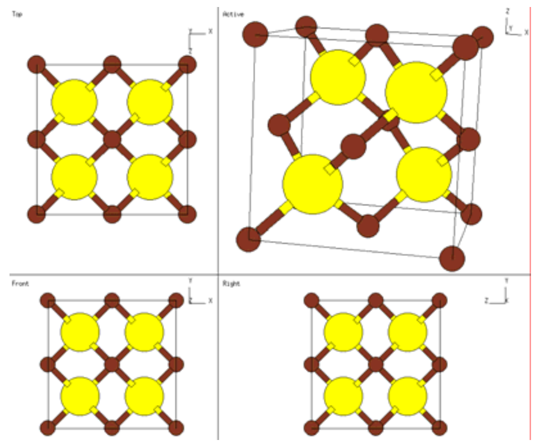




http://cst-www.nrl.navy.mil/lattice

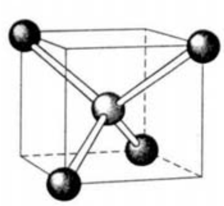
Zincblende Crystal Structure



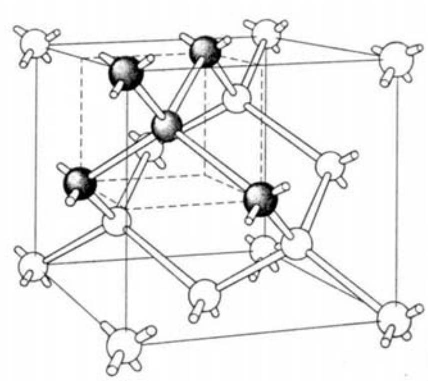


http://cst-www.nrl.navy.mil/lattice

Diamond Crystal Structure: Silicon

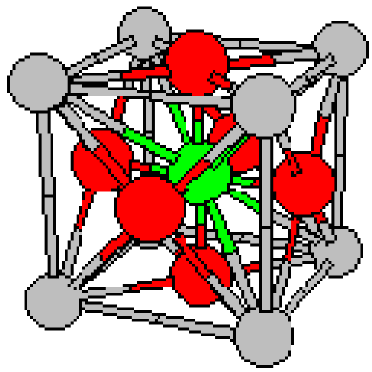


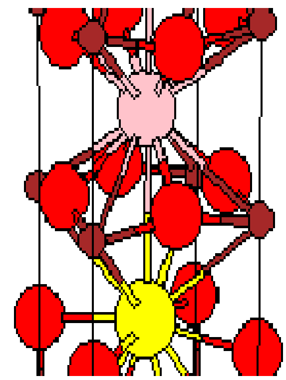
Bond angle = 109.5º



- 2 atom basis to a FCC Lattice
- Tetrahedral bond arrangement
- Each atom has 4 nearest neighbors and
  12 next nearest neighbors

Perovskite and Related Structures





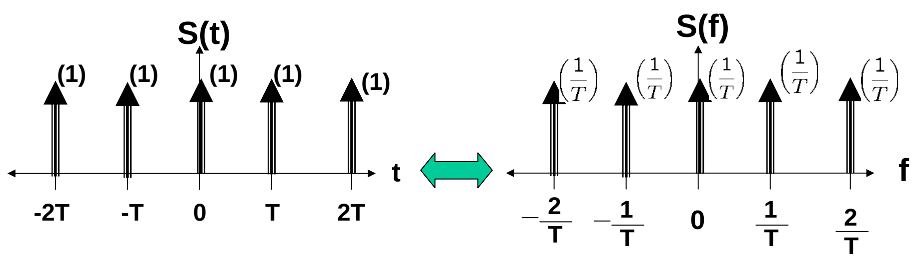
$YBa_2Cu_3O_{7-x}$
High-T_c Structure

Fourier Transform Review

EE-convention for Fourier Transforms

$$A(t) = \int_{-\infty}^{\infty} A(f) e^{j2\pi ft} df \Longleftrightarrow A(f) = \int_{-\infty}^{\infty} A(t) e^{-j2\pi ft} dt$$

$$S(t) = \sum_{n=-\infty}^{+\infty} \delta(t - nT) \Longleftrightarrow S(f) = \frac{1}{T} \sum_{m=-\infty}^{+\infty} \delta(f - \frac{m}{T})$$



Physics Convention for Fourier Transforms

$$A(t) = \int_{-\infty}^{\infty} A(\omega) e^{-i\omega t} \frac{d\omega}{2\pi} \iff A \quad (\omega) = \int_{-\infty}^{\infty} A(t) e^{i\omega t} dt$$

$$A(x) = \int_{-\infty}^{\infty} A(q) e^{iqx} \frac{dq}{2\pi} \quad \iff \quad A(q) = \int_{-\infty}^{\infty} A(x) e^{-iqx} dx$$

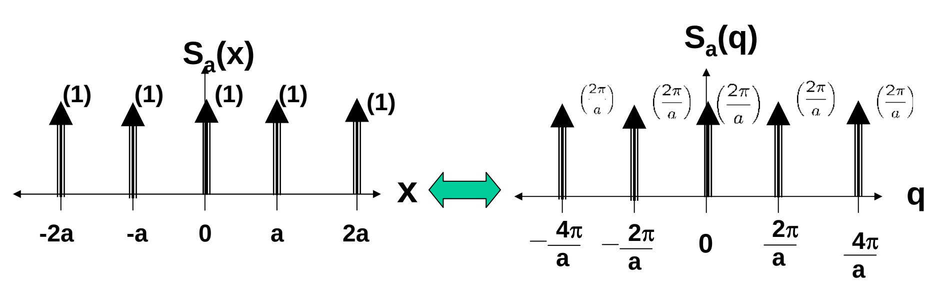
In general,

$$A(x,t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dq}{2\pi} \frac{d\omega}{2\pi} e^{i(qx-\omega t)} A(q,\omega)$$

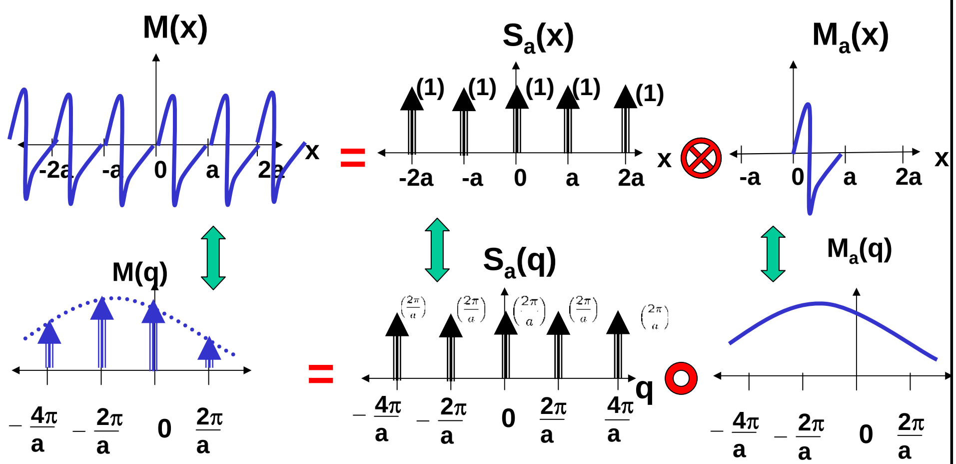
$$A(q,\omega) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx\, dt\, A(x,t) e^{-i(qx-\omega t)} dx$$

1D Periodic Crystal Structures

$$S_a(x) = \sum_{n=-\infty}^{+\infty} \delta(x-na) \iff S_a(q) = \frac{2\pi}{a} \sum_{m=-\infty}^{+\infty} \delta(q-\frac{2\pi}{a}m)$$



1D Periodic Crystal Structures



$$M(q) = M_a(q) \sum_{m=-\infty}^{\infty} \frac{2\pi}{a}\delta(q-\frac{2\pi}{a}m) = \sum_{m=-\infty}^{\infty} \frac{2\pi}{a} M_a(\frac{2\pi}{a}m)\delta(q-\frac{2\pi}{a}m)$$

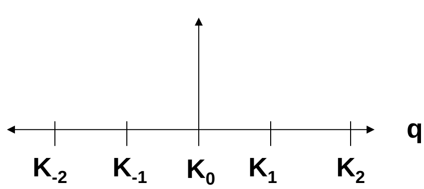
$$M(x) = \int_{-\infty}^{\infty} M(q)e^{iqx}\frac{dq}{2\pi} = \sum_{m=-\infty}^{\infty} \frac{1}{a} M_a(\frac{2\pi}{a}m)e^{i\frac{2\pi}{a}mx}$$

6.730
PSSA

Reciprocal Lattice Vectors

1. The Fourier transform in q-space is also a lattice
2. This lattice is called the **reciprocal lattice**
3. The lattice constant is 2 π / a
4. The **Reciprocal Lattice Vectors** are

$$K_m = m\frac{2\pi}{a} \qquad \text{where} \qquad m = 0, \pm 1, \pm 2$$



6.730
PSSA

Periodic Function as a Fourier Series

Recall that a periodic function and its transform are

$$M(q) = M_a(q)\sum_{m=-\infty}^{\infty}\frac{2\pi}{a}\delta(q-K_m) = \sum_{m=-\infty}^{\infty}\frac{2\pi}{a}M_a(K_m)\delta(q-K_m)$$

$$M(x) = \int_{-\infty}^{\infty} M(q)e^{iqx}\frac{dq}{2\pi} = \sum_{m=-\infty}^{\infty}\frac{1}{a}M_a(K_m)e^{iK_m x}$$

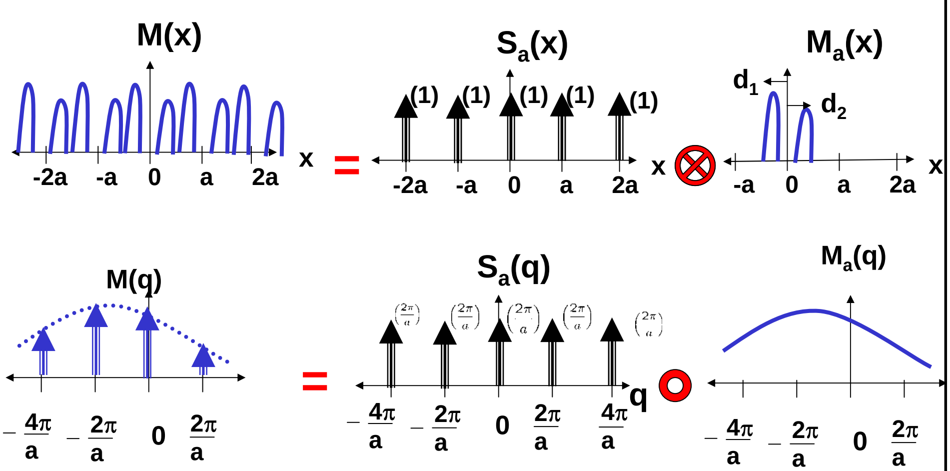
Define $M[K_m] = \frac{1}{a}M_a(K_m)$ **then the above is a Fourier Series:**

$$\boxed{M(x) = \sum_{m=-\infty}^{\infty} M[K_m]e^{iK_m x}} \qquad M[K_m] = \frac{1}{a}\int_0^a M(x)e^{-iK_m x}dx$$

and the equivalent Fourier transform is

$$M(q) = 2\pi\sum_{m=-\infty}^{\infty} M[K_m]\delta(q-K_m)$$

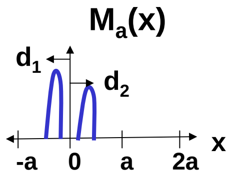
1D Periodic Crystal Structures with a basis



$$M(q) = \sum_{m=-\infty}^{\infty}\frac{2\pi}{a}M_a\left(\frac{2\pi}{a}m\right)\delta\left(q-\frac{2\pi}{a}m\right)$$

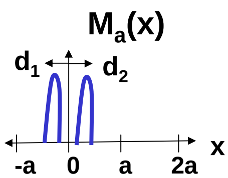
Delta functions still only occur where the reciprocal lattice is, independent of the basis. But the basis determines the weights.

Atomic Form Factors & Geometrical Structure Factors



Different Atoms (1) and (2)

$$\underbrace{M_a(K_m)}_{\text{Structure Factor}} = \underbrace{f_a^{(1)}(K_m)}_{\text{Atomic Form Factor}} e^{-iK_m d_1} + f_a^{(2)}(K_m) e^{-iK_m d_2}$$



Same atoms at d_1 and d_2

$$M_a(K_m) = \underbrace{f_a(K_m)}_{\text{Atomic Form Factor}} \cdot \underbrace{\left[e^{iK_m d_1} + e^{iK_m d_2}\right]}_{\text{Geometrical Structure Factor } \mathcal{S}(K_m)}$$