

$$\Rightarrow \frac{\hbar^2 k^2}{m} g_k + \frac{1}{V} \sum_{k'} U_{k-k'} g_{k'} = E g_k \quad \left. \begin{array}{l} \text{Bethe} \\ \text{- Goldstone} \\ \text{equation} \end{array} \right\}$$

$$g_k = 0 \quad \text{for } |\vec{k}| < k_F$$

using $\epsilon_k = \frac{\hbar^2 k^2}{2m}$ we have

$$(E - 2\epsilon_k) g_k = \frac{1}{V} \sum_{k'} U_{k-k'} g_{k'}$$

This is very difficult to solve for a general $U_{k-k'}$.
To simplify, we make a crude approximation:

$$U_{k-k'} = \begin{cases} -U_0 & \text{if } \epsilon_k, \epsilon_{k'} \text{ within } \overbrace{\hbar\omega_D}^{\text{max phonon energy}} \text{ of } \epsilon_F \\ 0 & \text{otherwise} \end{cases}$$

$$\Rightarrow g_k = \frac{-U_0 \left(\frac{1}{V} \sum_{k'} g_{k'} \right)}{E - 2\epsilon_k} \quad \text{where } \Sigma' \text{ means a sum over } \vec{k}' \text{ such that } |\vec{k}'| > k_F \text{ and } \frac{\hbar^2 k'^2}{2m} < \epsilon_F + \hbar\omega_D$$

Now sum both sides over \vec{k}

$$\left(\sum_k g_k \right) = -U_0 \left(\frac{1}{V} \sum_{k'} g_{k'} \right) \left(\sum_k \frac{1}{E - 2\epsilon_k} \right)$$

cancel $\sum g_k$ from both sides to get

$$1 = -U_0 \frac{1}{V} \sum_k' \frac{1}{E - 2\varepsilon_k}$$

$$\Rightarrow 1 = -U_0 \int_{\varepsilon_F}^{\varepsilon_F + \hbar\omega_D} d\varepsilon \frac{g(\varepsilon)}{E - 2\varepsilon} \quad g(\varepsilon) \text{ is density of states.}$$

$$\approx -U_0 g(\varepsilon_F) \int_{\varepsilon_F}^{\varepsilon_F + \hbar\omega_D} d\varepsilon \frac{1}{E - 2\varepsilon}$$

where we assumed $g(\varepsilon)$ varied slowly from ε_F to $\varepsilon_F + \hbar\omega_D$ (true since $\hbar\omega_D \ll \varepsilon_F$)

$$\Rightarrow 1 = \frac{U_0 g(\varepsilon_F)}{2} \ln \left(\frac{2\varepsilon_F - E + 2\hbar\omega_D}{2\varepsilon_F - E} \right)$$

solve above for the energy E

$$E = 2\varepsilon_F - \frac{2\hbar\omega_D}{e^{2/g(\varepsilon_F)U_0} - 1}$$

For a weak potential, $U_0 g(\varepsilon_F) \ll 1$, we have

$$E - 2\varepsilon_F = -2\hbar\omega_D e^{-2/g(\varepsilon_F)U_0}$$

Since the pair of electrons, in the absence of the attractive potential U , would have a minimum energy of $2\varepsilon_F$, the binding energy of the pair is

$$E' = 2\varepsilon_F - E = 2\hbar\omega_D e^{-2/g(\varepsilon_F)U_0} > 0$$

\Rightarrow bound state E has a lower energy than $2\varepsilon_F$

Note that the binding energy $\sim e^{-2/g(E_F)U_0}$ is a non-analytic function of U_0 , i.e. it cannot be expanded in powers of U_0 . This means that we could never have gotten this result by using perturbation theory!

Conclusion: pairs of electrons at the Fermi surface E_F can lower their energy by binding together into such a "Cooper pair". \Rightarrow The filled Fermi sphere ~~can no longer~~ is unstable to the formation of Cooper pairs and so can no longer be the true ground state. The new ground state was obtained by BCS starting from this idea of Cooper pairs, and became the basis for understanding superconductivity.

Back to the Cooper pair wavefunction:

$$g_{\vec{k}} \sim \frac{U_0 \times \text{constant}}{2E_{\vec{k}} - E} \quad \begin{array}{l} \text{depends on } \vec{k} \\ \text{only via } E_{\vec{k}} \end{array}$$

\Rightarrow Solution is spherically symmetric \Rightarrow Cooper pairs bind in an s-wave state.

The maximum $g_{\vec{k}}$ occurs for the smallest $E_{\vec{k}}$, i.e. at $|\vec{k}| = k_F$. Using $E = 2E_F - E'$ we get

$$g_k \sim \frac{U_0}{2(\epsilon_k - \epsilon_F) + E'}$$

The distribution g_k as function of k has a width given by

$$\epsilon_k - \epsilon_F \approx E' \ll \hbar \omega_D$$

Since only states within E' of ϵ_F are important in making the bound state, and $E' \ll \hbar \omega_D$, this suggests that the detailed structure of U_k is not so crucial and so our approximation might not be so terrible.

The size of a Cooper pair is ~~greater than~~ can be estimated as follows:

$$\xi_0 \sim \frac{\hbar v_F}{E'}$$

$$\xi_0 \sim \Delta R \sim \frac{1}{\Delta k} = \frac{1}{\frac{dR}{dE} \Delta E} = \frac{dE}{dR} \frac{1}{\Delta E} = \frac{\hbar v_F}{E'}$$

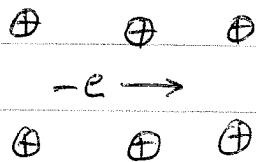
where we used that width in k -space was determined by $\epsilon_k - \epsilon_F \approx E'$.

$$\xi_0 \sim \frac{\hbar v_F}{E'} \gg r_s \quad \left(\frac{4\pi r_s^3}{3} = \frac{1}{n} \right)$$

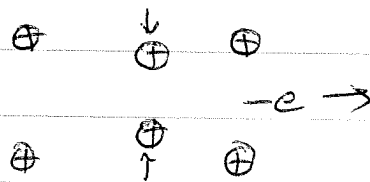
So the spatial extent of a Cooper pair is very much larger than the spacing between electrons

What is the origin of the attractive $e-e$ interaction that leads to Cooper pairing?

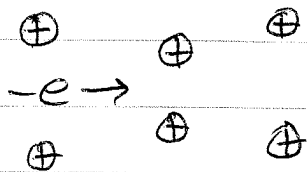
It is a time-delayed ionic screening effect!



electron passes by



ions get attracted to electron and deform. Net (+) charge builds up where $-e$ passed by, but now the $-e$ electron has moved on!



The excess (+) charge where the ions have deformed then attracts a new electron to the place where the first electron had been. This leads to an effective (but time delayed) attractive correlation between the electrons.

Crucial to this picture is that the ions move much more slowly than the electrons, so the ^{ion} deformation that attracts the 2nd electron, remains after the 1st electron has past. That is how the two (-) electrons can still attract!

Crystal Structures { Kittel Chpt 1 Ashcroft + Mermin Chpt 4

In most solids, the ions sit at the sites of a well defined periodic lattice of points. We now seek to describe ~~this lattice of ions~~ the geometric structure of this lattice of ions.

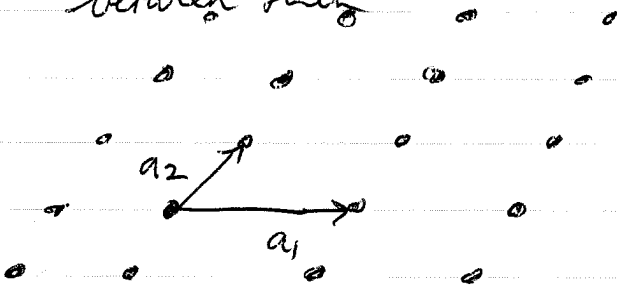
Bravais lattice - specifies the periodic ~~of~~ array in which the ~~units~~ units of the crystal are organized. Two equivalent definitions of the Bravais lattice are:

a) An infinite array of discrete points where the arrangement and orientation appears exactly the same upon whichever point the array is ~~not~~ viewed -

b) A 3-dimensional Bravais lattice consists of all points $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$ where $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are not all in the same plane, and n_1, n_2, n_3 are any integers.

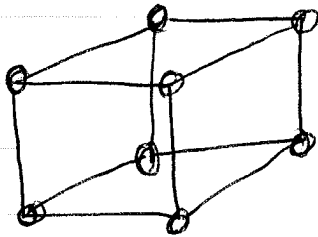
$\vec{a}_1, \vec{a}_2, \vec{a}_3$ are called the primitive vectors of the Bravais lattice - they are not unique. (primitive vectors sometimes called the basis vectors)

An example of a 2-d Bravais lattice with no special symmetry is given by \vec{a}_1, \vec{a}_2 of different lengths, with a angle $\alpha \neq \frac{2\pi}{\text{integer}}$ between them.

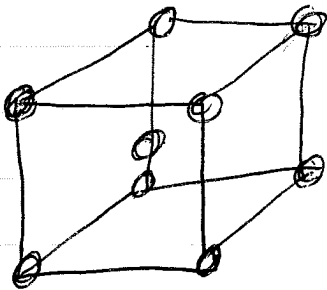


Examples of Bravais lattices

3D simple cubic lattice $\vec{a}_1 = a\hat{x}, \vec{a}_2 = a\hat{y}, \vec{a}_3 = a\hat{z}$



3D Body centered cubic (bcc)



take simple cubic and put an extra atom in the center of each cubic cell

looks like two interpenetrating simple cubic lattices

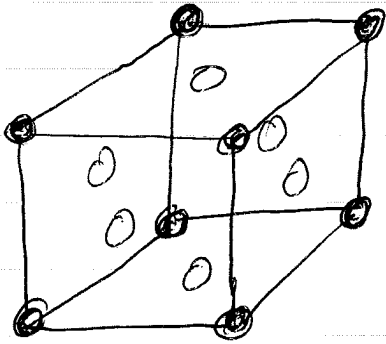
primitive vectors:

$$\vec{a}_1 = a\hat{x}, \vec{a}_2 = a\hat{y}, \vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y} + \hat{z})$$

or a more symmetric choice:

$$\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z} - \hat{x}), \vec{a}_2 = \frac{a}{2}(\hat{z} + \hat{x} - \hat{y}), \vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$

3D face centered cubic (fcc)



take a single cubic lattice and add an atom to the center of every face of each cubic cell

primitive vectors

$$\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{z} + \hat{x})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y})$$

bcc and fcc are very common lattice structures. single cubic is very rare (only α -phase of polonium under normal conditions)

fcc: Ar, Ag, Al, Au, Ca, Ce, β -Co, Cu, Ir, Kr, La, Ne, Ni, Pb, Pd, Pr, Pt, S-Pu, Rh, Sc, Sr, Th, Xe, Yb
lattice constant $a \sim 3-6 \text{ \AA}$

bcc: Ba, Cr, Cs, Fe, K, Li, Mo, Na, Nb, Rb, Ta, Tl, V, W
 $a \sim 3-6 \text{ \AA}$

Bravais Lattice - this term can refer to either the set of points, or the set of vectors

$$\vec{R} = \sum_i n_i \vec{a}_i$$

coordination number - the number of points in a Bravais lattice that are closest to a given point is the coordination number z . These closest points are the "nearest neighbors" of the given point. Each point has the same coordination number

$$\text{s.c. } z = 6$$

$$\text{b.c.c. } z = 8$$

$$\text{fcc } z = 12$$

primitive cell - a volume of space, that when translated by all vectors \vec{R} in the Bravais lattice, will fill all of space without any overlaps or voids.

The primitive cell is not unique just as the choice of primitive vectors \vec{a}_i ~~are~~ is not unique.

For a given set of primitive vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$ then the volume swept out by the set of points

$$\vec{r} = x_1 \vec{a}_1 + x_2 \vec{a}_2 + x_3 \vec{a}_3$$

with $0 \leq x_i \leq 1$, is an example of a primitive cell.

Since the primitive cell must contain only one Bravais lattice point, the volume

v of a primitive cell must be such that

$$V = Nv \quad N = \text{total number of lattice points}$$

$$V = \text{total volume}$$

$$\Rightarrow v = \frac{V}{N} = \frac{1}{n} \quad n = \text{density of BL points.}$$

v is independent of choice of the primitive cell

The primitive cell need not have the full symmetry of the crystal

unit cell or conventional cell - a volume that fills up all space without overlaps or voids when translated by some particular subset of vectors of the Bravais lattice. The unit cell is bigger than the primitive cell, and usually chosen for convenience with the symmetry of the lattice.

For example, for bcc or fcc one can take as the unit cell the simple cubic cell which is decorated to form the bcc or fcc structure. The parameters that specify the size of the unit cell are called the lattice constants

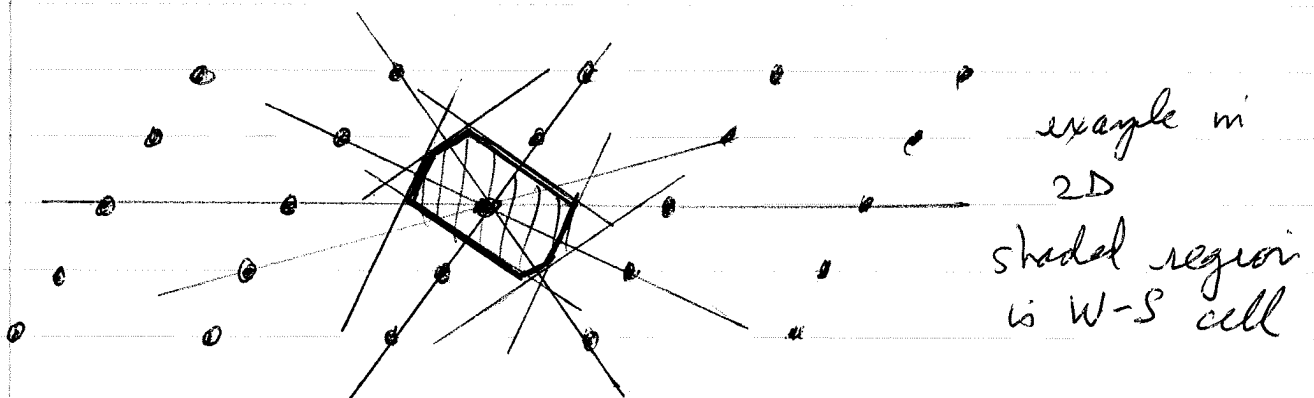
Wigner Seitz cell

This is a uniquely defined choice for a primitive cell that has the full symmetry of the Bravais lattice. We define it as follows:

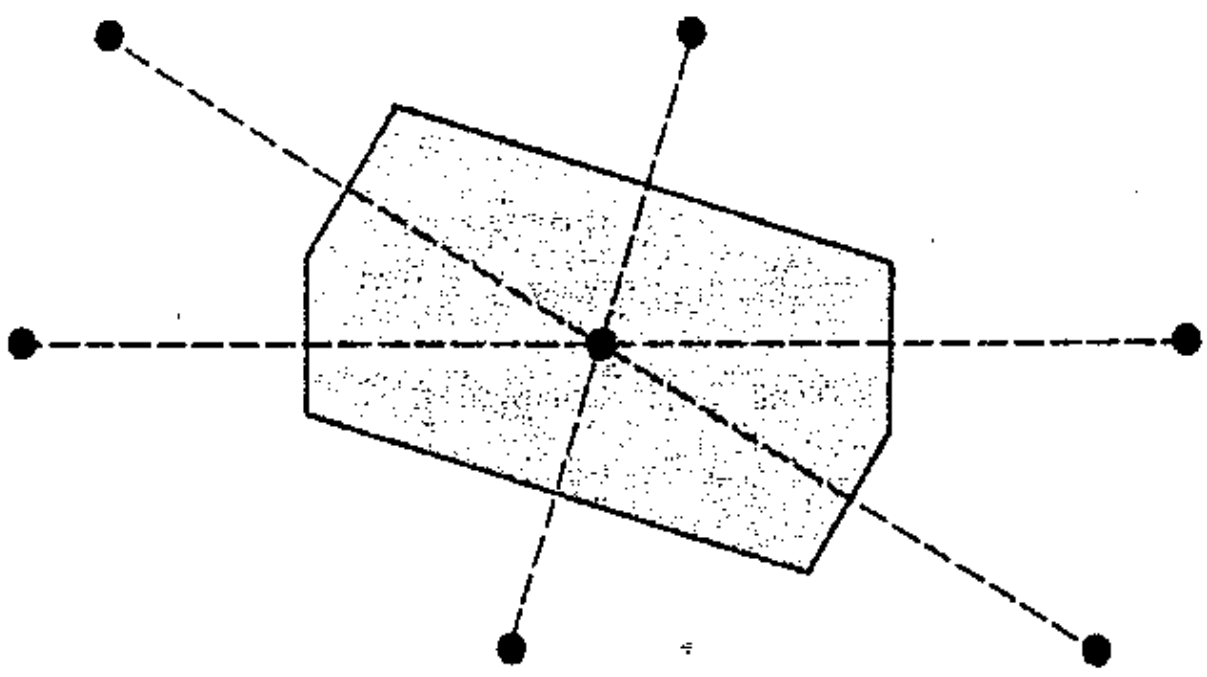
Choose a point \vec{P} in the Bravais lattice. The region of space closer to \vec{P} than to any other point \vec{P}' in the Bravais lattice is the Wigner Seitz cell.

Since above definition makes no reference to any particular set of primitive vectors, the W-S cell has all the same symmetries of the Bravais lattice.

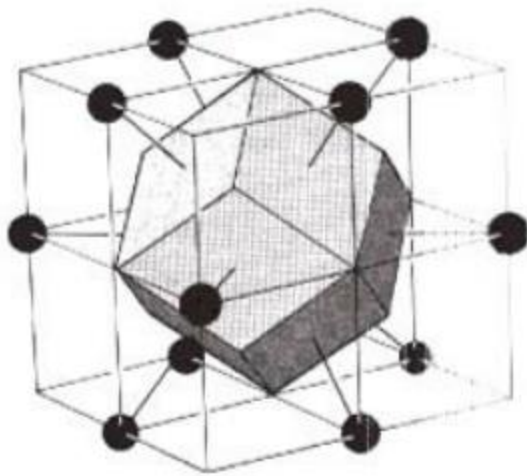
To construct the W-S cell, draw lines from \vec{P} to all other points \vec{P}' in the Bravais lattice. Bisect each such line with a plane. The inner envelope of these planes is the surface of the W-S cell.



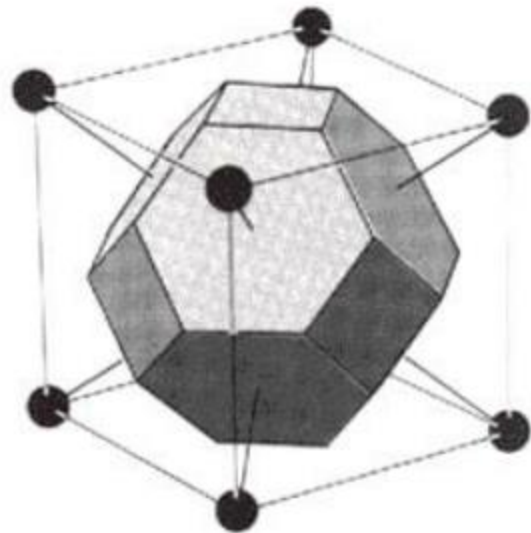
see Kittel or AM for W-S cells of 3D BL



Wigner-Seitz Cell - 3D

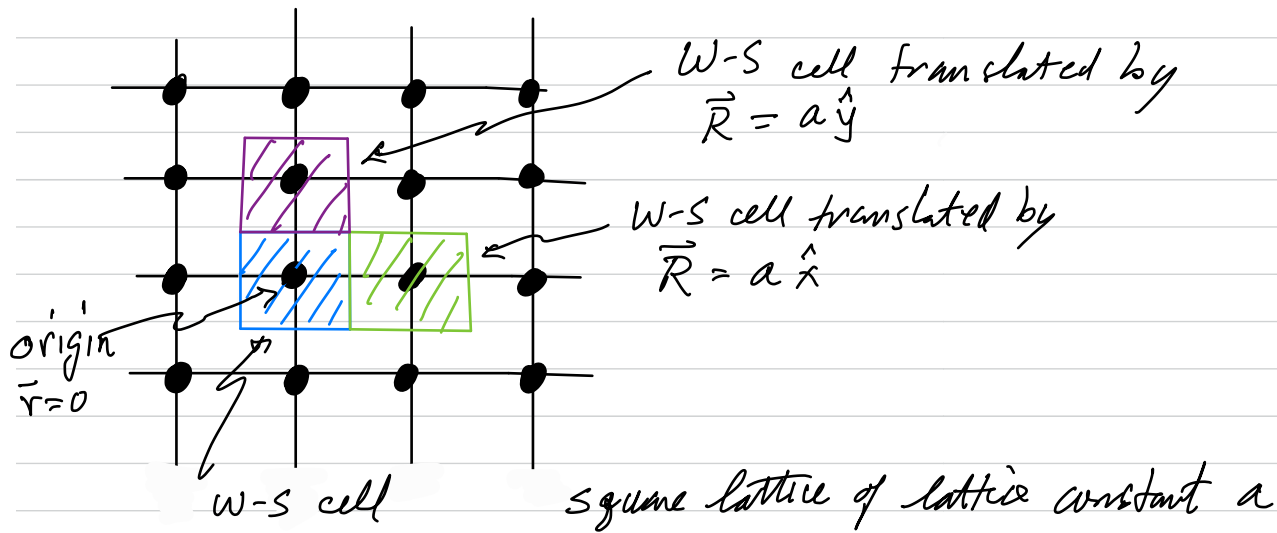


f.c.c Wigner-Seitz cell



b.c.c Wigner-Seitz cell

How do we know that the Wigner-Seitz cell is a primitive cell?



Let $\{\vec{r}_0\}$ be the set of positions in the W-S cell. These are the points in space closer to $\vec{r} = 0$ than to any other point \vec{R} in the Bravais lattice.

Now consider the set of positions $\{\vec{r}_0 + \vec{R}\}$ obtained by translating the W-S cell by the B-L vector \vec{R} . These are the positions that are closer to \vec{R} than to any other point in the B-L.

The set of $\{\vec{r}_0 + \vec{R}\}$ as \vec{R} varies over all B-L vectors \vec{R} is then the set of positions occupied by all translations of the W-S cell by B-L vectors \vec{R} .

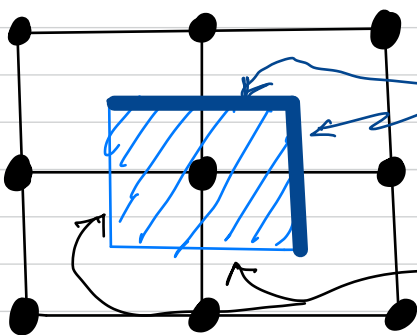
To show that the W-S cell is a primitive cell we want to show that the set of $\{\vec{r}_0 + \vec{R}\}$ fill all space without any voids or overlaps.

Consider a point in space \vec{r} . Clearly it is closer to one particular \vec{R}_0 than to any other. It is therefore

contained in the set $\{\vec{r}_0 + \vec{R}_0\}$ and it is not contained in any other set $\{\vec{r}_0 + \vec{R}\}$. Hence the sets $\{\vec{r}_0 + \vec{R}\}$ cover all space (\Rightarrow no voids) and no \vec{r} belongs to more than one such set (\Rightarrow no overlaps). So the W-S cell is a primitive cell of the B-L.

A technicality

If a point \vec{r} happens to lie exactly midway between two B-L vectors, say \vec{R}_1 and \vec{R}_2 , then it is ambiguous whether it should belong to $\{\vec{r}_0 + \vec{R}_1\}$ or $\{\vec{r}_0 + \vec{R}_2\}$. Such is the case, for example, for all points on the surface of the W-S cell. We can fix this by convention by choosing half the points on the W-S surface to belong to the W-S cell, and the other half not.



these points we take as included in the W-S cell

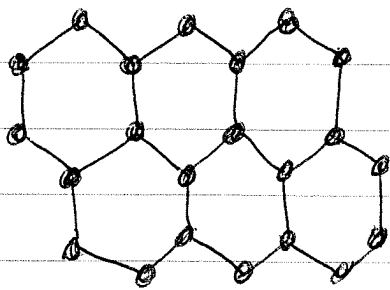
these points not in the W-S cell

Crystal Structure - Bravais lattice with a basis

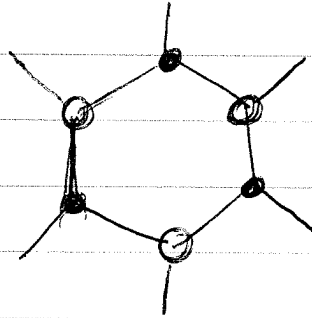
Crystals can form periodic structures which are NOT Bravais lattices - all points are not equivalent, ~~either~~ either due to positioning of atoms or because different atoms occupy different sites

Such structures are called a lattice with a basis and are described by an underlying B-L plus a set of basis vectors that give the positions of the atoms with respect to each B-L site \vec{R} .

example: honeycomb lattice in 2D



← This is not a Bravais-lattice!

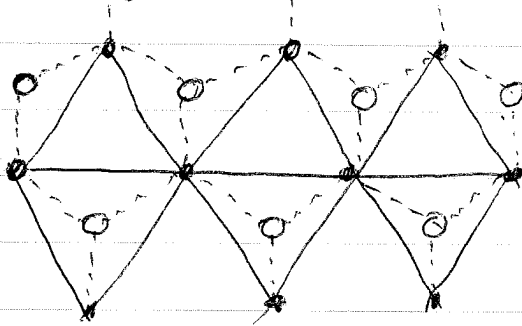


the \bullet sites are all equivalent and the \circ ~~sites~~ sites are all equivalent, but

The \bullet sites are NOT equivalent to the \circ sites!

Note: \circ sites all have a \bullet neighbor to the upper right whereas \bullet sites do not - they have a neighbor to the lower left \circ . Hence the orientational environment of \bullet sites is different from that of \circ sites

But we can describe the honeycomb lattice as a 2D triangular lattice with a two point basis.
 Let the \bullet sites describe the sites \vec{R} of a triangular B-L.



dashed lines show the honeycomb structure.
 solid lines show the underlying triangular B-L

primitive vectors $\begin{cases} \vec{a}_1 = a \hat{x} & \longrightarrow \\ \vec{a}_2 = a \left(\frac{\hat{x}}{2} + \frac{\sqrt{3}}{2} \hat{y} \right) & \nearrow \end{cases}$

basis vectors $\begin{cases} \vec{d}_1 = 0 & \text{gives } \bullet \text{ sites} \\ \vec{d}_2 = \frac{2}{\sqrt{3}} a \hat{y} & \text{gives } \circ \text{ sites} \end{cases}$

sites of honeycomb lattice given by

$$\{ \vec{R} + \vec{d}_1, \vec{R} + \vec{d}_2 \} \quad \text{with } \vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2, \\ n_1, n_2 \text{ integers}$$

We could describe the fcc and bcc Bravais lattices as a single cubic lattice with a basis

$$\Rightarrow \text{primitive vectors} \begin{cases} \vec{a}_1 = a\hat{x} \\ \vec{a}_2 = a\hat{y} \\ \vec{a}_3 = a\hat{z} \end{cases}$$

$$\text{basis vectors bcc:} \begin{cases} \vec{d}_1 = 0 \\ \vec{d}_2 = \frac{a}{2}(\hat{x} + \hat{y} + \hat{z}) \end{cases}$$

2 point basis

$$\text{basis vectors fcc:} \begin{cases} \vec{d}_1 = 0 \\ \vec{d}_2 = \frac{a}{2}(\hat{x} + \hat{y}) \\ \vec{d}_3 = \frac{a}{2}(\hat{y} + \hat{z}) \\ \vec{d}_4 = \frac{a}{2}(\hat{z} + \hat{x}) \end{cases}$$

4 point basis

Diamond structure

Two interpenetrating fcc lattices displaced along the body diagonal of the cubic unit cell by $1/4$ the length of the diagonal
(See Ashcroft + Mermin Fig 4.18)

fcc Bravais lattice with two point basis

$$\vec{d}_1 = 0 \\ \vec{d}_2 = \frac{a}{4}(\hat{x} + \hat{y} + \hat{z})$$

coordination number $z = 4$ - tetrahedral bonds
examples: C, Si, Ge, α -Sn

Bond lengths from atom at $\vec{d}_1 = \frac{a}{4}(\hat{x} + \hat{y} + \hat{z})$ to origin and faces are the same.

$$|\vec{d}_1| = \frac{\sqrt{3}}{4} a$$

$$|\vec{d}_1 - \frac{a}{2}(\hat{x} + \hat{y})| = \left| -\frac{a}{4}\hat{x} - \frac{a}{4}\hat{y} + \frac{a}{4}\hat{z} \right| = \frac{\sqrt{3}}{4} a$$

$$|\vec{d}_1 - \frac{a}{2}(\hat{x} + \hat{z})| = \left| -\frac{a}{4}\hat{x} + \frac{a}{4}\hat{y} - \frac{a}{4}\hat{z} \right| = \frac{\sqrt{3}}{4} a$$

$$|\vec{d}_1 - \frac{a}{2}(\hat{y} + \hat{z})| = \left| \frac{a}{2}\hat{x} - \frac{a}{2}\hat{y} - \frac{a}{2}\hat{z} \right| = \frac{\sqrt{3}}{4} a$$

each atom of diamond structure has 4 equal length bonds to 4 nearest neighbors. These bonds form the edges of a tetrahedron.

