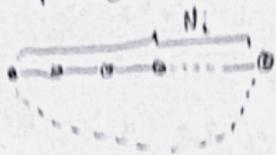


* Bohr - Von Karman condition \Rightarrow boundary number of electrons per unit cell

Bohr - Von Karman

The boundary condition is the condition that implies the wavefunction was eigenstate of \hat{H} are periodic



$$N(\vec{r} + N_i \vec{a}_i) = \psi(\vec{r}) \quad (*)$$

\uparrow
primitive vector \vec{a}_i

$$N_1 N_2 N_3 = N$$

number of primitive cells in the crystal

the largest portion that's we can go from vector \vec{a}_i

$$(*) \Leftrightarrow e^{i \vec{K} N_i \vec{a}_i} = 1 \quad \Rightarrow \quad \vec{K} = \sum \frac{2\pi i}{N_i} \vec{b}_i$$

\Rightarrow The smallest volume that contains one point K is

$$\Delta K = \frac{1}{N_1 N_2 N_3} \underbrace{b_1 \cdot (b_2 \times b_3)}$$

V_{BZ} : volume of the

$$= \frac{V_{BZ}}{N}$$

\rightarrow In the Brillouin zone, number of K points that's we can have

$$\frac{V_{BZ}}{\Delta K} = N$$

* In the class, we mentioned about number of valence electrons. what the teacher means is number of valence electrons per unit cell

In total, number of valence electrons that's we have

so

$$n_e \cdot N_{\text{unit-cell}} = N$$

- inside the Brillouin zone, we have all of k -points
- in our k space, because the points that's outside this volume have the correspondence inside this region.
so that,
- we for each band to full fill, we just need 1 valence electron.

below

- in the class, Lilia showed the Fermi level, we have 3 band, so that if we have more than 6 valence electrons
fill band that's we will go the higher than the Fermi level