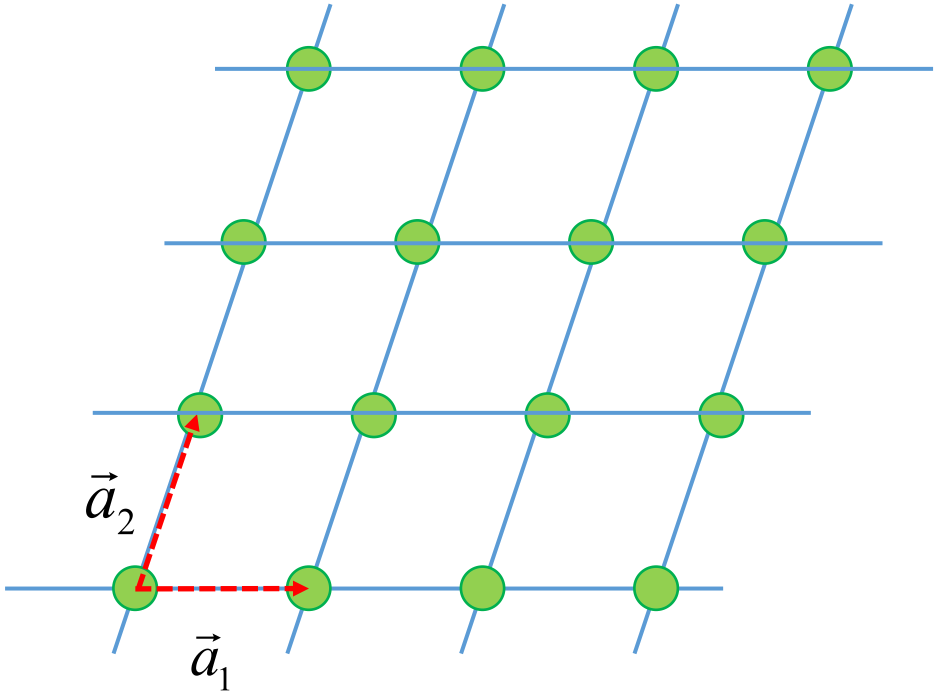
Take-home Exam !!!

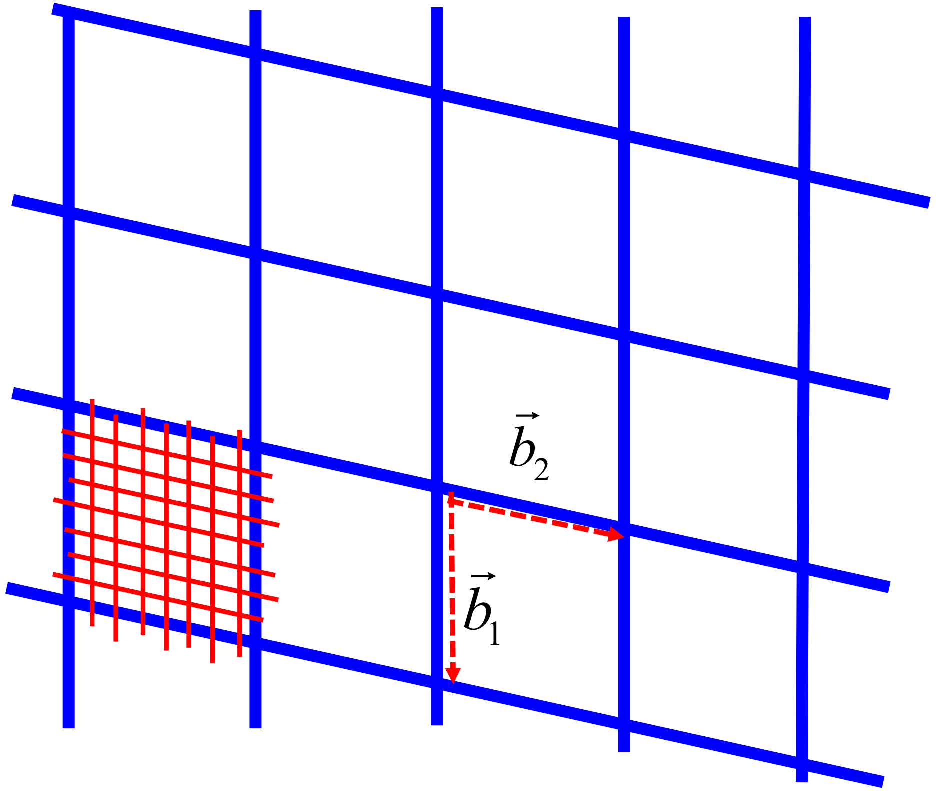
- Everybody solves this problem.

- Randomly select one you, who may present this in the next-week class time !!!

Lattice and reciprocal lattice

For example, a triangular lattice





$\vec{a}_1 = (a,0,0)$, $\vec{a}_2 = a(1/2, \sqrt{3}/2, 0)$, $\vec{a}_3 = (0,0,c)$

$$\vec{b}_1 = \frac{2\pi}{V}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{a}(1, -\frac{1}{\sqrt{3}}, 0)$$

$$\vec{b}_2 = \frac{2\pi}{V}(\vec{a}_3 \times \vec{a}_1) = \frac{2\pi}{a}(0, \frac{2}{\sqrt{3}}, 0)$$

k-point sampling

- In actual computation of solid states, we perform the Brillouin zone integration through the discrete k-point sampling, in most of cases, we make uniform discrete k-point sampling.
- Based on the Born-von-Karman boundary conditions, show that the number of sampled k-points in the Brillouin zone is the same as the number of cells in the position space.

Number cells = number of k-points

Consider a Bloch state $\psi_{\vec{k}}(\vec{r})$ with $\vec{k} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3$

The translation eigen state $\psi_{\vec{k}}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}\psi_{\vec{k}}(\vec{r})$

Born-von-Karman with very large N_1 : $\psi_{\vec{k}}(\vec{r}+N_1\vec{a}_1) = e^{i\vec{k}\cdot N_1\vec{a}_1}\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}(\vec{r})$

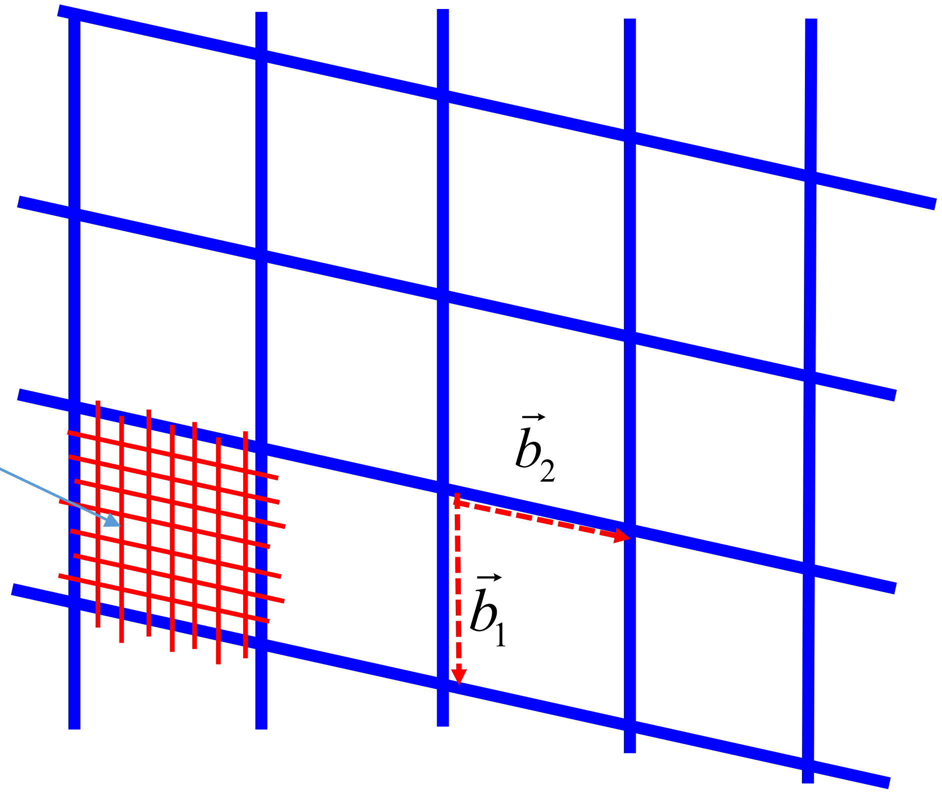
We have $k_1 = \dfrac{l}{N_1}$.

In the same wave, we have discretely sampled k-points

$$\vec{k} = \frac{l}{N_1}\vec{b}_1 + \frac{m}{N_2}\vec{b}_2 + \frac{n}{N_3}\vec{b}_3$$

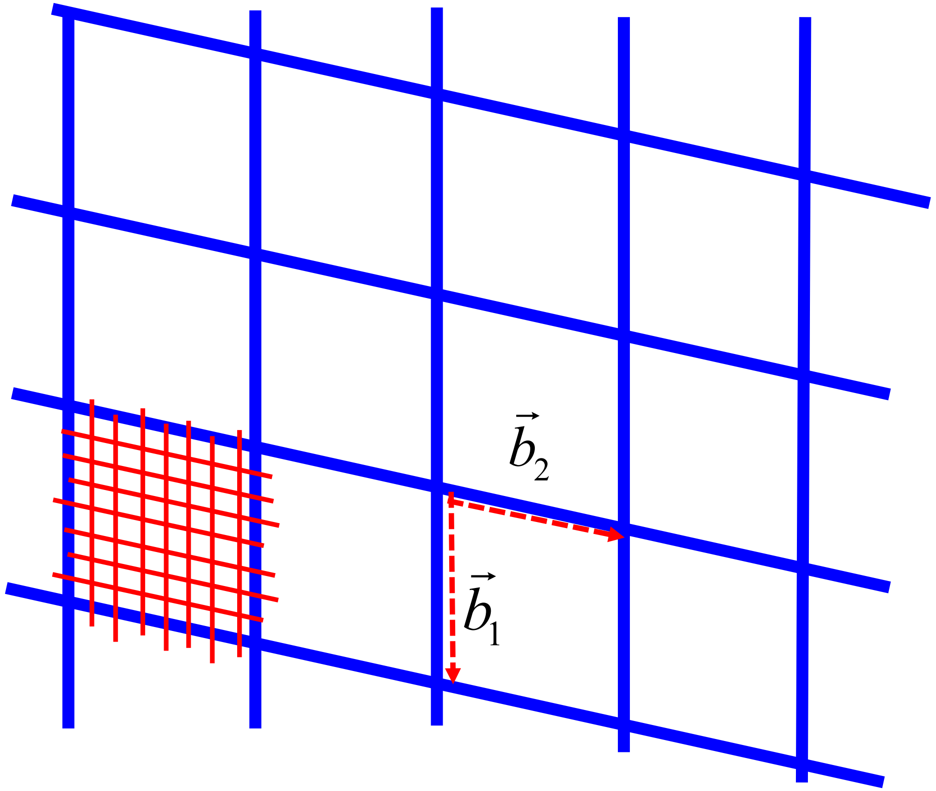
The volume per k-point

$$d^3\vec{k} = \frac{1}{N_1 N_2 N_3}\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)$$



The number of sampled k-points

$$N_{k-point} = \frac{\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)}{d^3\vec{k}} = \frac{1}{N_1 N_2 N_3}$$



What's wrong in this page ???

Implication

- Suppose we have an insulator with N electron per unit cell.

$$\left(\frac{1}{2}(-i\nabla+\vec{k})^2+V(\vec{r})\right)u_{n,\vec{k}}(\vec{r})=E_n(\vec{k})u_{n,\vec{k}}(\vec{r})$$

- How many bands are occupied by the electron ?

Implication

- Think of construction of the density from the wavefunctions, the energy-momentum eigenfunctions, of an insulator.

$$\rho(\vec{r}) = \sum_{i=1}^{N_k}\sum_{n=1}^{N} W(\vec{k})\left|\psi_{n,\vec{k}}(\vec{r})\right| = \sum_{i=1}^{N_k}\sum_{n=1}^{N} W(\vec{k})\left|u_{n,\vec{k}}(\vec{r})\right|$$

- What is N ?, what is $W(\vec{k})$???

Hamoon, present this page, for five minutes, next-week, lecture time ?