Notes:

- **Office hours:** Monday & Wednesday 11:30-12:30, **Thursday** 1PM.
- I sent **email** yesterday. **If you didn’t get my email let me know.** (Or also let me know if you prefer a different email address than the one I used).
Reciprocal Lattice:

- Composed of plane waves having symmetry of lattice: \( e^{i\vec{K} \cdot (\vec{r} + \vec{R})} = e^{i\vec{K} \cdot \vec{r}} \)
- To construct: \( \vec{K} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3 \) with \( \vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij} \)

Find (3D case):

- \( \vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \)
- \( \vec{b}_2 = \frac{2\pi \vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \)
- \( \vec{b}_3 = \frac{2\pi \vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \)
Cubic Bravais Lattice systems & primitive cells

white parallelepipeds: cell edges \( \vec{a}_1, \vec{a}_2, \vec{a}_3 \)

BCC (body center)
2 sites / cubic cell
Examples: Iron, Na

FCC (face center)
4 sites / cubic cell
Examples: Cu, Al, Ni, Silicon*, NaCl*, etc
* These are FCC with basis

Find: FCC lattice reciprocal is BCC lattice
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- To construct: \( \vec{K} = h\vec{b}_1 + kB_2 + \ell\vec{b}_3 \) with \( \vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij} \)

- Find (3D case):
  \[
  \begin{align*}
  \vec{b}_1 &= 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \\
  \vec{b}_2 &= 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \\
  \vec{b}_3 &= 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}
  \end{align*}
  \]

Results:

- Wavefronts of \( e^{i\vec{K} \cdot \vec{R}} \) are Bragg planes (lattice planes);

  shows that \( \frac{2\pi}{d} \hat{n} \) is a \( K \) vector; \( h, k, \ell \leftrightarrow h, k, \ell \)

- Reciprocal lattice is itself a Bravais lattice; “dual” to direct lattice. Also reciprocal of reciprocal lattice = direct lattice.

- \( K \) vectors: \( k \)-space Fourier components of direct-space lattice.
Reciprocal Lattice:

Results:

- Wavefronts of $e^{i\vec{K} \cdot \vec{R}}$ are Bragg planes (lattice planes);
  
  shows that $\frac{2\pi}{d} \hat{n}$ is a $K$ vector; $h, k, \ell \leftrightarrow h, k, \ell$

- Reciprocal lattice is itself a Bravais lattice; “dual” to direct lattice. Also reciprocal of reciprocal lattice = direct lattice.

- $K$ vectors: $k$-space Fourier components of direct-space lattice (complete set).

\[
n(\vec{r}) = \sum_{\vec{K}} n_{\vec{K}} \exp[i\vec{K} \cdot \vec{r}] \quad n_{\vec{K}} = \frac{1}{V_{\text{cell}}} \int d^3r \ n(r) \exp[-i\vec{K} \cdot \vec{r}]
\]

Also:  
  - Wigner-Seitz reciprocal cell = $1^{\text{st}}$ Brillouin Zone.  
  - Volume = \( \frac{(2\pi)^3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \)