Today's Outline - February 25, 2020

- Information about:

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- Information about:
  (a) Final presentation

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- Information about:
  (a) Final presentation
  (b) Final project

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- Lattice & basis functions

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Homework Assignment #03:
Chapter 3:1,3,4,6,8
due Thursday, February 27, 2020

Final presentation

1. Choose paper for presentation

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2. Clear it with me!

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3. Do some background research on the technique

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3. Do some background research on the technique
4. Prepare a 15 minute presentation

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4. Prepare a 15 minute presentation
5. Be ready for questions!

Final project

1. Come up with a potential experiment

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5. Lay out proposed experiment (you can ask for help!)

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6. Make sure to give reasonable answers forall the questions

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7. Put me as one of the investigators of the proposal

Scattering from ordered crystals

Liquid scattering and small angle scattering provide structural information about highly disordered systems and long length scales, respectively.

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We will now proceed to develop a model for this kind of scattering starting with some definitions in 2D space.

Types of lattice vectors

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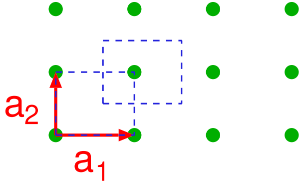

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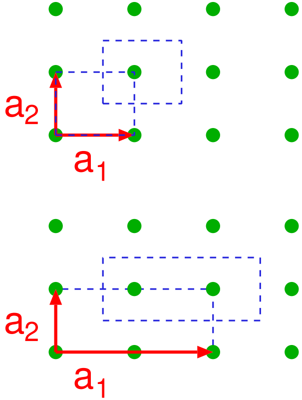

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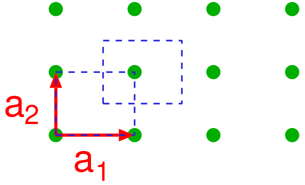
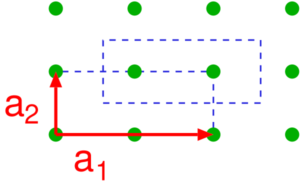
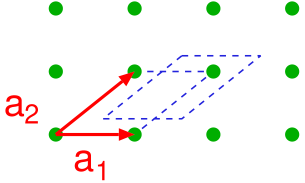


primitive

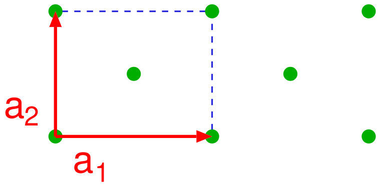


non-primitive



non-conventional

More about lattice vectors



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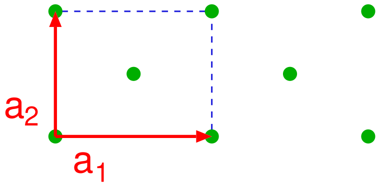

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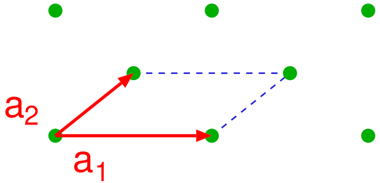
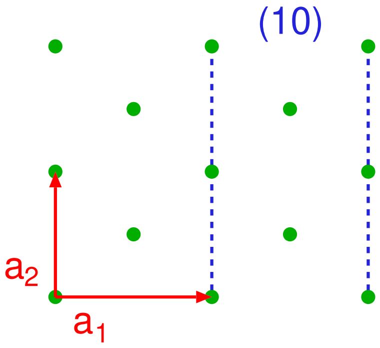


...are not primitive

Miller indices



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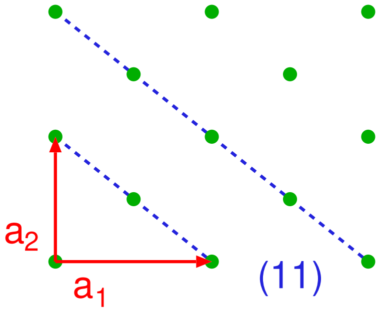

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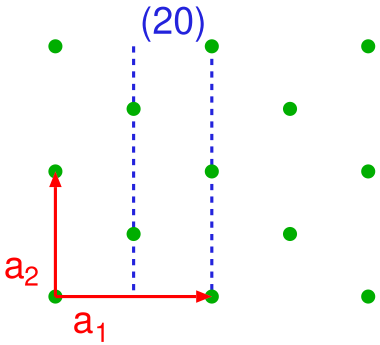

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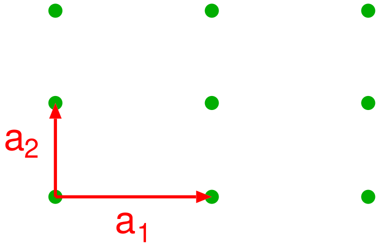
for a lattice with orthogonal unit vectors

$$\frac{1}{d_{hk}^2} = \frac{h^2}{a_1^2} + \frac{k^2}{a_2^2}$$

Reciprocal lattice



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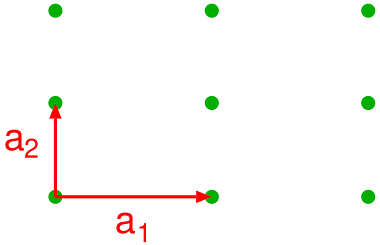

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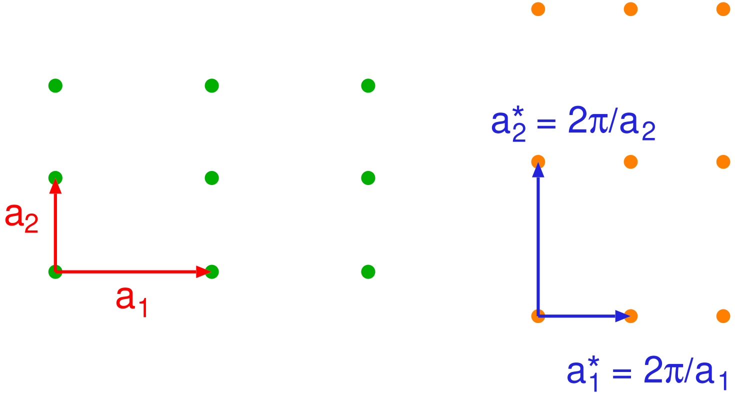

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Scattering amplitude

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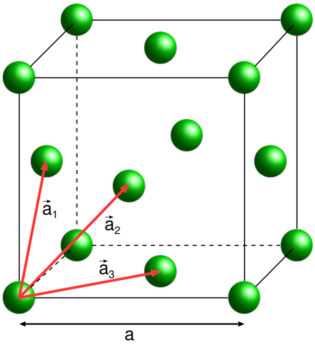
$$\therefore\ \vec{Q} = \vec{G}_{hkl}$$

The FCC reciprocal lattice

The primitive lattice vectors of the face-centered cubic lattice are



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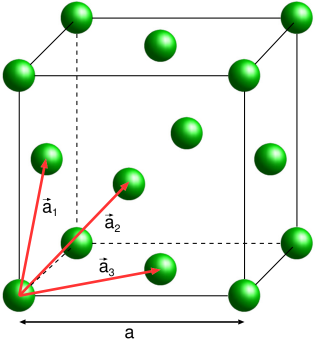

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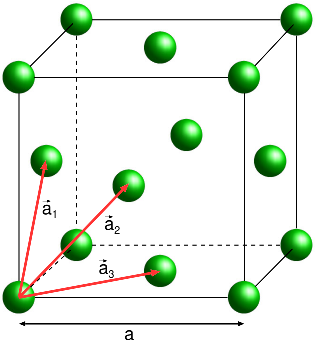

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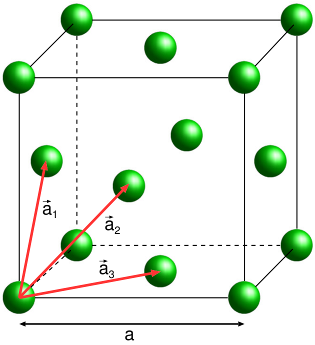

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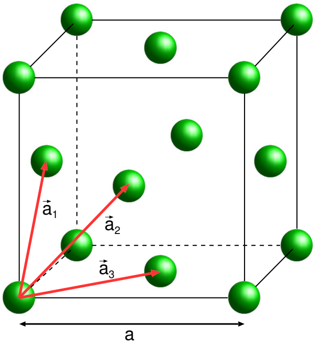

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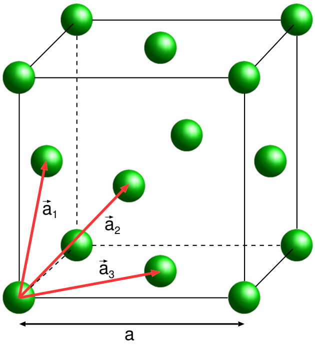

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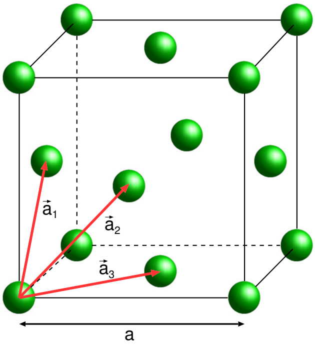

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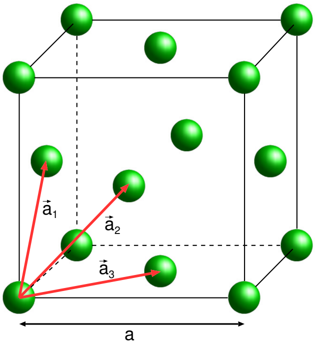

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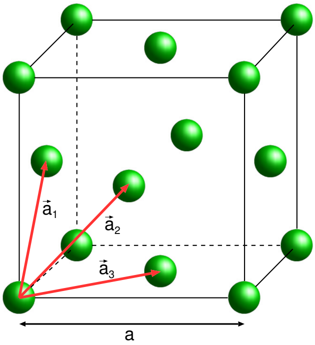

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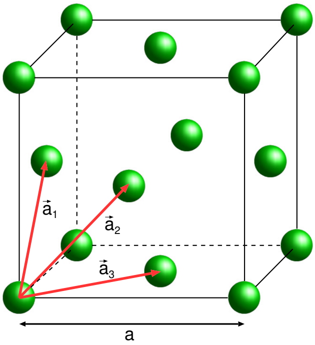

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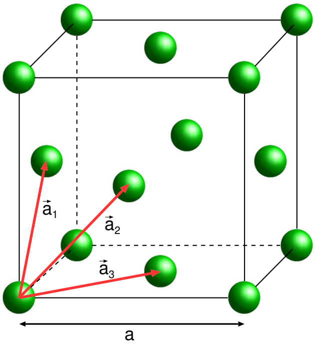

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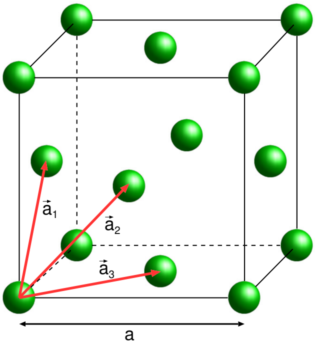

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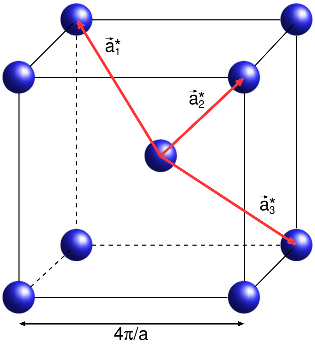

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for very large N, the lattice sum approaches a delta function and since $Q = [h+\xi]a^*$ we have

$$|S_N(\xi)| \to \delta(\xi) \qquad\qquad \xi = \frac{Q - ha^*}{a^*} = \frac{Q - G_h}{a^*}$$

$$|S_N(Q)| \to a^* \sum_{G_h} \delta(Q - G_h) = \sum_{n=0}^{N-1} e^{iQna}$$

Lattice sum in 1D

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since $\delta(a^*\xi) = \delta(\xi)/a^*$

Lattice sum modulus

the 1D modulus squared

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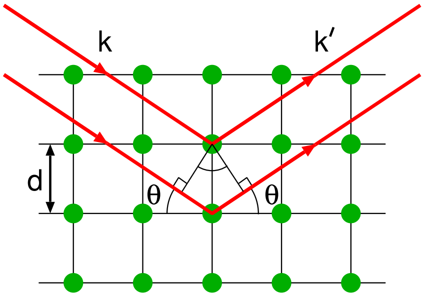
$$\left|S_N(\vec{Q})\right|^2 \rightarrow NV_c^* \sum_{\vec{G}_{hkl}} \delta(\vec{Q} - \vec{G}_{hkl})$$

Bragg condition



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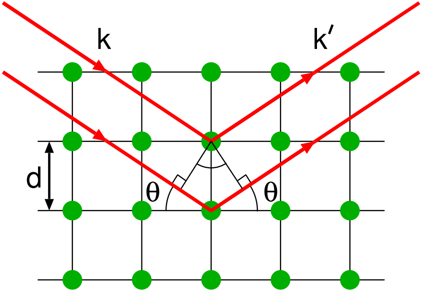
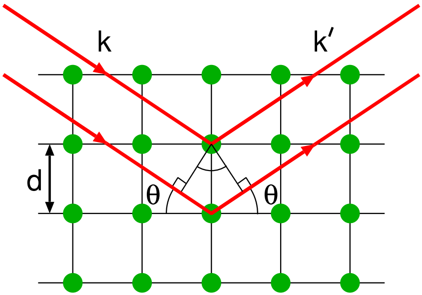


The Bragg condition for diffraction is derived by assuming specular reflection from parallel planes separated by a distance d.

Bragg condition



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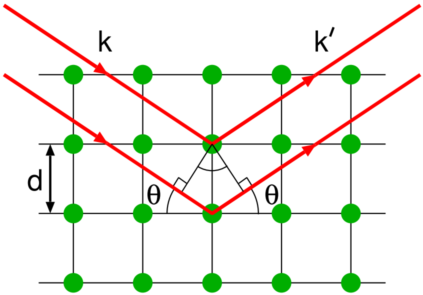

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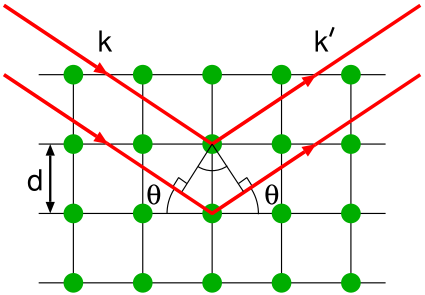

$$2d \sin\theta = \lambda$$

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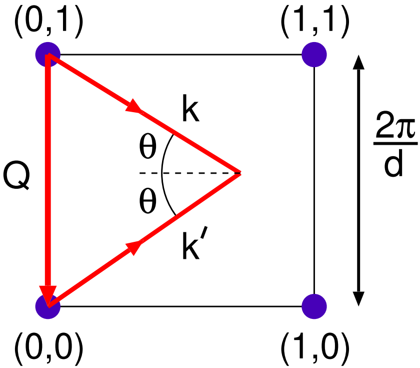
Laue condition

The Laue condition states that the scattering vector must be equal to a reciprocal lattice vector



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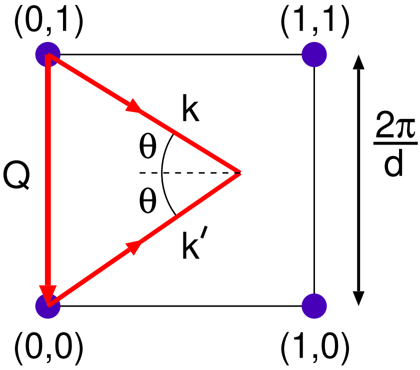

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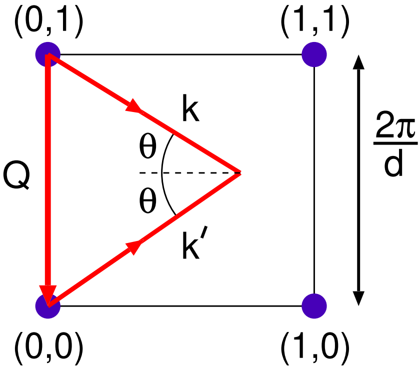

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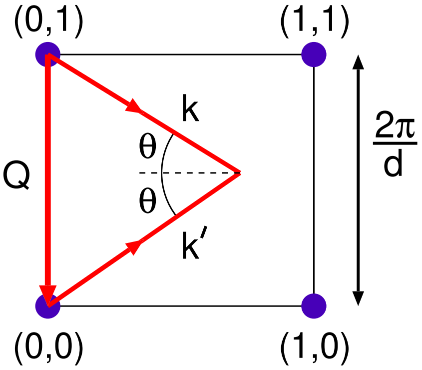

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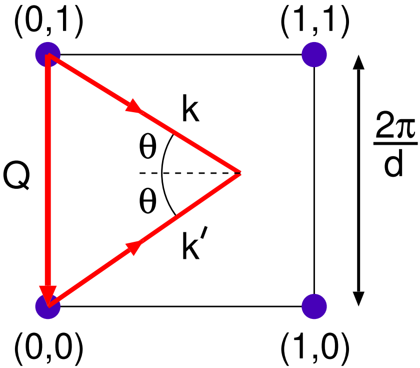

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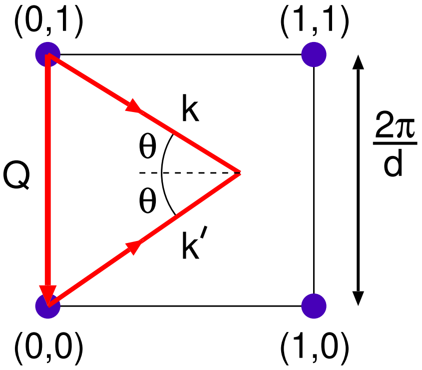

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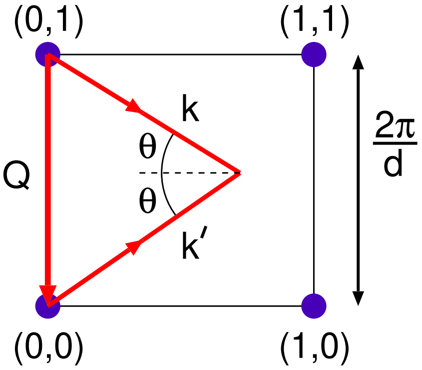

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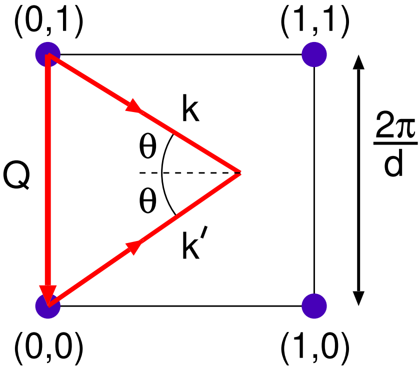
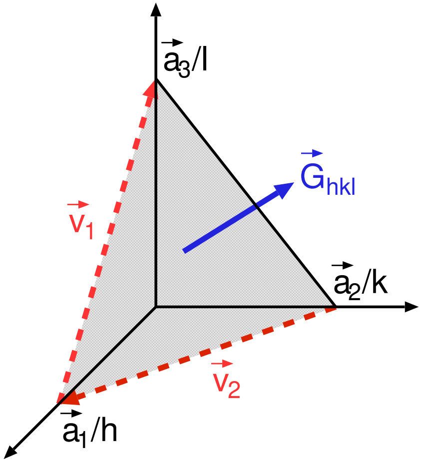


Thus the Bragg and Laue conditions are equivalent

General proof of Bragg-Laue equivalence



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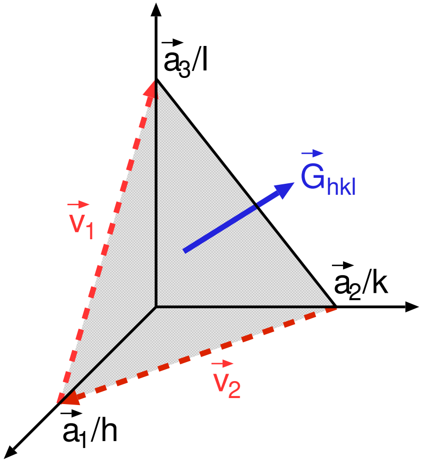

Must show that for each point in reciprocal space, there exists a set of planes in the real space lattice such that:

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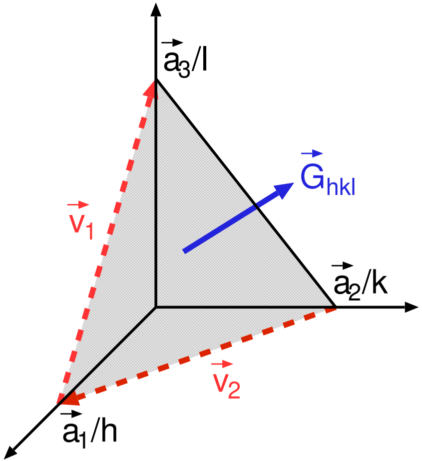

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$\vec{G}_{hkl}$ is perpendicular to the planes with Miller indices (hkl)

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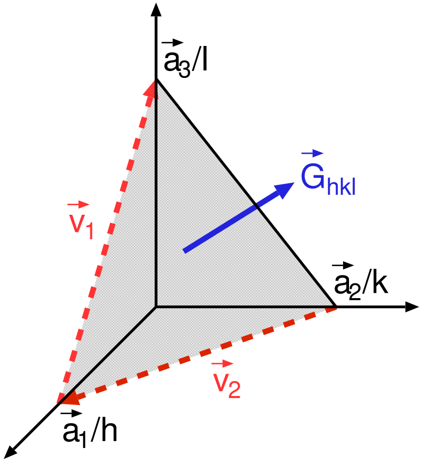

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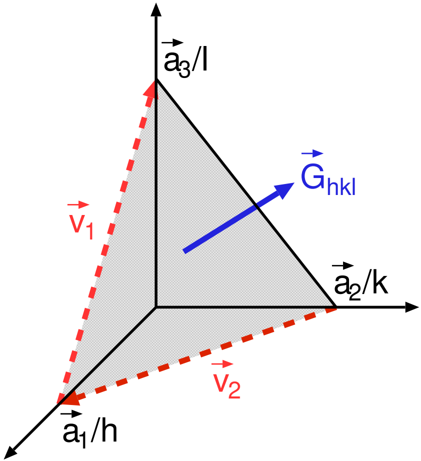

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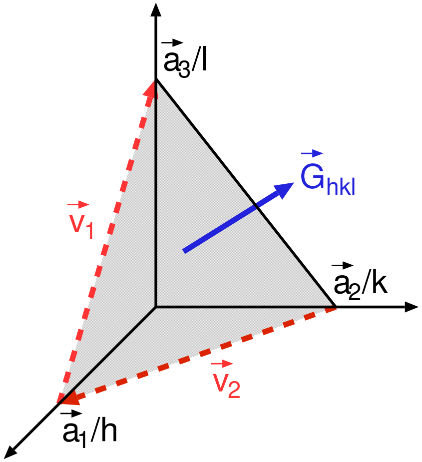

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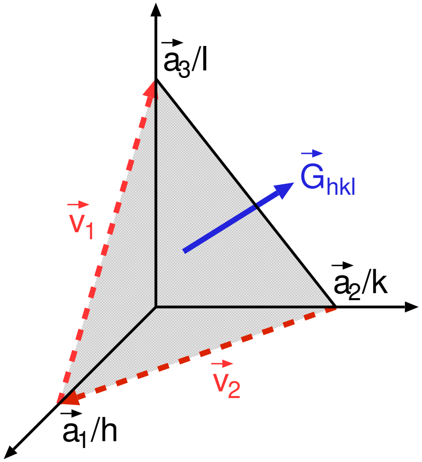

The plane with Miller indices (hkl) intersects the three basis vectors of the lattice at a_1/h, a_2/k, and a_3/l

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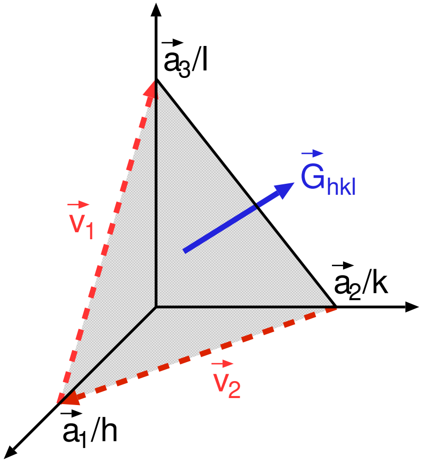

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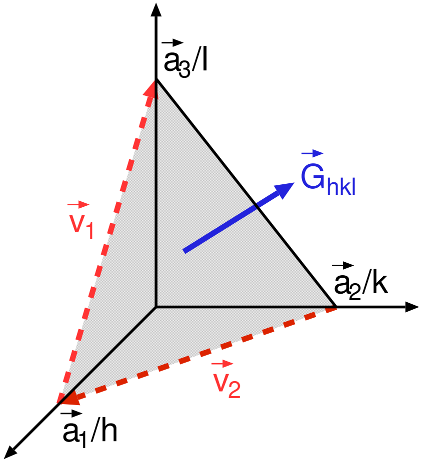

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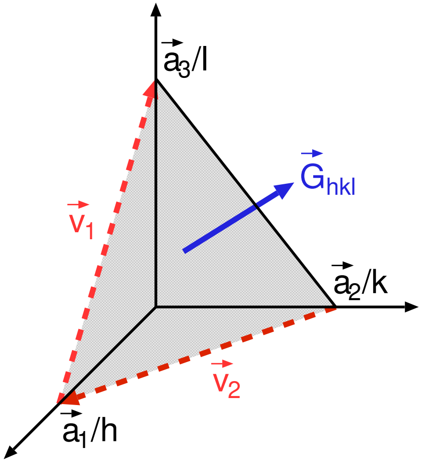

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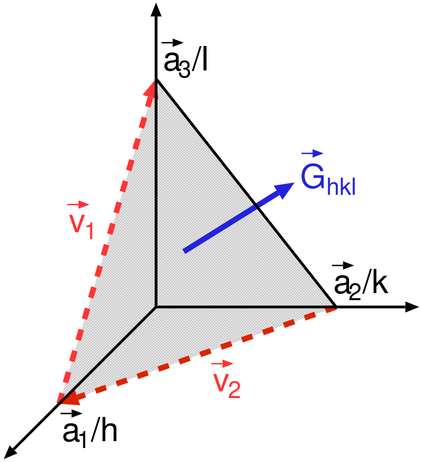

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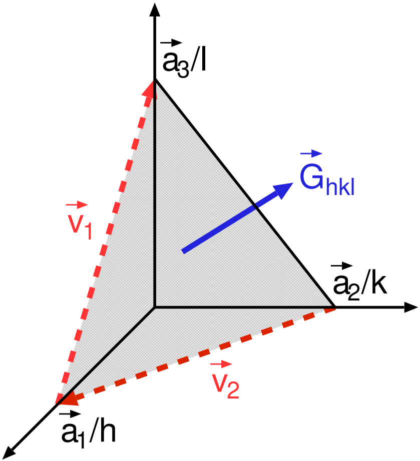

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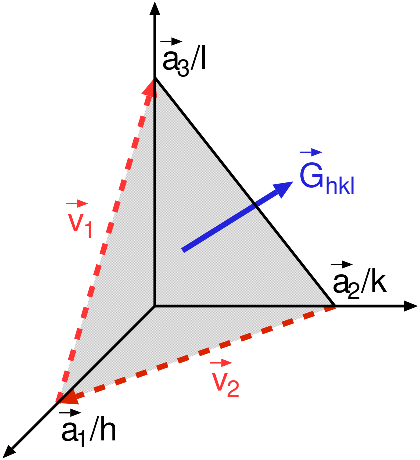
$$\vec{G}_{hkl} \cdot \vec{v} = (h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*) \cdot \left((\epsilon_2 - \epsilon_1)\frac{\vec{a}_1}{h} - \epsilon_2 \frac{\vec{a}_2}{k} + \epsilon_1 \frac{\vec{a}_3}{l} \right)$$

General proof of Bragg-Laue equivalence



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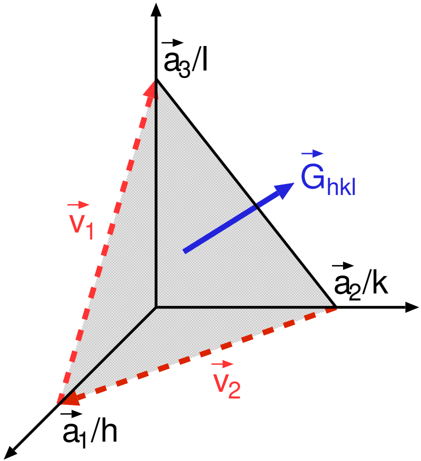

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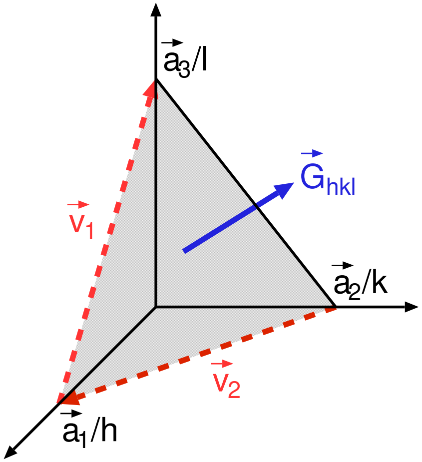
Thus $\vec{G}_{hkl}$ is indeed normal to the plane with Miller indices (hkl)

General proof of Bragg-Laue equivalence



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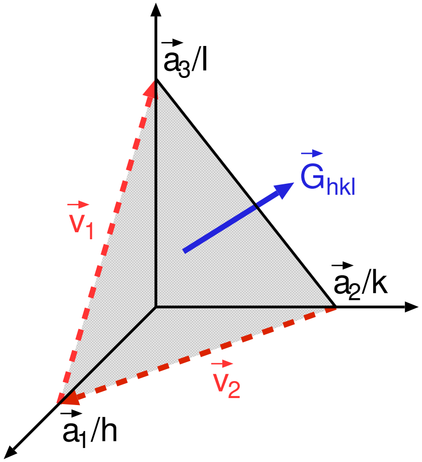
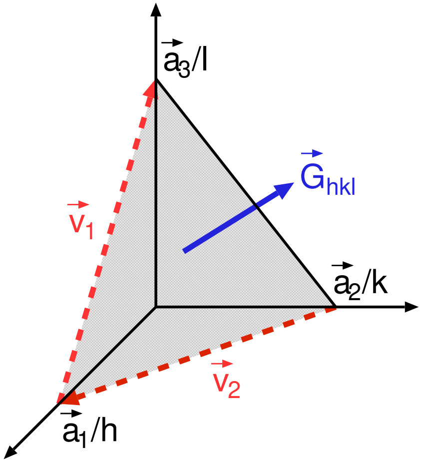


The spacing between planes (hkl) is simply given by the distance from the origin to the plane along a normal vector

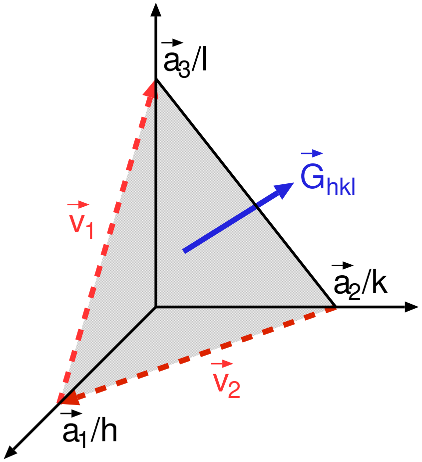
General proof of Bragg-Laue equivalence



The spacing between planes (hkl) is simply given by the distance from the origin to the plane along a normal vector

This can be computed as the projection of any vector which connects the origin to the plane onto the unit vector in the $\vec{G}_{hkl}$ direction. In this case, we choose, $\vec{a}_1/h$

General proof of Bragg-Laue equivalence



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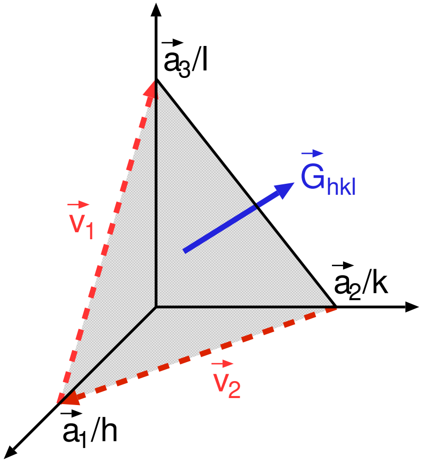

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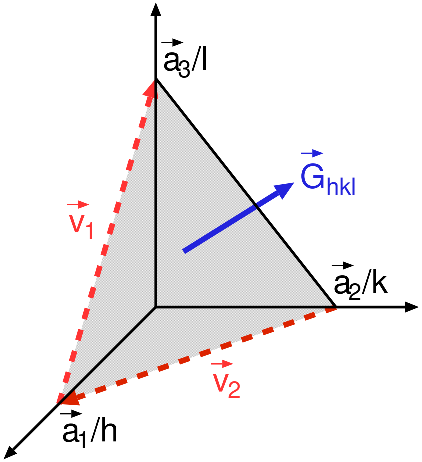

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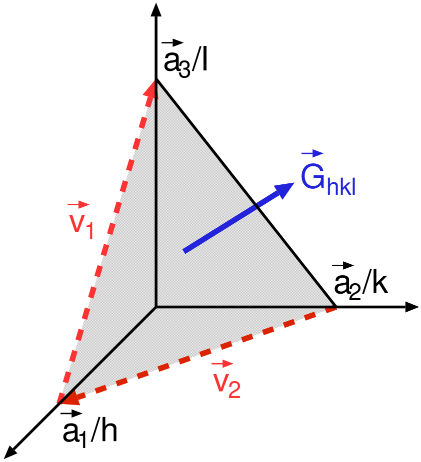
General proof of Bragg-Laue equivalence



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This can be computed as the projection of any vector which connects the origin to the plane onto the unit vector in the $\vec{G}_{hkl}$ direction. In this case, we choose, $\vec{a}_1/h$

$$\hat{G}_{hkl} = \frac{\vec{G}_{hkl}}{|\vec{G}_{hkl}|}$$

$$\hat{G}_{hkl} \cdot \frac{\vec{a}_1}{h} = \frac{(h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*)}{|\vec{G}_{hkl}|} \cdot \frac{\vec{a}_1}{h} = \frac{2\pi}{|\vec{G}_{hkl}|} = d_{hkl}$$