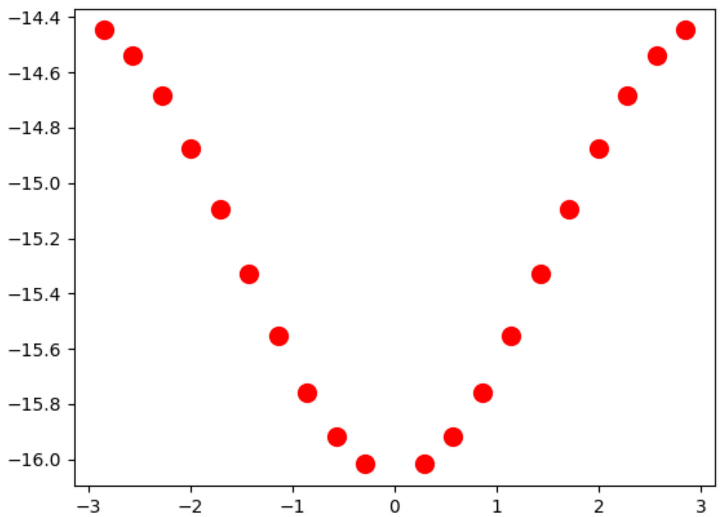
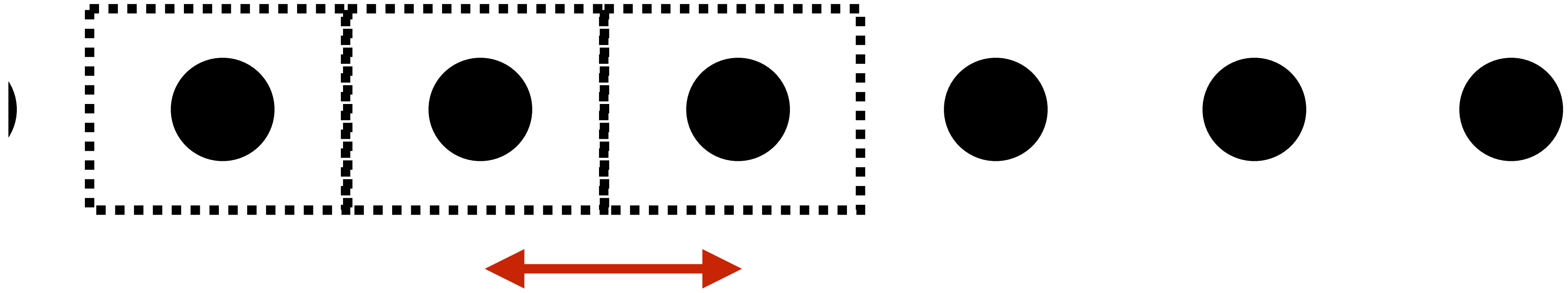
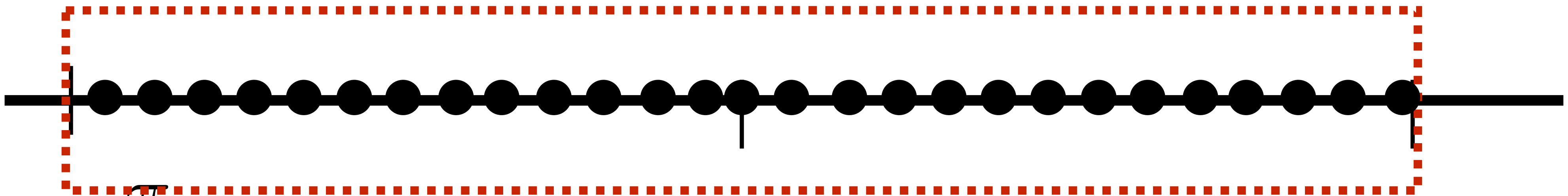


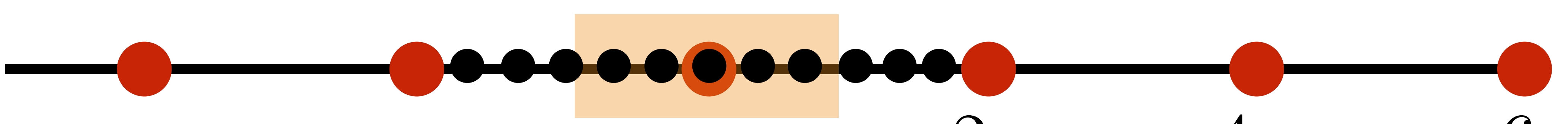
unit cell





$$k = -\frac{\pi}{a} \qquad\qquad k = \frac{\pi}{a}$$

First Brillouin Zone

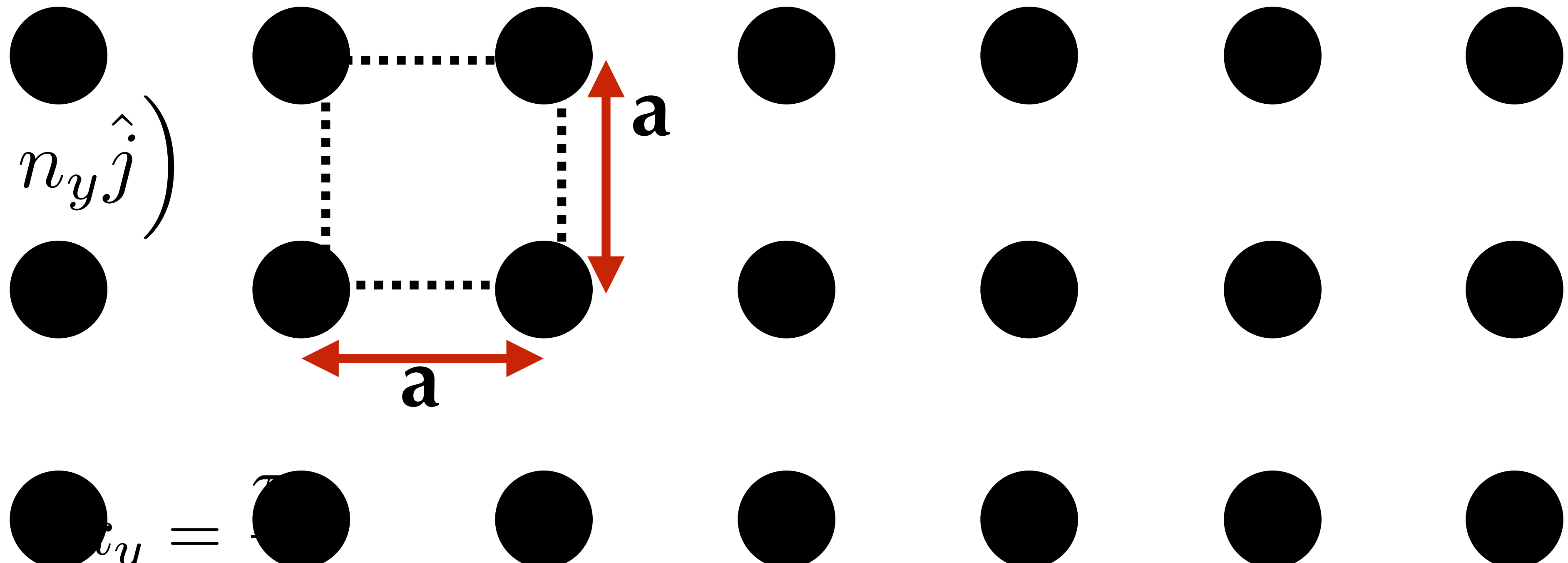


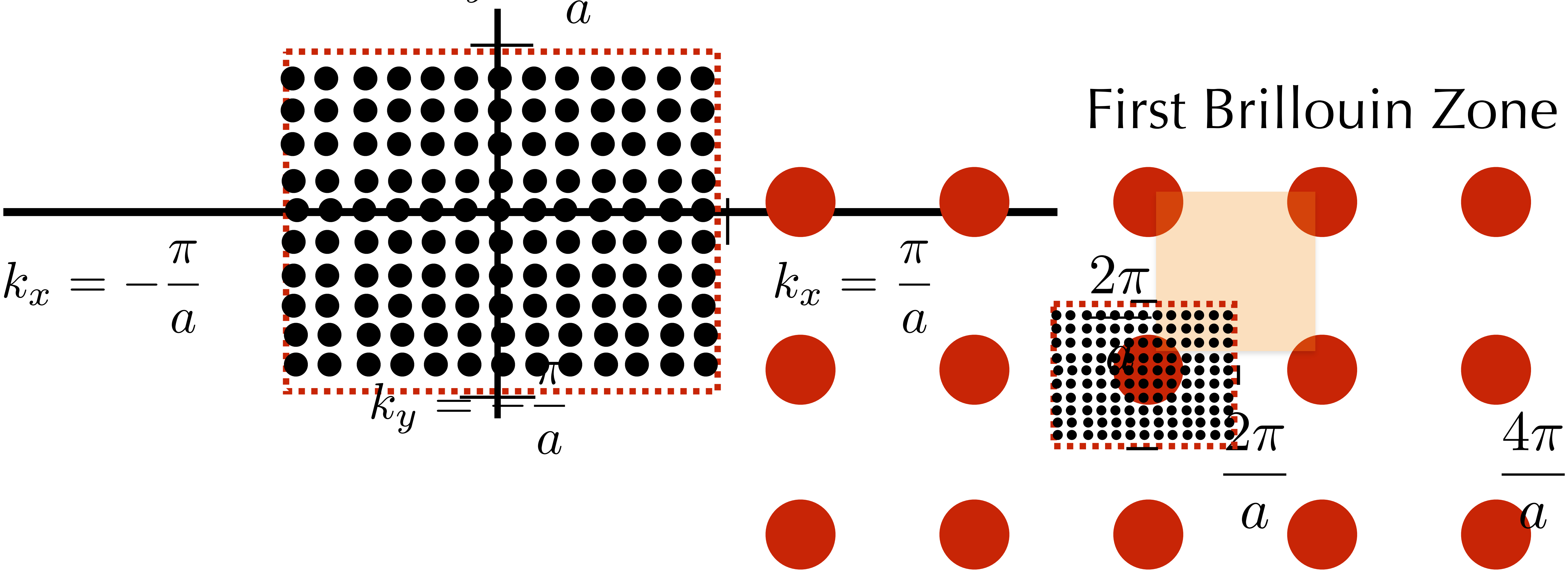
$$\frac{-2\pi}{a} \qquad 0 \qquad \frac{2\pi}{a} \qquad \frac{4\pi}{a} \qquad \frac{6\pi}{a}$$

A repeating atomic configuration in real space leads to a solution that repeats in k-space.

$$\Psi(x) = e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$\mathbf{k} = \frac{2\pi}{L}\left(n_x\hat{i} + n_y\hat{j}\right)$$

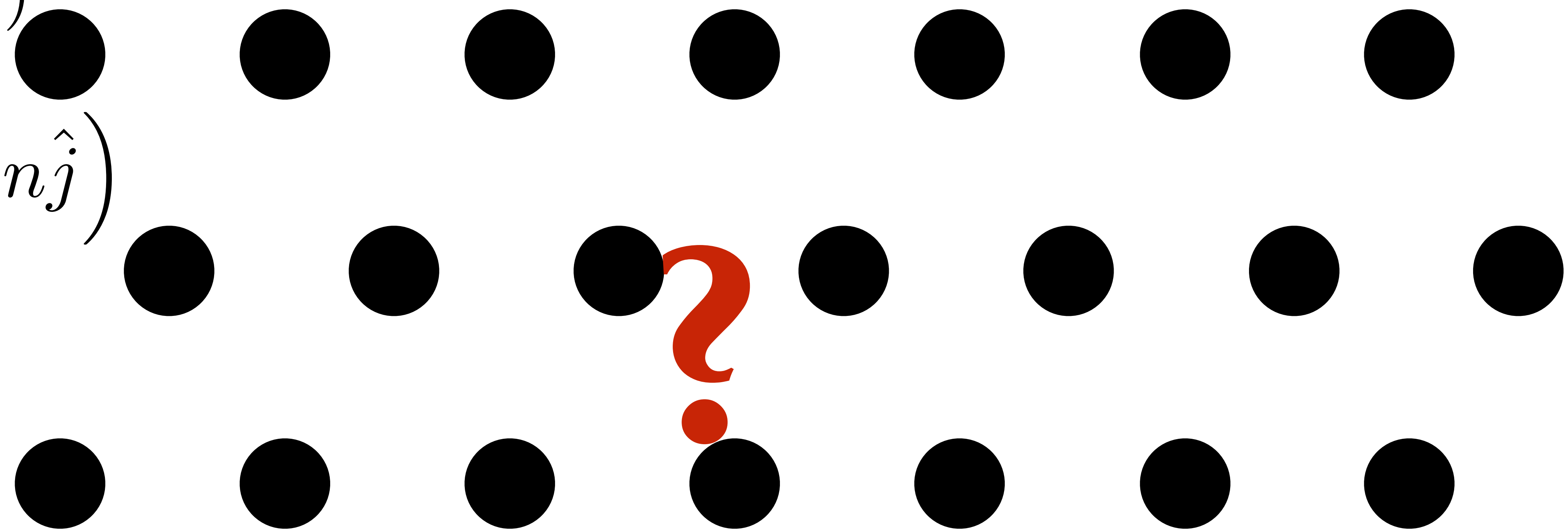


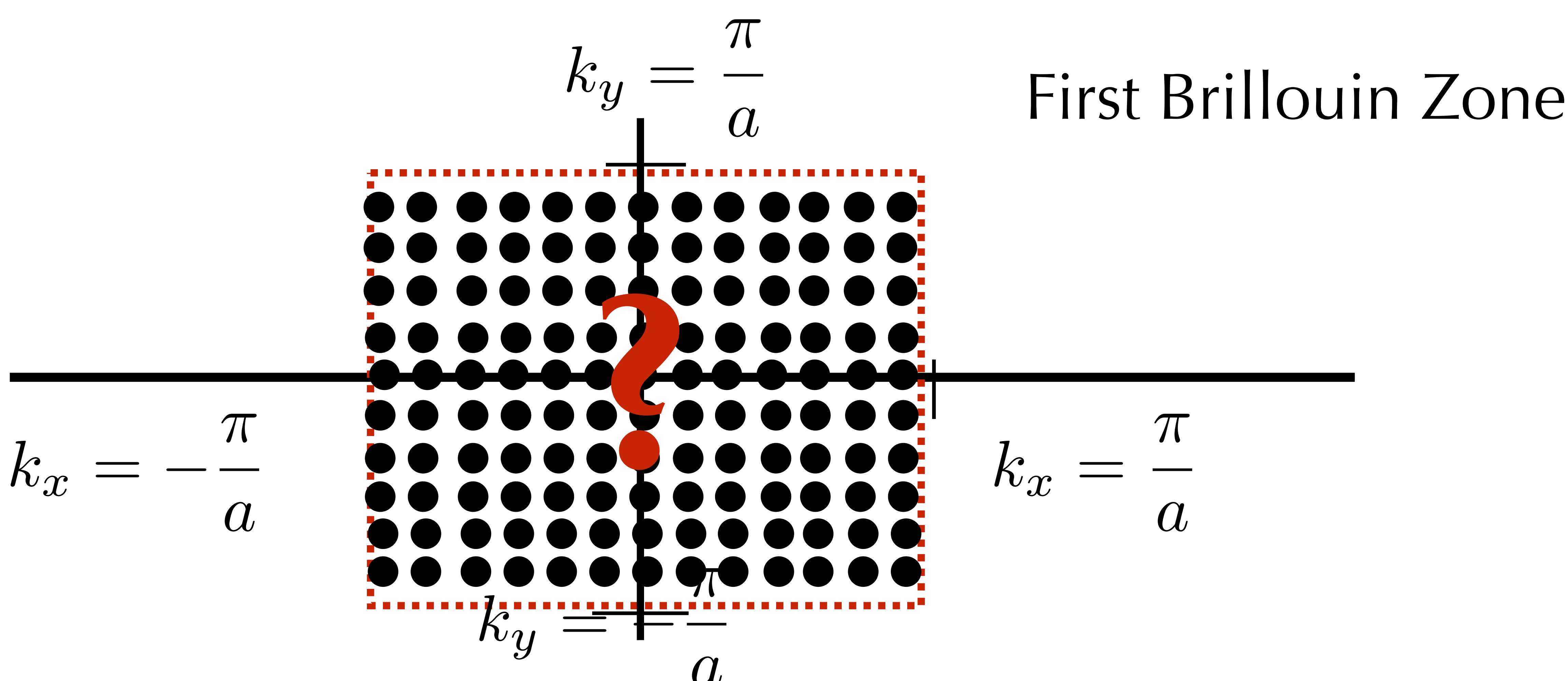


A repeating atomic configuration in real space leads to a solution that repeats in k-space.

$$\Psi(x) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r})$$

$$\mathbf{k} = \frac{2\pi}{Na}\left(m\hat{i} + n\hat{j}\right)$$





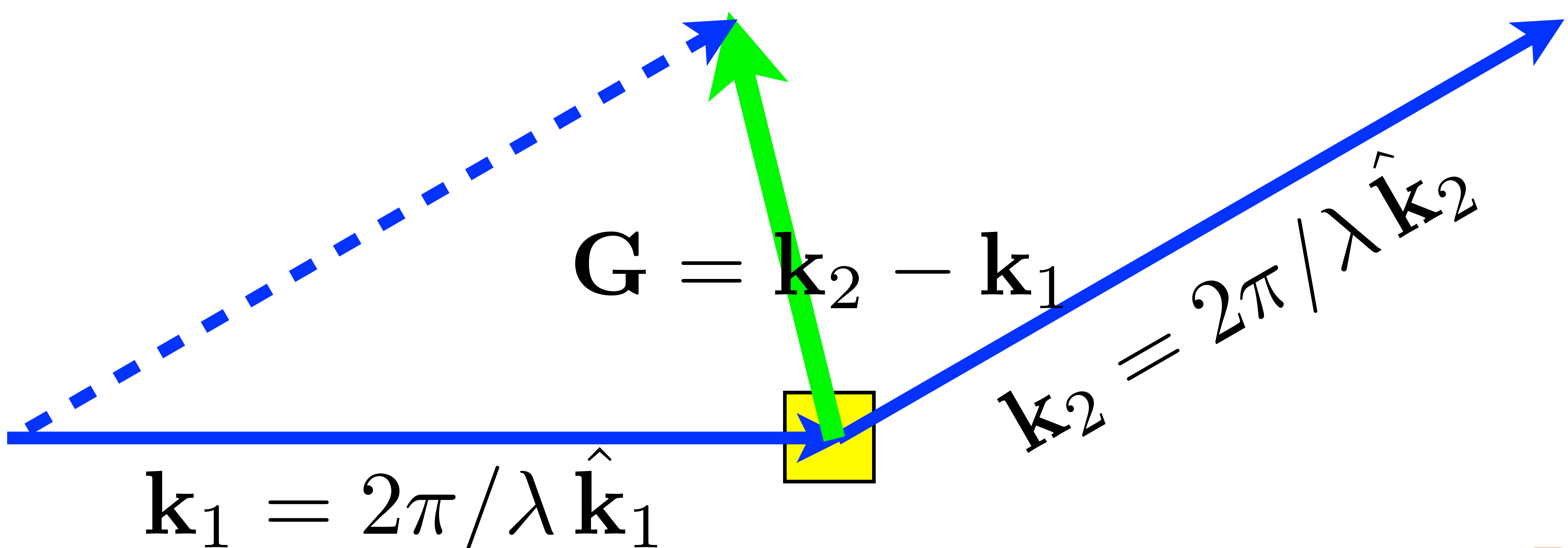
Reciprocal lattice review

$$R\cos\theta_1 + R\cos\theta_2 = n\lambda$$

$$kR\cos\theta_1 + kR\cos\theta_2 = nk\lambda$$

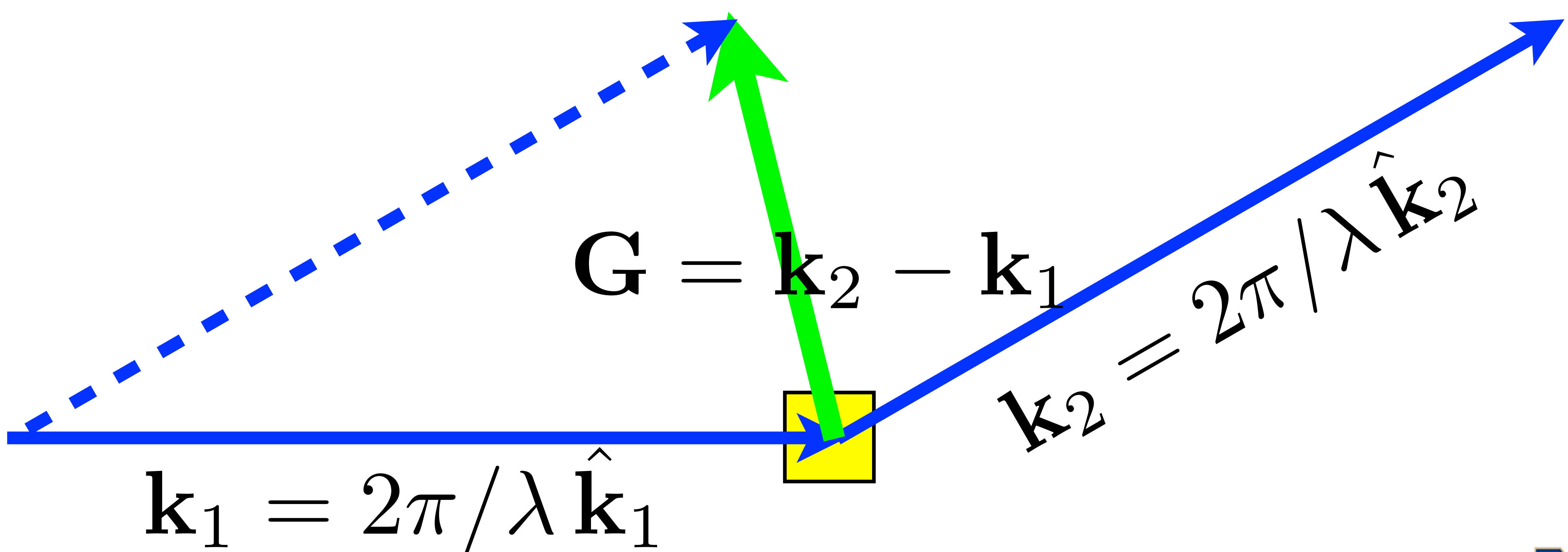
$$-\mathbf{R}\cdot\mathbf{k}_1 \qquad \mathbf{R}\cdot\mathbf{k}_2$$

$$\mathbf{R}\cdot\mathbf{G} = 2\pi n$$



Reciprocal lattice review

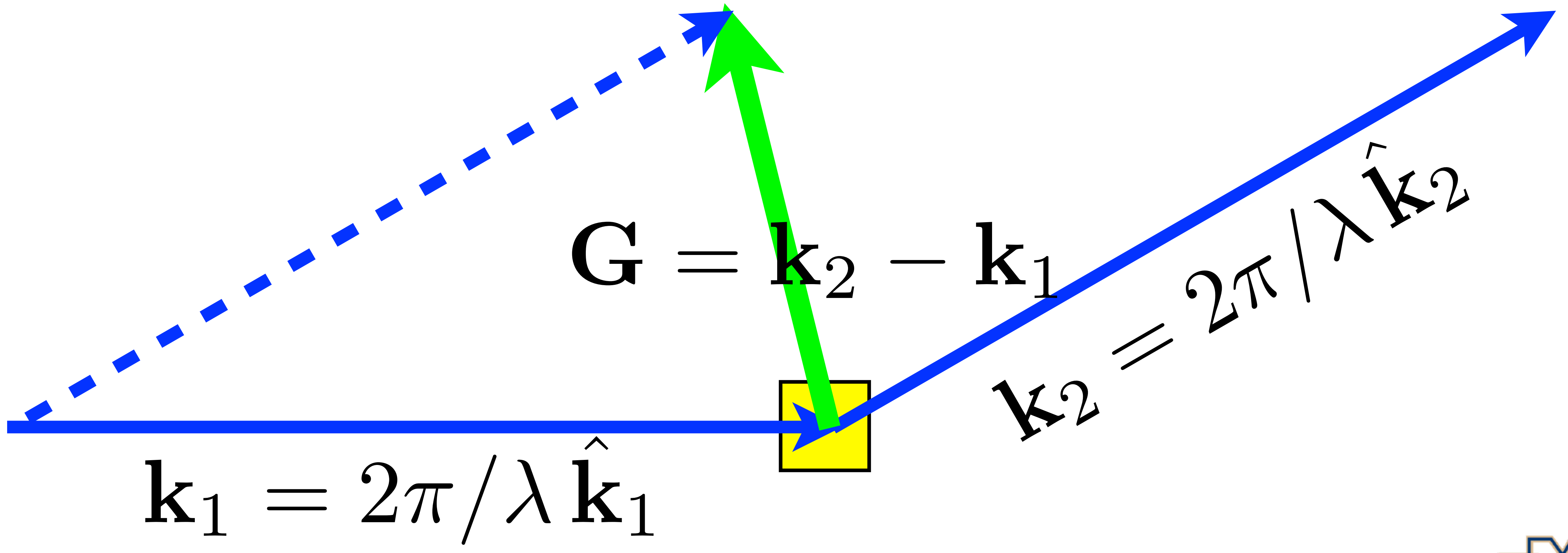
$$\mathbf{R} \cdot \mathbf{G} = 2\pi n$$



Reciprocal lattice review

$$\mathbf{R} \cdot \mathbf{G} = 2\pi n$$

$$\mathbf{R} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3$$



Reciprocal lattice review

$$\mathbf{R}\cdot\mathbf{G}=2\pi n$$

$$\mathbf{R}=m_1\mathbf{a}_1+m_2\mathbf{a}_2+m_3\mathbf{a}_3$$

$$\mathbf{G}=n_1\mathbf{b}_1+n_2\mathbf{b}_2+n_3\mathbf{b}_3$$

Reciprocal lattice review

$$\mathbf{R} \cdot \mathbf{G} = 2\pi n$$

$$\mathbf{R} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3$$

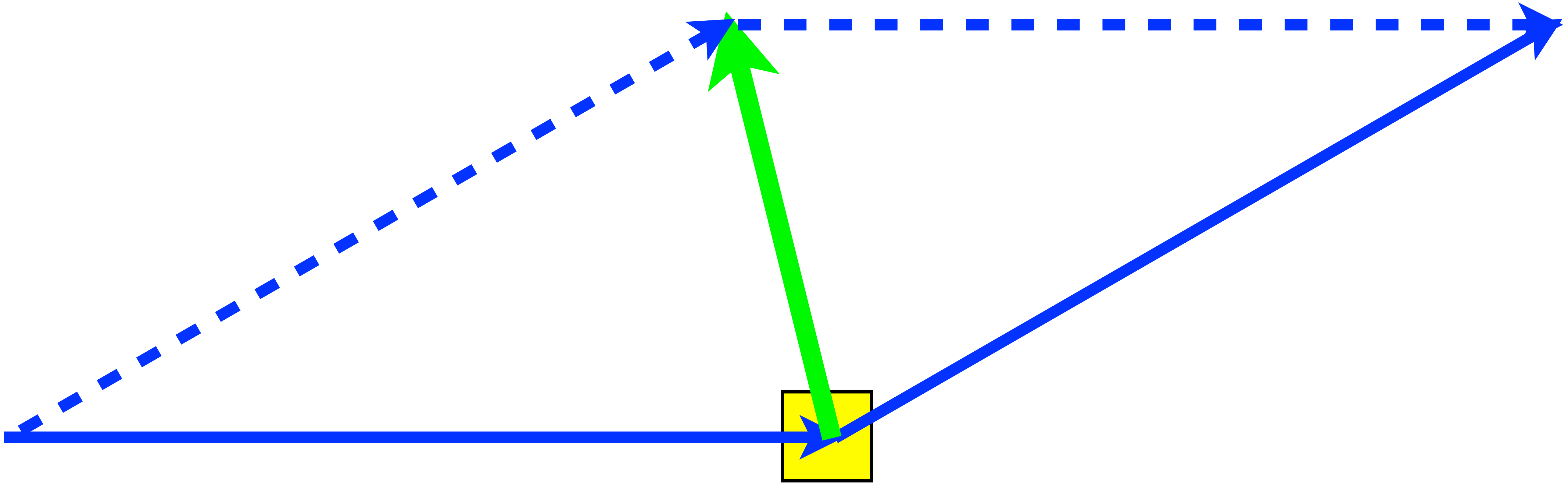
$$\mathbf{G} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3$$

$$\mathbf{b}_i = 2\pi \frac{(\mathbf{a}_j \times \mathbf{a}_k)}{\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k)}$$

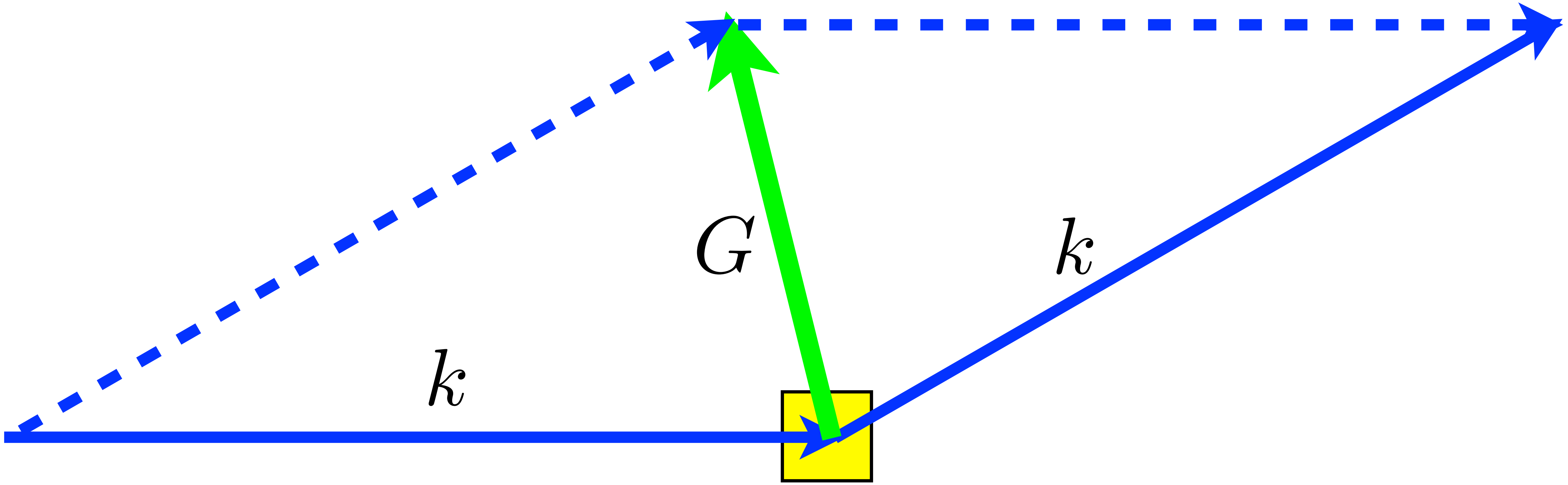
What is all this good for?

What is all this good for? General Bragg's Law!

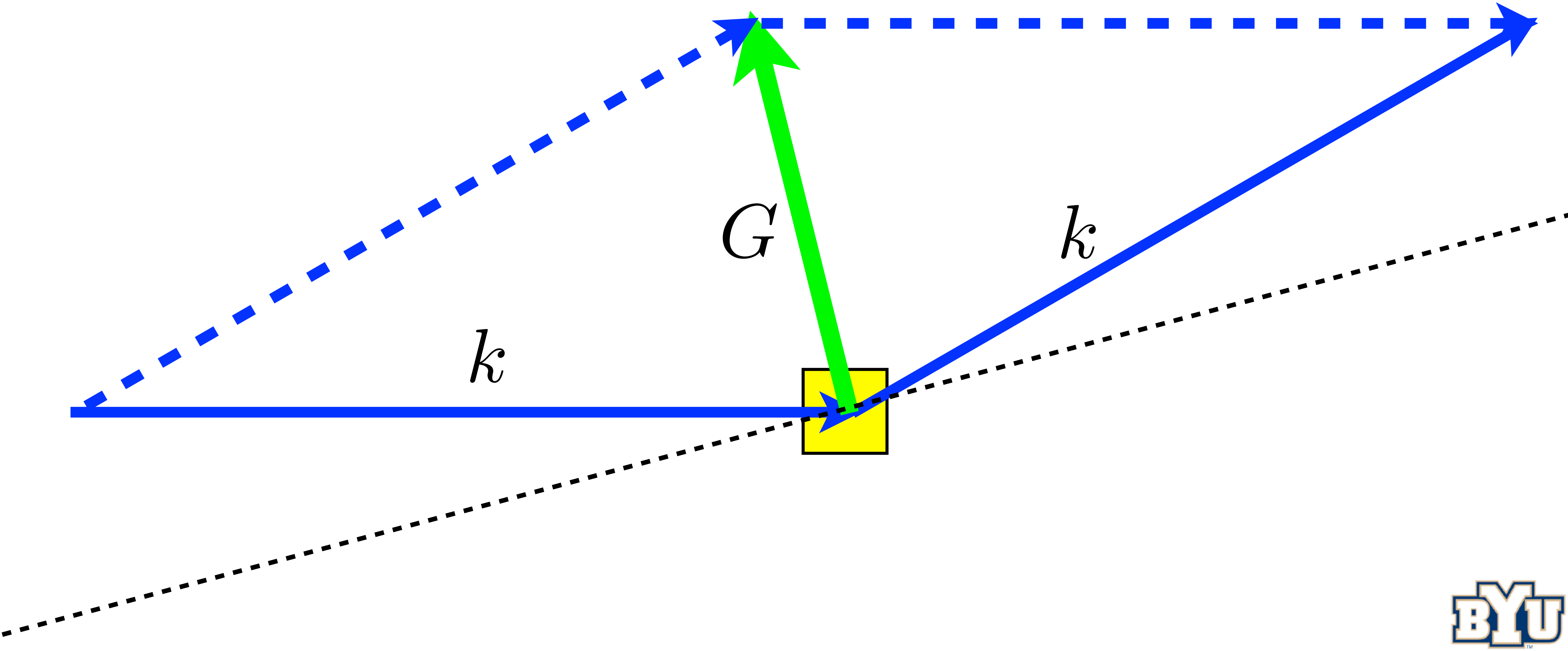
What is all this good for? General Bragg's Law!



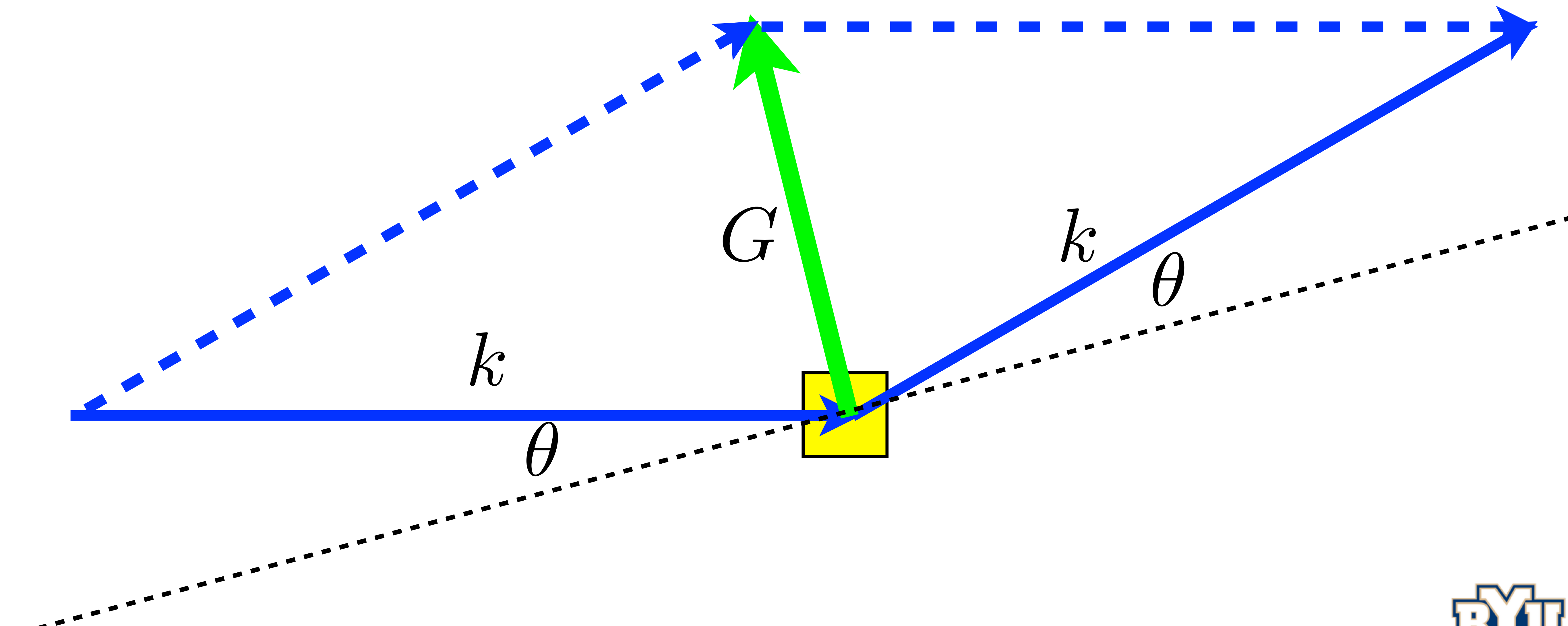
What is all this good for?
General Bragg's Law!



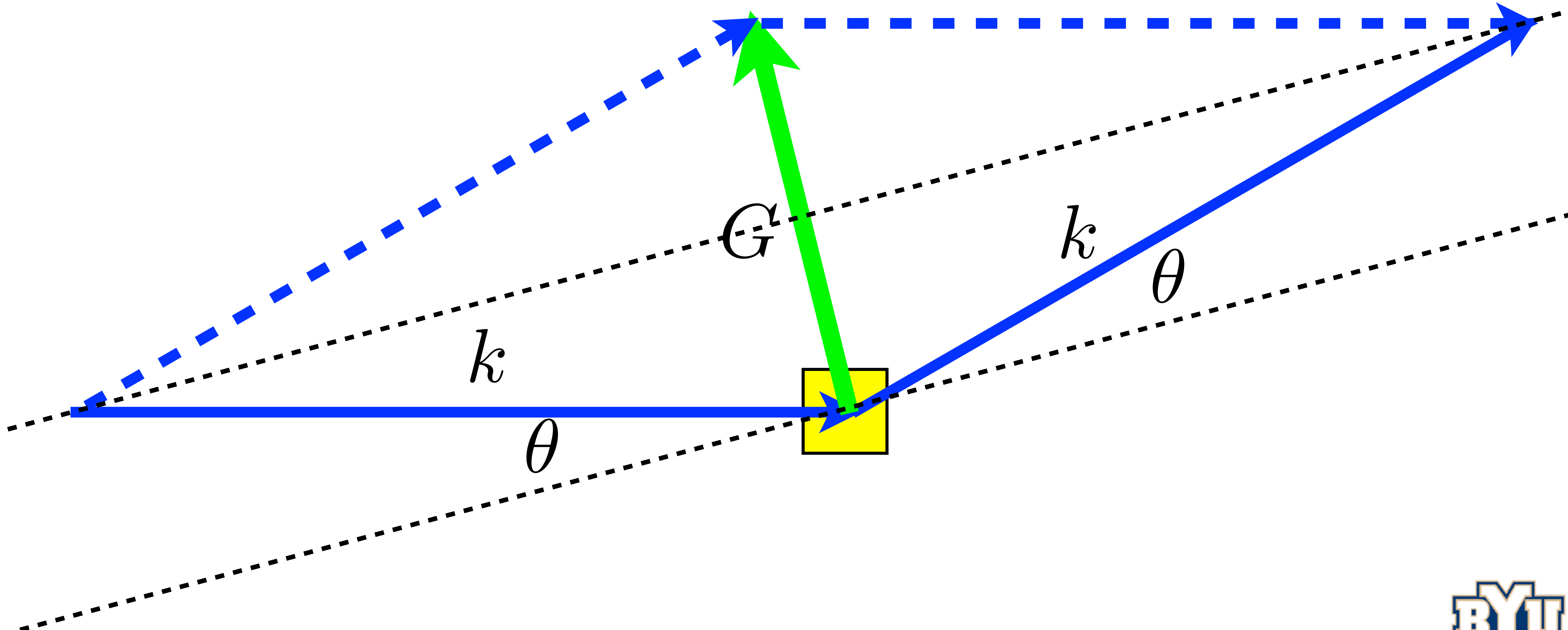
What is all this good for? General Bragg's Law!



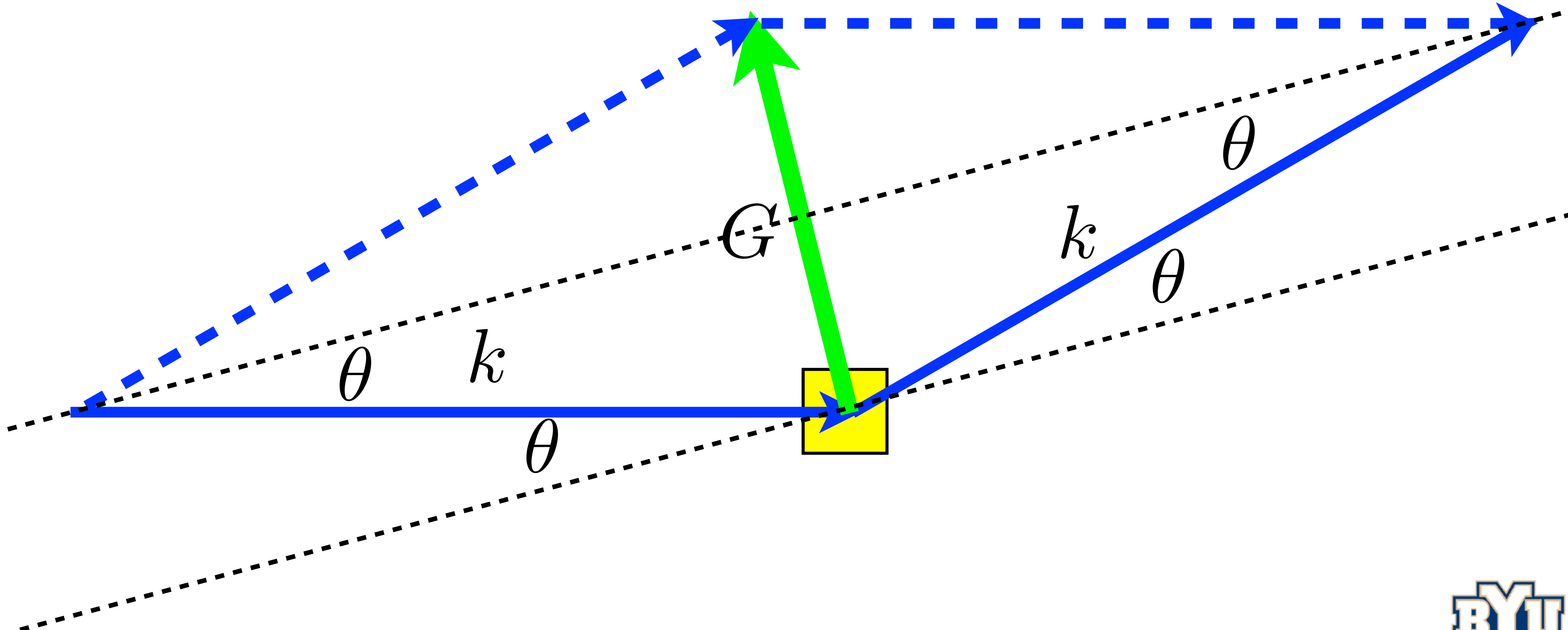
What is all this good for? General Bragg's Law!



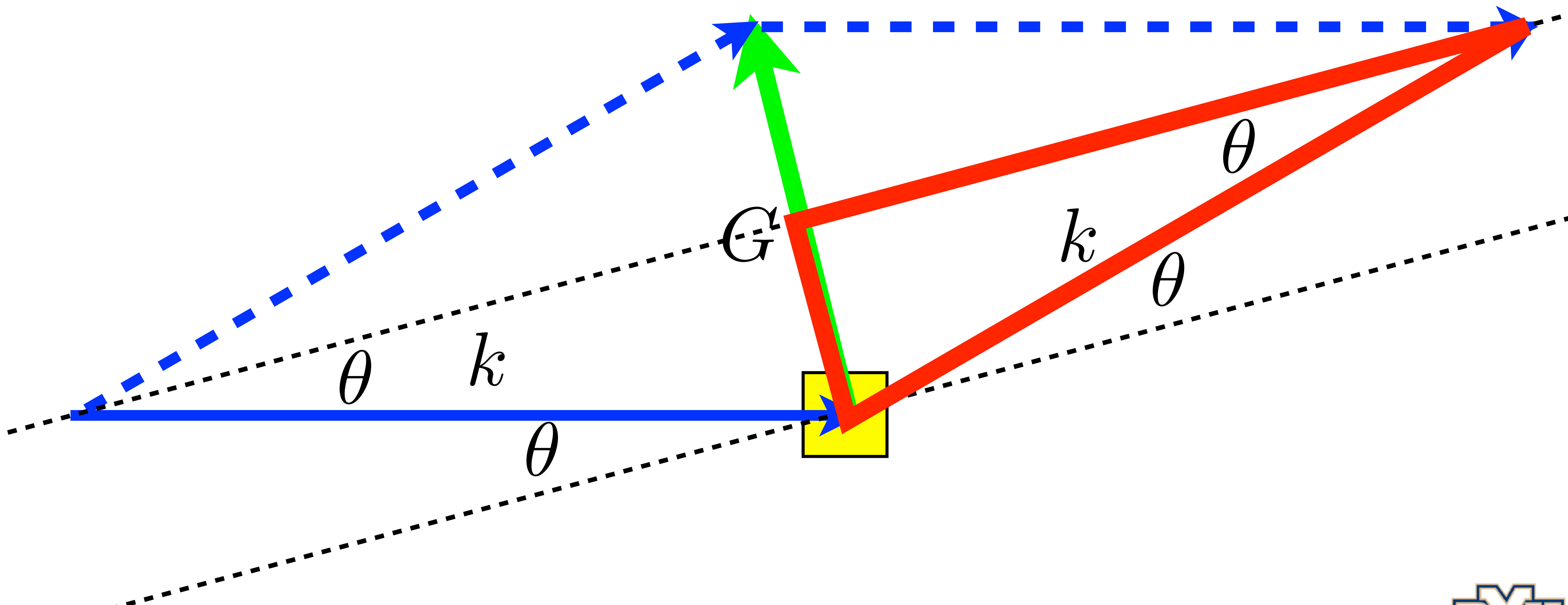
What is all this good for? General Bragg's Law!

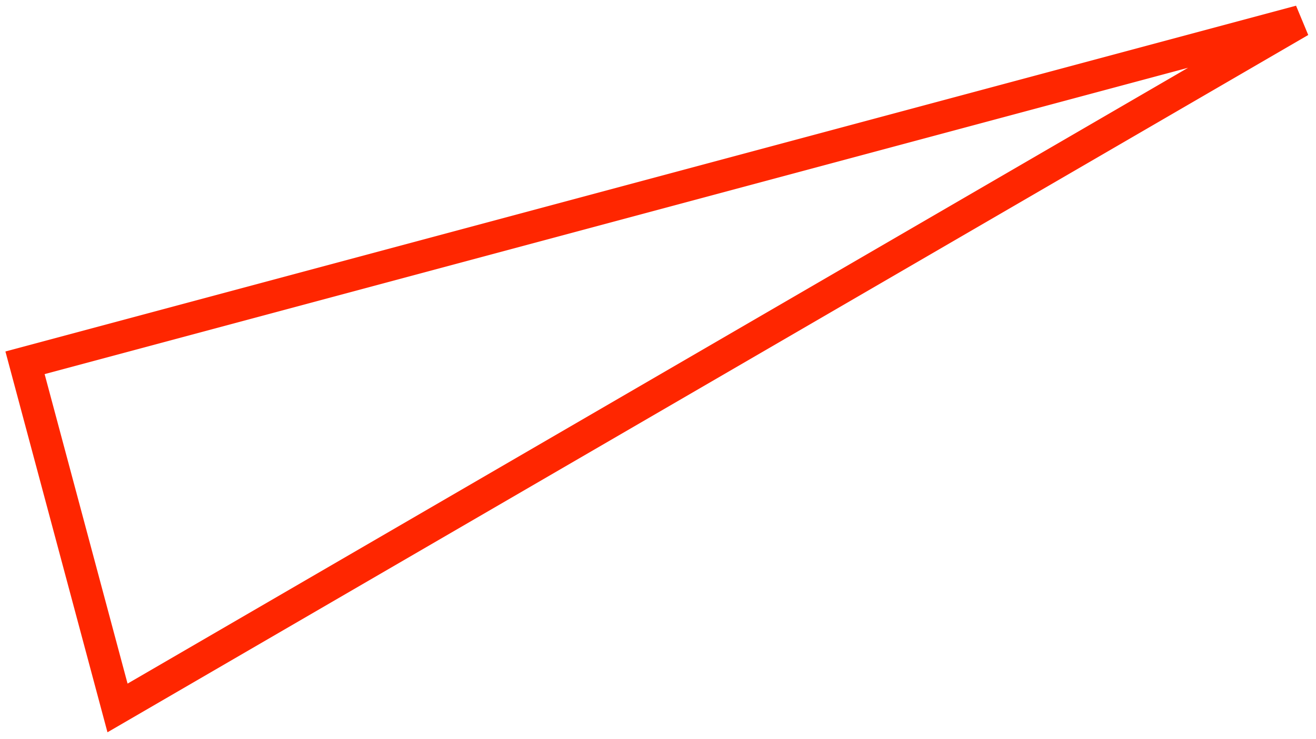


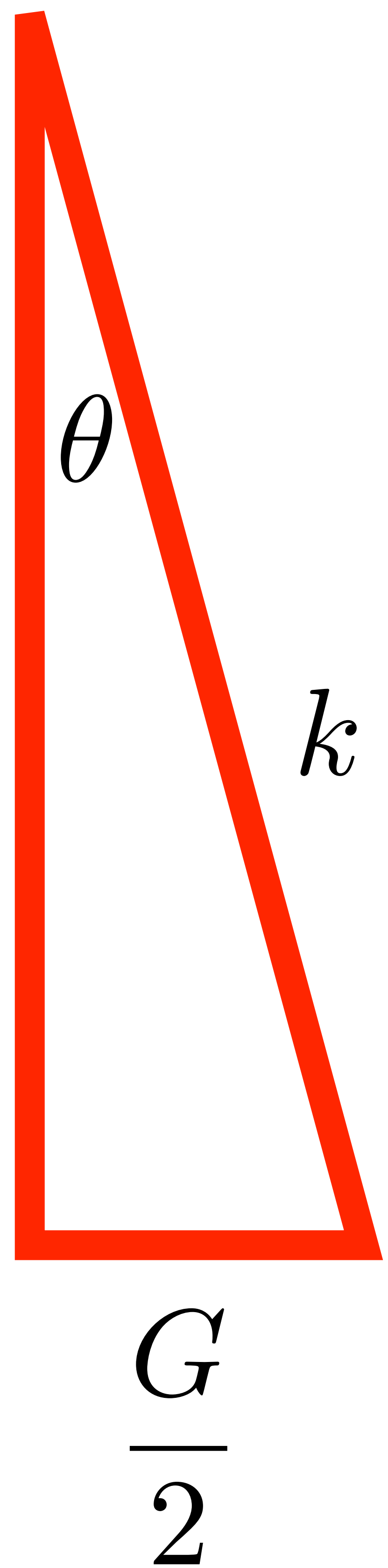
What is all this good for? General Bragg's Law!



What is all this good for? General Bragg's Law!

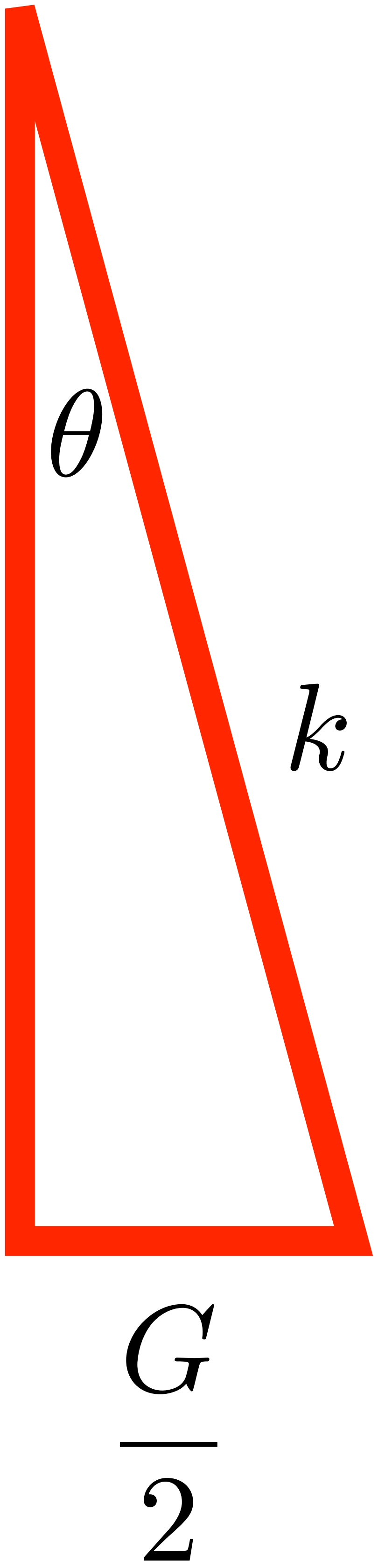






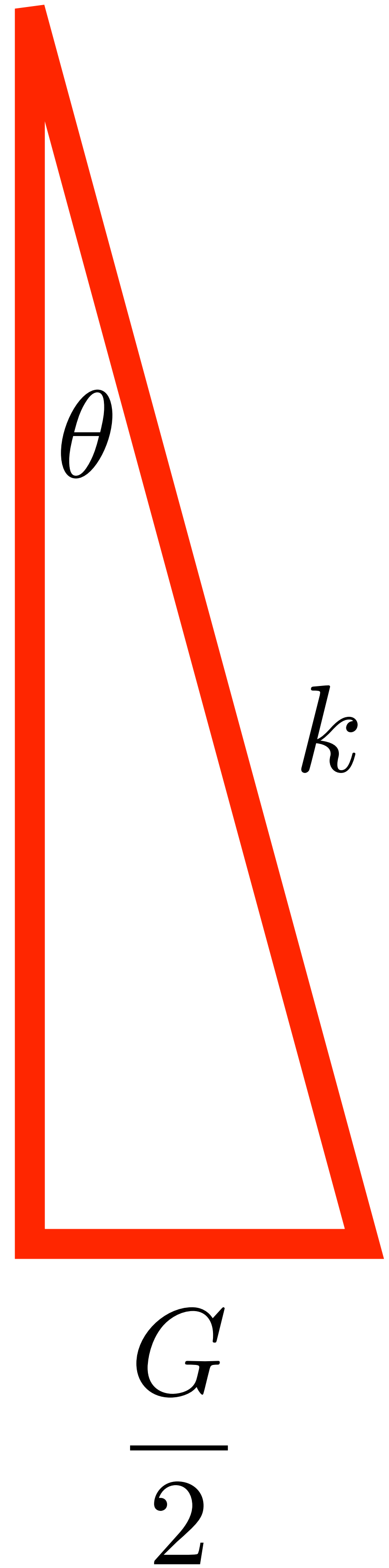
θ
k
$\frac{G}{2}$

$$\frac{G}{2k} = \sin\theta$$



$$\frac{G}{2k} = \sin\theta$$

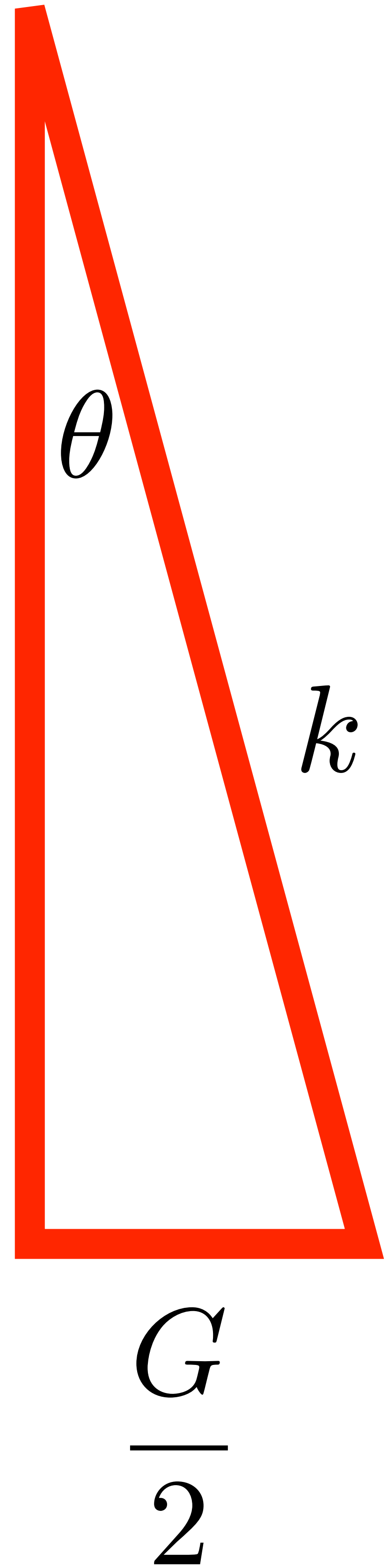
$$G \leq 2k$$

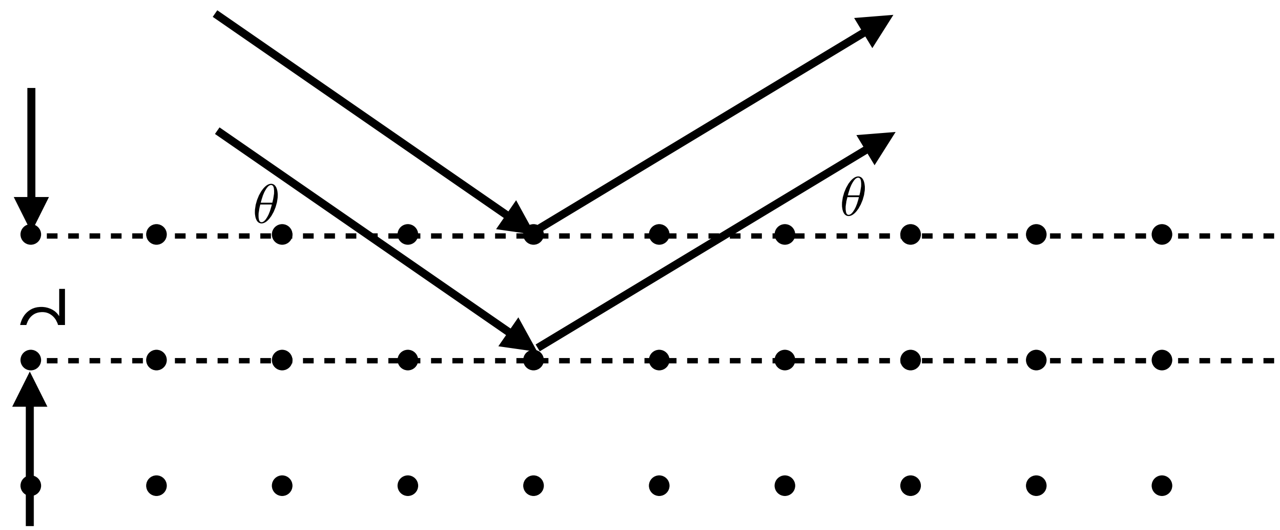


$$\mathbf{G} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3$$

$$\frac{G}{2k} = \sin\theta$$

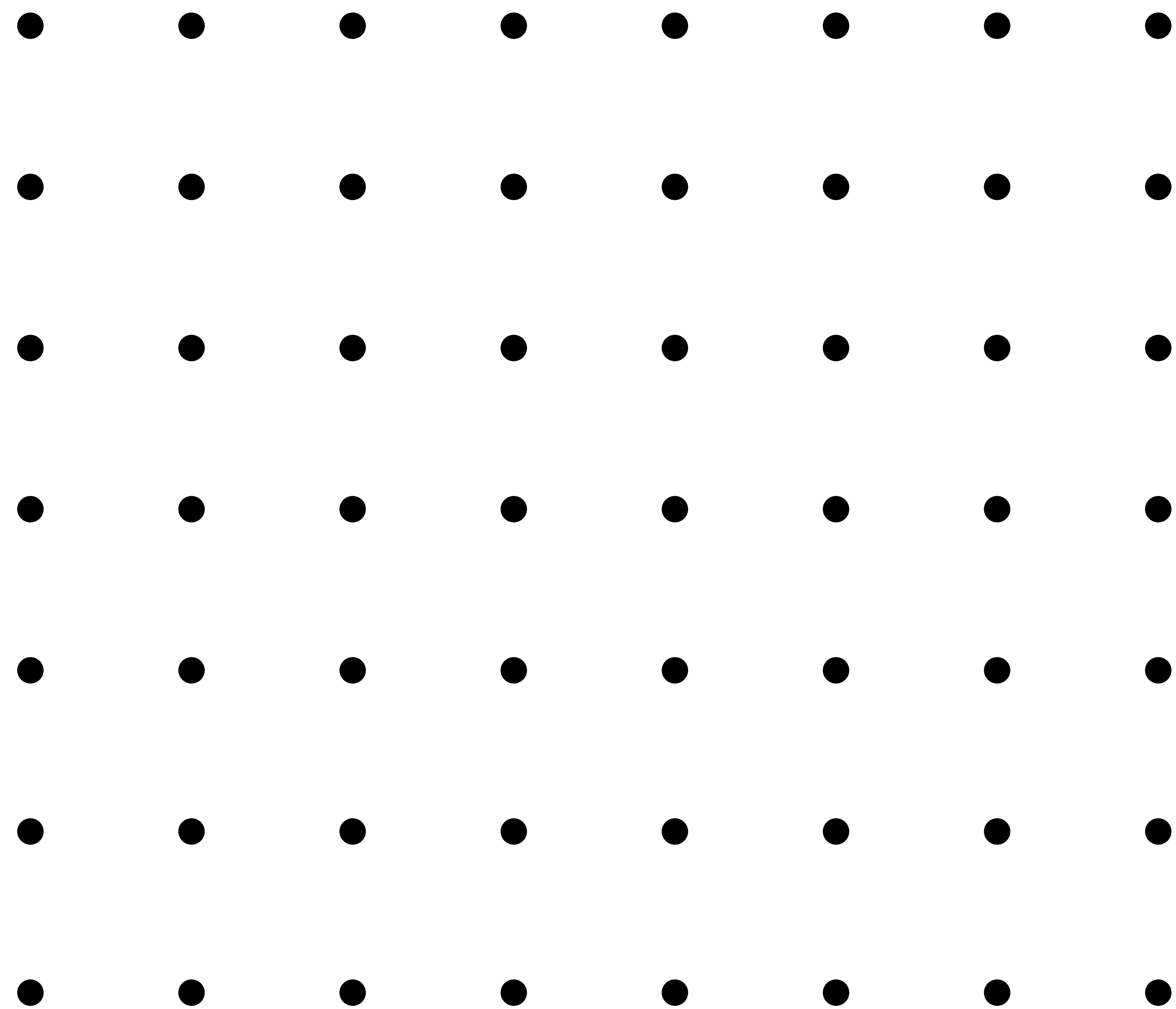
$$G \leq 2k$$





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

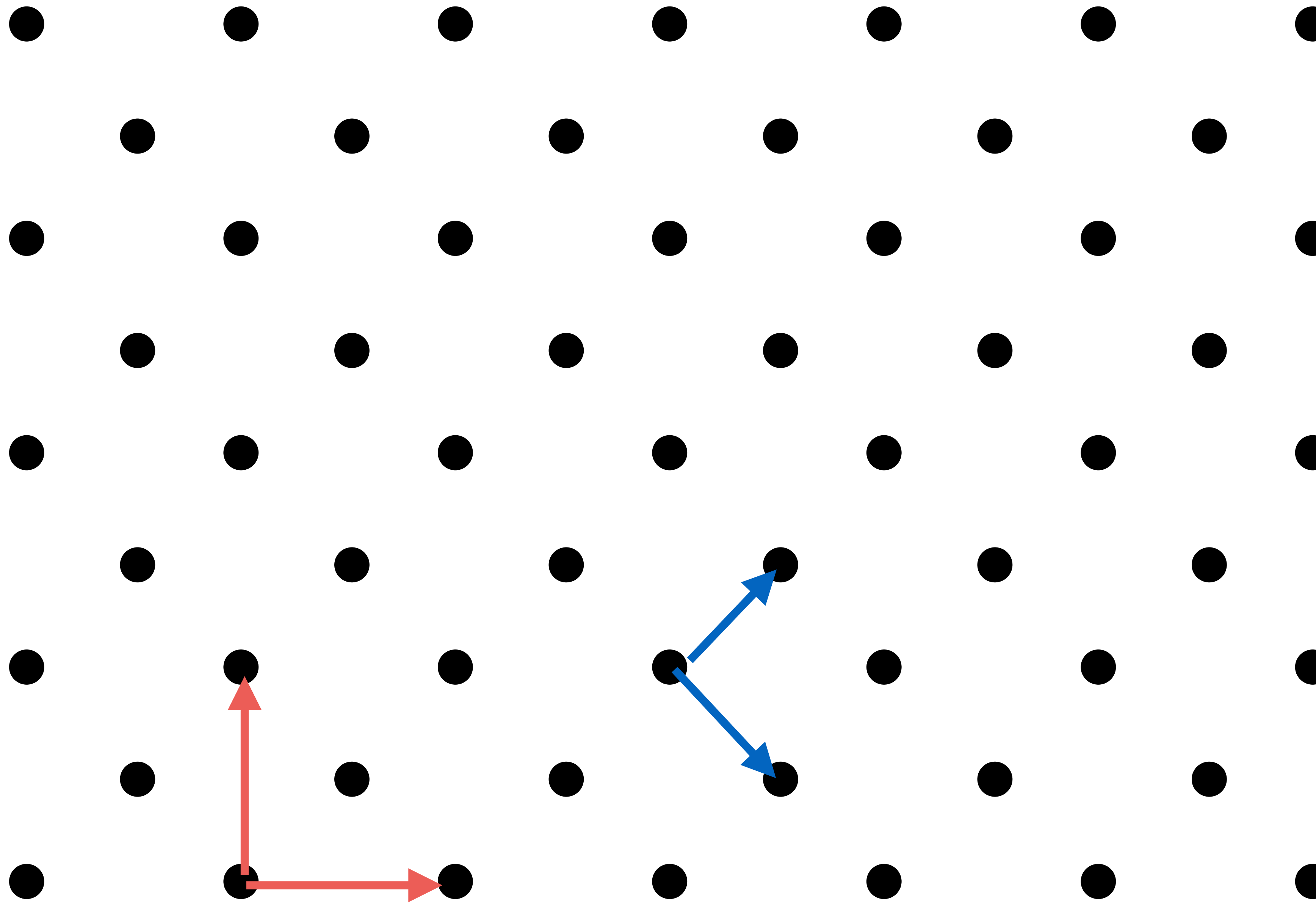
$$G = 2k \sin \theta$$



$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\Delta\mathbf{k}} \right] \boxed{\sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p\cdot\Delta\mathbf{k}}}$$

$$\lambda = 1.542 \text{ Å}$$

$$a = 3.61 \text{ Å}$$



$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)}$$

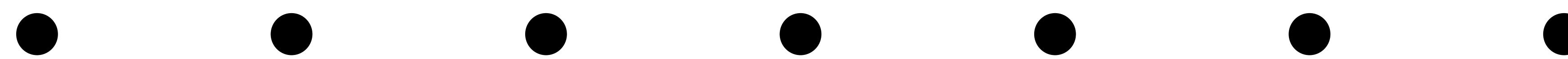
$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$

$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\Delta\mathbf{k}} \right] \boxed{\sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p\cdot\Delta\mathbf{k}}}$$

$$\lambda = 1.542 \text{ Å}$$

$$a = 3.61 \text{ Å}$$

h



TableForm=

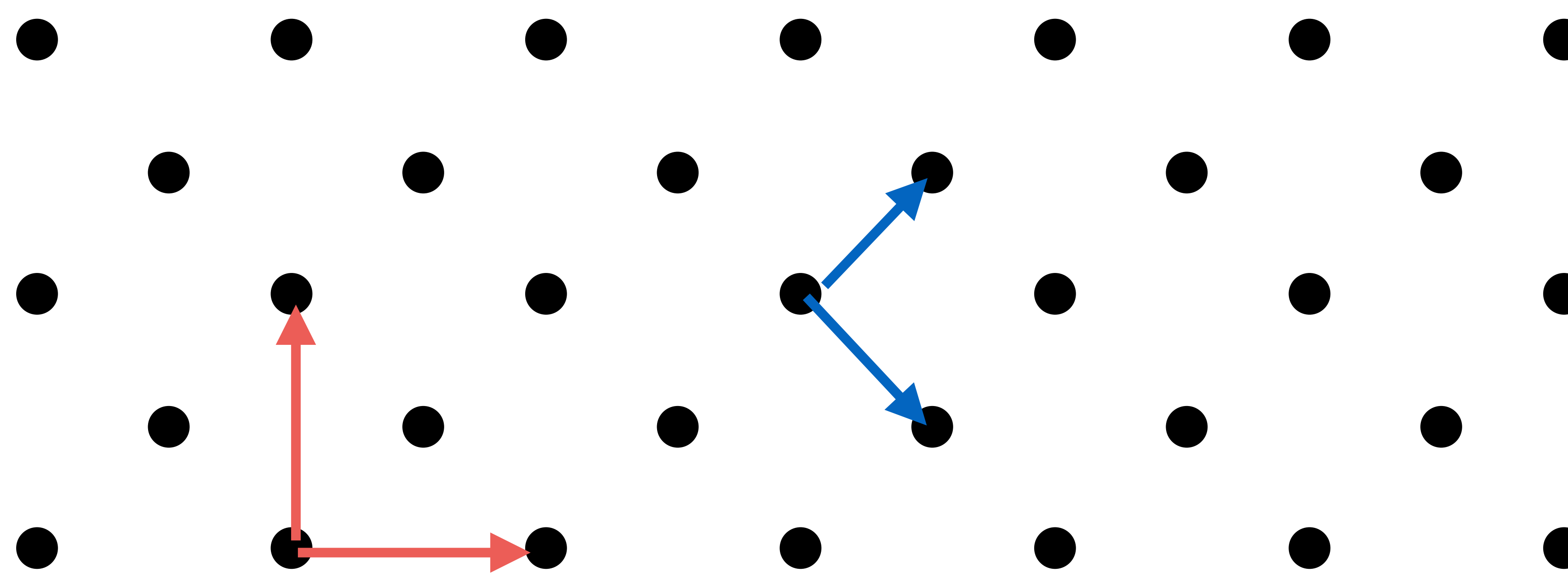
k

0.	17.5801	37.1624	64.9739	90. − 36.3554 i
17.5801	25.2866	42.4835	72.7711	90. − 39.3563 i
37.1624	42.4835	58.6818	90. − 23.9993 i	90. − 46.6866 i
64.9739	72.7711	90. − 23.9993 i	90. − 42.0372 i	90. − 55.662 i
90. − 36.3554 i	90. − 39.3563 i	90. − 46.6866 i	90. − 55.662 i	90. − 64.7129 i

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)}$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$



$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\Delta\mathbf{k}} \right] \boxed{\sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p\cdot\Delta\mathbf{k}}}$$

$$\lambda = 1.542 \text{ Å}$$

$$a = 3.61 \text{ Å}$$

h

k

0.	12.3318	25.2866	39.8455	58.6818
12.3318	17.5801	28.5265	42.4835	61.7131
25.2866	28.5265	37.1624	50.3584	72.7711
39.8455	42.4835	50.3584	64.9739	90. - 20.9914 i
58.6818	61.7131	72.7711	90. - 20.9914 i	90. - 36.3554 i

h

TableForm=

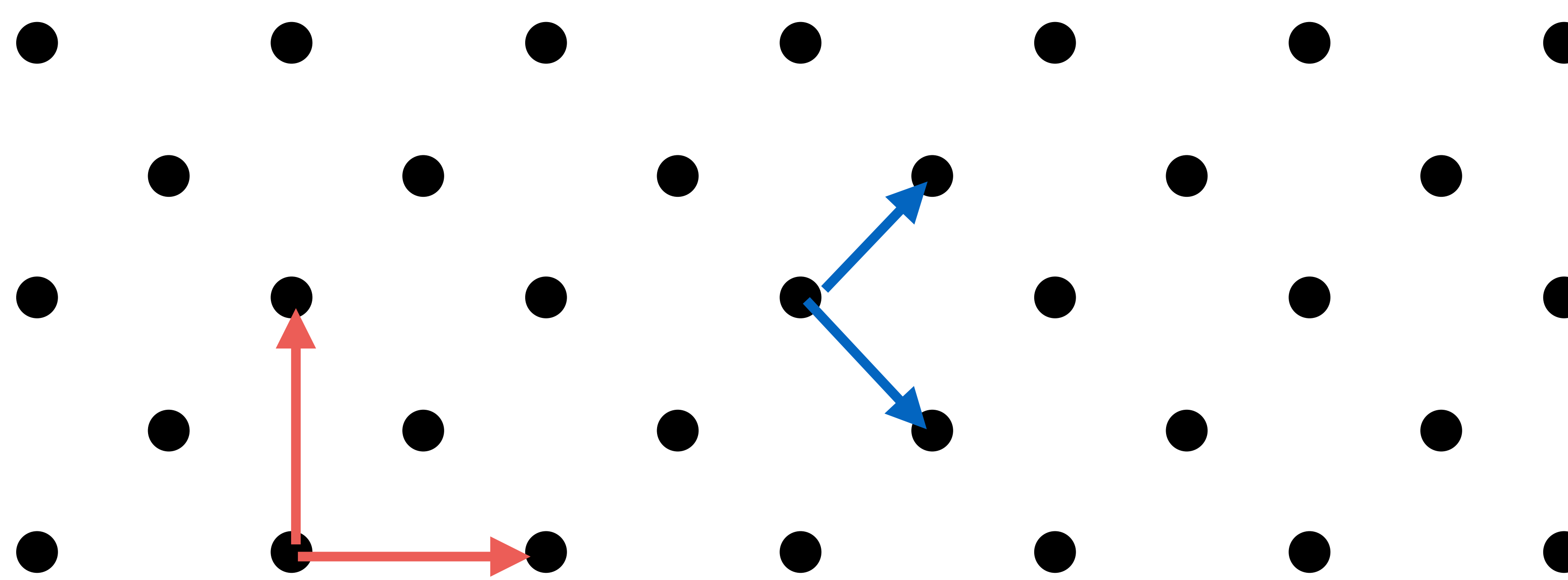
k

0.	17.5801	37.1624	64.9739	90. - 36.3554 i
17.5801	25.2866	42.4835	72.7711	90. - 39.3563 i
37.1624	42.4835	58.6818	90. - 23.9993 i	90. - 46.6866 i
64.9739	72.7711	90. - 23.9993 i	90. - 42.0372 i	90. - 55.662 i
90. - 36.3554 i	90. - 39.3563 i	90. - 46.6866 i	90. - 55.662 i	90. - 64.7129 i

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)}$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$



$$\mathcal{E} \propto f_e(\theta)\left[\sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\Delta\mathbf{k}}\right]\boxed{\sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p\cdot\Delta\mathbf{k}}}$$

$$\lambda = 1.542\ \text{Å}$$

$$a = 3.61\ \text{Å}$$

h

k

0.	~~12.3318~~	25.2866	~~39.8455~~	58.6818
~~12.3318~~	17.5801	~~28.5265~~	42.4835	~~61.7131~~
25.2866	~~28.5265~~	37.1624	~~50.3584~~	72.7711
~~39.8455~~	42.4835	~~50.3584~~	64.9739	90. - 20.9914 i
58.6818	~~61.7131~~	72.7711	90. - 20.9914 i	90. - 36.3554 i

h

TableForm=

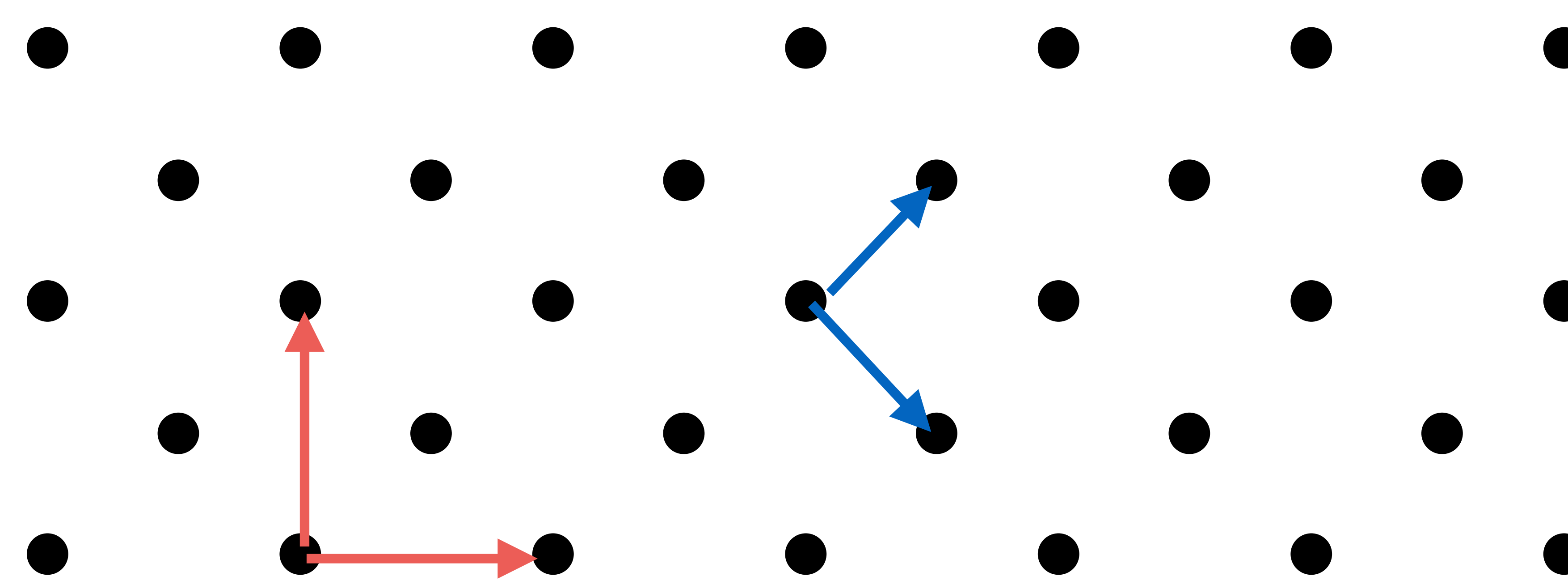
k

0.	17.5801	37.1624	64.9739	90. - 36.3554 i
17.5801	25.2866	42.4835	72.7711	90. - 39.3563 i
37.1624	42.4835	58.6818	90. - 23.9993 i	90. - 46.6866 i
64.9739	72.7711	90. - 23.9993 i	90. - 42.0372 i	90. - 55.662 i
90. - 36.3554 i	90. - 39.3563 i	90. - 46.6866 i	90. - 55.662 i	90. - 64.7129 i

$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1\cdot(\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2\cdot(\mathbf{a}_3 \times \mathbf{a}_1)}$$

$$\mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3\cdot(\mathbf{a}_1 \times \mathbf{a}_2)}$$



$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\Delta\mathbf{k}} \right] \boxed{\sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p\cdot\Delta\mathbf{k}}}$$

$$\lambda = 1.542 \text{ Å}$$

$$a = 3.61 \text{ Å}$$

h

k

0.	~~12.3318~~	25.2866	~~39.8455~~	58.6818
~~12.3318~~	17.5801	~~28.5265~~	42.4835	~~61.7131~~
25.2866	~~28.5265~~	37.1624	~~50.3584~~	72.7711
~~39.8455~~	42.4835	~~50.3584~~	64.9739	90. - 20.9914 i
58.6818	~~61.7131~~	72.7711	90. - 20.9914 i	90. - 36.3554 i

h

TableForm=

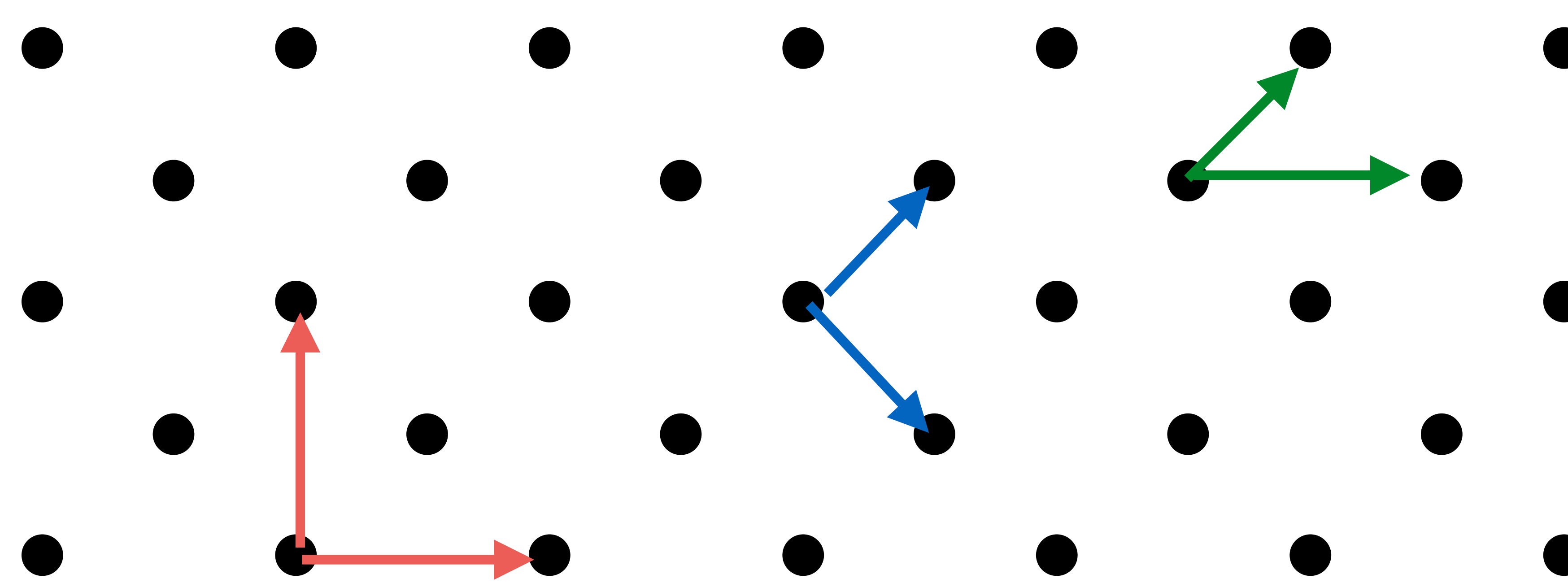
k

0.	17.5801	37.1624	64.9739	90. - 36.3554 i
17.5801	25.2866	42.4835	72.7711	90. - 39.3563 i
37.1624	42.4835	58.6818	90. - 23.9993 i	90. - 46.6866 i
64.9739	72.7711	90. - 23.9993 i	90. - 42.0372 i	90. - 55.662 i
90. - 36.3554 i	90. - 39.3563 i	90. - 46.6866 i	90. - 55.662 i	90. - 64.7129 i

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)}$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$



$$\mathcal{E} \propto f_e(\theta)\left[\sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\Delta\mathbf{k}}\right]\boxed{\sum_{\mathbf{r}_p} f_{ap}(\theta)e^{i\mathbf{r}_p\cdot\Delta\mathbf{k}}}$$

$$\lambda = 1.542\ \text{Å}$$

$$a = 3.61\ \text{Å}$$

h ↓ k →

0.	~~12.3318~~	25.2866	~~39.8455~~	58.6818
~~12.3318~~	17.5801	~~28.5265~~	42.4835	~~61.7131~~
25.2866	~~28.5265~~	37.1624	~~50.3584~~	72.7711
~~39.8455~~	42.4835	~~50.3584~~	64.9739	90. − 20.9914 i
58.6818	~~61.7131~~	72.7711	90. − 20.9914 i	90. − 36.3554 i

h ↓ k →

TableForm=

0.	17.5801	37.1624	64.9739	90. − 36.3554 i
17.5801	25.2866	42.4835	72.7711	90. − 39.3563 i
37.1624	42.4835	58.6818	90. − 23.9993 i	90. − 46.6866 i
64.9739	72.7711	90. − 23.9993 i	90. − 42.0372 i	90. − 55.662 i
90. − 36.3554 i	90. − 39.3563 i	90. − 46.6866 i	90. − 55.662 i	90. − 64.7129 i

0.	25.2866	58.6818	90. − 42.0372 i
17.5801	17.5801	42.4835	90. − 23.9993 i
37.1624	25.2866	37.1624	72.7711
64.9739	42.4835	42.4835	64.9739
90. − 36.3554 i	72.7711	58.6818	72.7711

$$\mathcal{E} \propto f_e(\theta)\left[\sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\Delta\mathbf{k}}\right]\boxed{\sum_{\mathbf{r}_p} f_{ap}(\theta)\, e^{i\mathbf{r}_p\cdot\Delta\mathbf{k}}}$$

$$\lambda = 1.542\ \text{Å}$$

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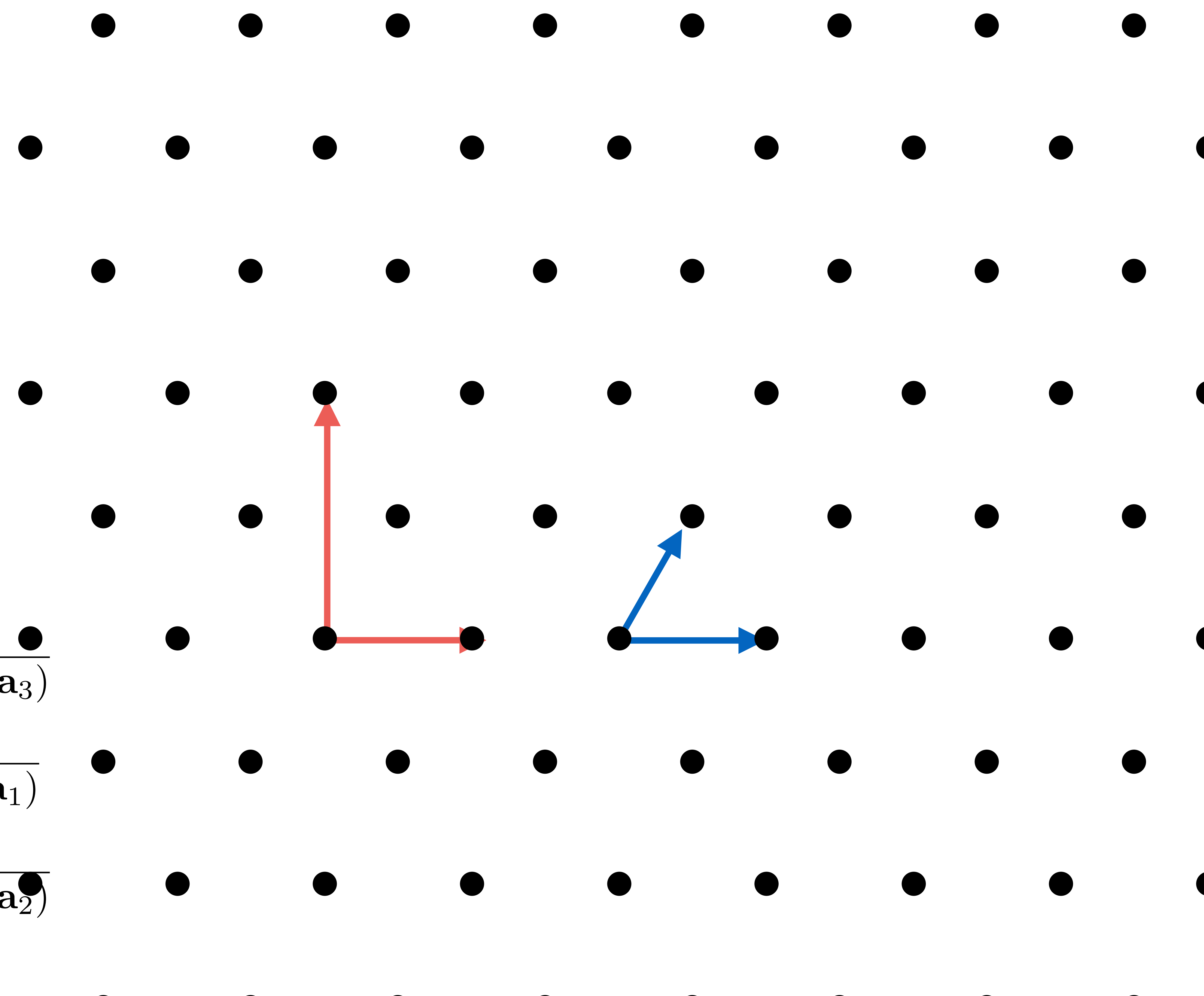


$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

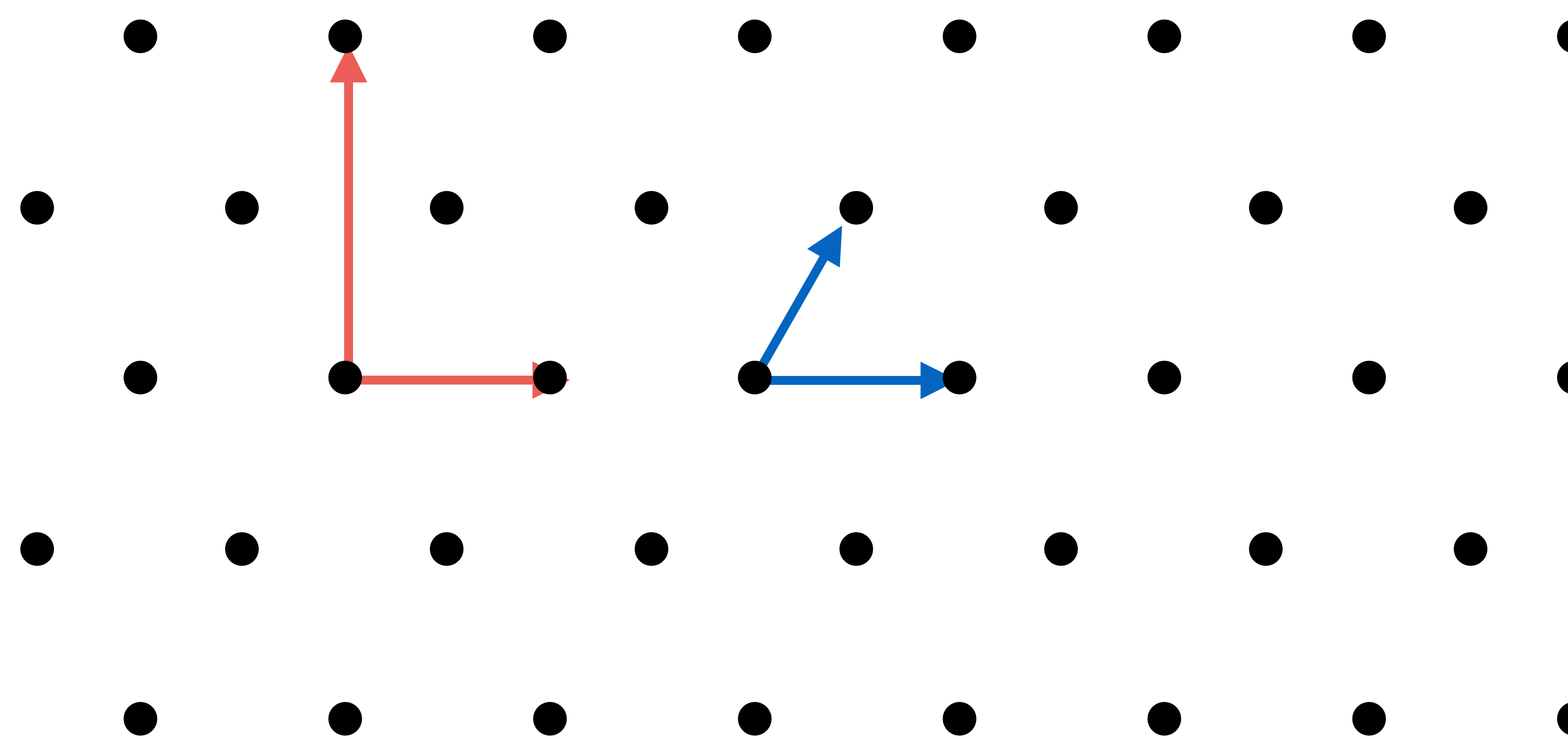
$$\mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)}$$

$$\mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$

$$\mathcal{E} \propto f_e(\theta)\left[\sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\Delta\mathbf{k}}\right]\boxed{\sum_{\mathbf{r}_p} f_{ap}(\theta)\, e^{i\mathbf{r}_p\cdot\Delta\mathbf{k}}}$$

$$\lambda = 1.542\ \text{Å}$$
$$a = 3.61\ \text{Å}$$

0.	16.5921	34.8277	58.9444	90. - 30.2067 i
14.8864	14.8864	28.5957	48.1721	90. - 11.999 i
30.9177	25.2866	30.9177	45.494	73.1867
50.4176	41.0286	41.0286	50.4176	73.5869
90. - 13.4335 i	64.2575	58.6818	64.2575	90. - 13.4335 i



$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2\times\mathbf{a}_3}{\mathbf{a}_1\cdot(\mathbf{a}_2\times\mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3\times\mathbf{a}_1}{\mathbf{a}_2\cdot(\mathbf{a}_3\times\mathbf{a}_1)}$$

$$\mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1\times\mathbf{a}_2}{\mathbf{a}_3\cdot(\mathbf{a}_1\times\mathbf{a}_2)}$$

$$\mathcal{E} \propto f_e(\theta) \left[\sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\Delta\mathbf{k}} \right] \boxed{\sum_{\mathbf{r}_p} f_{ap}(\theta) e^{i\mathbf{r}_p\cdot\Delta\mathbf{k}}}$$

$\lambda = 1.542$ Å

$a = 3.61$ Å

0.	16.5921	34.8277	58.9444	90. − 30.2067 i
14.8864	14.8864	28.5957	48.1721	90. − 11.999 i
30.9177	25.2866	30.9177	45.494	73.1867
50.4176	41.0286	41.0286	50.4176	73.5869
90. − 13.4335 i	64.2575	58.6818	64.2575	90. − 13.4335 i

0.	8.20862	16.5921	25.3618	34.8277
12.3318	14.8864	20.8909	28.5957	37.5706
25.2866	26.7679	30.9177	37.2228	45.494
39.8455	41.0286	44.5453	50.4176	59.127
58.6818	60.0134	64.2575	72.8742	90. − 13.4335 i

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$

$$\mathcal{E} \propto f_e(\theta)\left[\sum_{\mathbf{R}} e^{i\mathbf{R}\cdot\Delta\mathbf{k}}\right]\boxed{\sum_{\mathbf{r}_p} f_{ap}(\theta)\, e^{i\mathbf{r}_p\cdot\Delta\mathbf{k}}}$$

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$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$