

Question #14

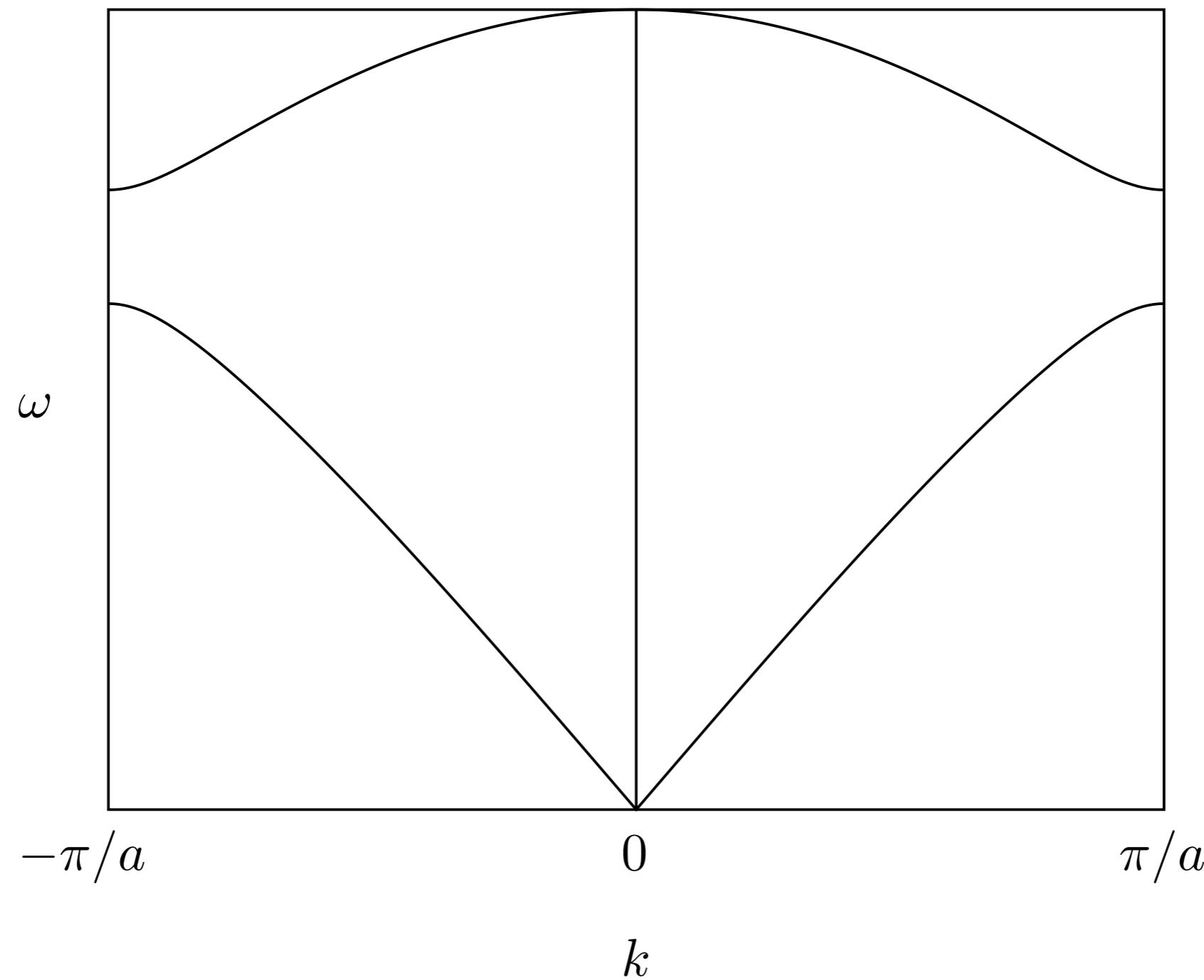
Consider lattice waves in a one-dimensional **diatomic** crystal. Inside the first Brillouin zone, the waves with the lowest frequencies have
(C) the shortest or
(D) the longest wavelengths.

Question #15

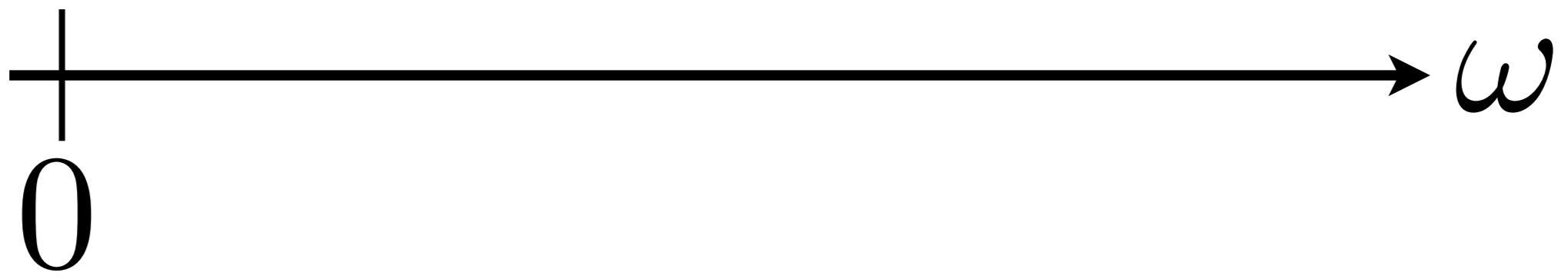
Consider lattice waves in a one-dimensional diatomic crystal. Inside the first Brillouin zone, the waves with the **highest** frequencies have

- (C) the shortest or
- (D) the longest wavelengths.

Phonon dispersion for diatomic crystal



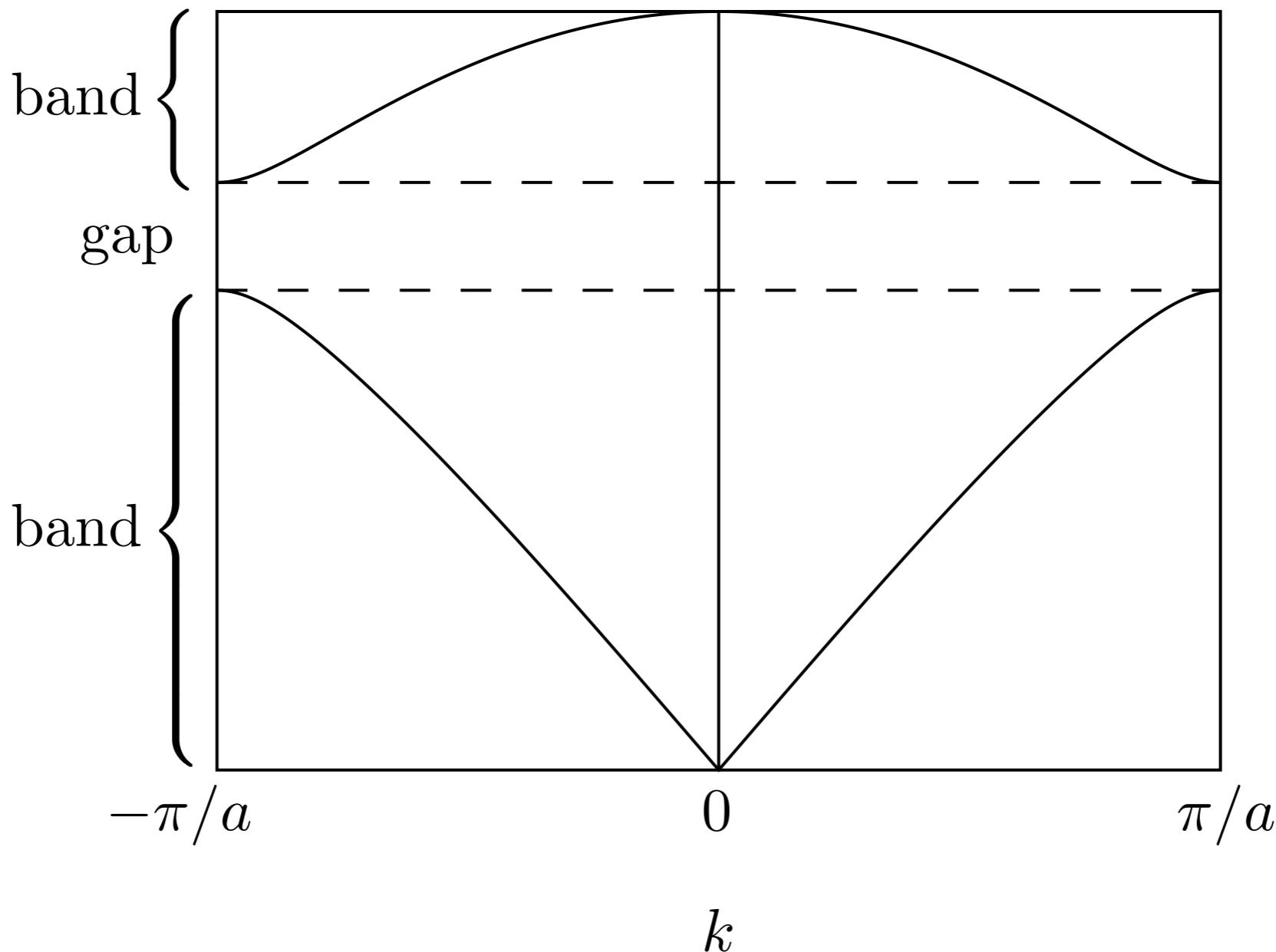
Gaps

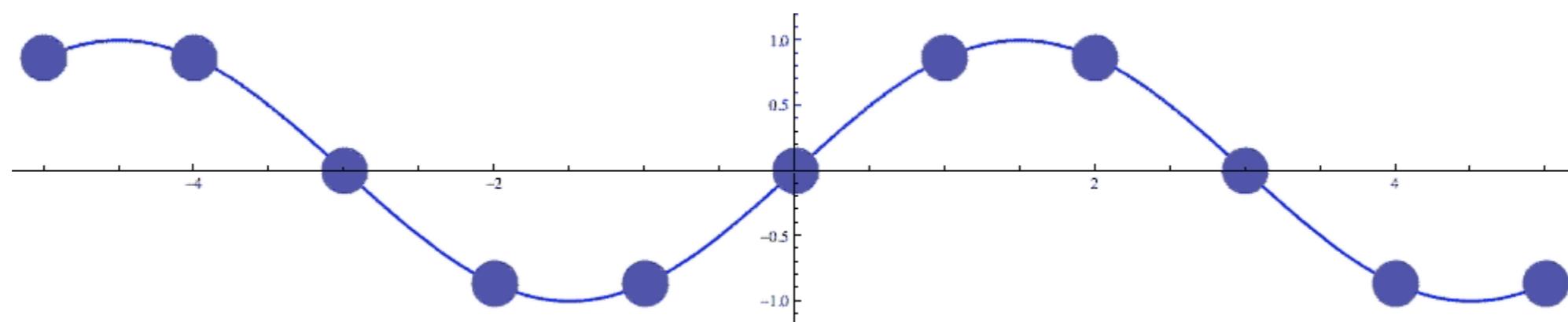
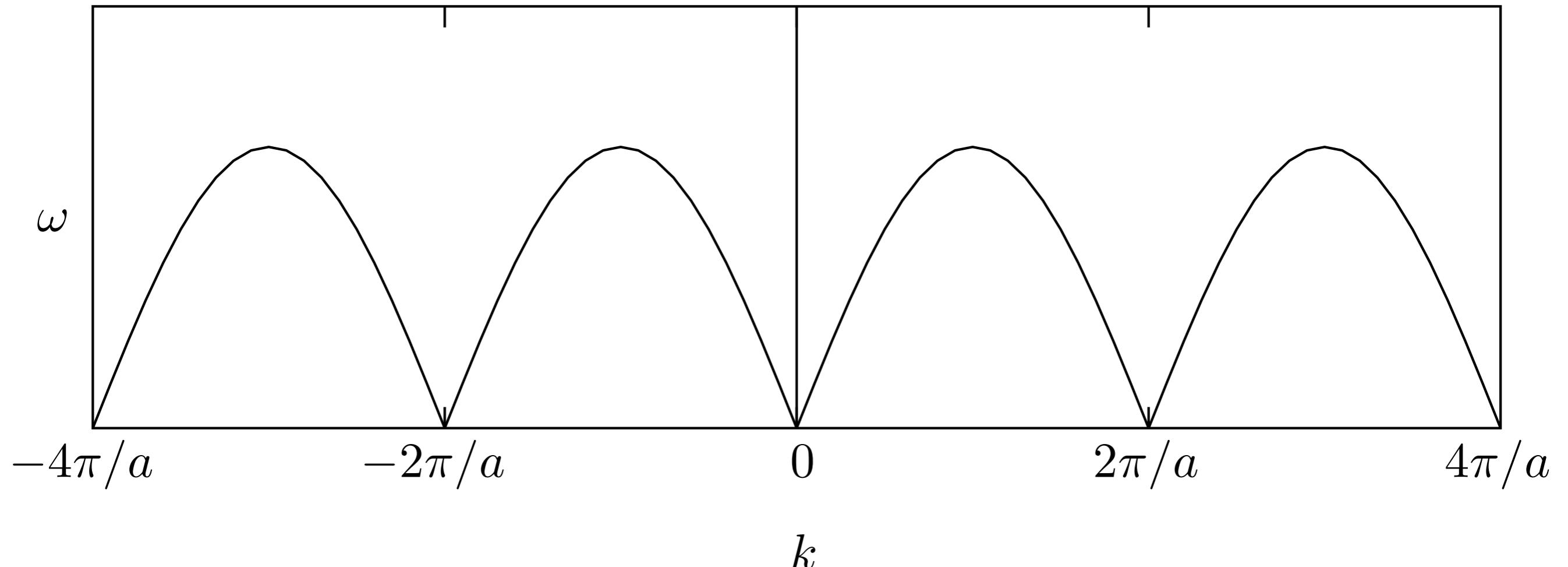


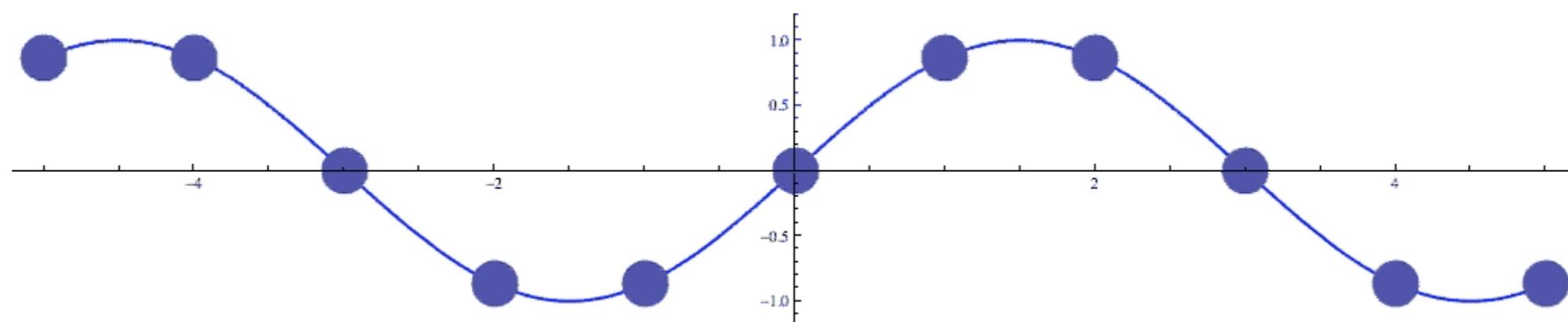
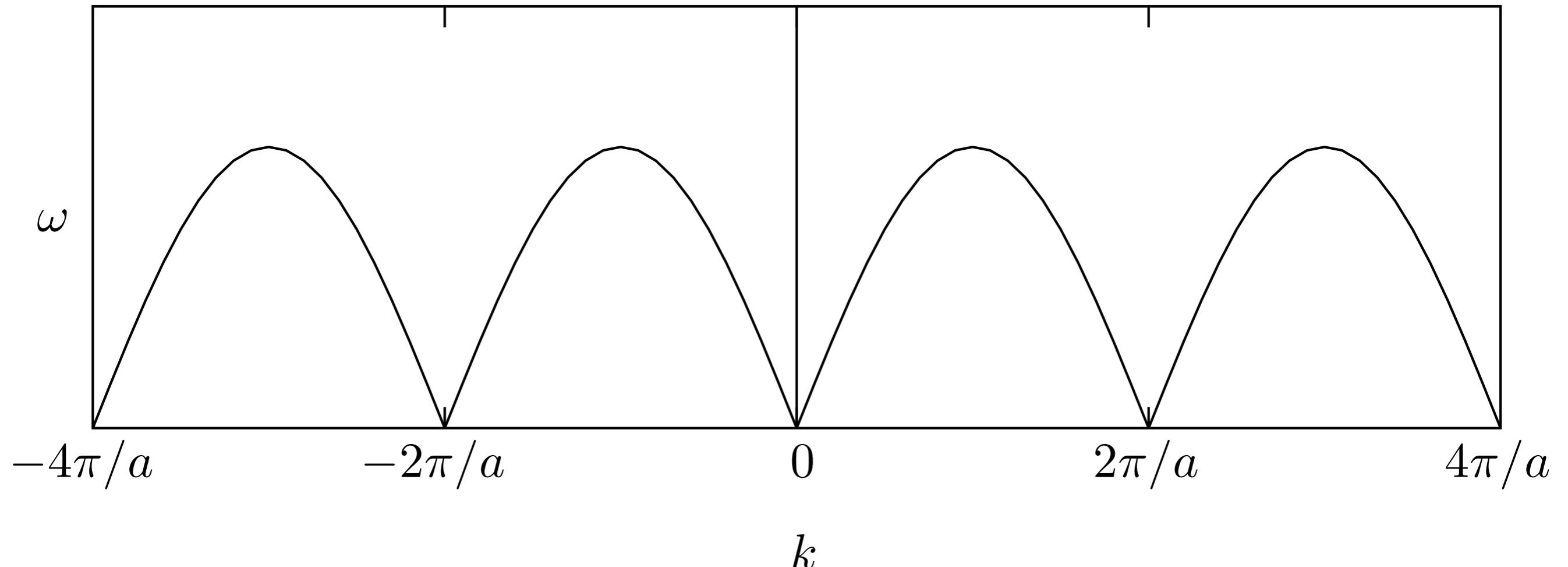
Gaps



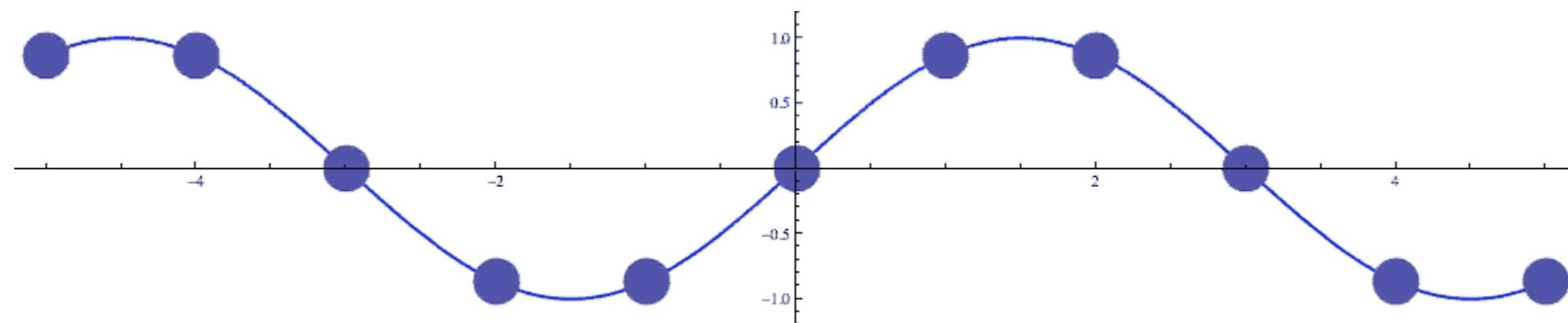
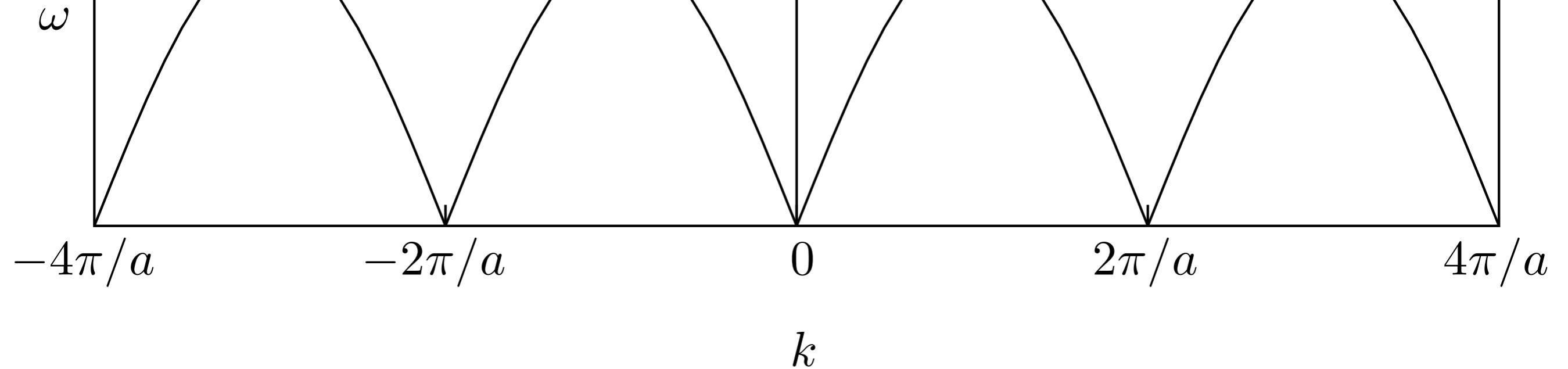
Gaps



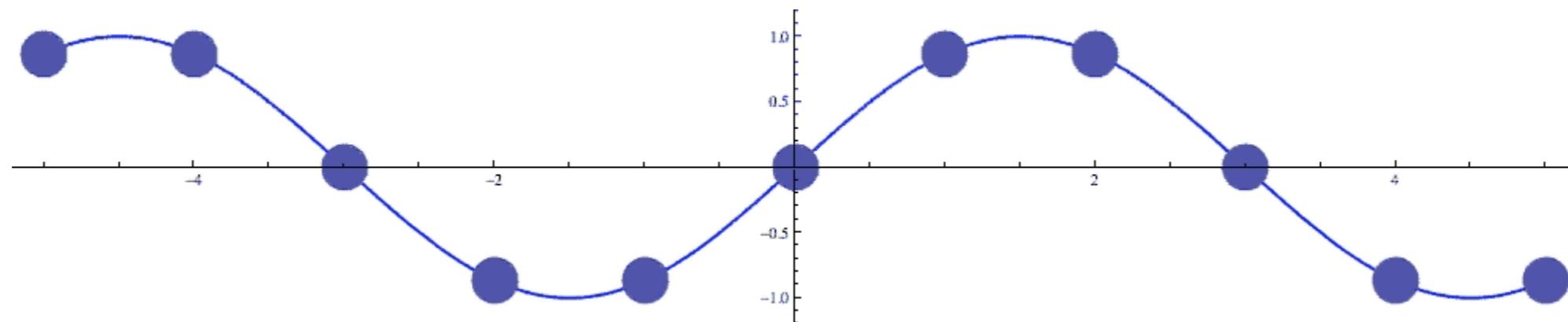
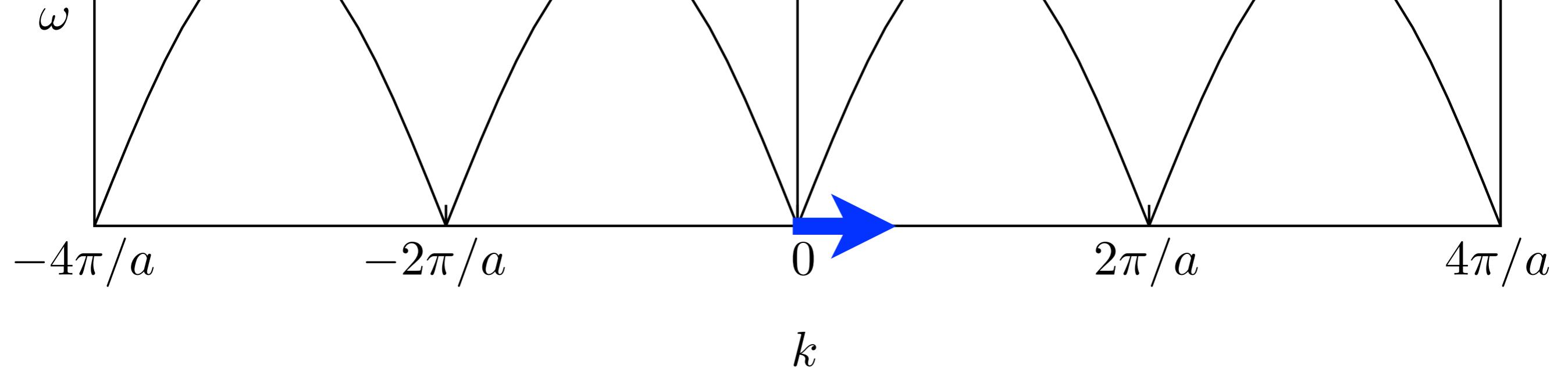




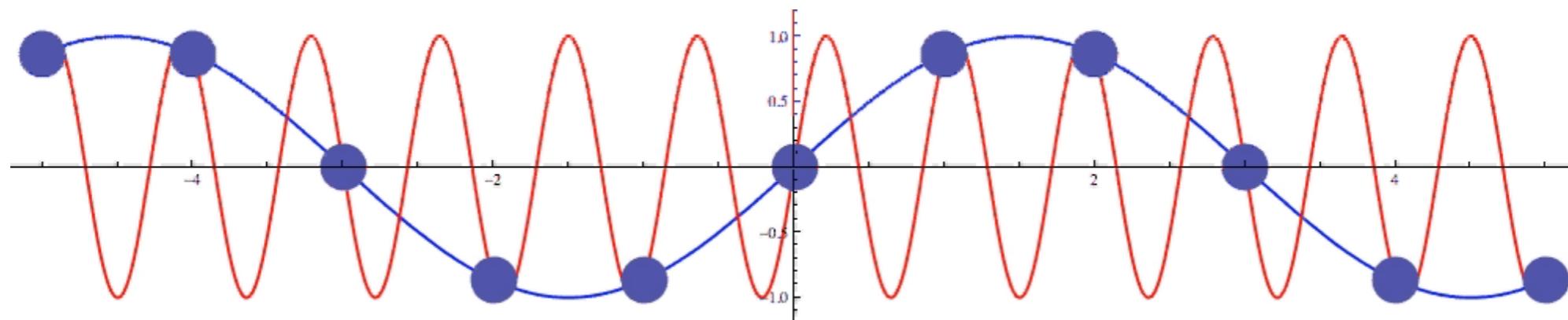
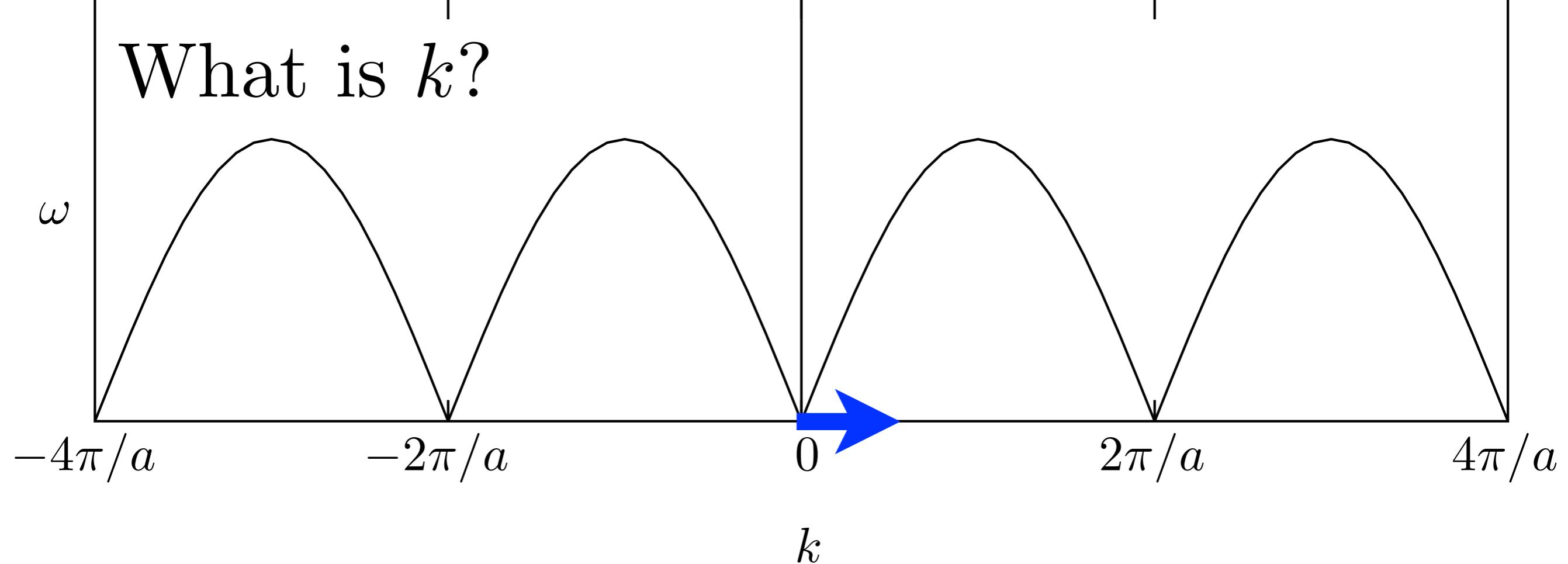
What is k ?



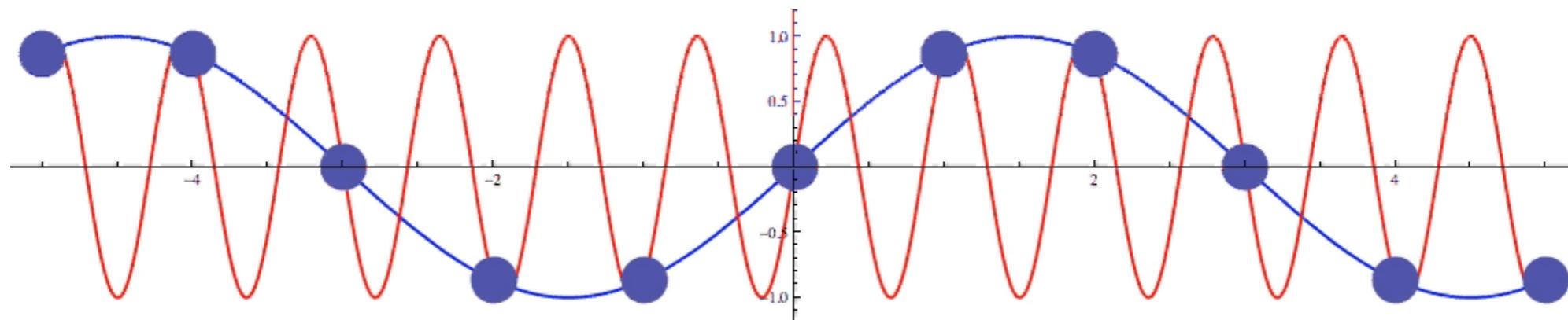
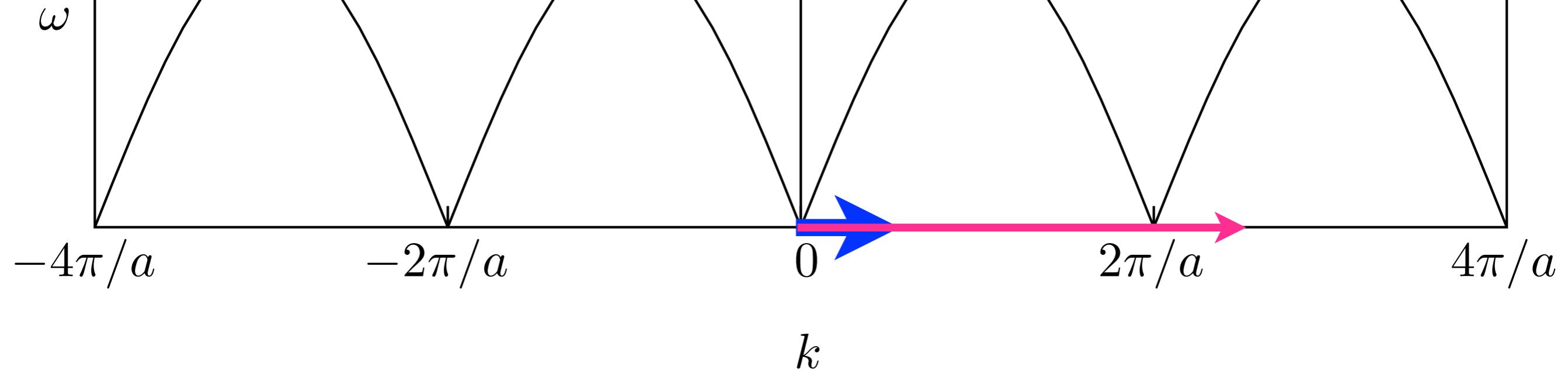
What is k ?



What is k ?



What is k ?

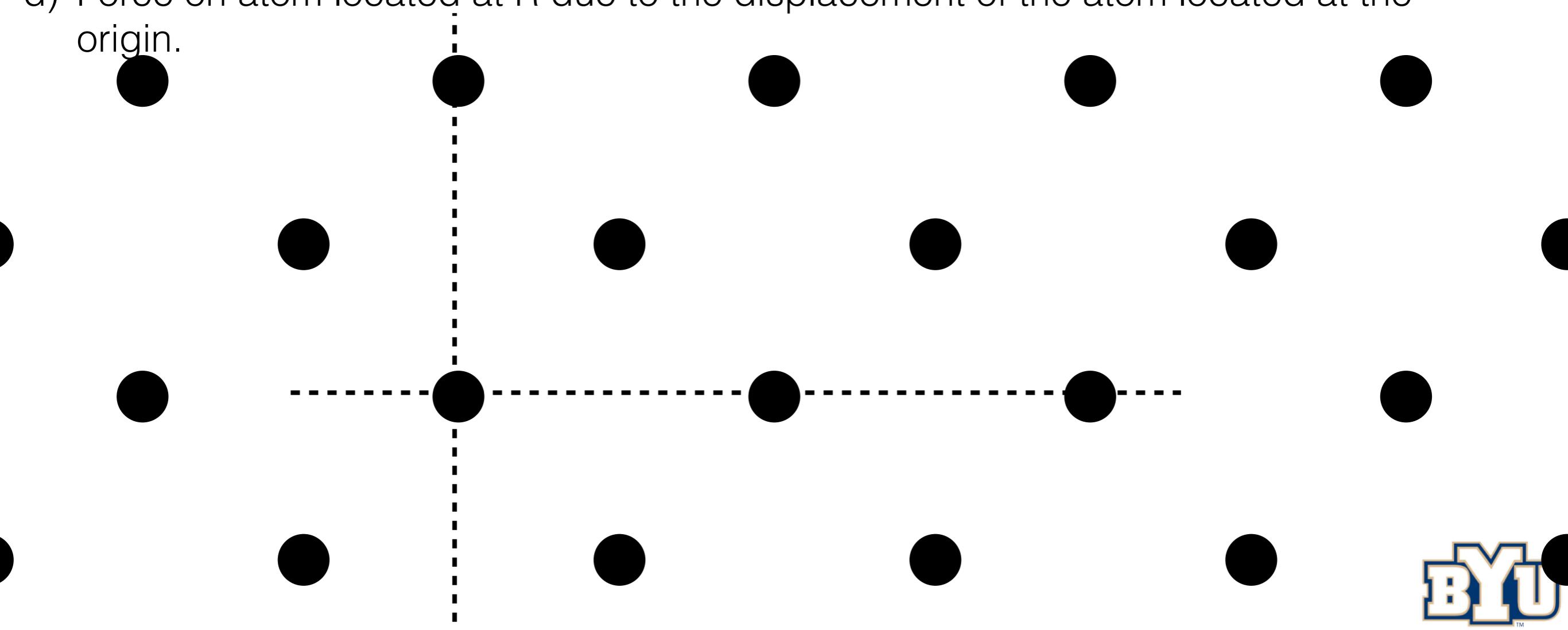


$$\mathbf{F} = -\alpha \left[\hat{\mathbf{R}} \cdot \mathbf{u}(000) - \hat{\mathbf{R}} \cdot \mathbf{u}(\mathbf{R}) \right] \hat{\mathbf{R}}$$

Question #16

What does this expression mean?

- a) Force on atom at the origin due to the displacement of the atom located at R.
- b) Force on atom located at R due to its displacement and the displacement of the atom located at the origin.
- c) Force on atom at the origin due to it's displacement and the displacement of the atom located at R.
- d) Force on atom located at R due to the displacement of the atom located at the origin.

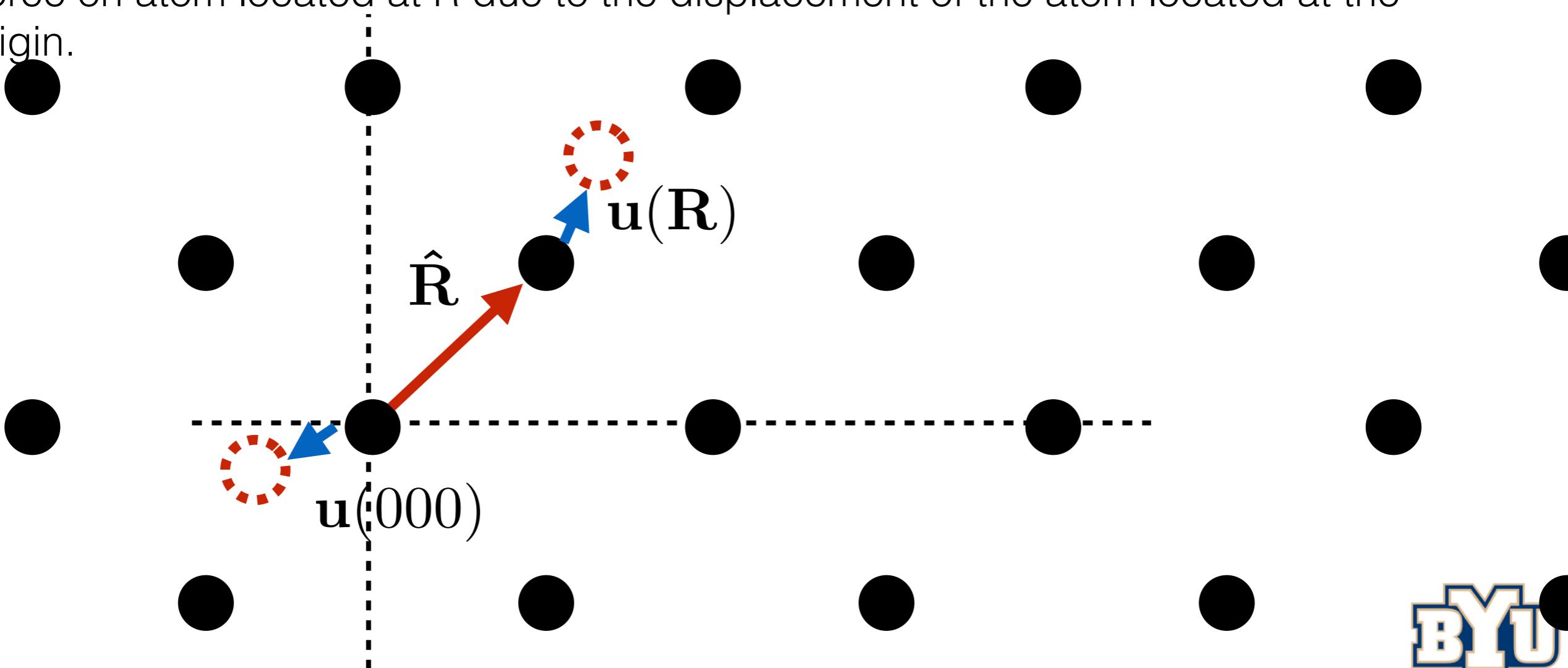


$$\mathbf{F} = -\alpha \left[\hat{\mathbf{R}} \cdot \mathbf{u}(000) - \hat{\mathbf{R}} \cdot \mathbf{u}(\mathbf{R}) \right] \hat{\mathbf{R}}$$

Question #16

What does this expression mean?

- a) Force on atom at the origin due to the displacement of the atom located at \mathbf{R} .
- b) Force on atom located at \mathbf{R} due to its displacement and the displacement of the atom located at the origin.
- c) Force on atom at the origin due to it's displacement and the displacement of the atom located at \mathbf{R} .
- d) Force on atom located at \mathbf{R} due to the displacement of the atom located at the origin.



$$\mathbf{F} = -\alpha \left[\hat{\mathbf{R}} \cdot \mathbf{u}(000) - \hat{\mathbf{R}} \cdot \mathbf{u}(\mathbf{R}) \right] \hat{\mathbf{R}}$$

Question #17

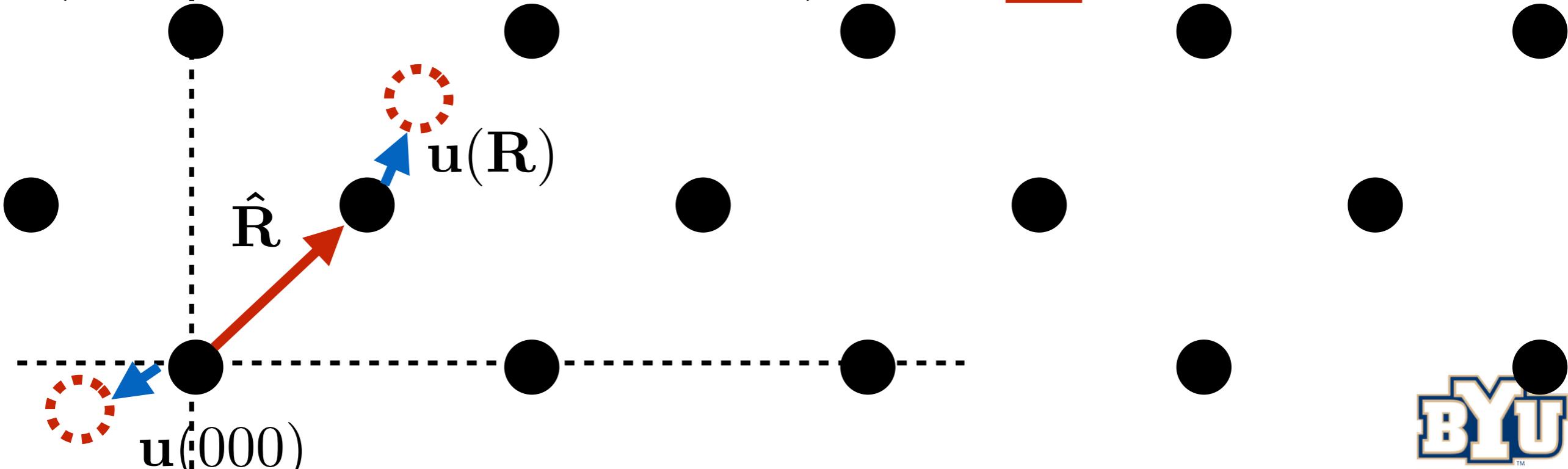
Evaluate this expression for $\mathbf{R} = \left(\frac{1}{2}a, \frac{1}{2}a, 0 \right)$

$$-\frac{\alpha}{\sqrt{2}} \left(u_x(000) + u_y(000) - u_x\left(\frac{1}{2}\frac{1}{2}0\right) - u_y\left(\frac{1}{2}\frac{1}{2}0\right) \right) \boxed{\mathbf{D}}$$

$$-\frac{\alpha}{\sqrt{2}} \left(u_x(000) + u_y(000) - u_x\left(\frac{1}{2}\frac{1}{2}0\right) - u_y\left(\frac{1}{2}\frac{1}{2}0\right) \right) (\hat{i} + \hat{j}) \boxed{\mathbf{B}}$$

$$-\frac{\alpha}{2} \left(u_x(000) + u_y(000) - u_x\left(\frac{1}{2}\frac{1}{2}0\right) - u_y\left(\frac{1}{2}\frac{1}{2}0\right) \right) (\hat{i} + \hat{j}) \boxed{\mathbf{A}}$$

$$-\frac{\alpha}{2} \left(u_x(000) + u_y(000) - u_x\left(\frac{1}{2}\frac{1}{2}0\right) + u_y\left(\frac{1}{2}\frac{1}{2}0\right) \right) (\hat{i} + \hat{j}) \boxed{\mathbf{C}}$$



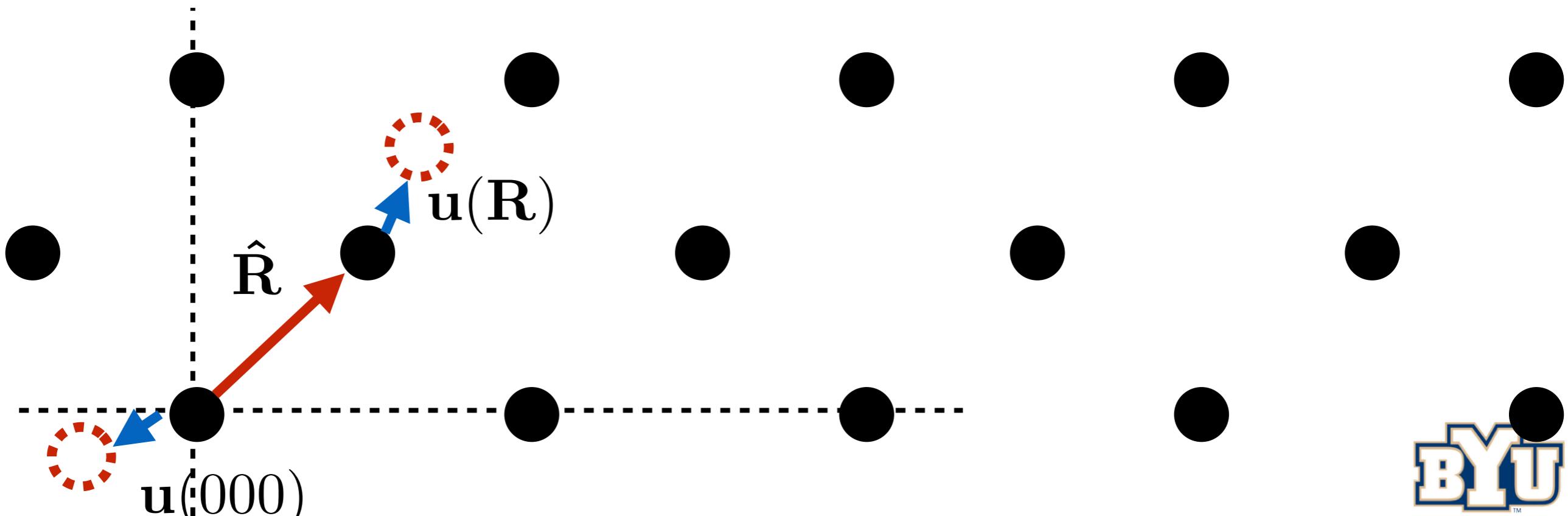
$$\mathbf{F} = -\alpha \left[\hat{\mathbf{R}} \cdot \mathbf{u}(000) - \hat{\mathbf{R}} \cdot \mathbf{u}(\mathbf{R}) \right] \hat{\mathbf{R}}$$

$$-\frac{\alpha}{2} \left(u_x(000) + u_y(000) - u_x\left(\frac{1}{2}\frac{1}{2}0\right) - u_y\left(\frac{1}{2}\frac{1}{2}0\right) \right) (\hat{i} + \hat{j})$$

$$\mathbf{u}_n = \mathbf{A} e^{i\mathbf{k} \cdot \mathbf{r}_n - i\omega t}$$

Let \mathbf{k} point in the [100] direction

$$\mathbf{F} = -\frac{\alpha}{2} \left(u_x(000) + u_y(000) - u_x(000)e^{\frac{ika}{2}} - u_y(000)e^{\frac{ika}{2}} \right) (\hat{i} + \hat{j})$$



$$\mathbf{F} = -\alpha \left[\hat{\mathbf{R}} \cdot \mathbf{u}(000) - \hat{\mathbf{R}} \cdot \mathbf{u}(\mathbf{R}) \right] \hat{\mathbf{R}}$$

$$-\frac{\alpha}{2} \left(u_x(000) + u_y(000) - u_x\left(\frac{1}{2}\frac{1}{2}0\right) - u_y\left(\frac{1}{2}\frac{1}{2}0\right) \right) (\hat{i} + \hat{j})$$

$$\mathbf{u}_n = \mathbf{A} e^{i\mathbf{k}\cdot\mathbf{r}_n-i\omega t}$$

$$\mathbf{u}(000) = \mathbf{A} e^{-i\omega t}$$

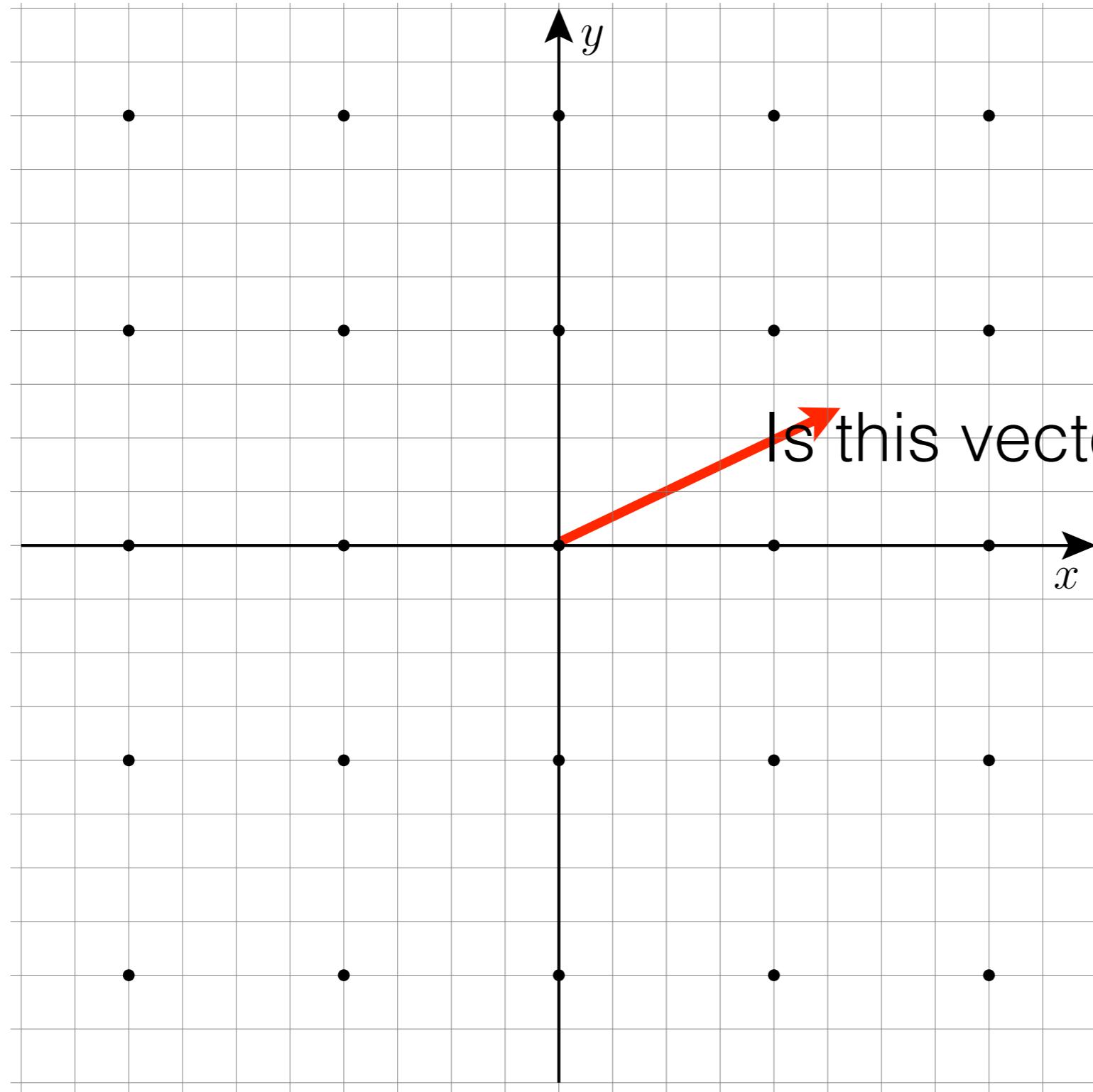
$$\mathbf{u}\left(\frac{1}{2}\frac{1}{2}0\right) = \mathbf{A} e^{\frac{ik_a}{2}} e^{-i\omega t} = \mathbf{u}(000) e^{\frac{ik_a}{2}}$$

$$\mathbf{F} = -\frac{\alpha}{2} \left(u_x(000) + u_y(000) - u_x(000)e^{\frac{ik_a}{2}} - u_y(000)e^{\frac{ik_a}{2}} \right) (\hat{i} + \hat{j})$$

$$\begin{pmatrix} (F_{x_1})_x & (F_{y_1})_x & (F_{z_1})_x \\ (F_{x_1})_y & (F_{y_1})_y & (F_{z_1})_y \\ (F_{x_1})_z & (F_{y_1})_z & (F_{z_1})_z \\ \dots & & \end{pmatrix} \begin{pmatrix} u_{x_1} \\ u_{y_1} \\ u_{z_1} \\ \dots \end{pmatrix} = m\omega^2 \begin{pmatrix} u_{x_1} \\ u_{y_1} \\ u_{z_1} \\ \dots \end{pmatrix}$$



$$k = (1.88, 0.95) \text{\AA}^{-1} = 2\pi/a(1.22, 0.62)$$

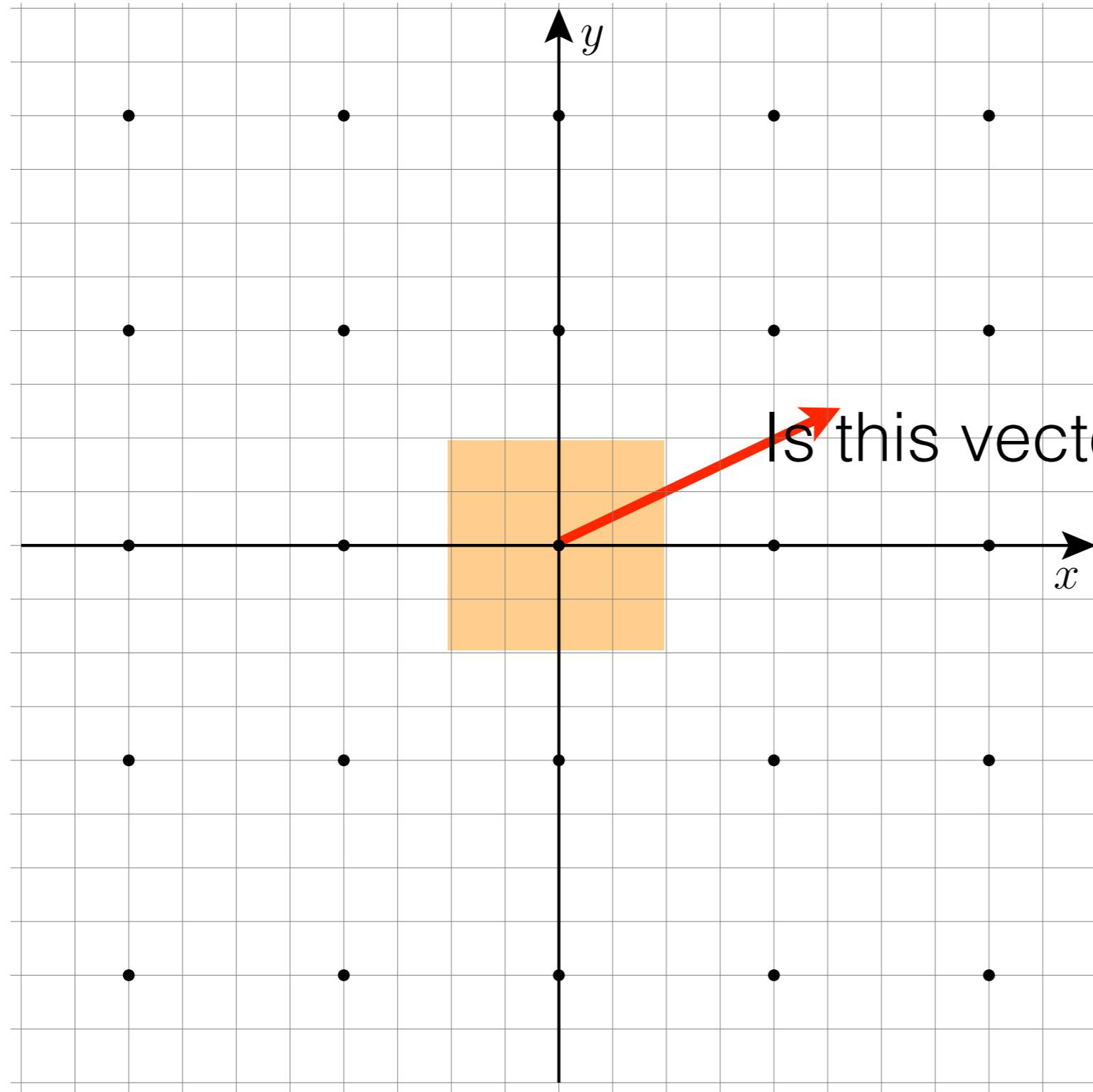


$$a_0 = 4.11 \text{\AA}$$

Question #18

- a) .
b) Yes
c) No

$$k = (1.88, 0.95) \text{\AA}^{-1} = 2\pi/a(1.22, 0.62)$$



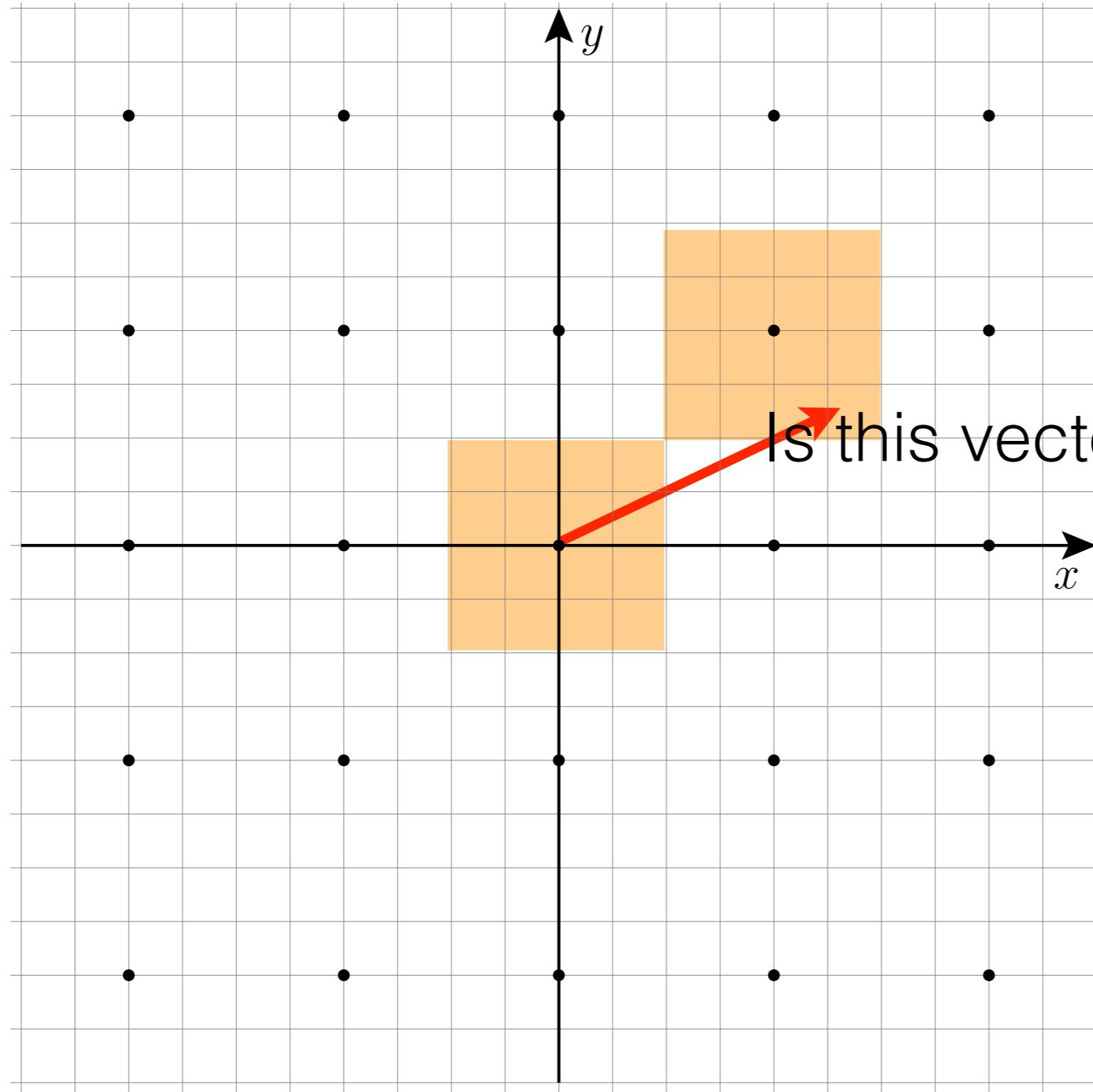
$$a_0 = 4.11 \text{\AA}$$

Question #18

Is this vector inside the first BZ?

- a) .
- b) Yes
- c) No

$$k = (1.88, 0.95) \text{\AA}^{-1} = 2\pi/a(1.22, 0.62)$$



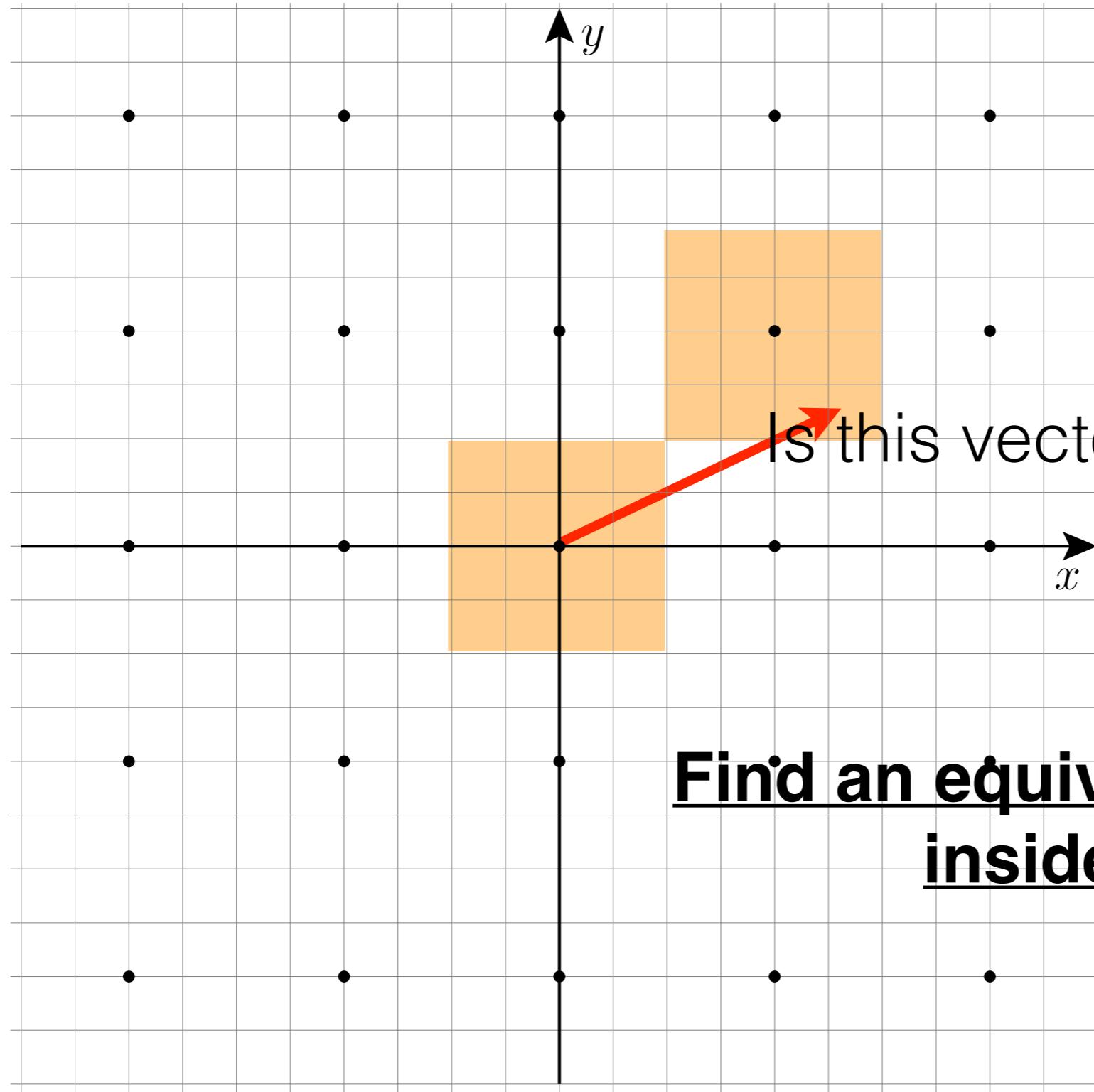
$$a_0 = 4.11 \text{\AA}$$

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Is this vector inside the first BZ?

- a) .
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$$k = (1.88, 0.95) \text{\AA}^{-1} = 2\pi/a(1.22, 0.62)$$



$$a_0 = 4.11 \text{\AA}$$

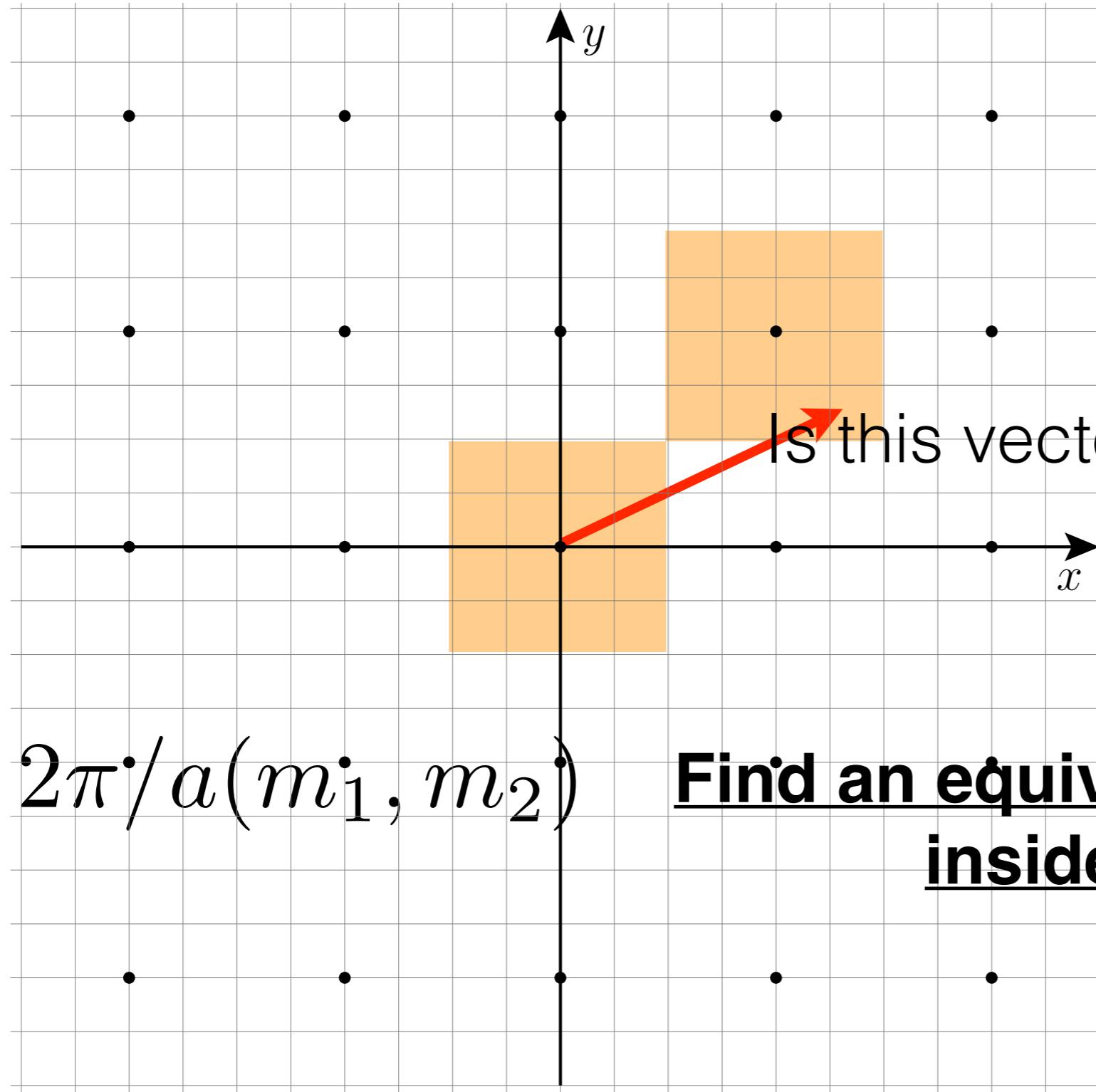
Question #18

Is this vector inside the first BZ?

- a) .
- b) Yes
- c) No

Find an equivalent vector that *is*
inside the first BZ.

$$k = (1.88, 0.95) \text{\AA}^{-1} = 2\pi/a(1.22, 0.62)$$



$$a_0 = 4.11 \text{\AA}$$

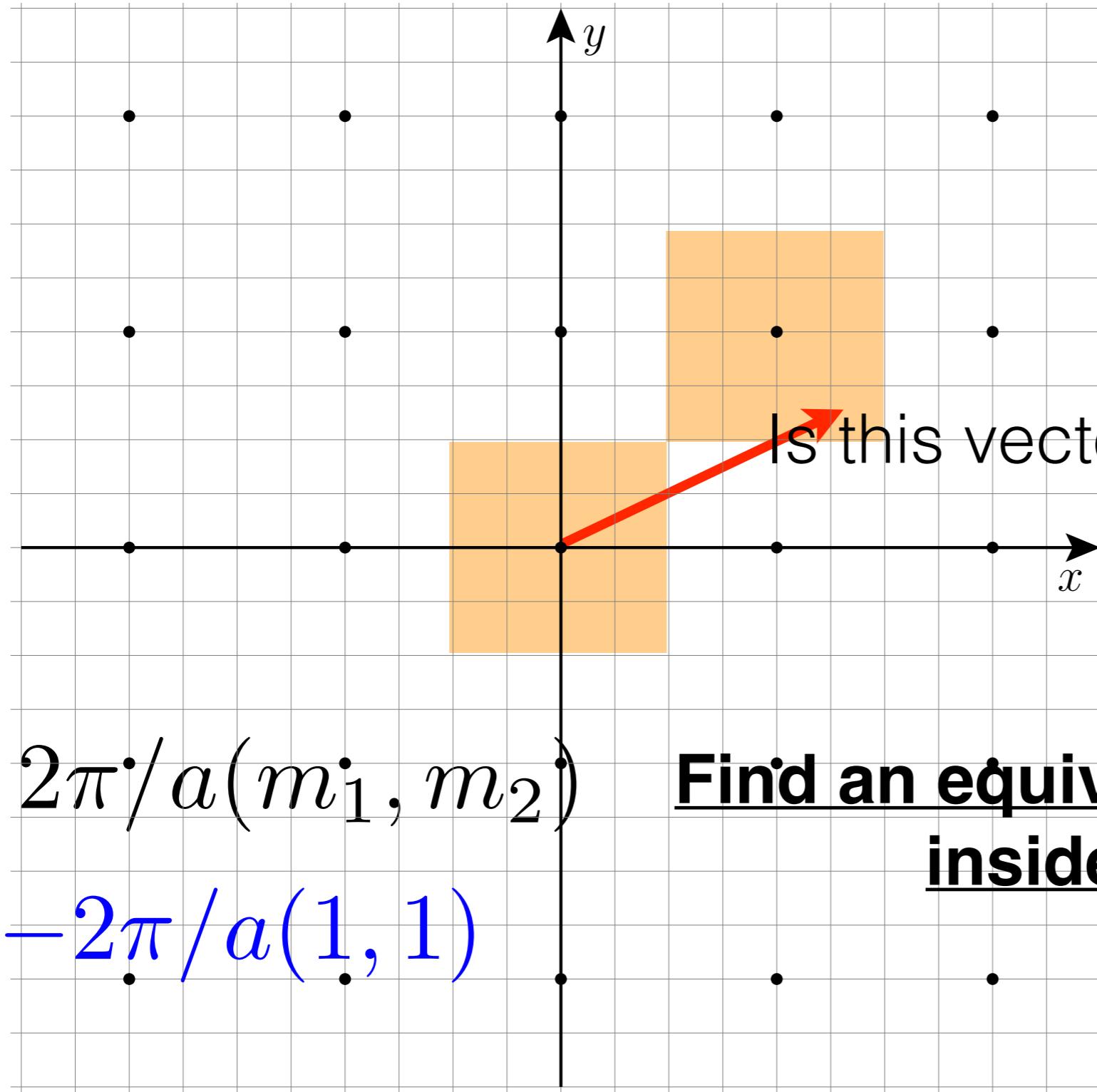
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Is this vector inside the first BZ?

- a) .
- b) Yes
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Find an equivalent vector that *is* inside the first BZ.

$$k = (1.88, 0.95) \text{\AA}^{-1} = 2\pi/a(1.22, 0.62)$$



$$2\pi/a(m_1, m_2)$$

$$-2\pi/a(1, 1)$$

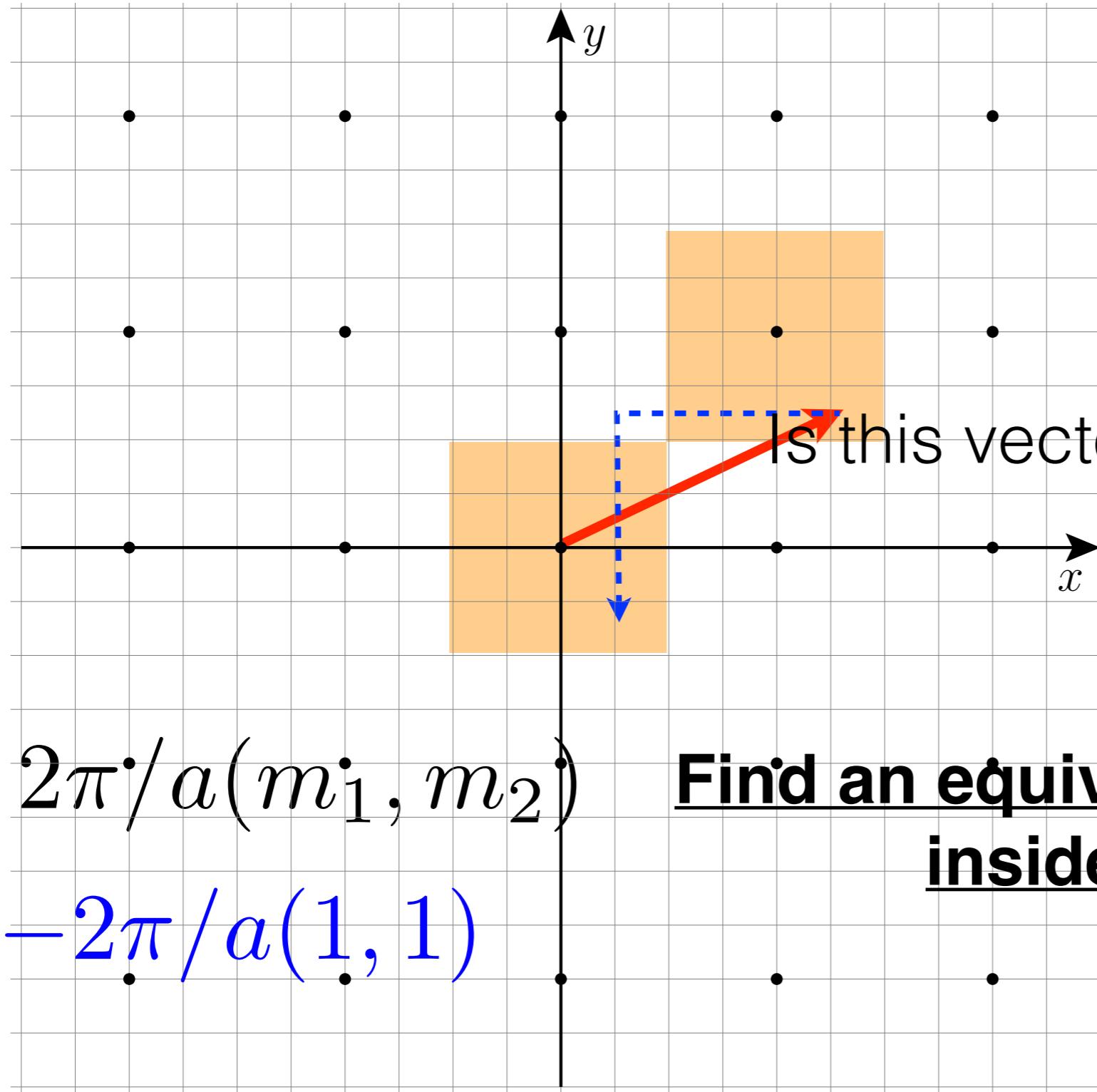
$$a_0 = 4.11 \text{\AA}$$

Question #18

Find an equivalent vector that ***is*** inside the first BZ.

- a) .
- b) Yes
- c) No

$$k = (1.88, 0.95) \text{\AA}^{-1} = 2\pi/a(1.22, 0.62)$$



$$a_0 = 4.11 \text{\AA}$$

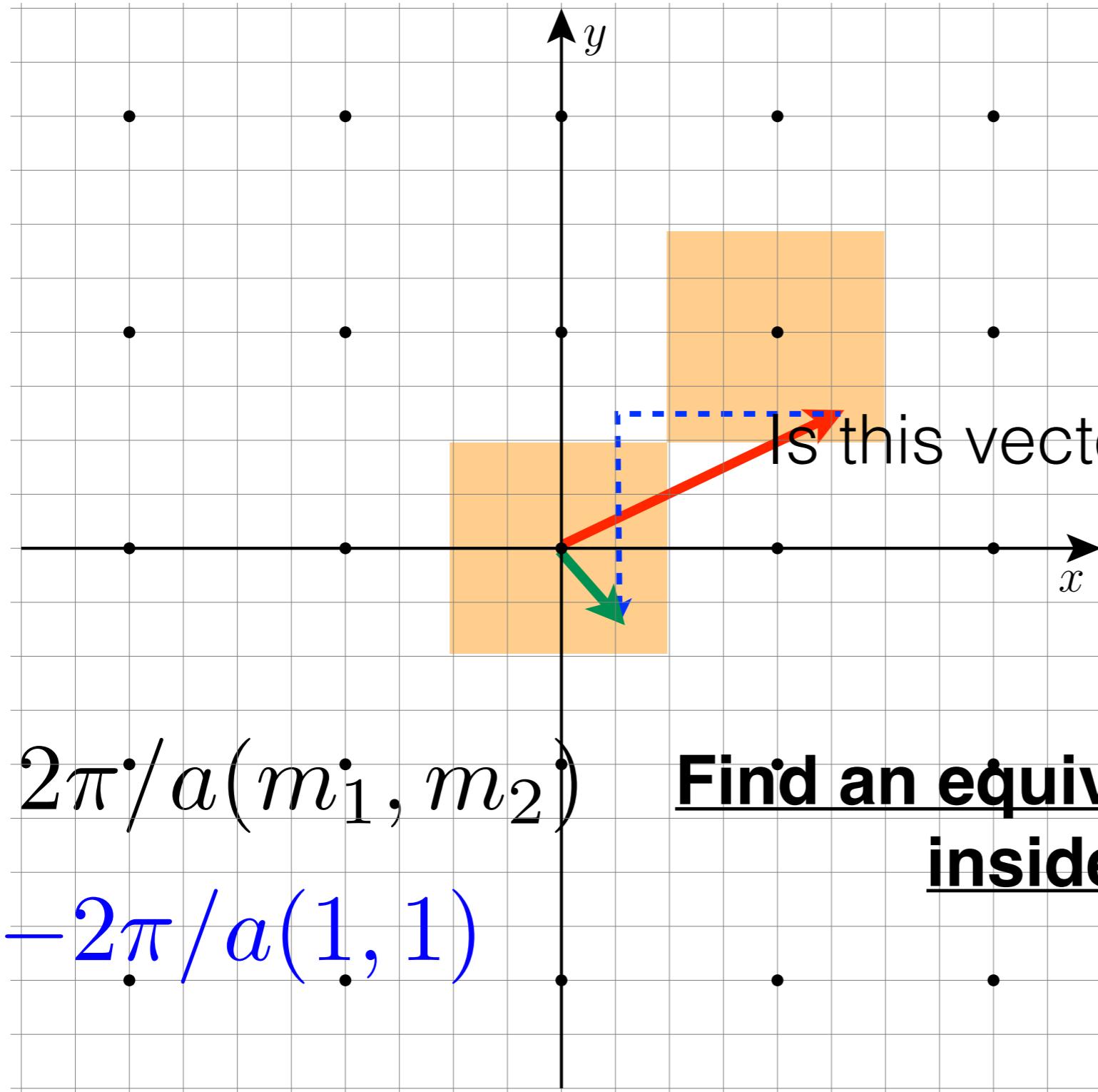
Question #18

Is this vector inside the first BZ?

- a) .
- b) Yes
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Find an equivalent vector that *is* inside the first BZ.

$$k = (1.88, 0.95) \text{\AA}^{-1} = 2\pi/a(1.22, 0.62)$$



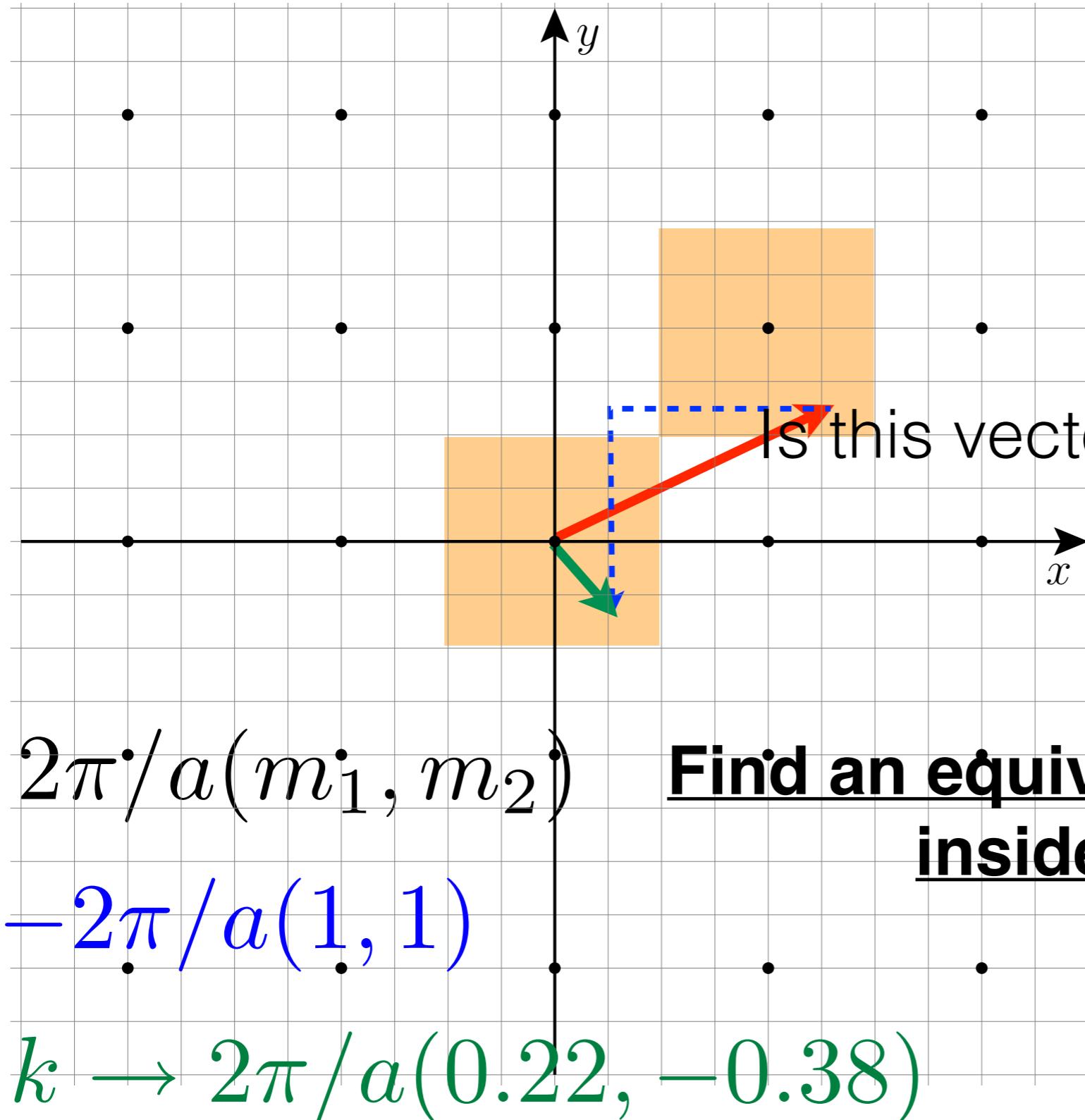
$$a_0 = 4.11 \text{\AA}$$

Question #18

- a) .
- b) Yes
- c) No

Find an equivalent vector that *is* inside the first BZ.

$$k = (1.88, 0.95) \text{ \AA}^{-1} = 2\pi/a(1.22, 0.62)$$

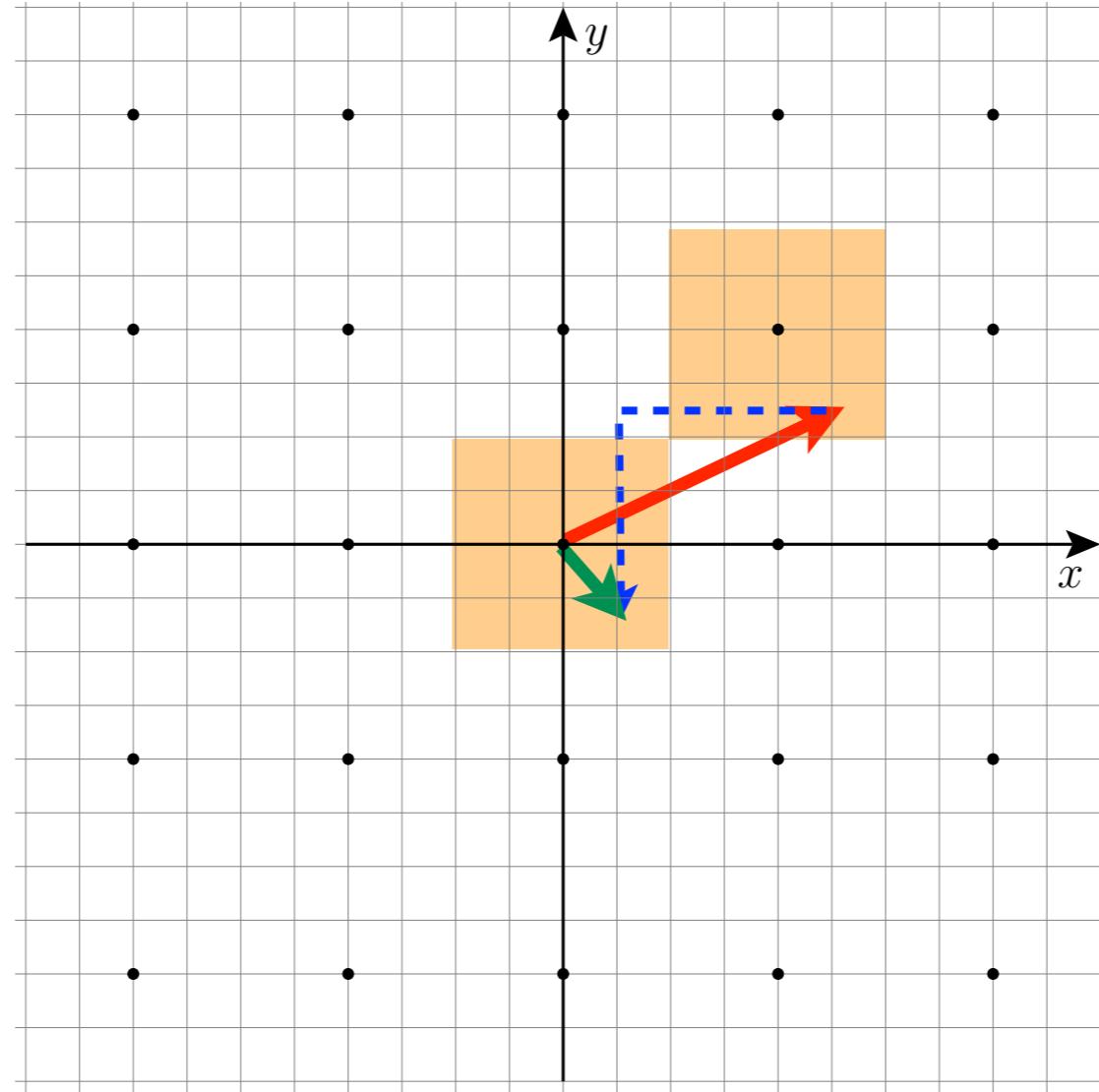


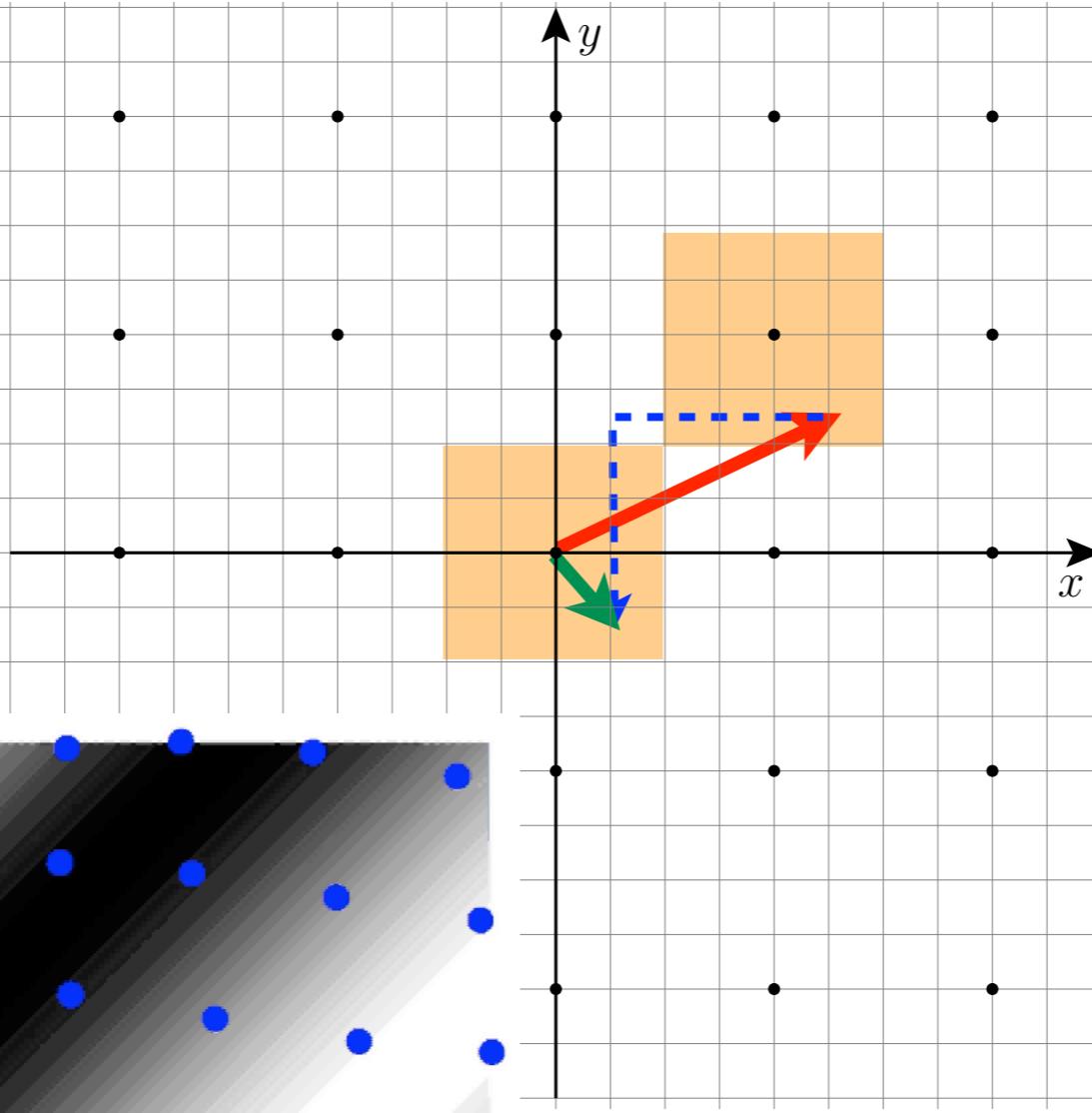
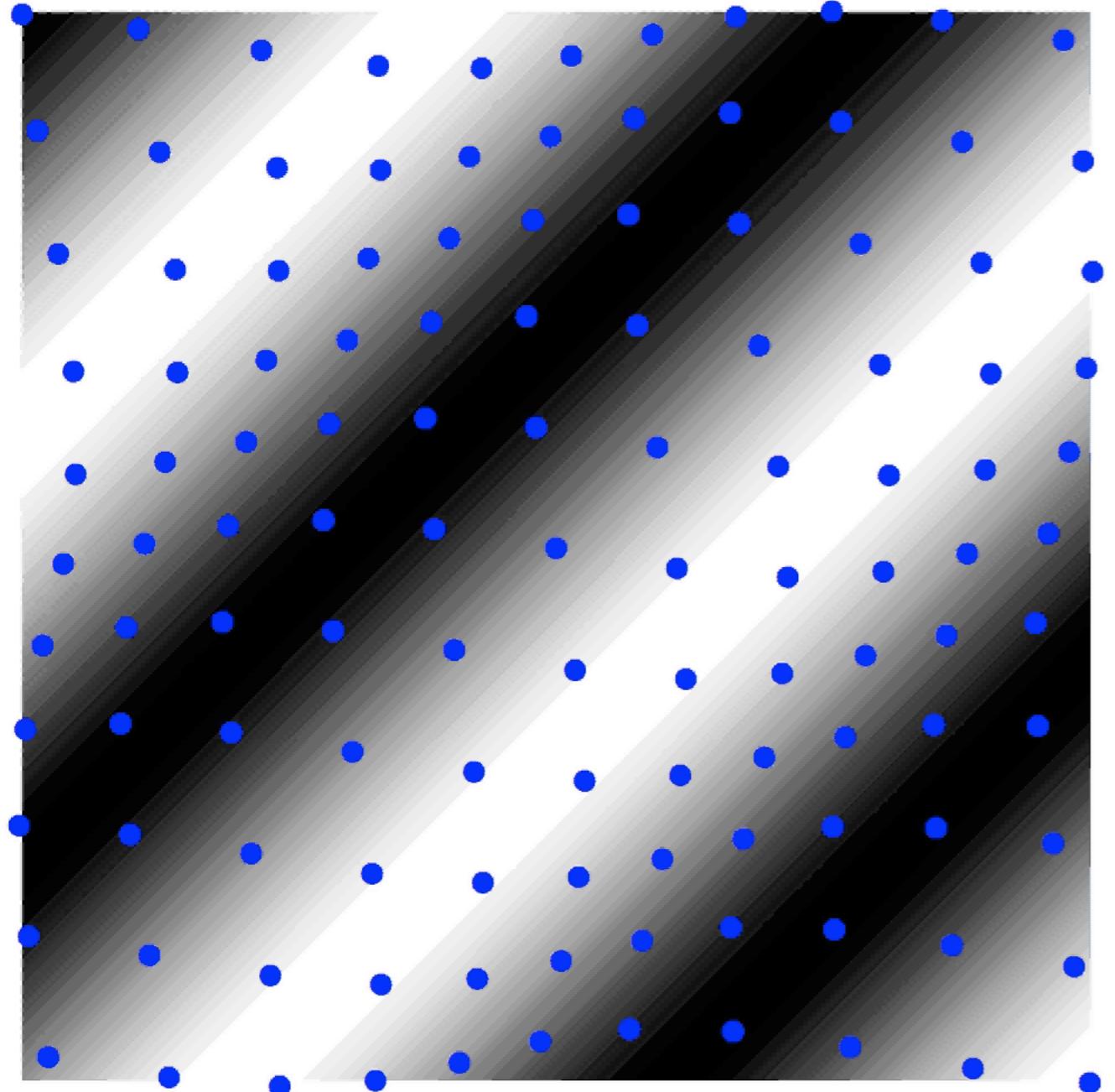
$$a_0 = 4.11 \text{ \AA}$$

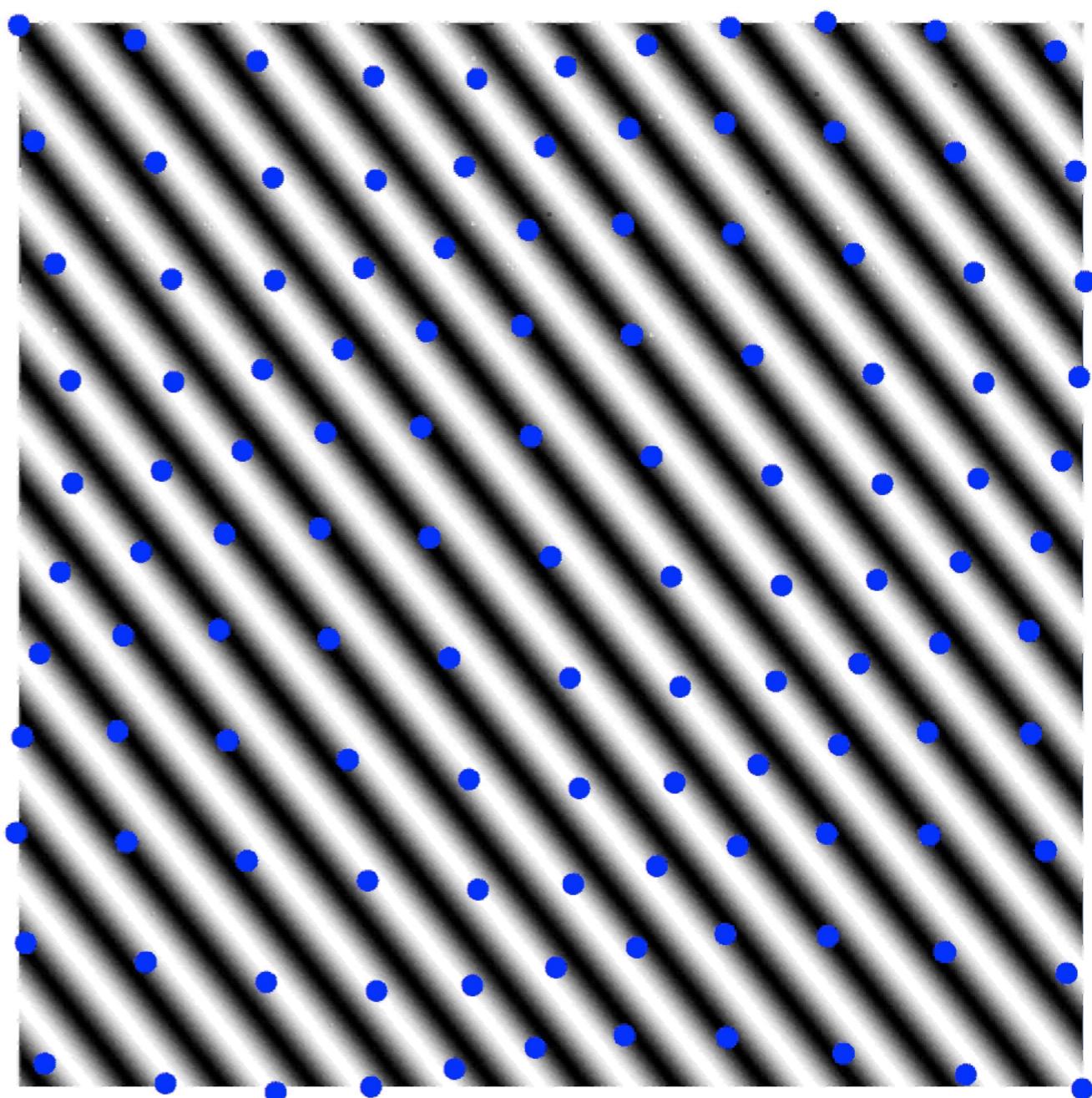
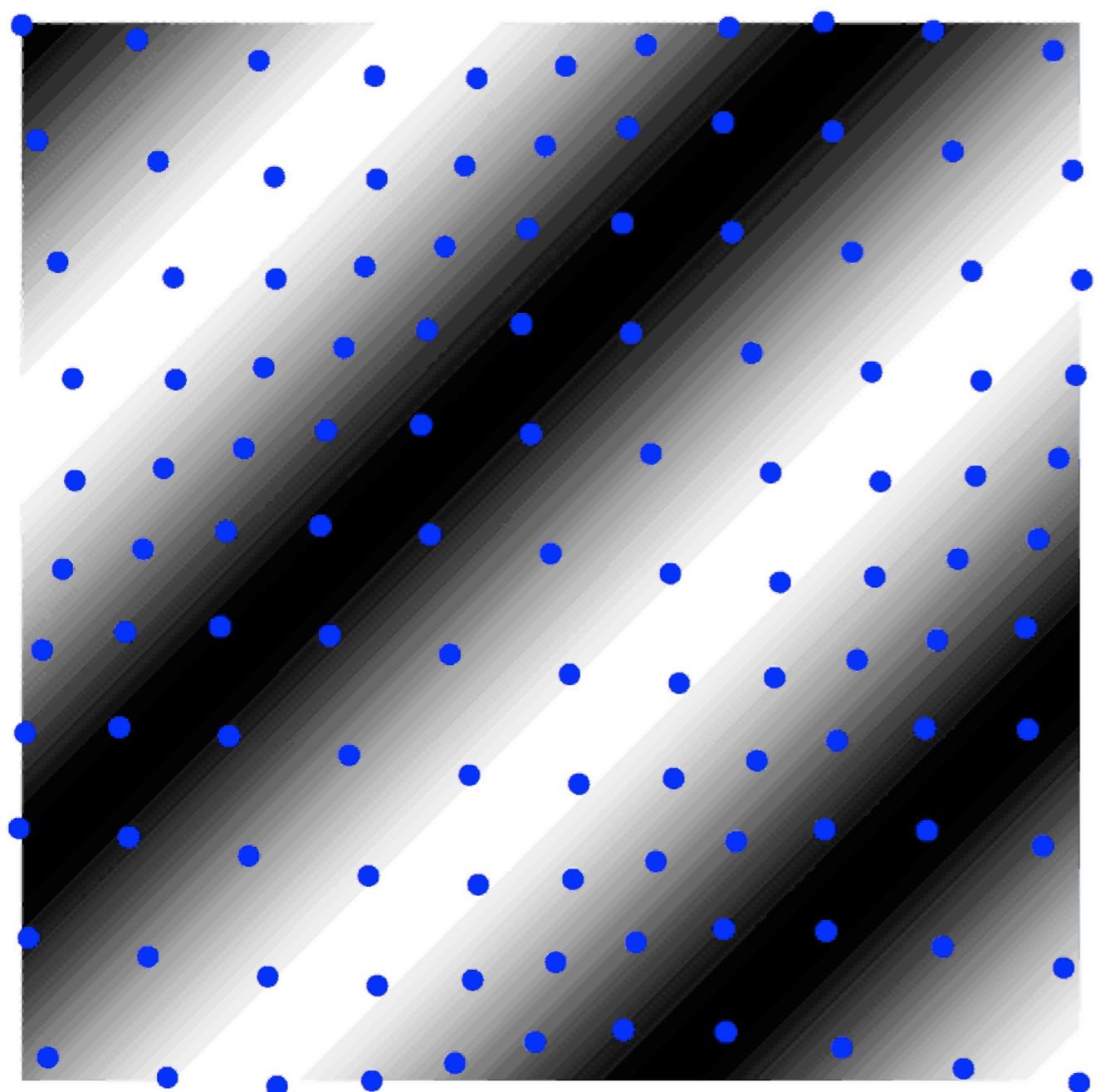
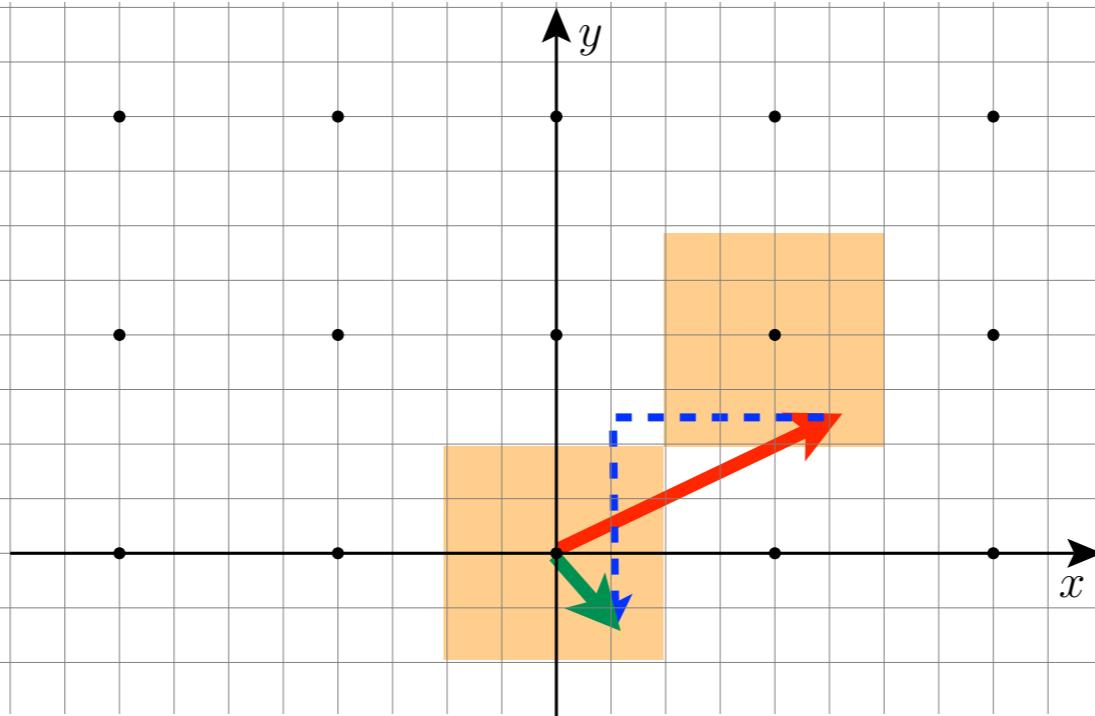
Question #18

Find an equivalent vector that ***is*** inside the first BZ.

a) .
b) Yes
c) No

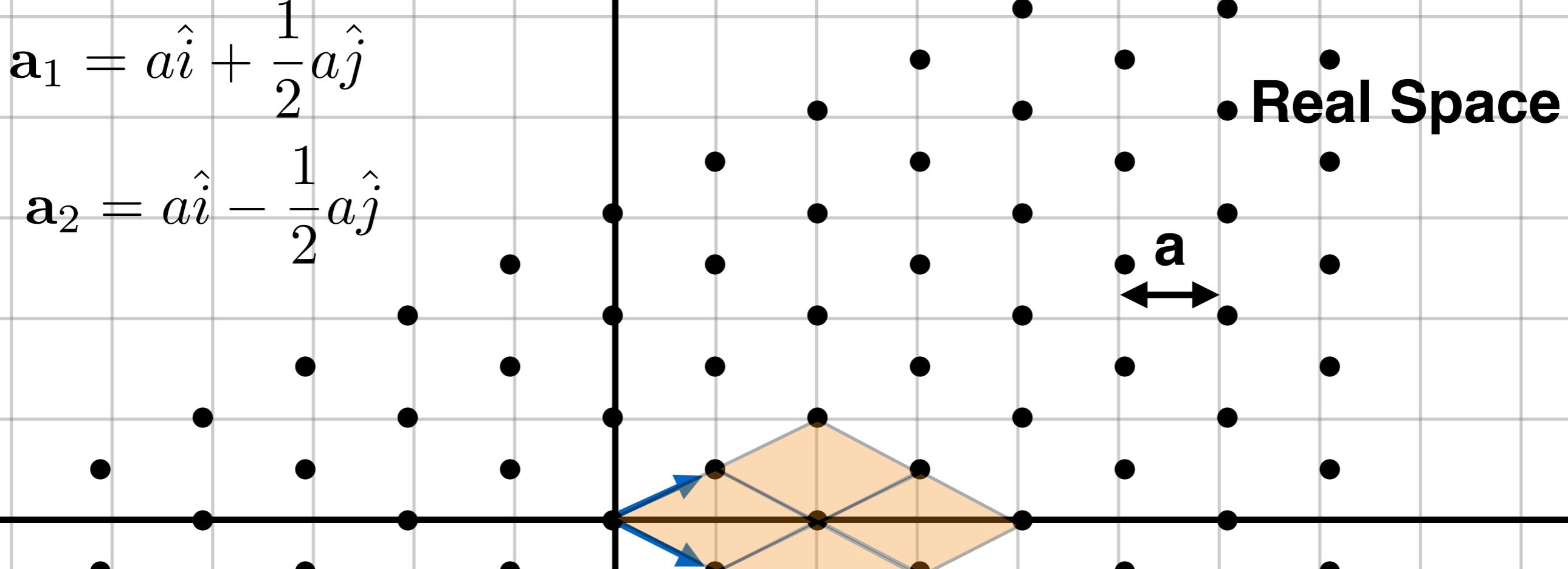






$$\mathbf{a}_1 = a\hat{i} + \frac{1}{2}a\hat{j}$$

$$\mathbf{a}_2 = a\hat{i} - \frac{1}{2}a\hat{j}$$



Is the vector below inside the first BZ (in reciprocal space)?

Question #1

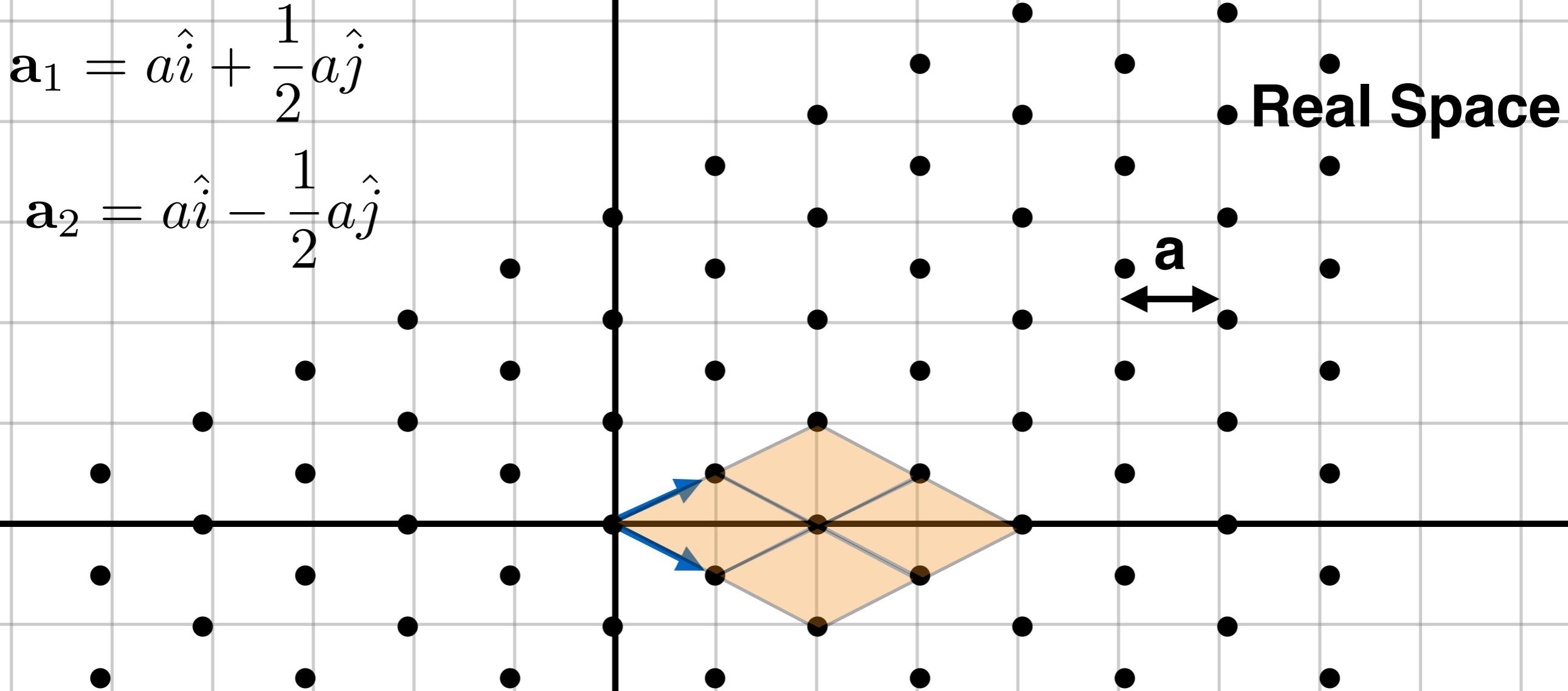
d) yes

$$\vec{k} = \frac{\pi}{a} (2.5, 2)$$

e) No

$$\mathbf{a}_1 = a\hat{i} + \frac{1}{2}a\hat{j}$$

$$\mathbf{a}_2 = a\hat{i} - \frac{1}{2}a\hat{j}$$



Which vector is equivalent to the one below but is found in the first BZ?

the first BZ?

Question #2

A)

$$\frac{\pi}{a} (-0.5, 0)$$

$$\frac{\pi}{a} (0.5, 1)$$

B)

$$\vec{k} = \frac{\pi}{a} (2.5, 2)$$

C)

$$\frac{\pi}{a} (2, -0.5)$$

D)

$$\frac{\pi}{a} (1, -0.5)$$

E)

$$\frac{\pi}{a} (1, 0.5)$$

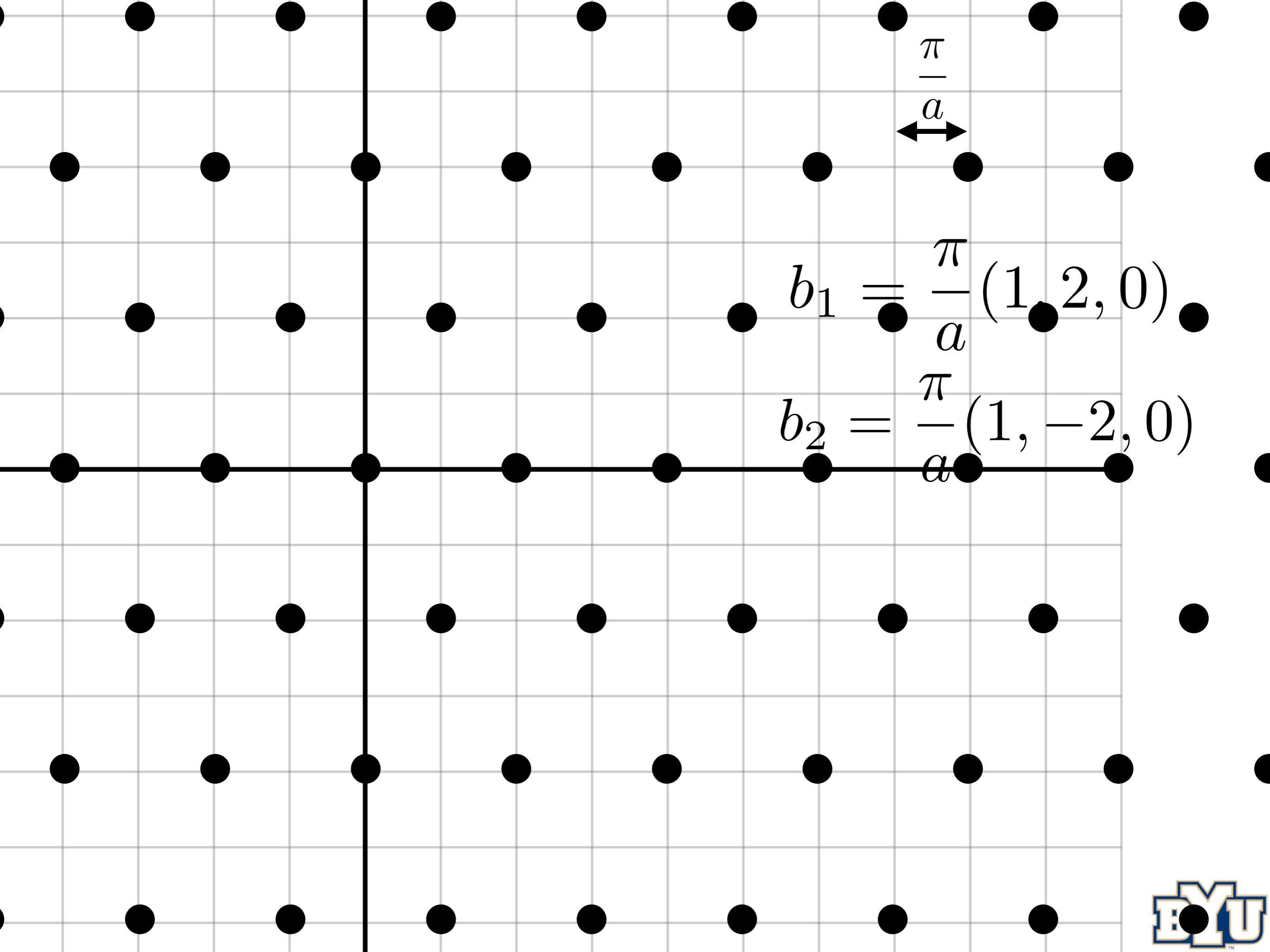
BYU

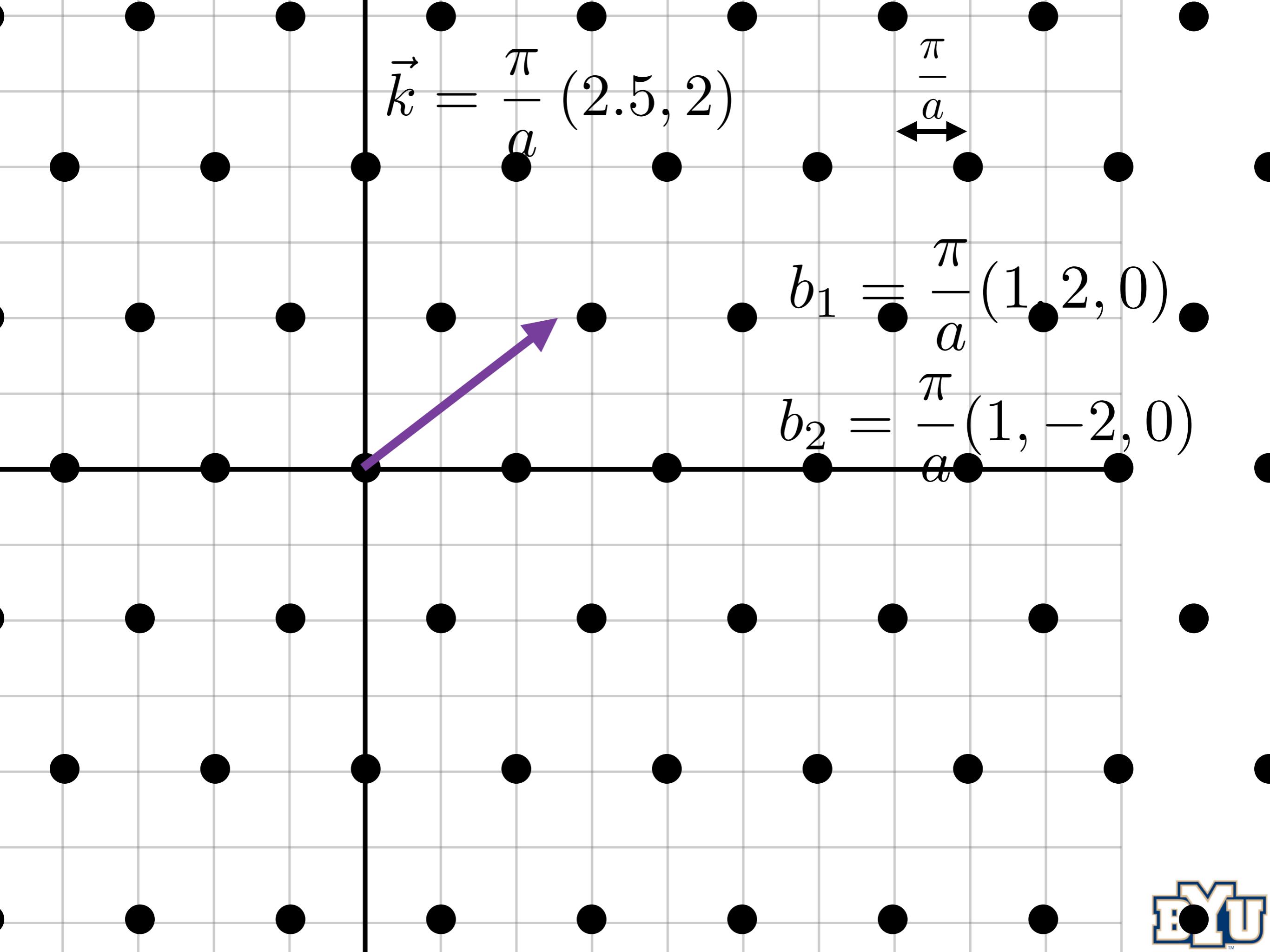
$$\frac{\pi}{a}$$

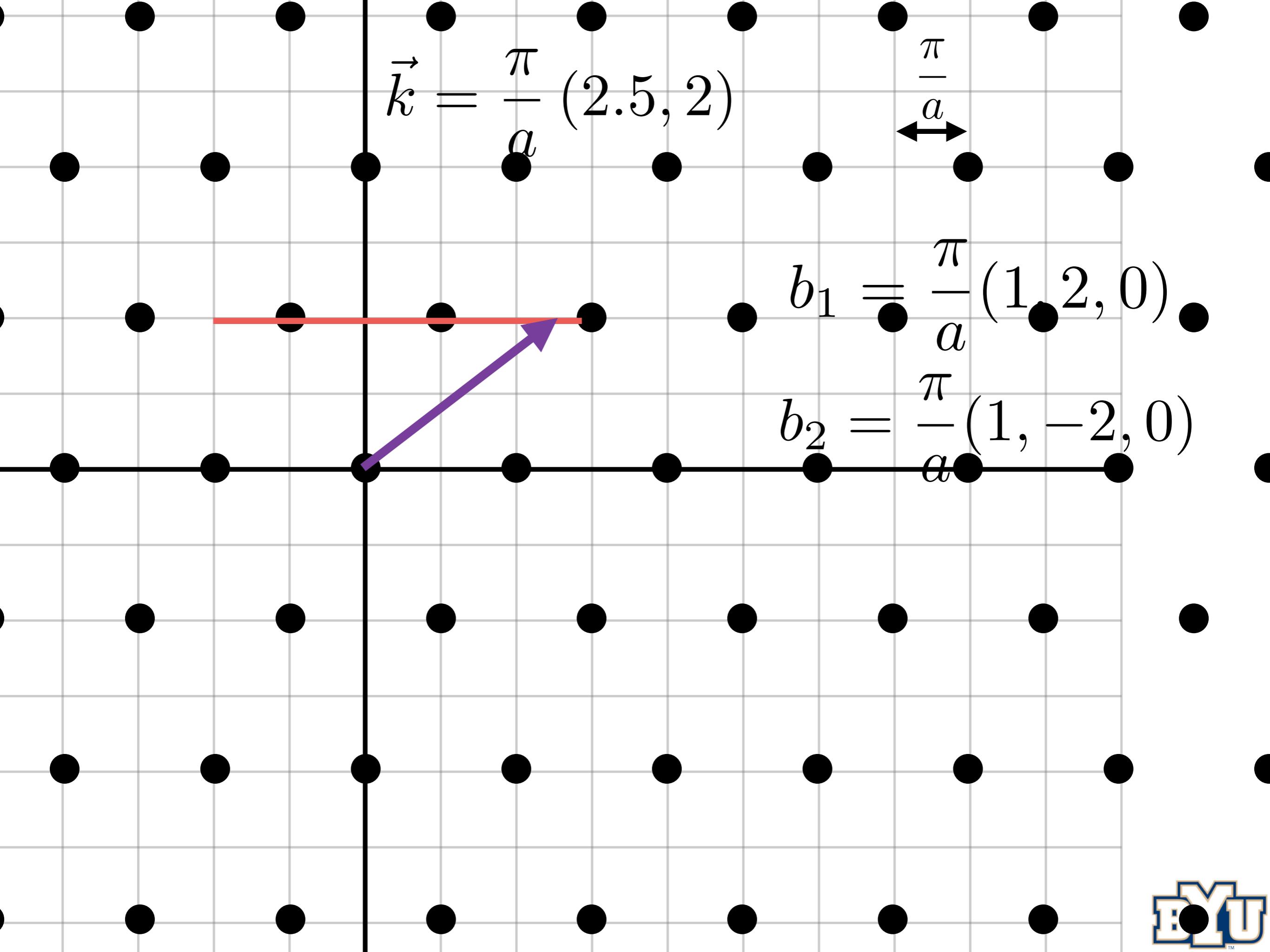
$$\frac{\pi}{a} \longleftrightarrow$$

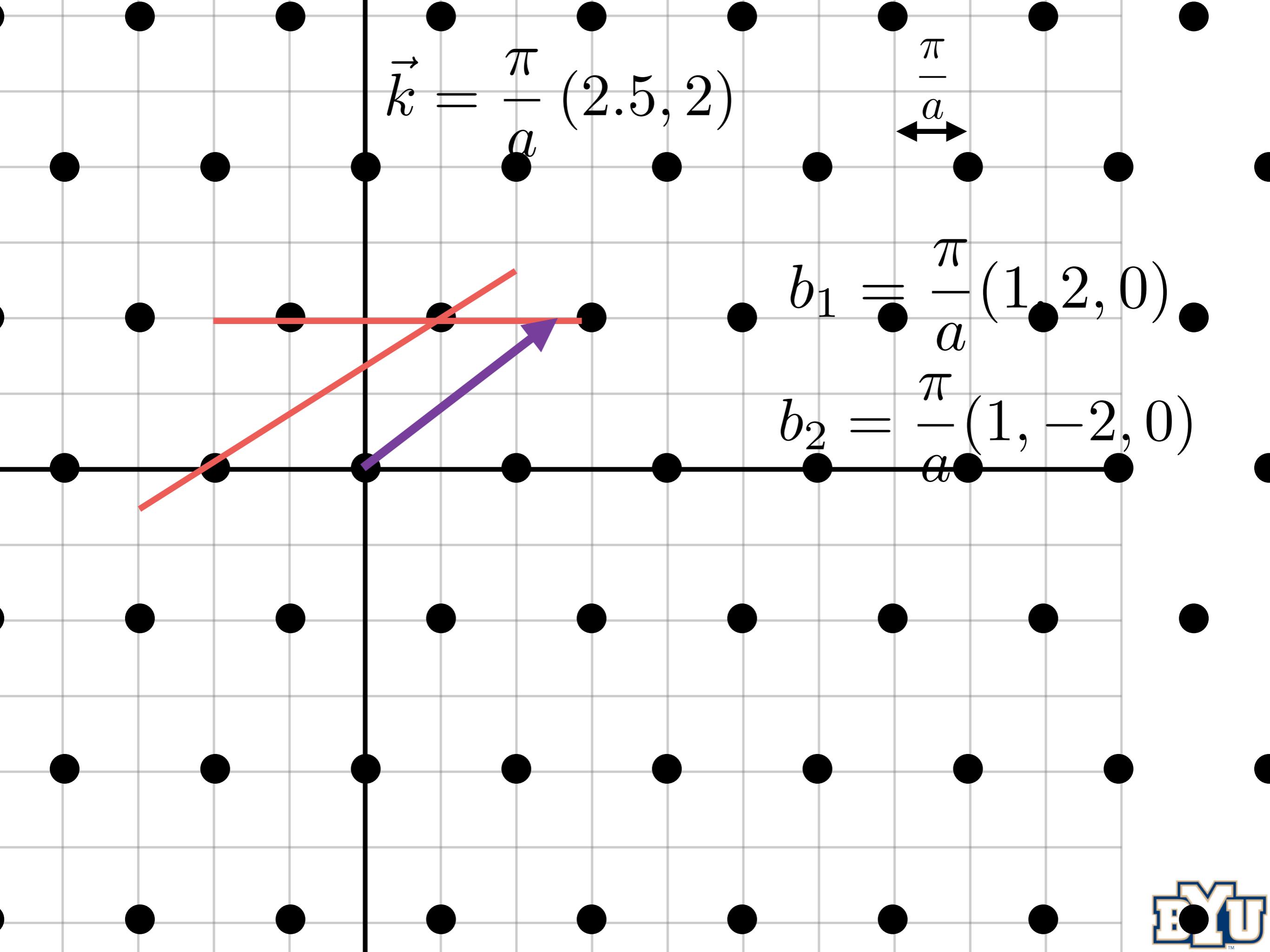
$$b_1 = \frac{\pi}{a} (1, 2, 0)$$

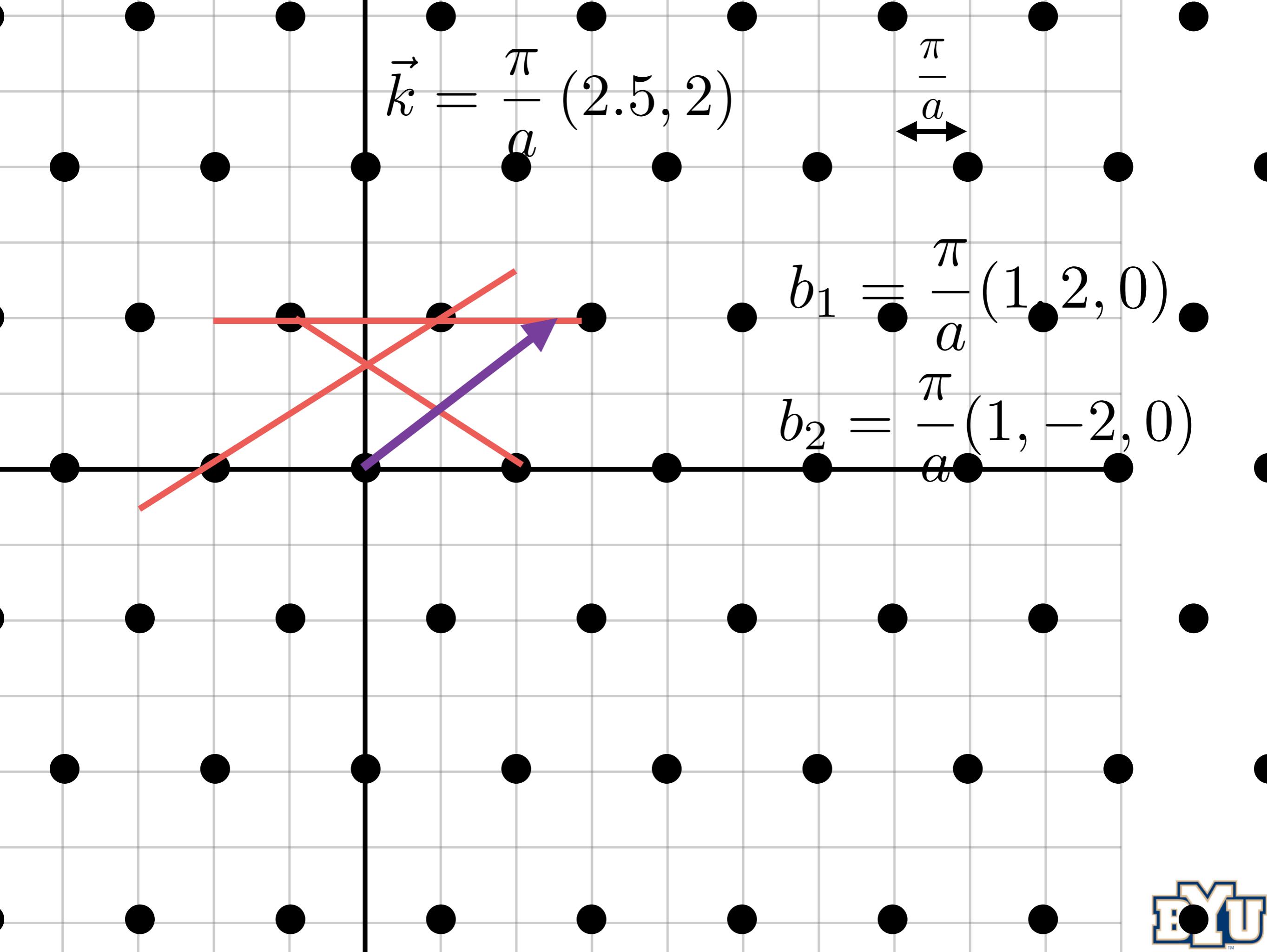
$$b_2 = \frac{\pi}{a} (1, -2, 0)$$

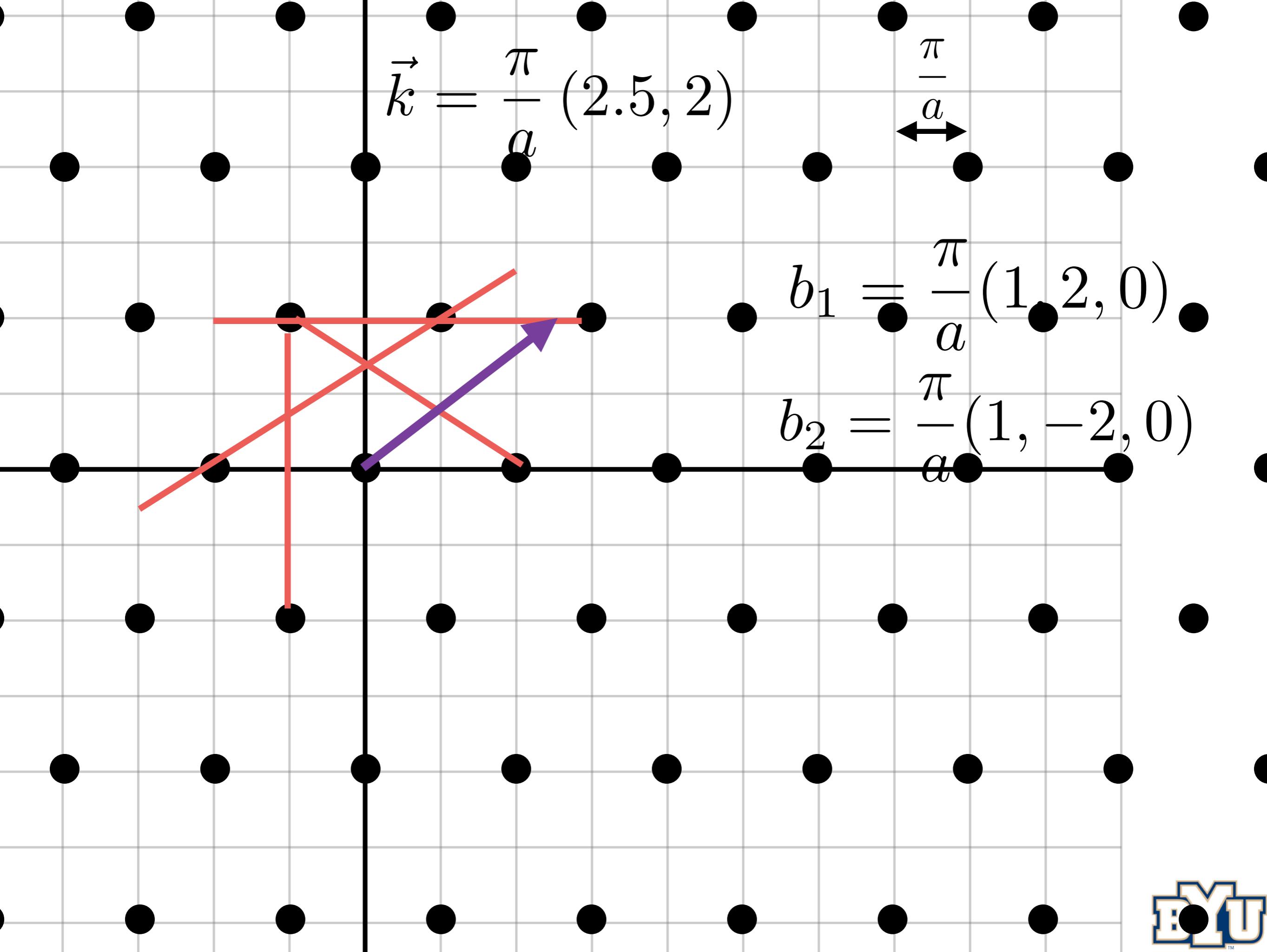


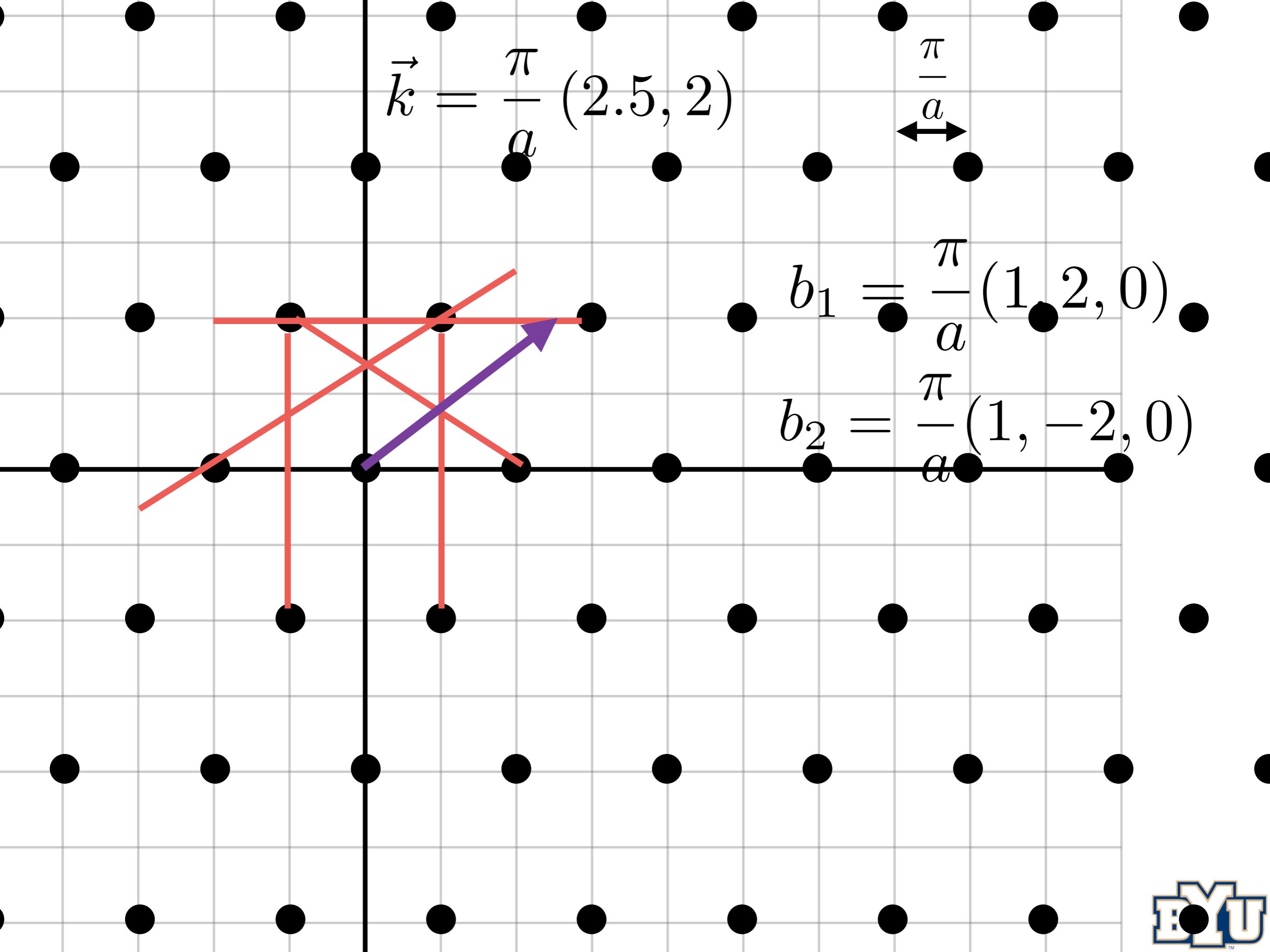


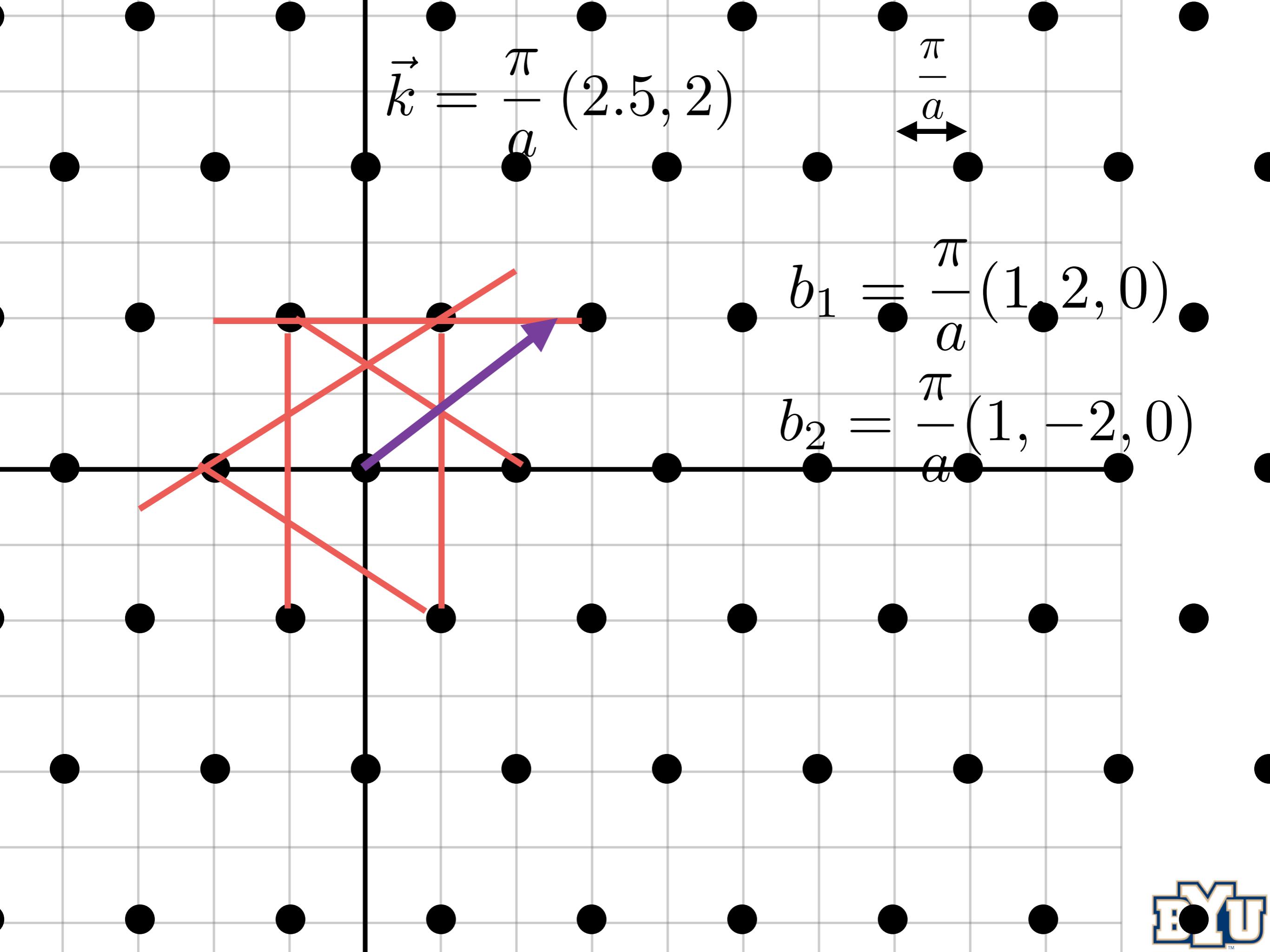


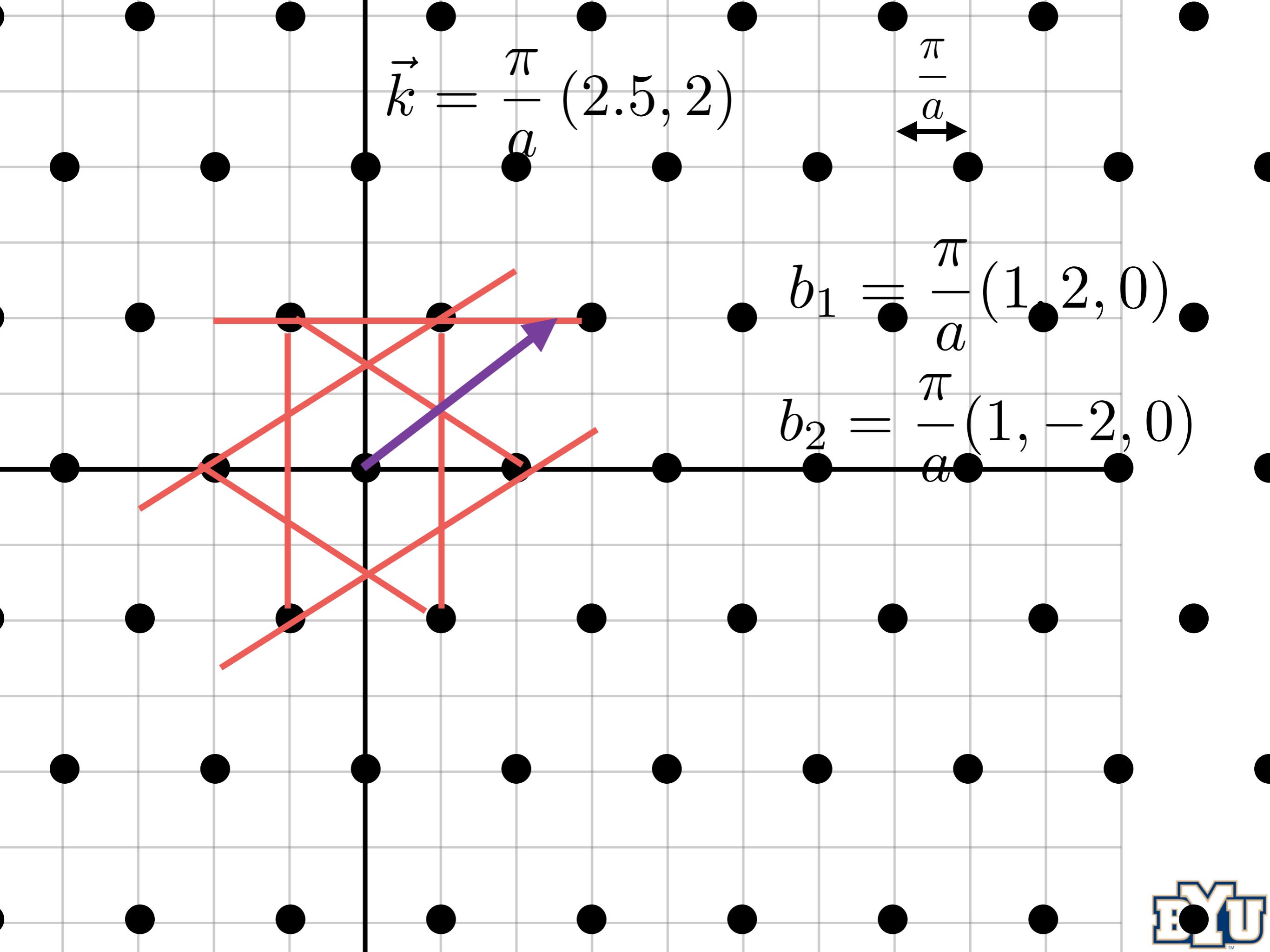


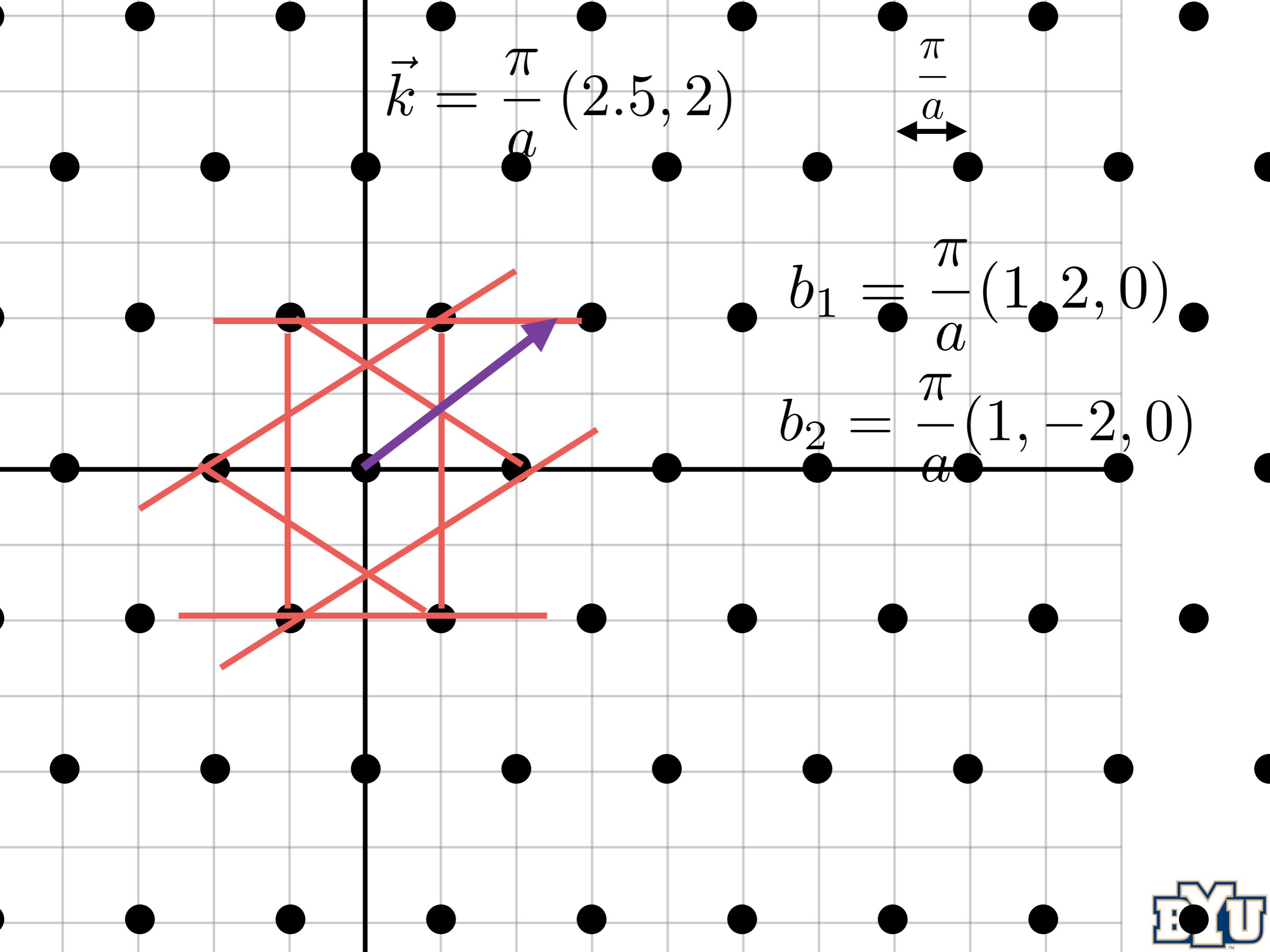


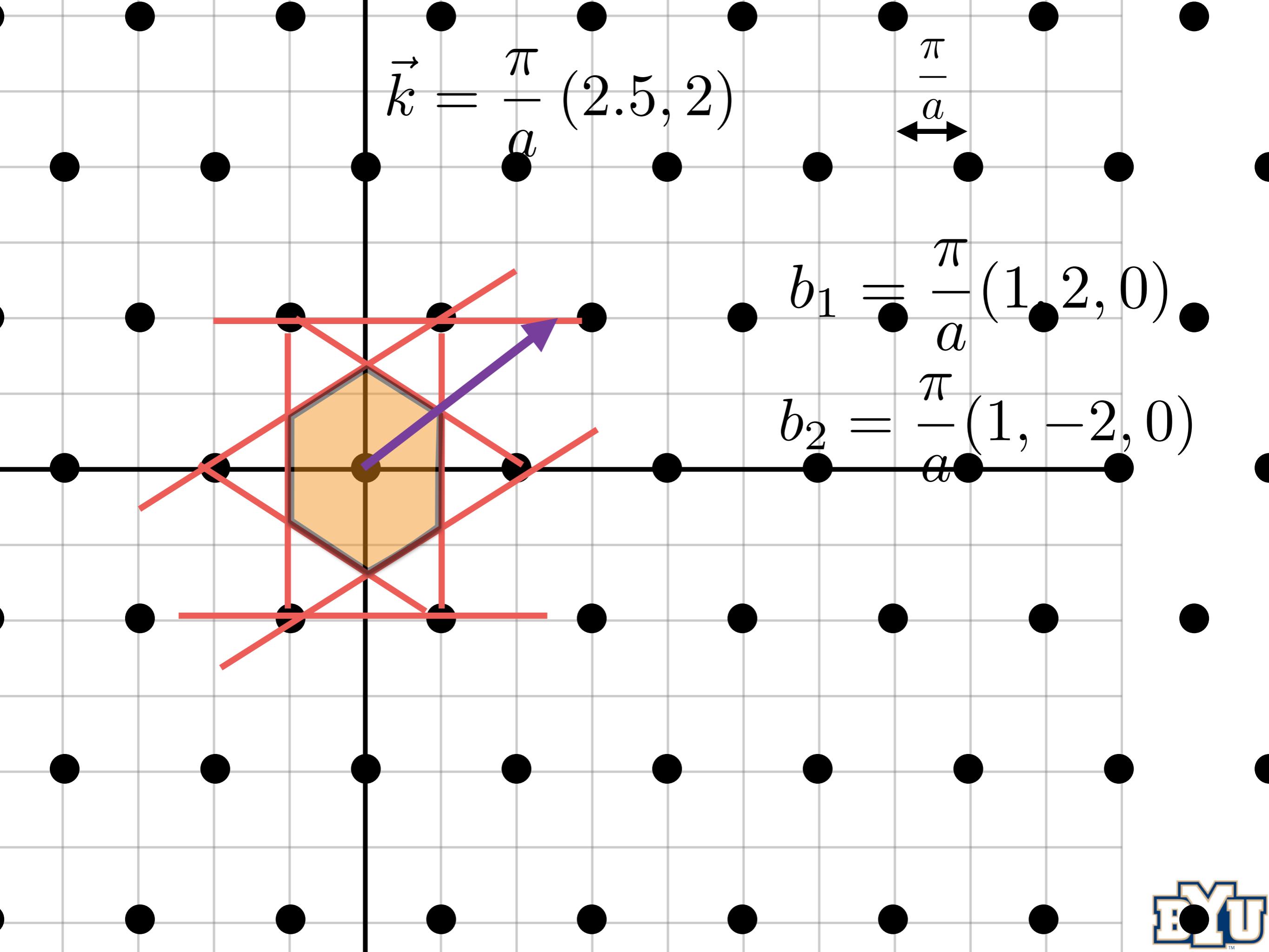


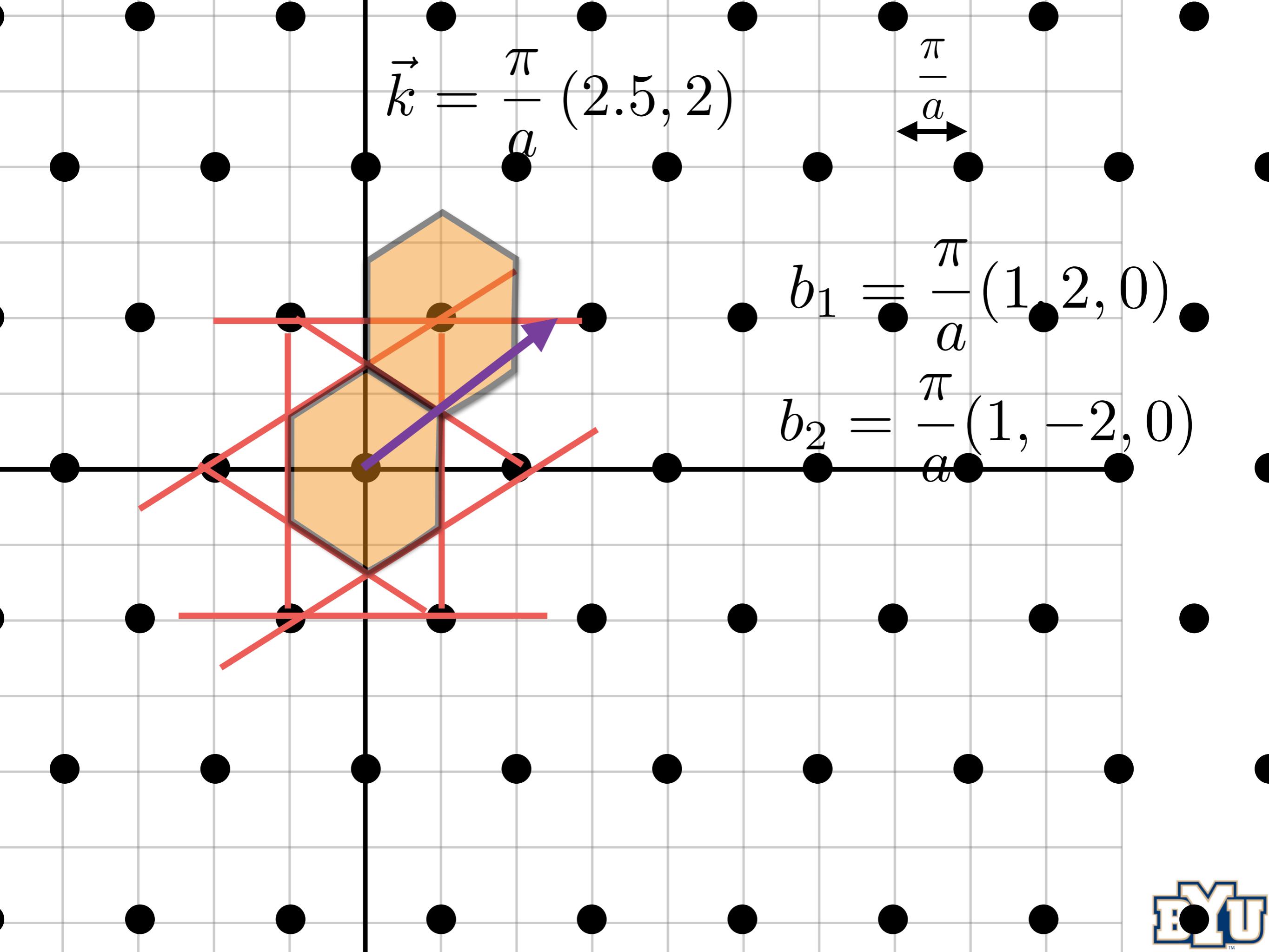


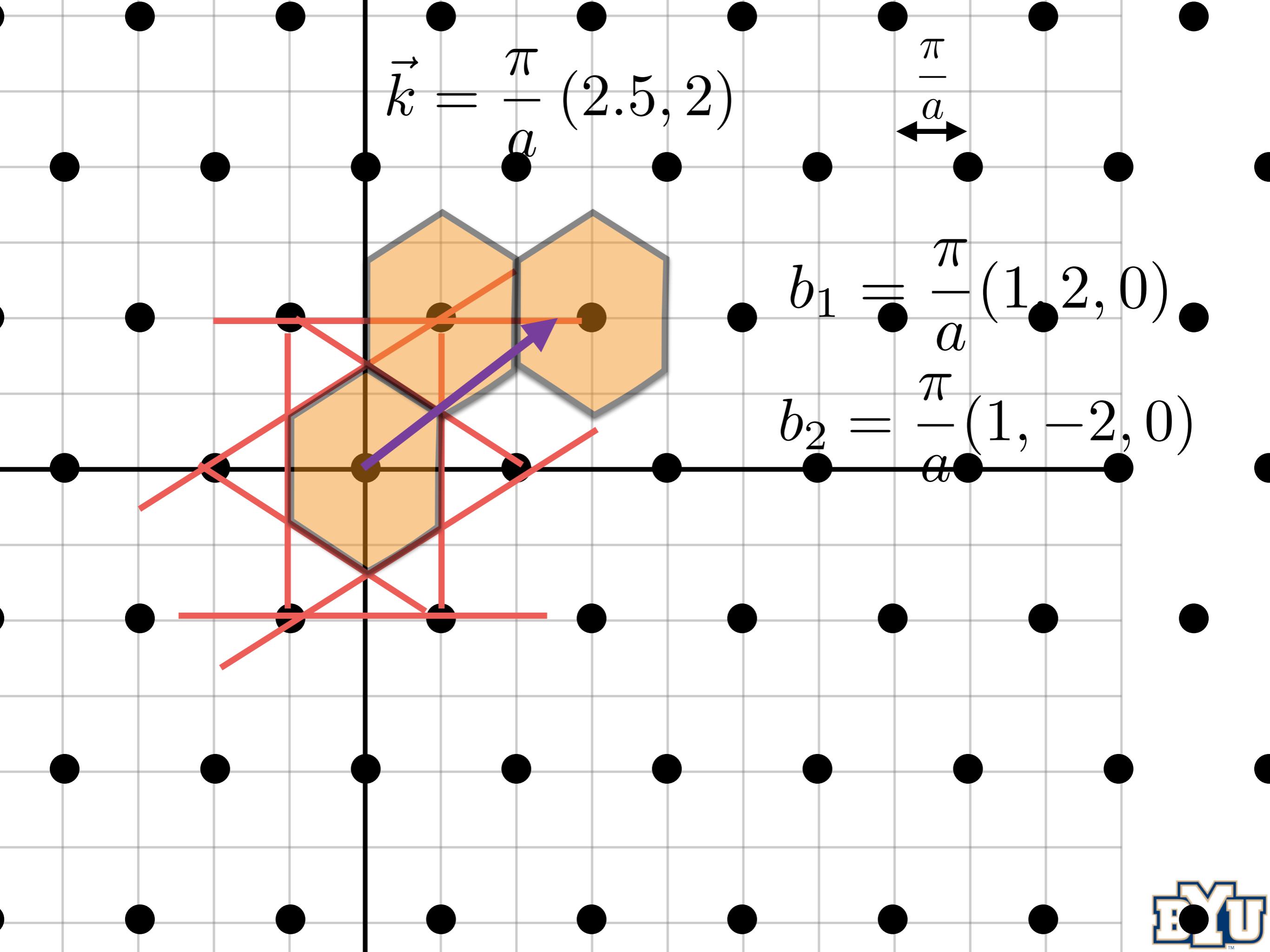


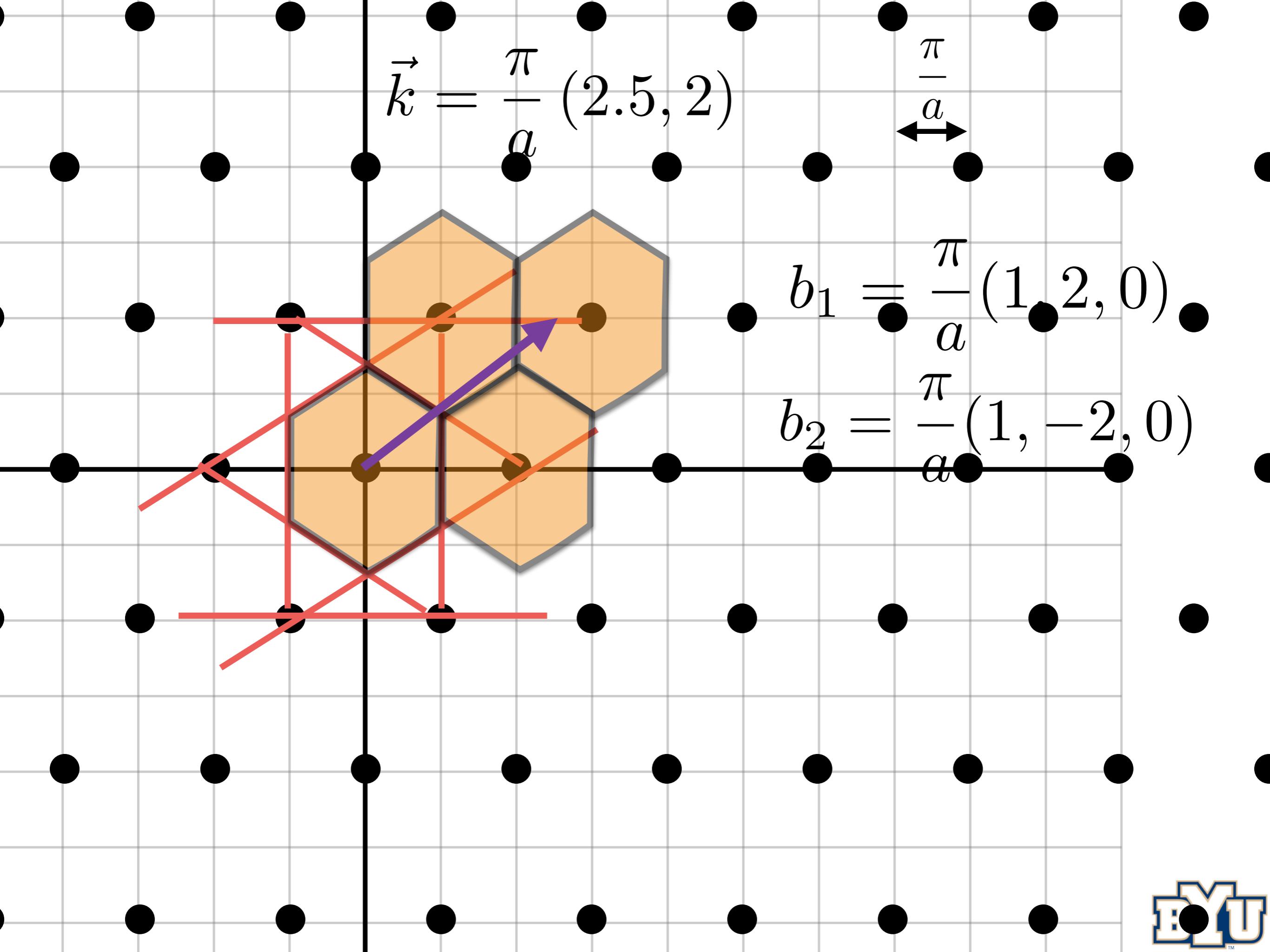


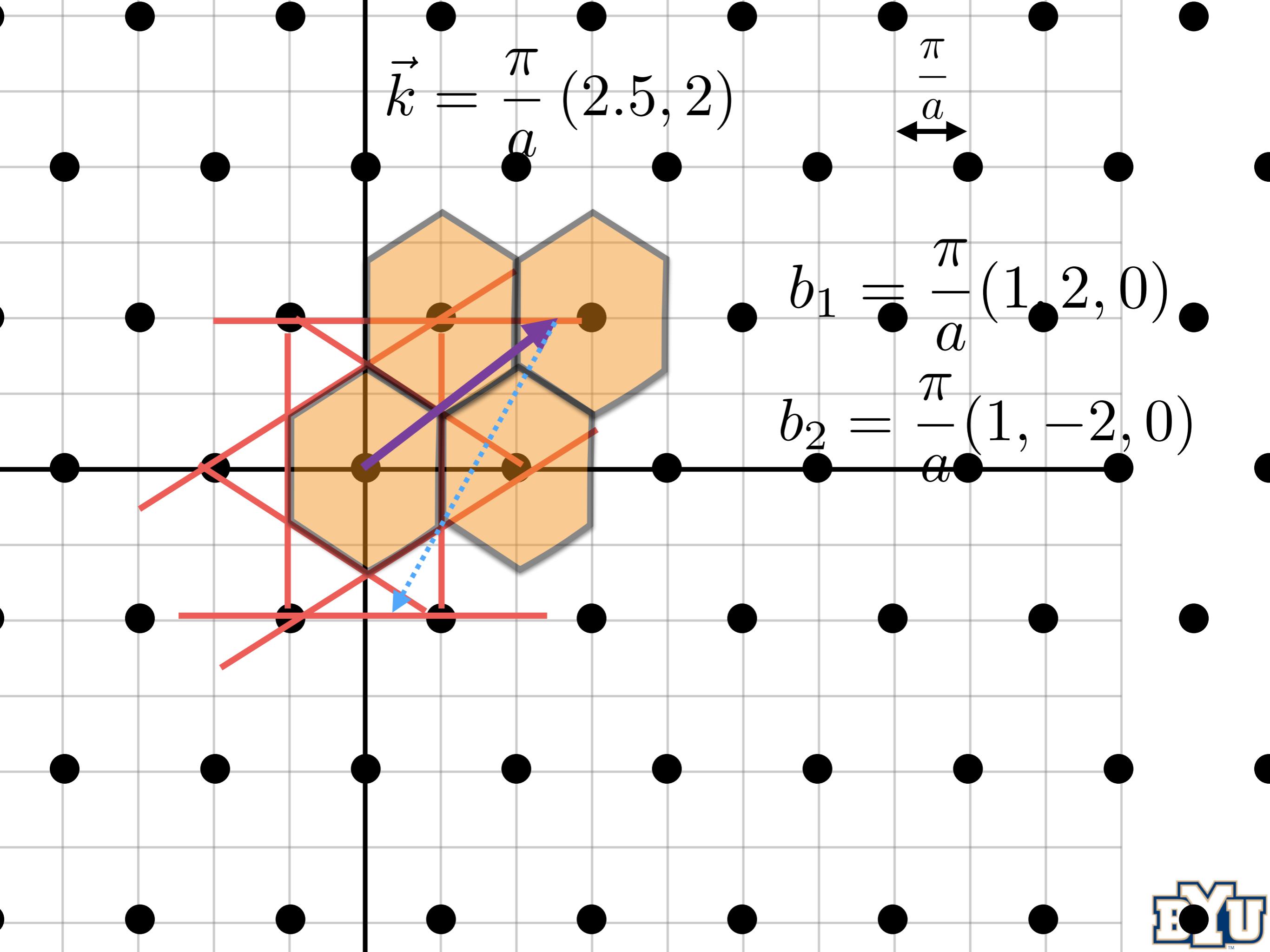


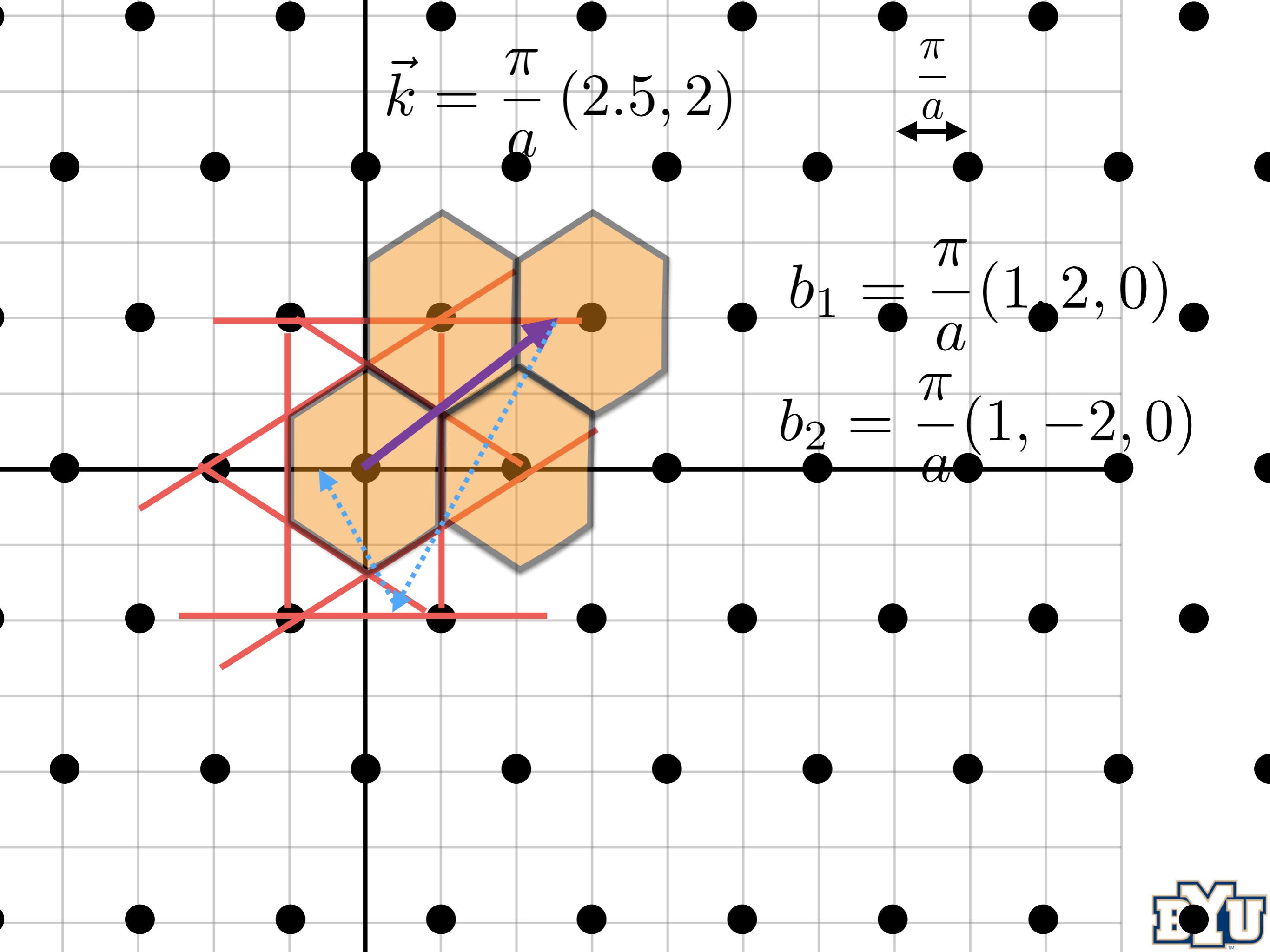












$$\vec{k} = \frac{\pi}{a} (2.5, 2)$$

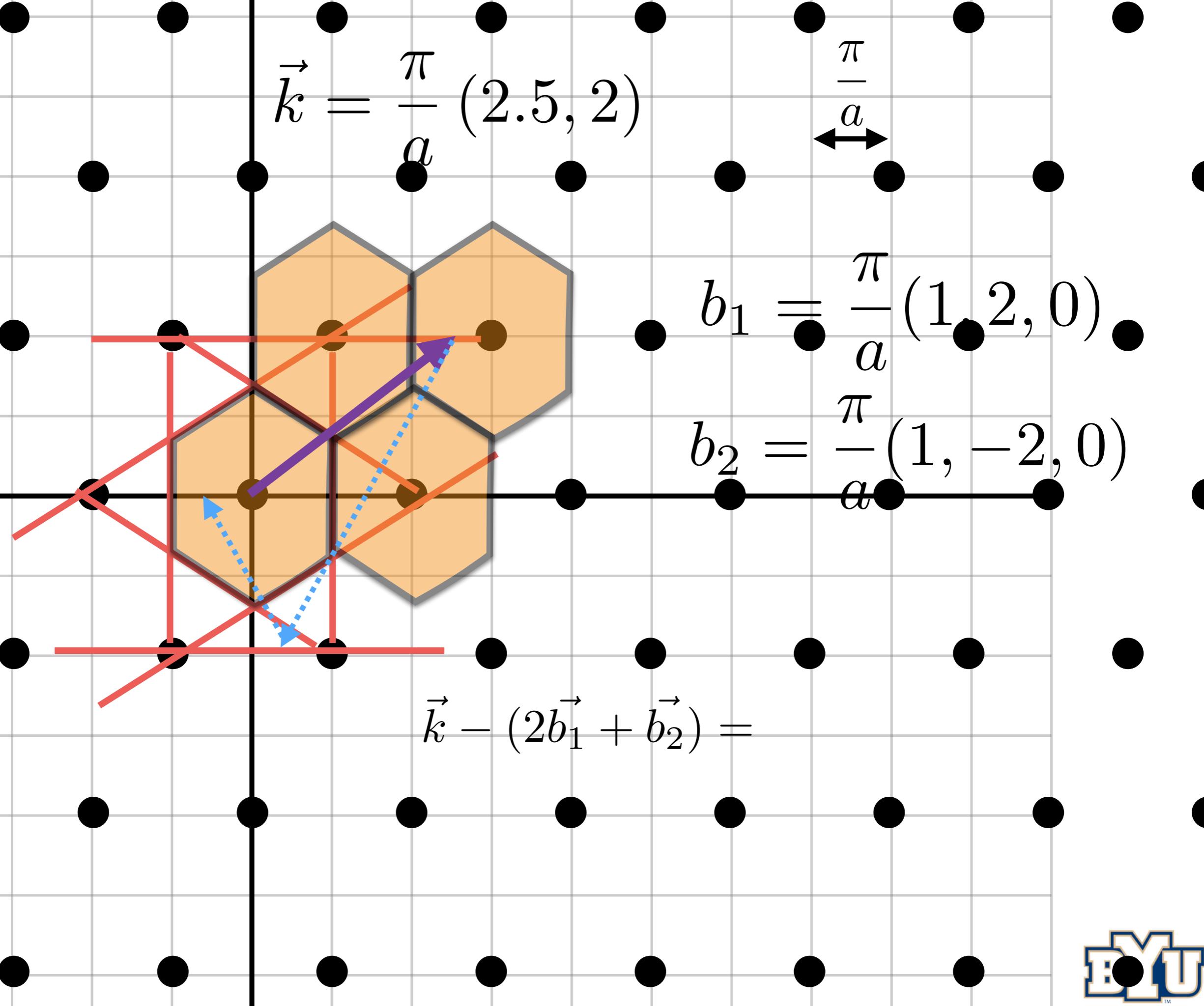
a

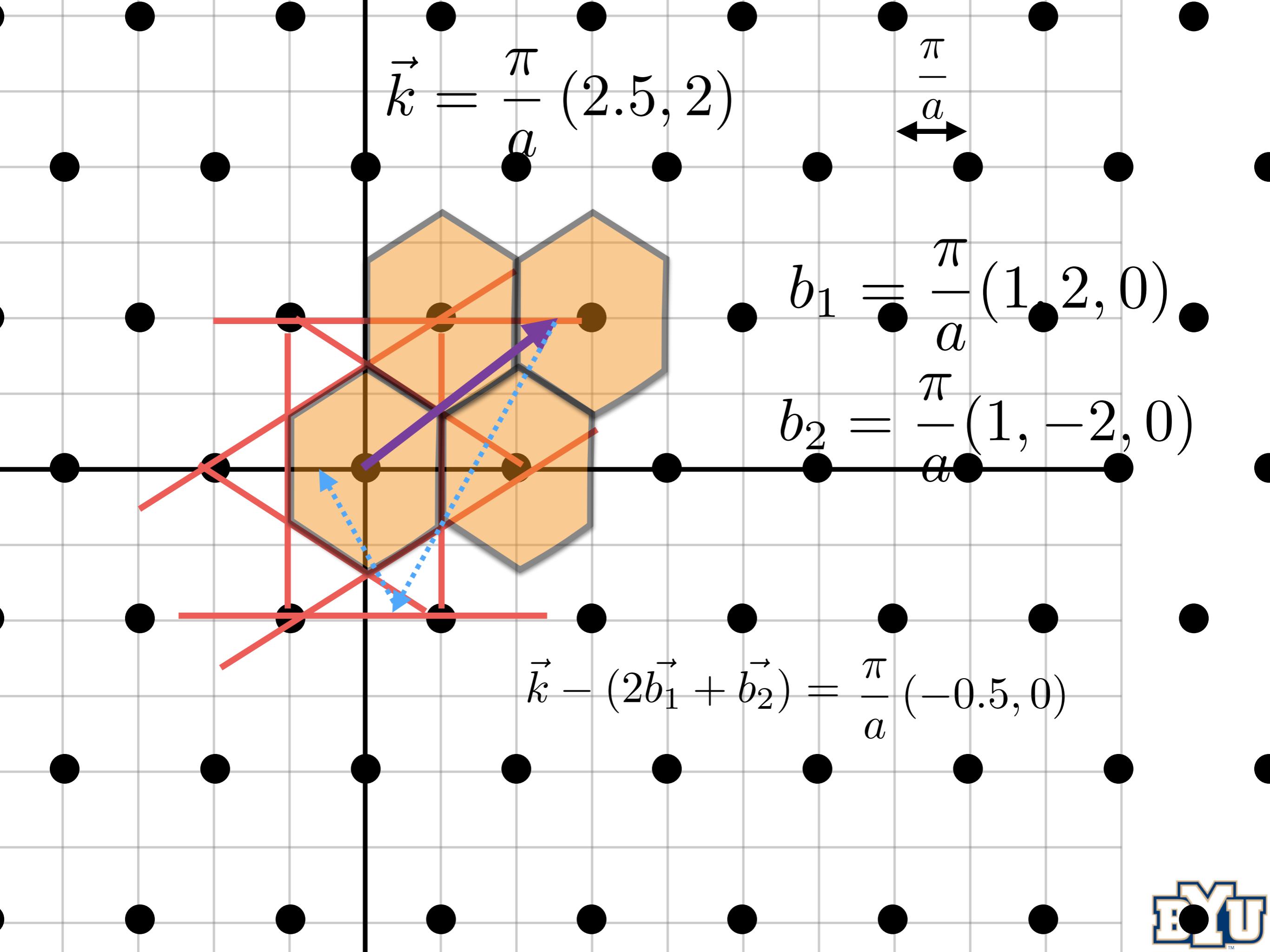
$$\frac{\pi}{a}$$

$$b_1 = \frac{\pi}{a} (1, 2, 0)$$

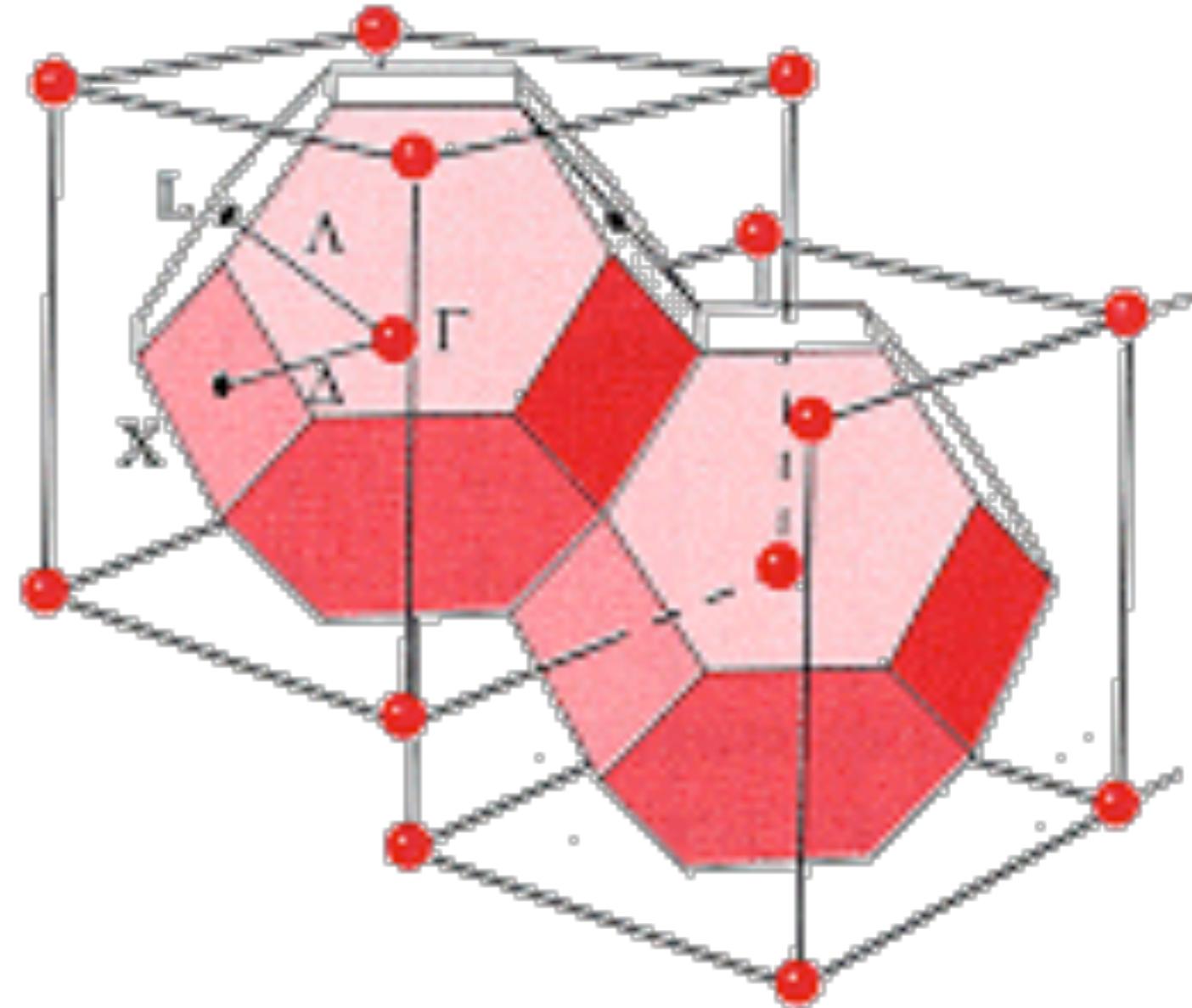
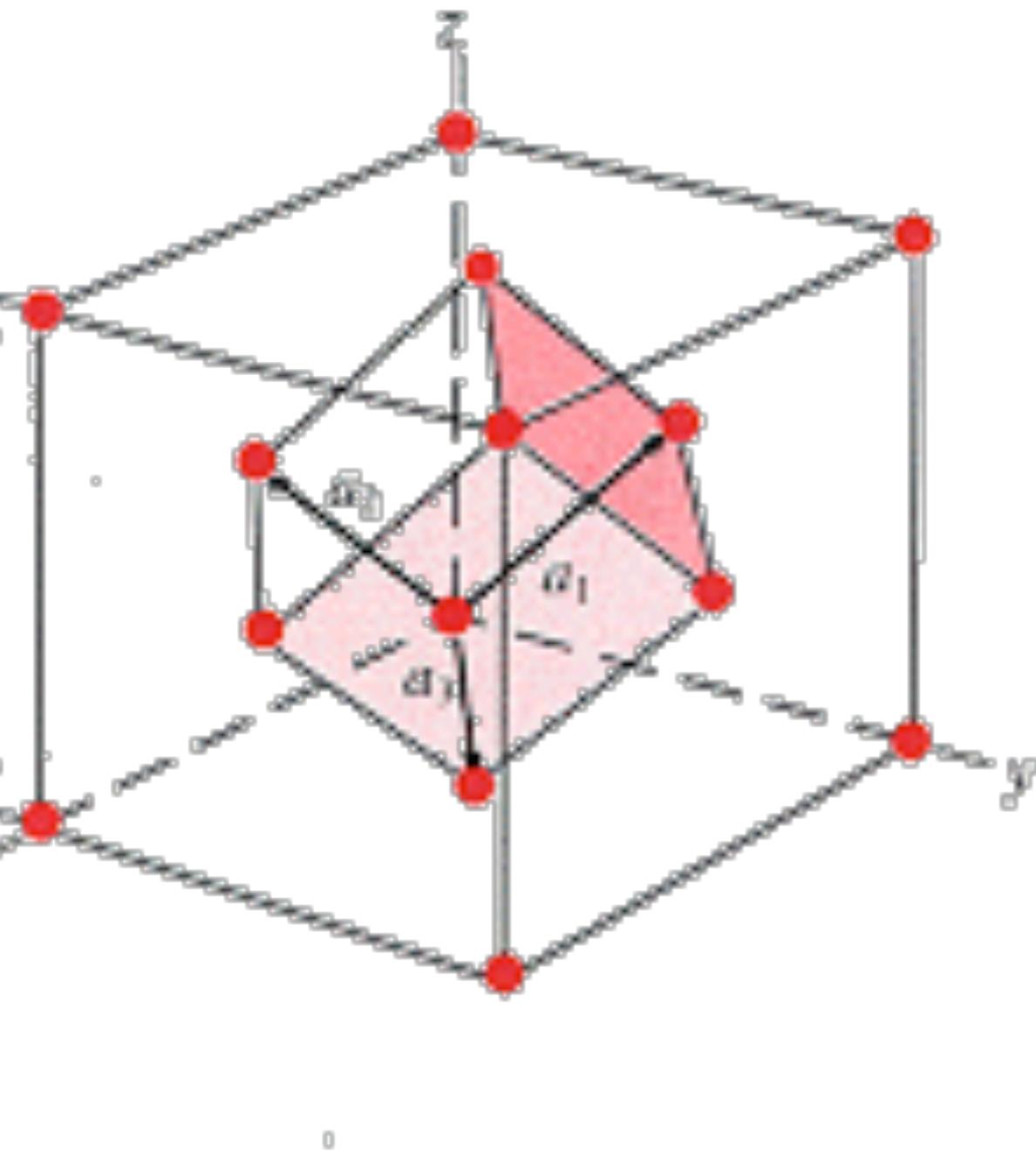
$$b_2 = \frac{\pi}{a} (1, -2, 0)$$

$$\vec{k} - (2\vec{b}_1 + \vec{b}_2) =$$

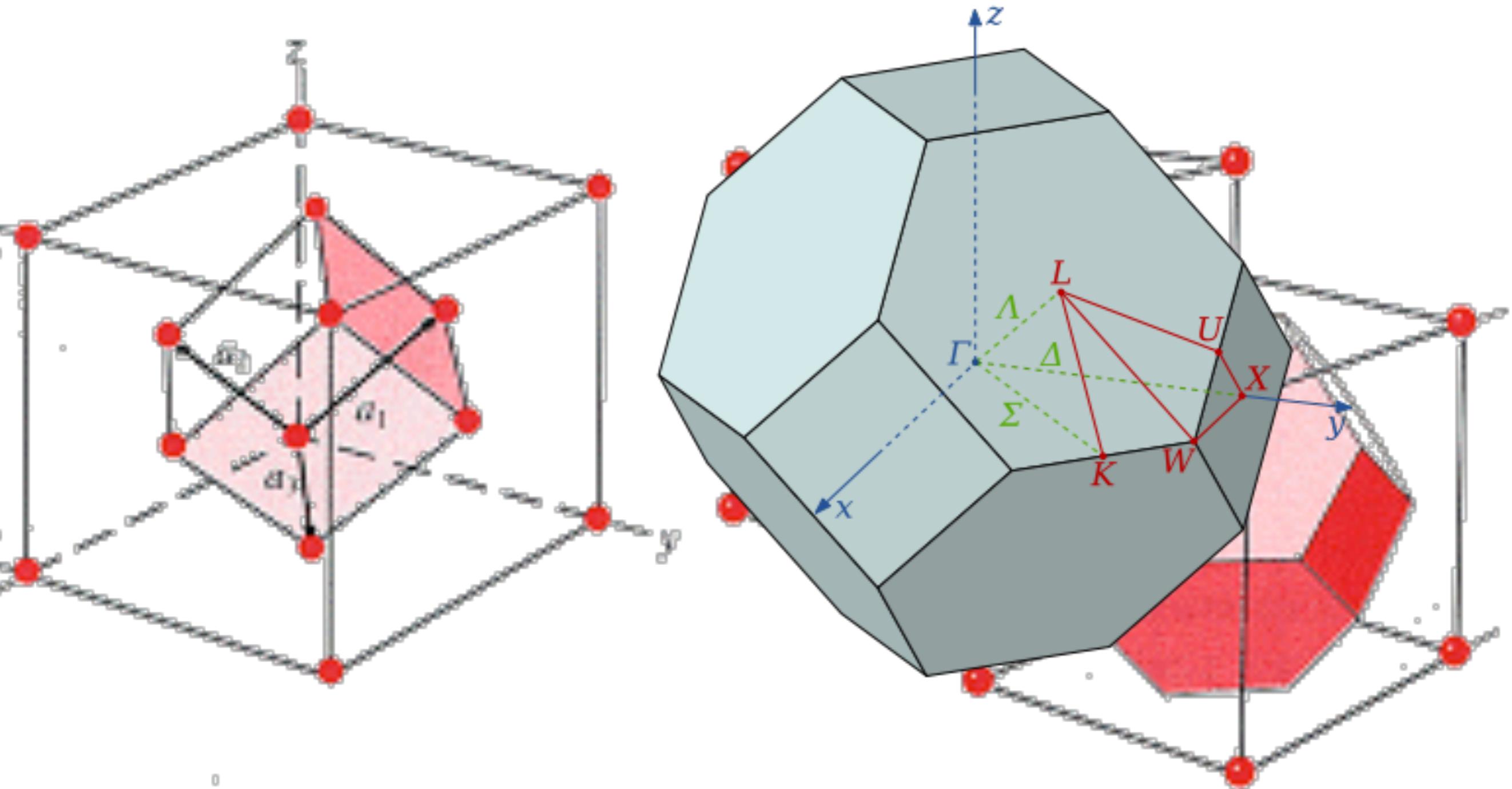




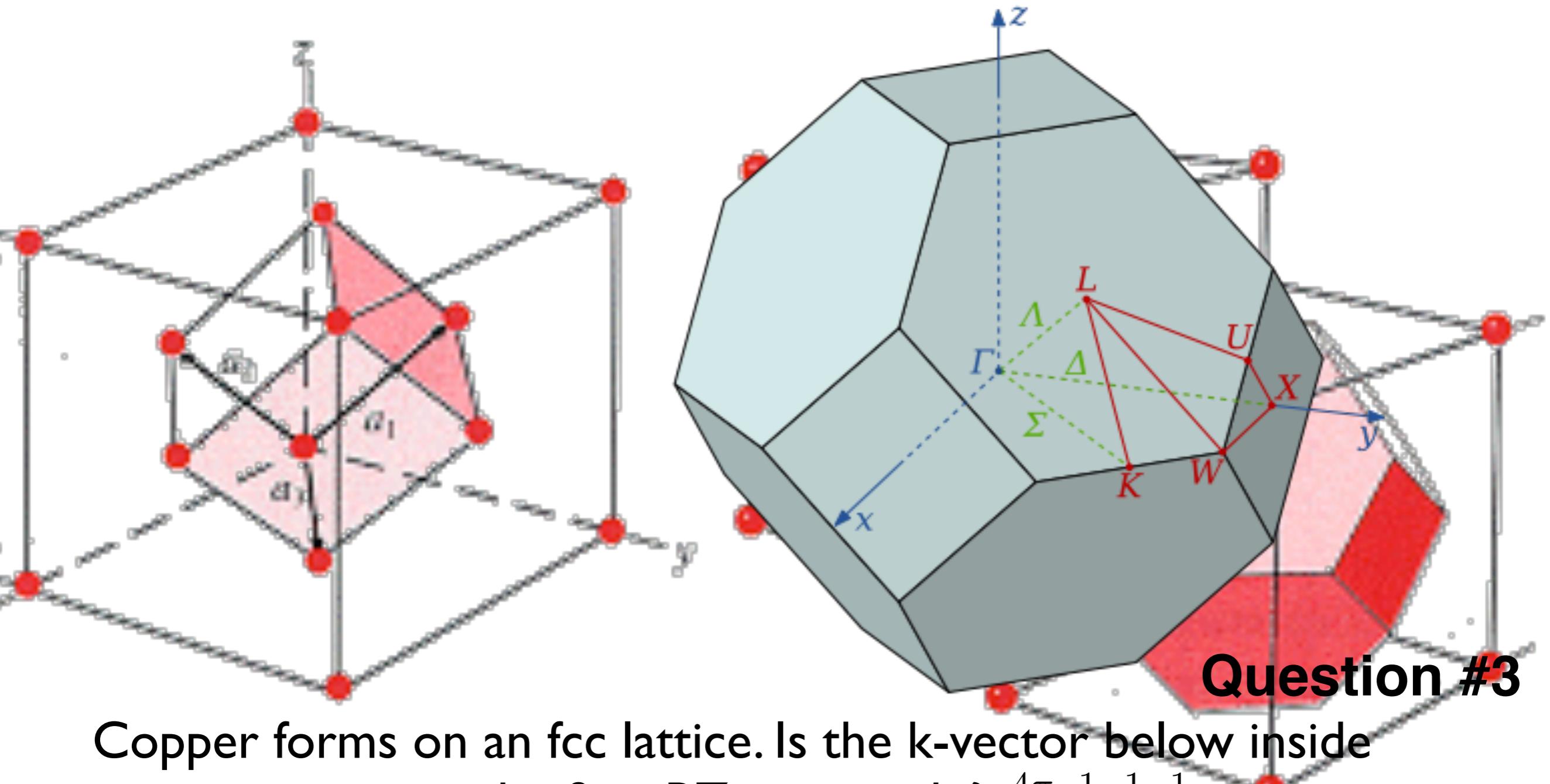
When the crystal forms a(n) _____ lattice, the reciprocal lattice is _____ with lattice parameter _____.



When the crystal forms a(n) _____ lattice, the reciprocal lattice is _____ with lattice parameter _____.



When the crystal forms a(n) _____ lattice, the reciprocal lattice is _____ with lattice parameter _____.

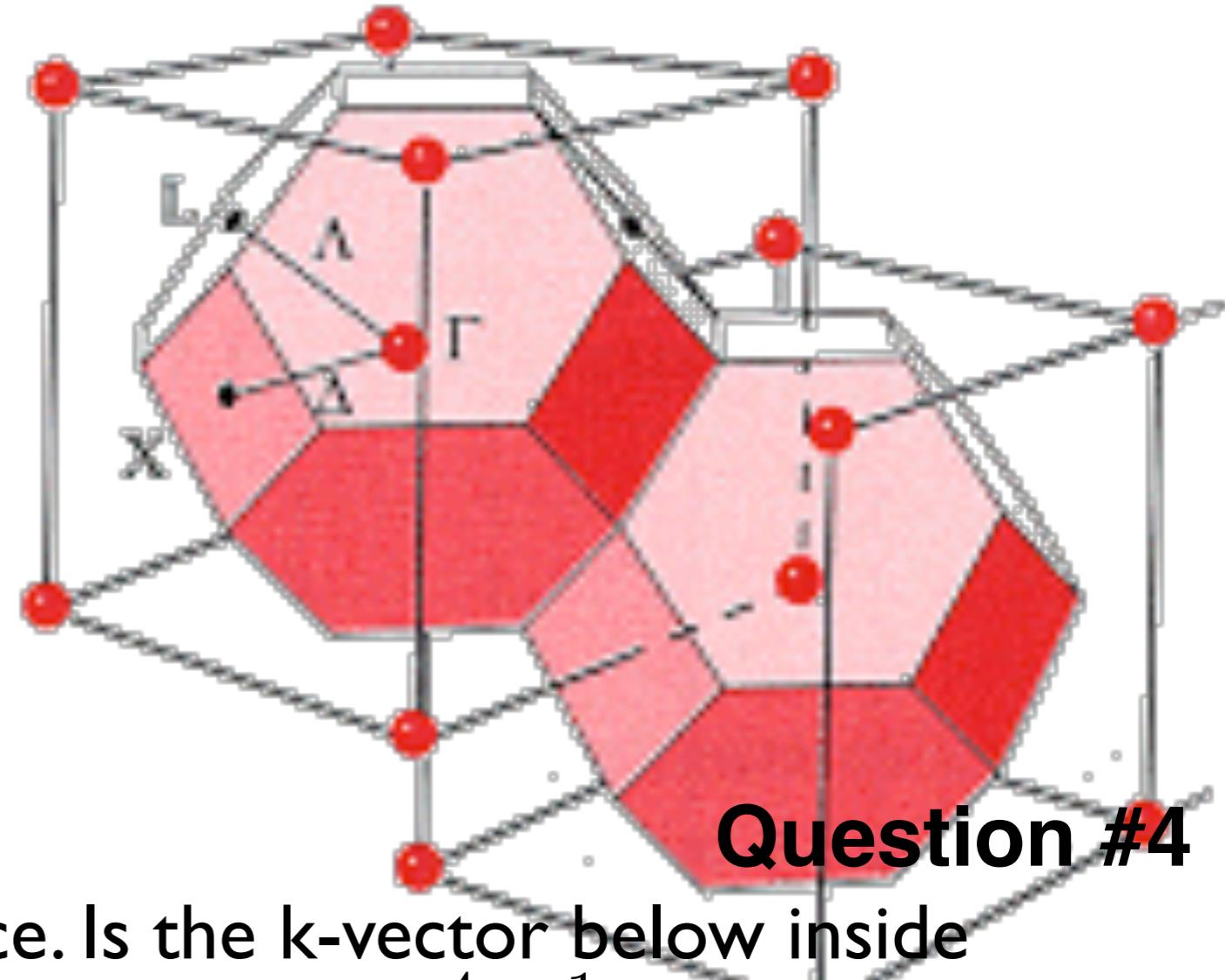
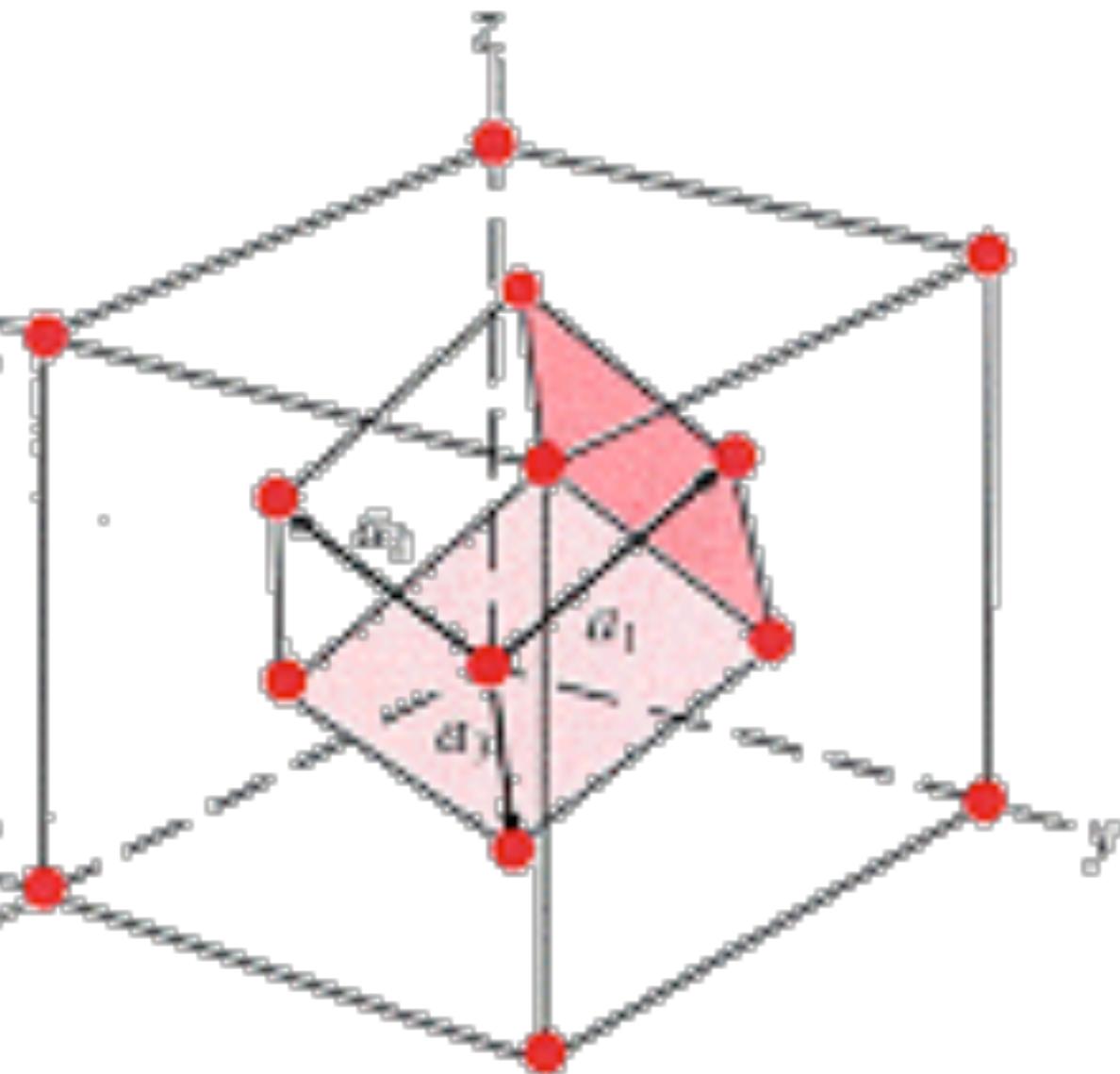


Copper forms on an fcc lattice. Is the k-vector below inside the first BZ or outside? $\frac{4\pi}{a}(\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$

c) inside

e) outside

When the crystal forms a(n) _____ lattice, the reciprocal lattice is _____ with lattice parameter _____.



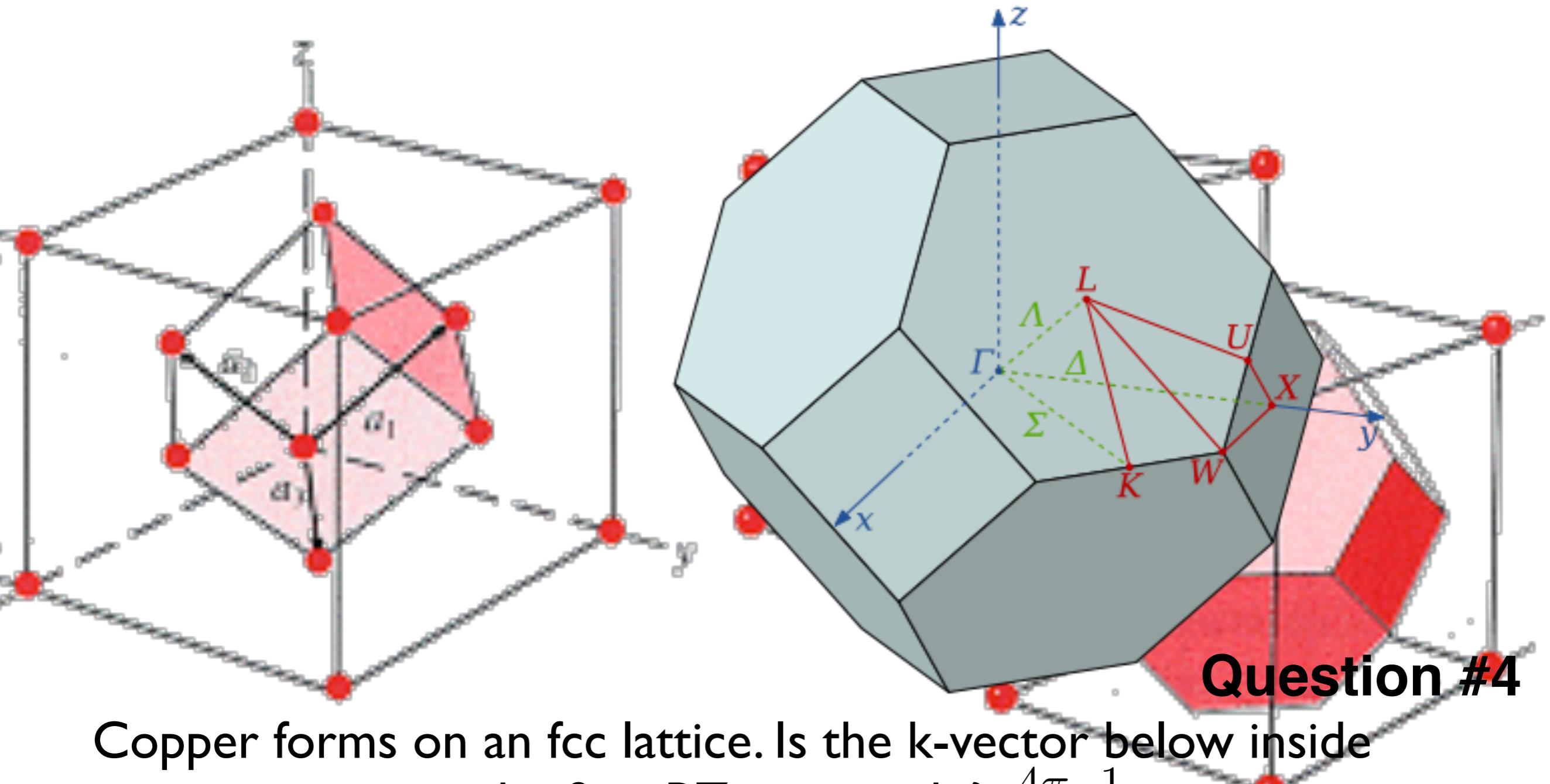
Question #4

Copper forms on an fcc lattice. Is the k-vector below inside the first BZ or outside? $\frac{4\pi}{a}(\frac{1}{4}, 0, 0)$

c) outside

d) inside

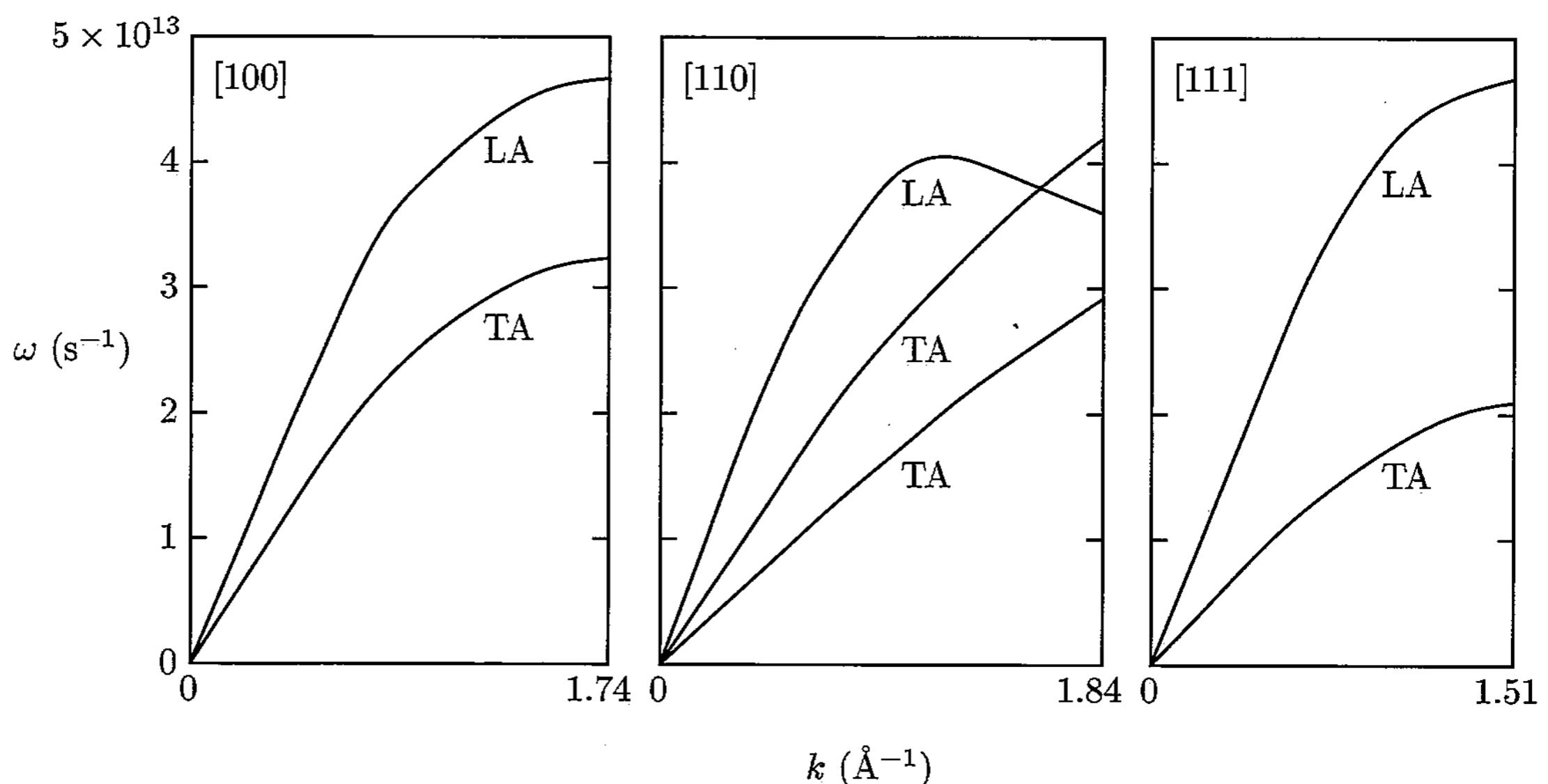
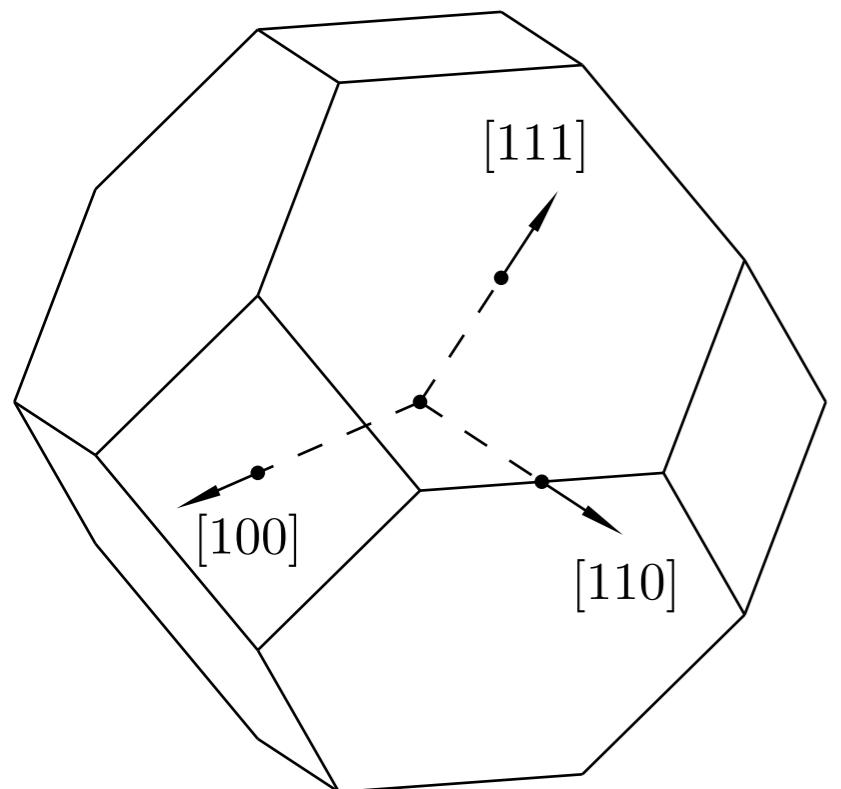
When the crystal forms a(n) _____ lattice, the reciprocal lattice is _____ with lattice parameter _____.

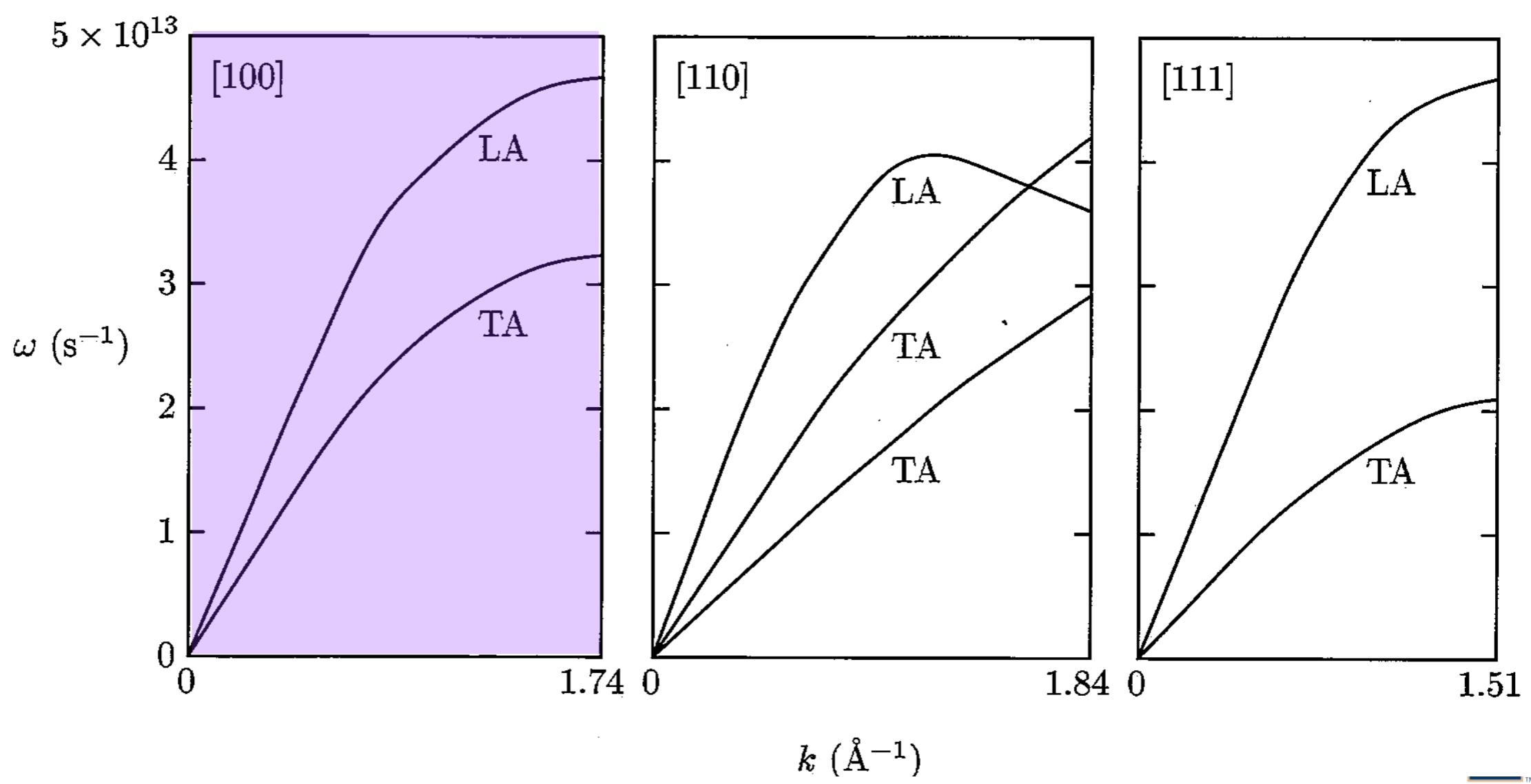
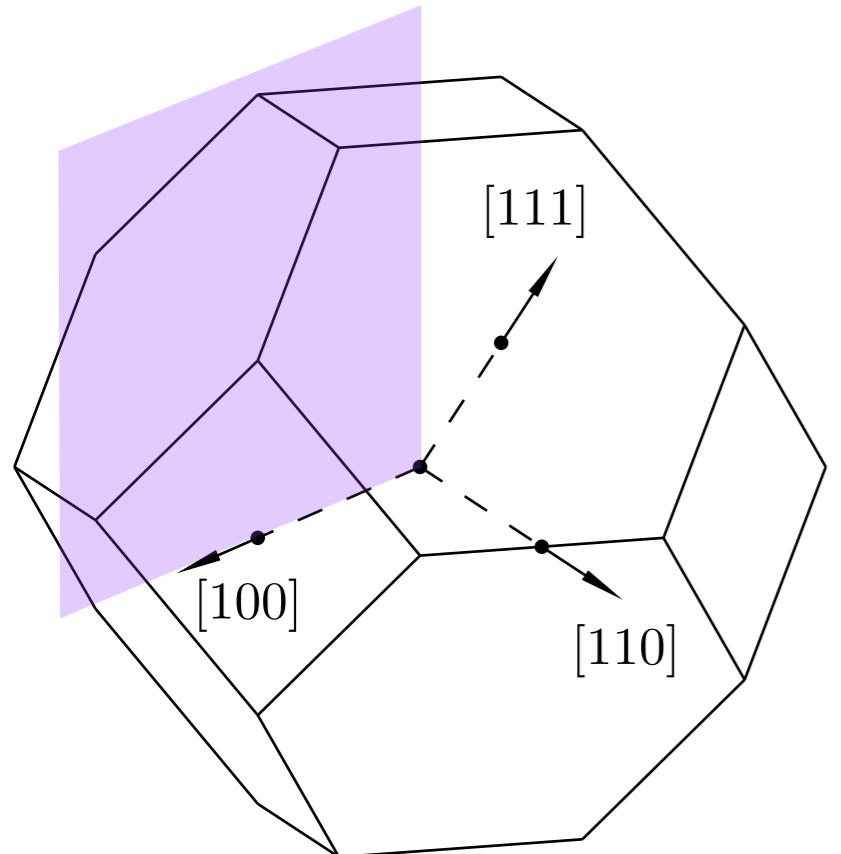


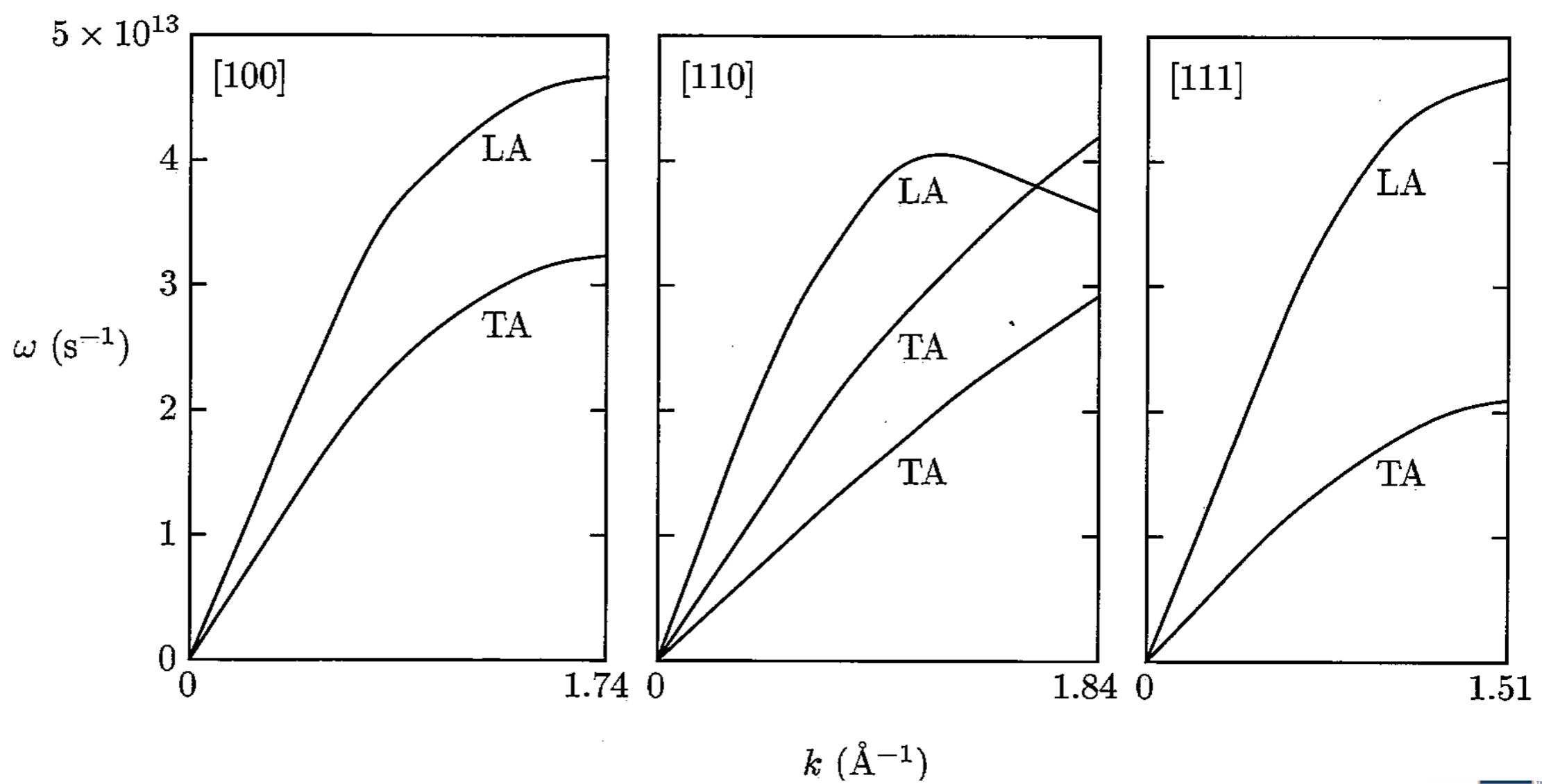
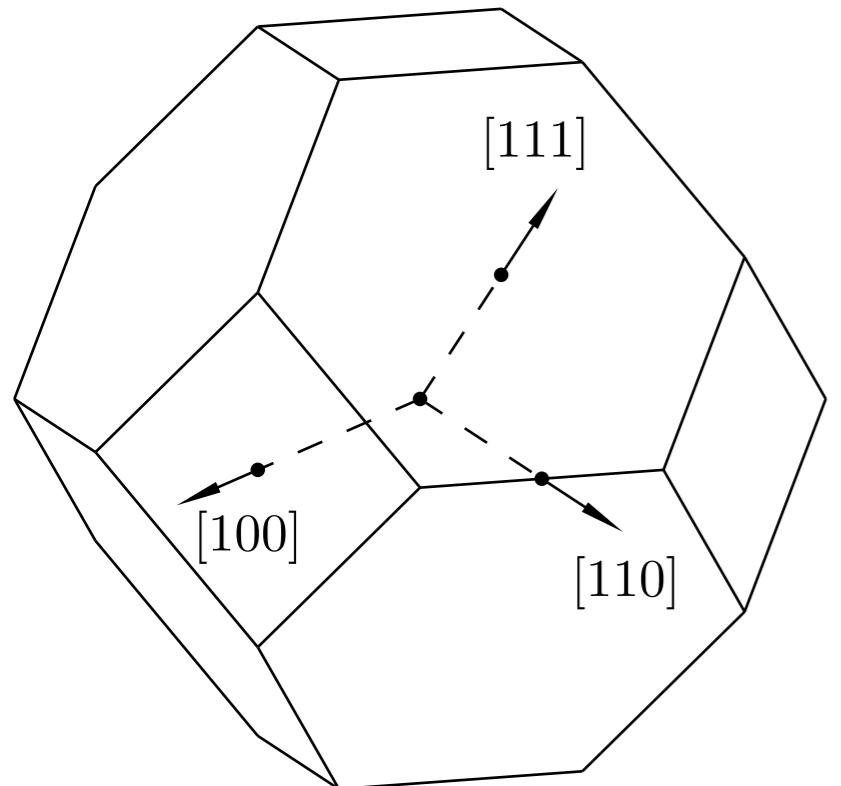
Copper forms on an fcc lattice. Is the k-vector below inside the first BZ or outside? $\frac{4\pi}{a}(\frac{1}{4}, 0, 0)$

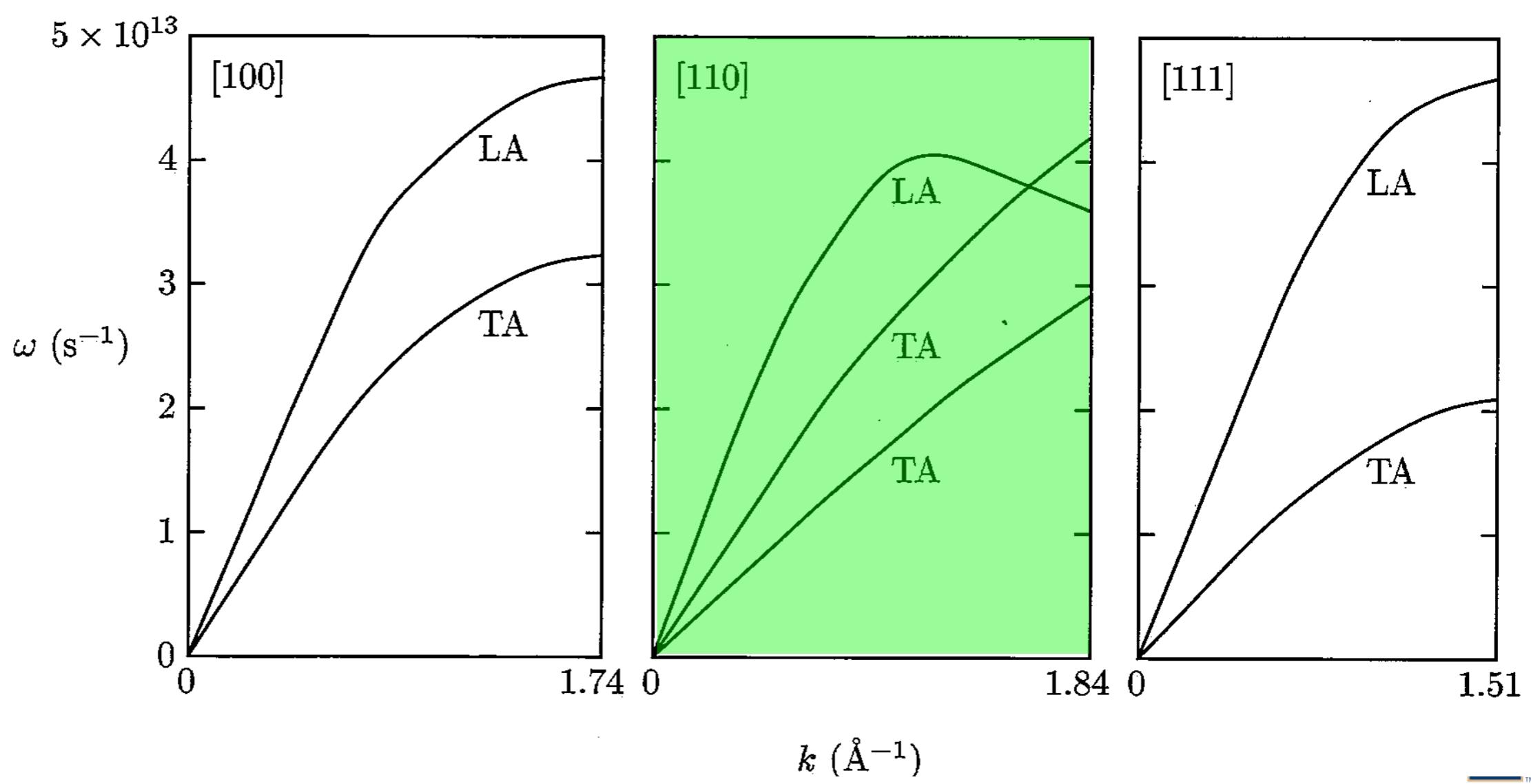
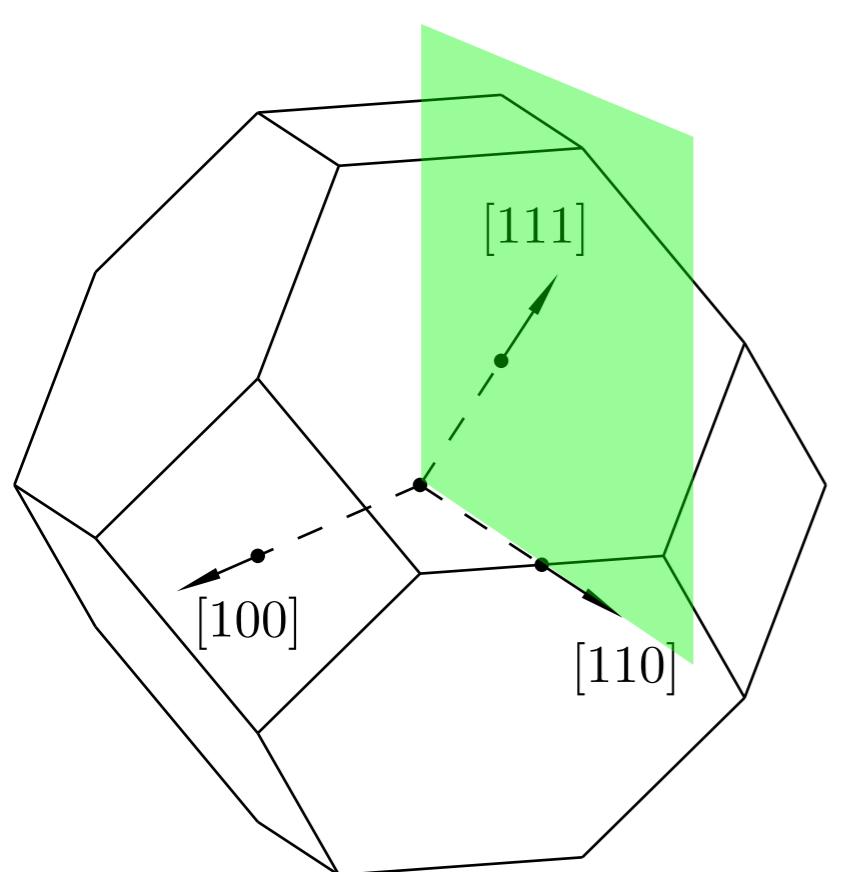
c) outside

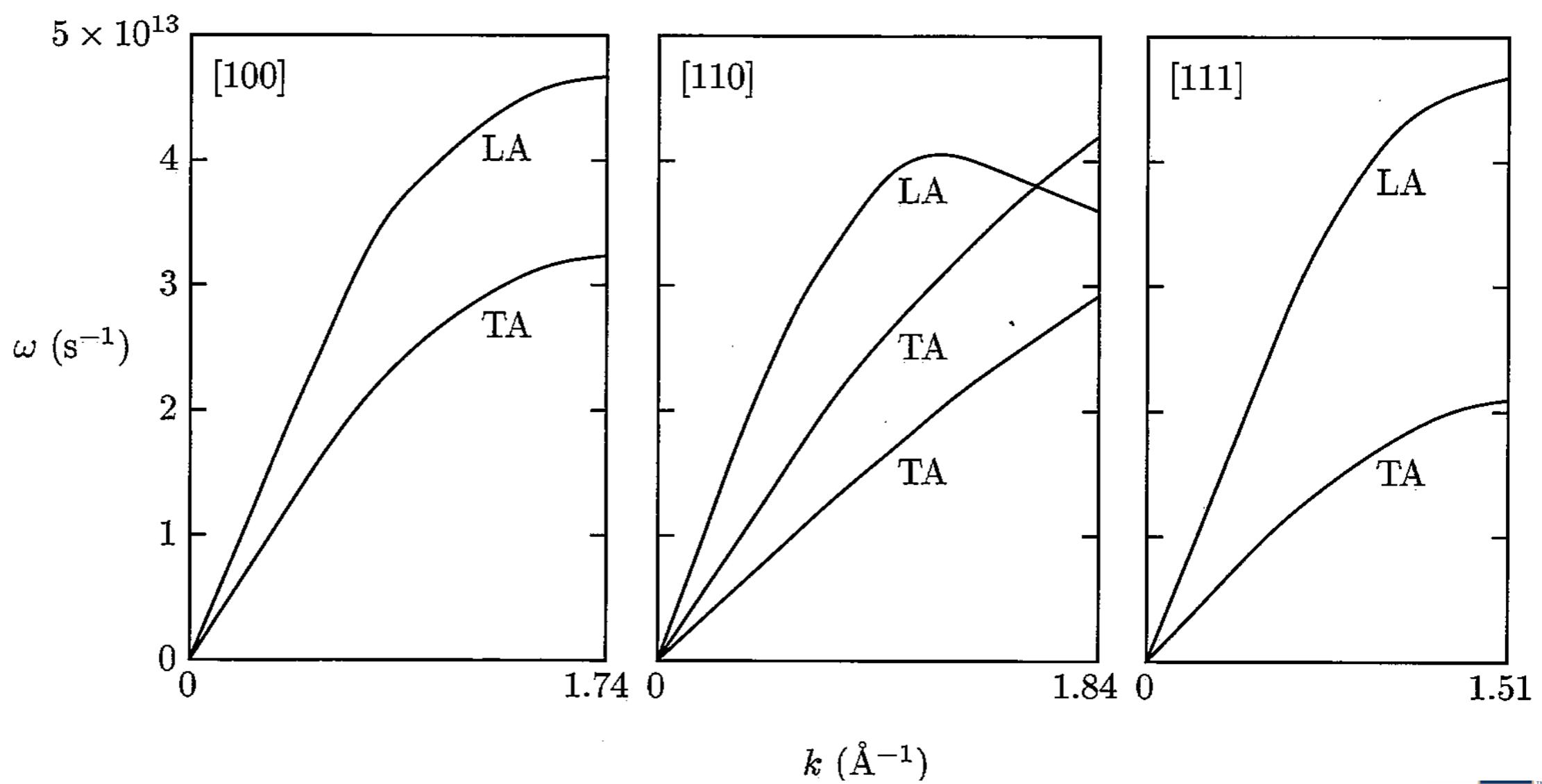
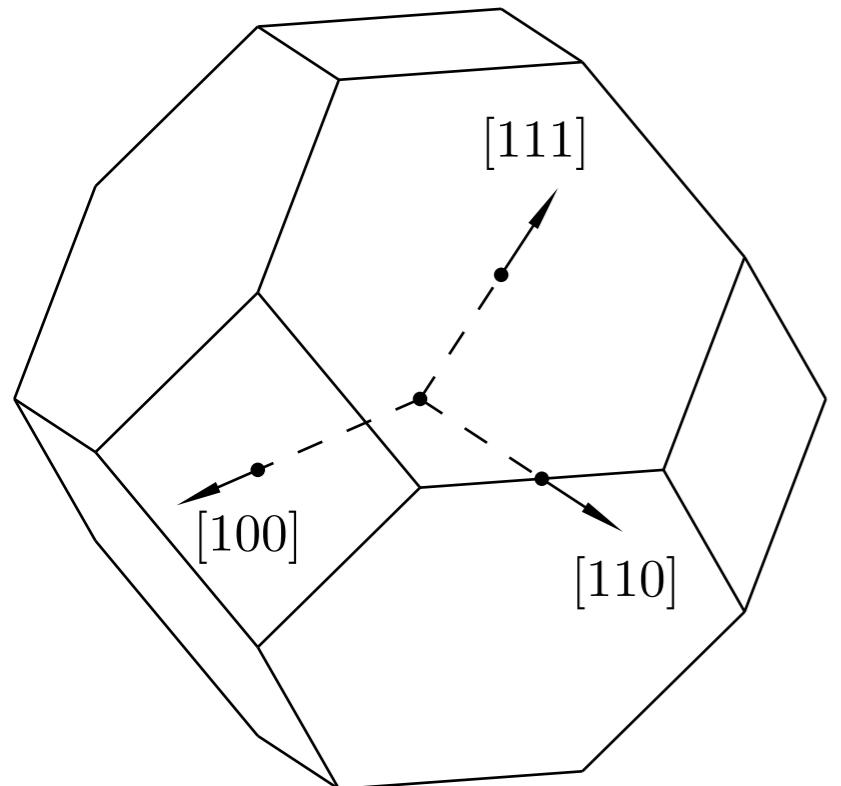
d) inside

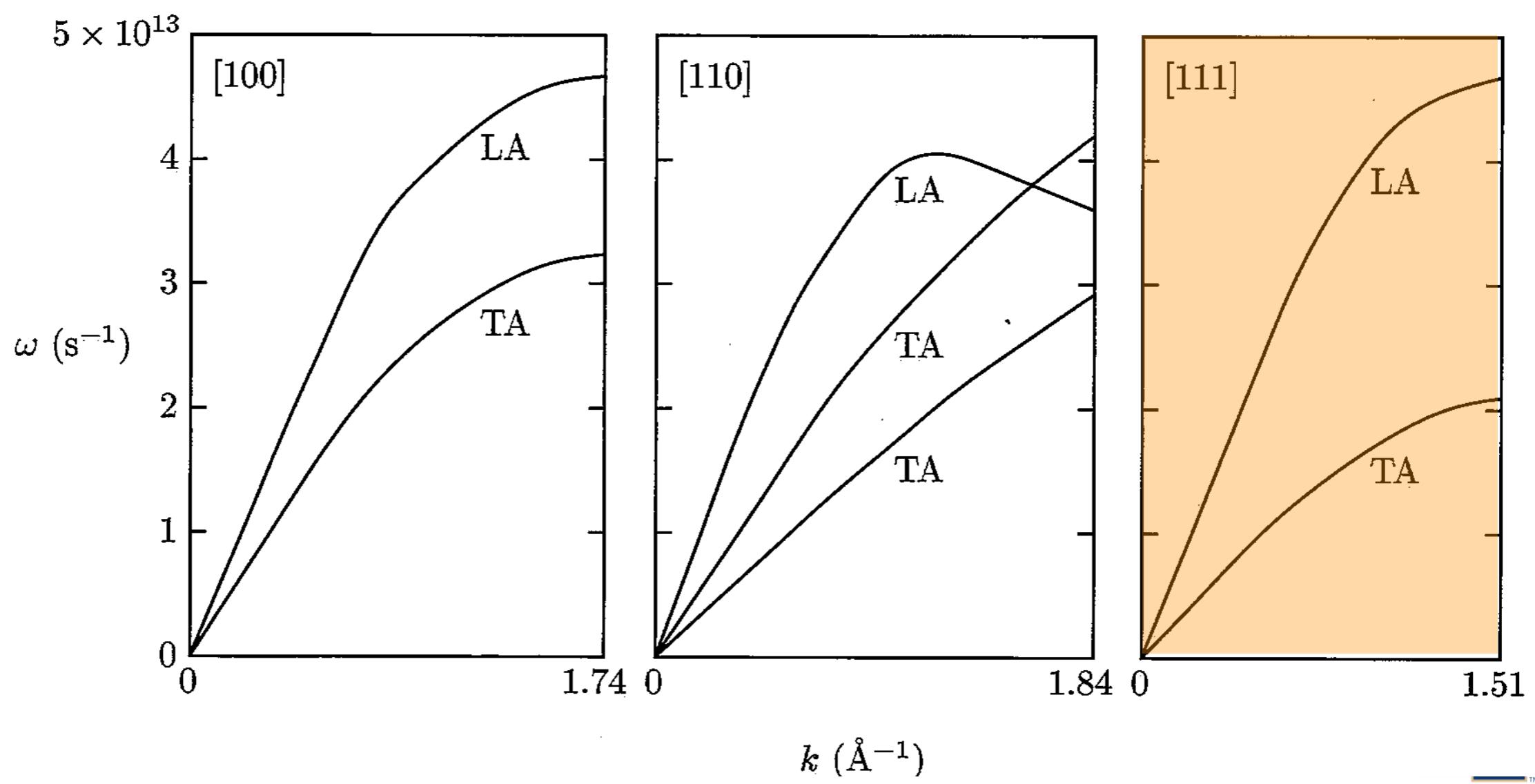
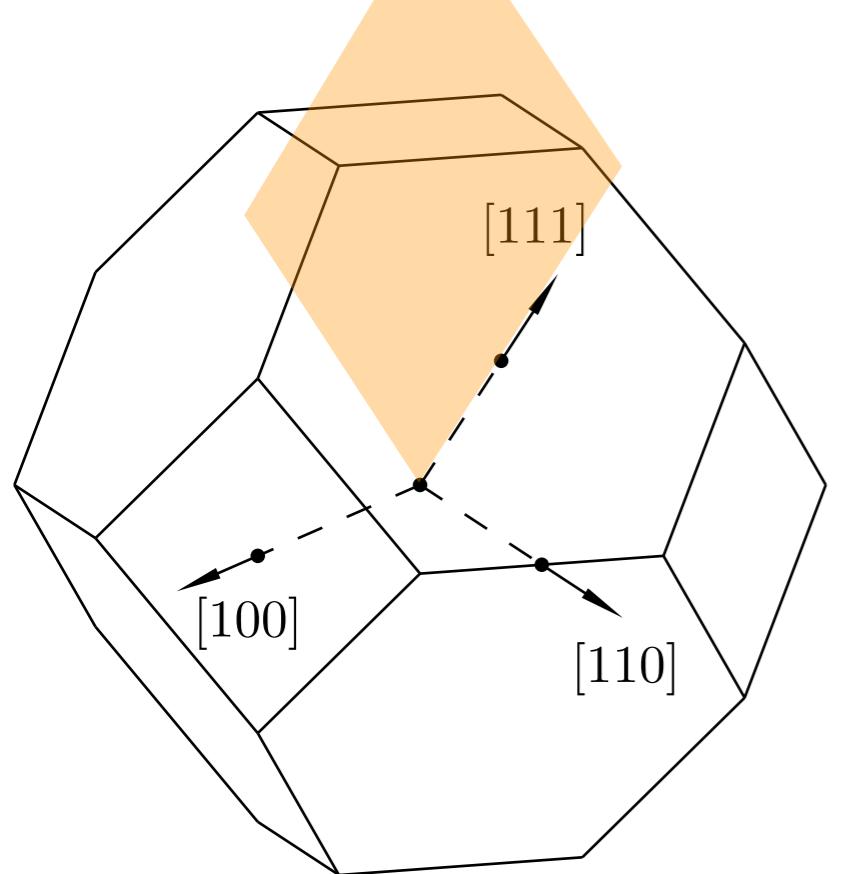


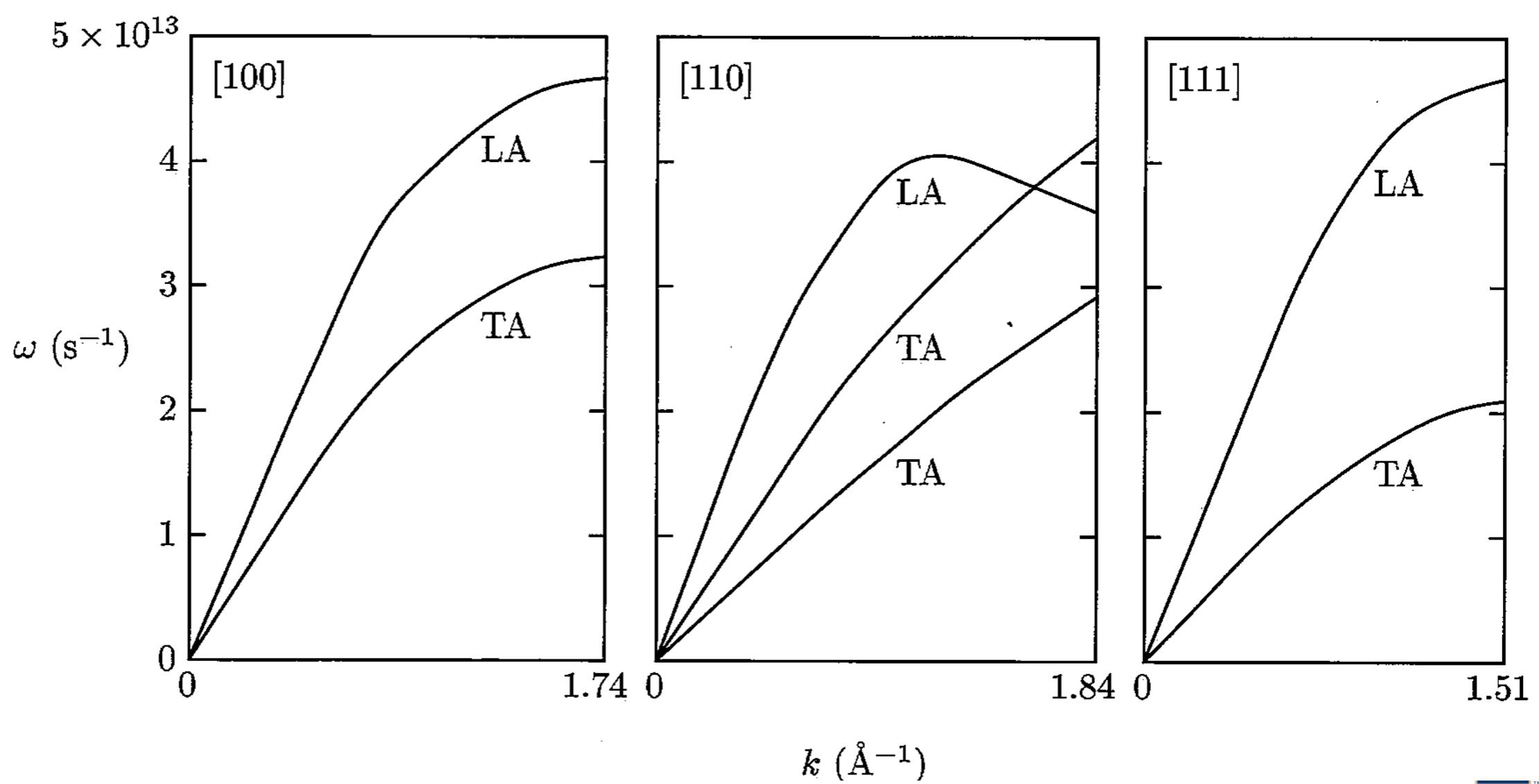
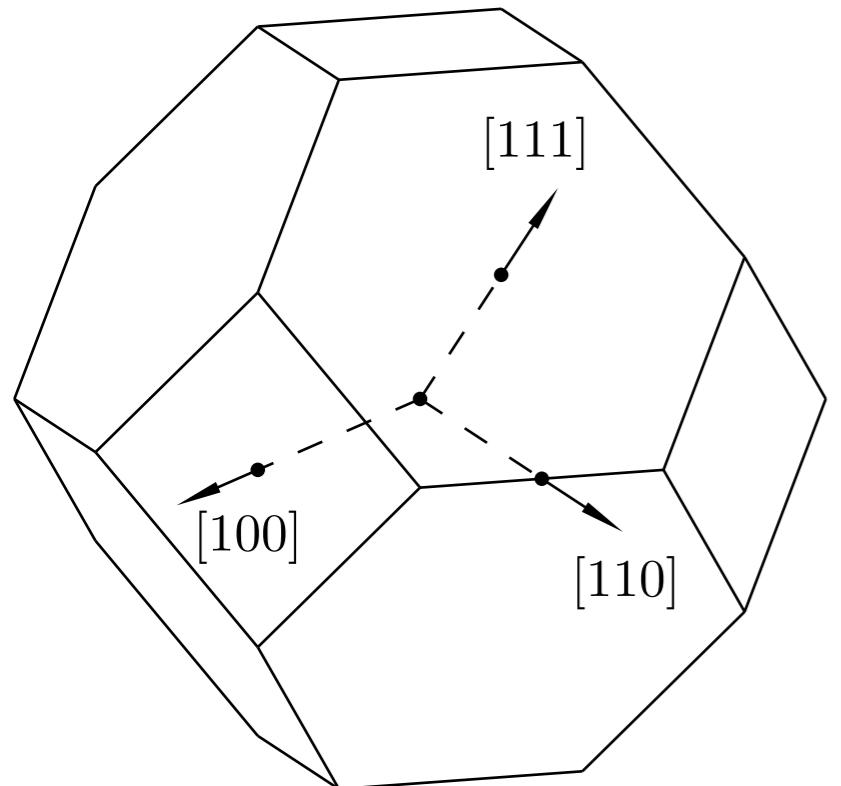


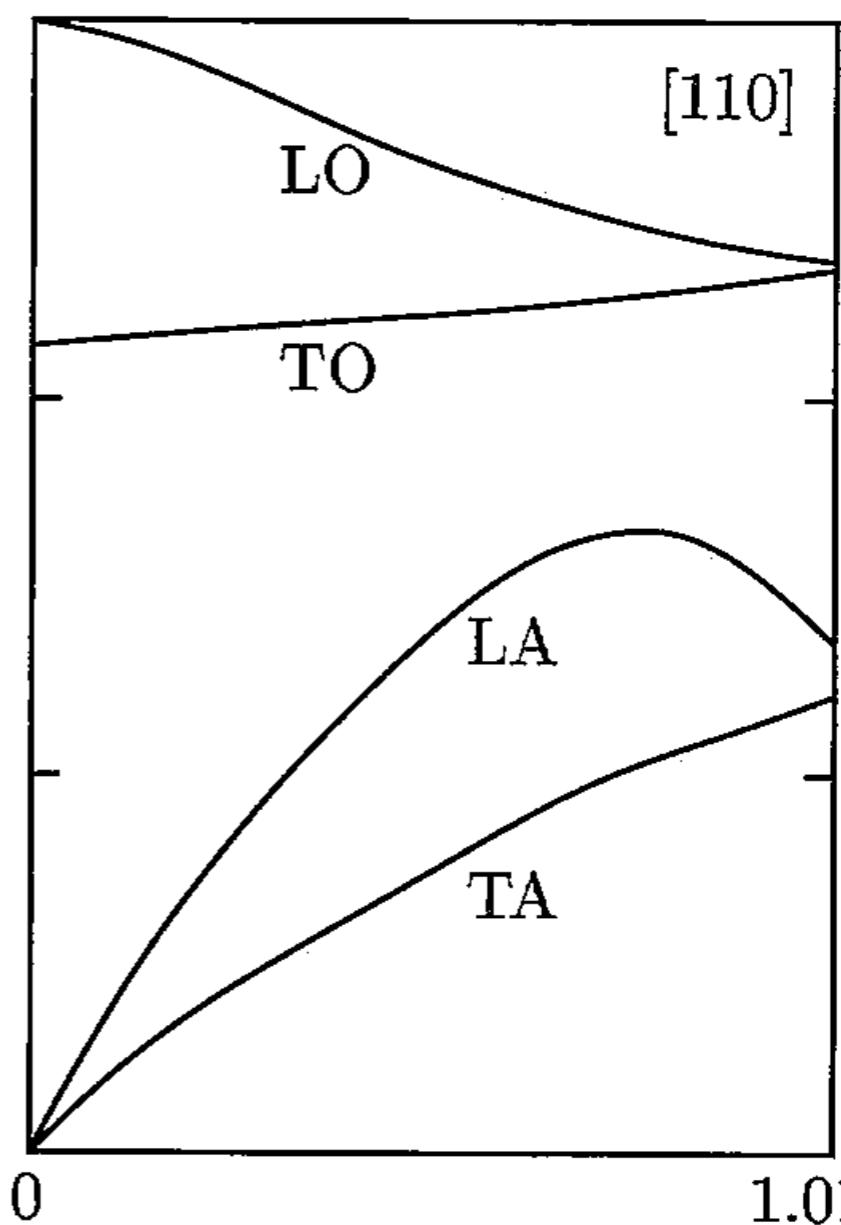
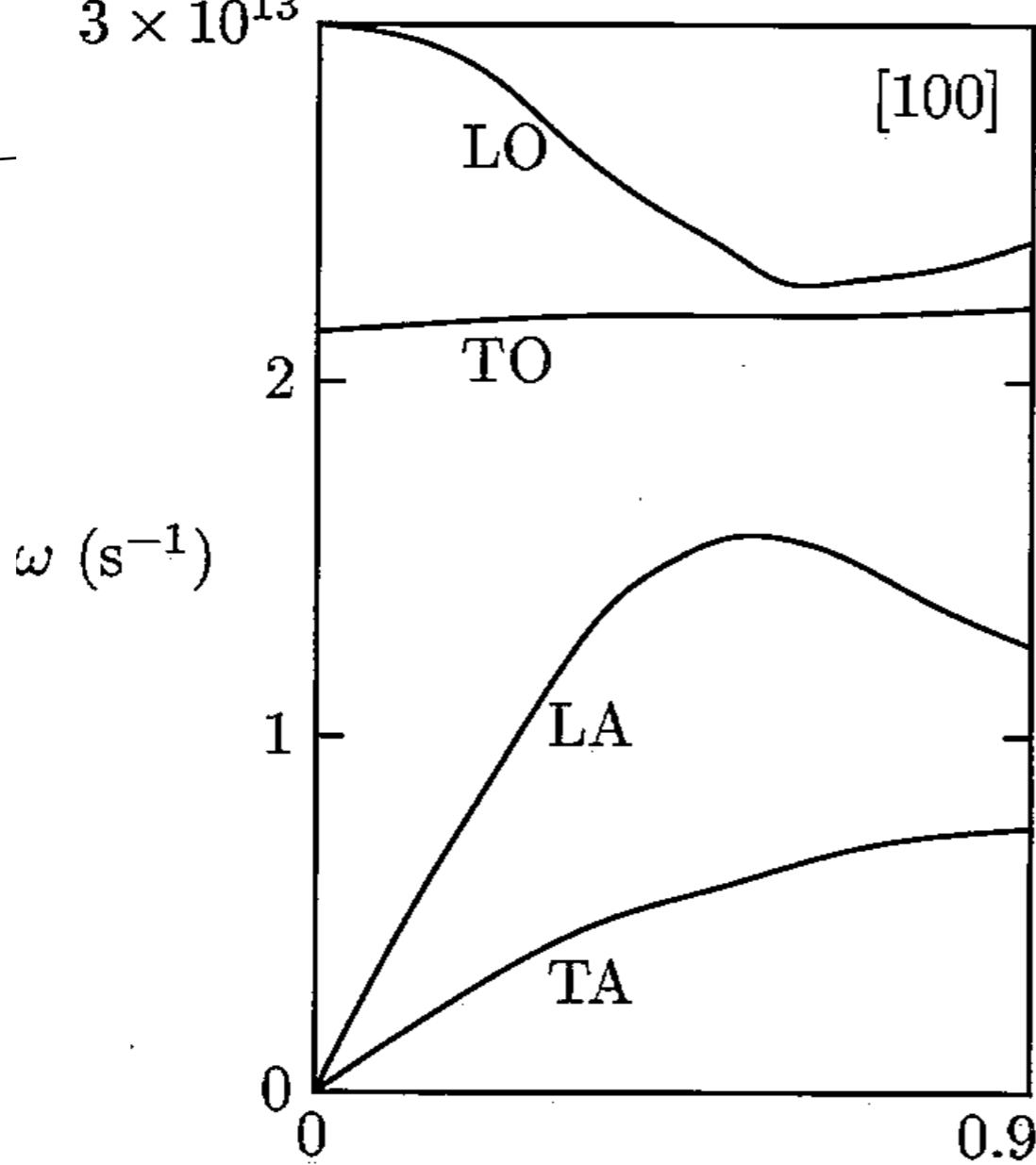
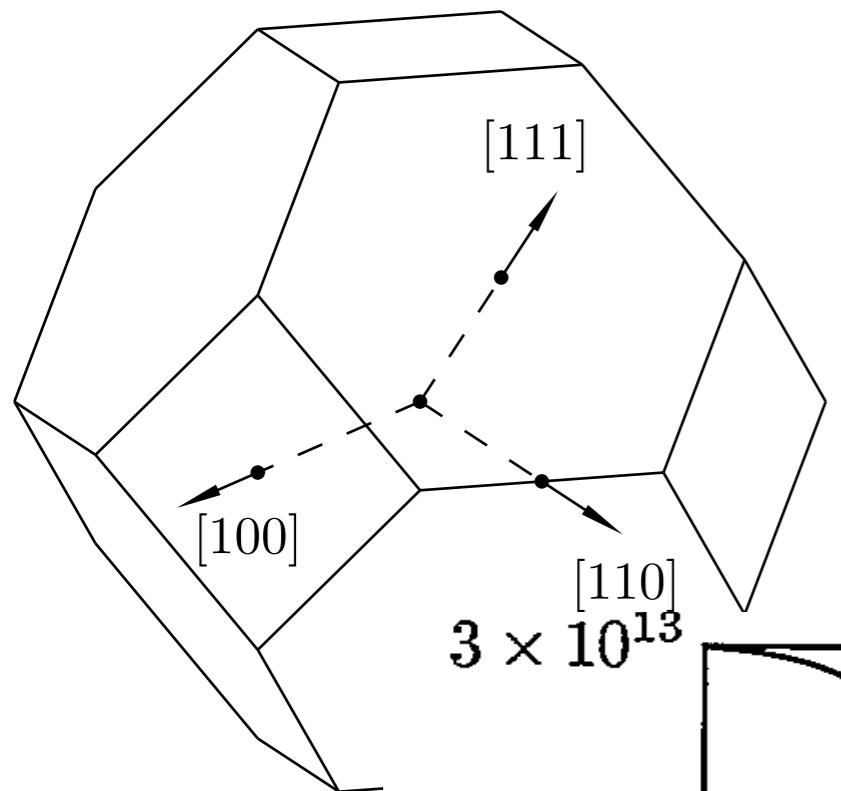


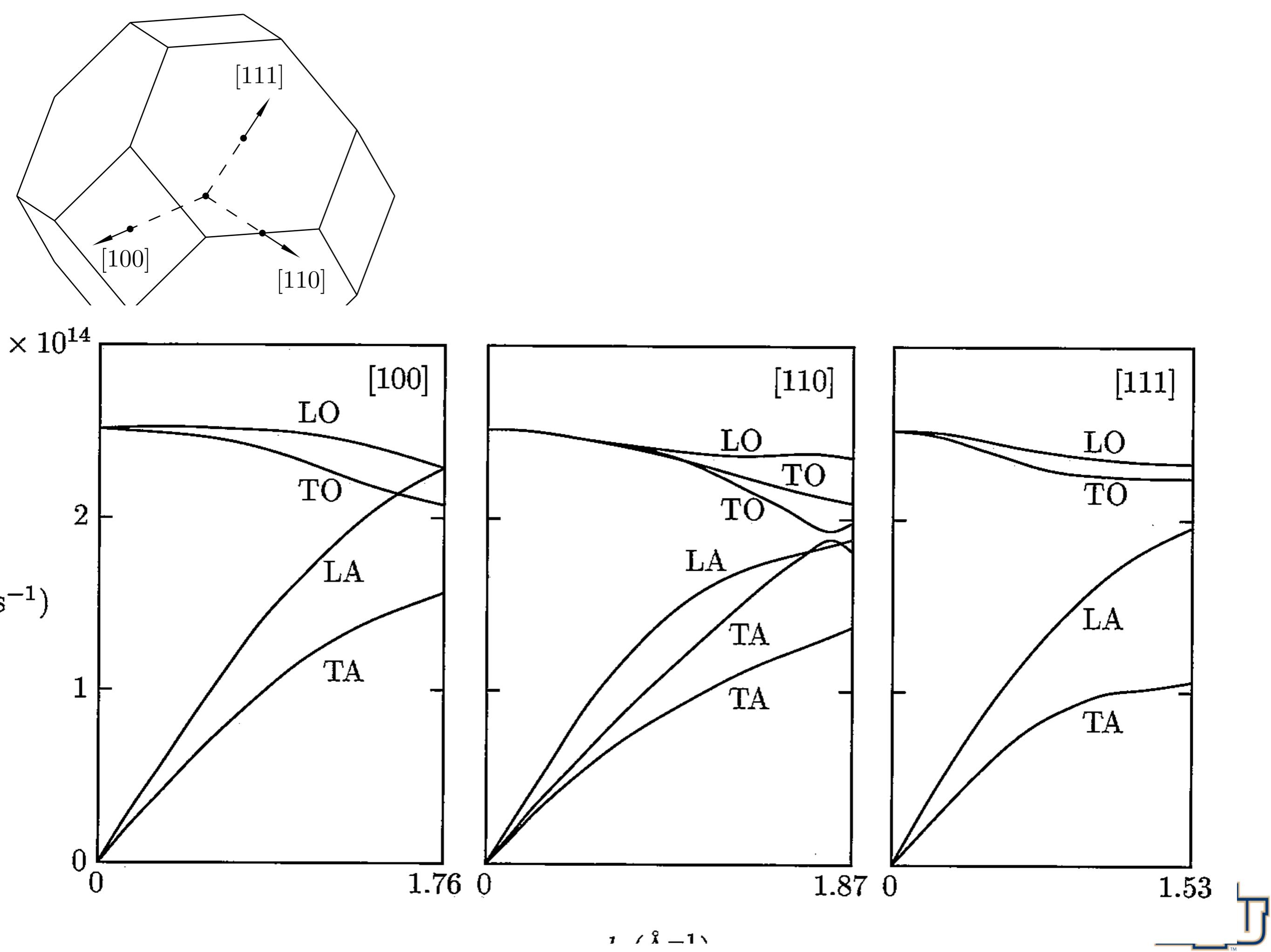






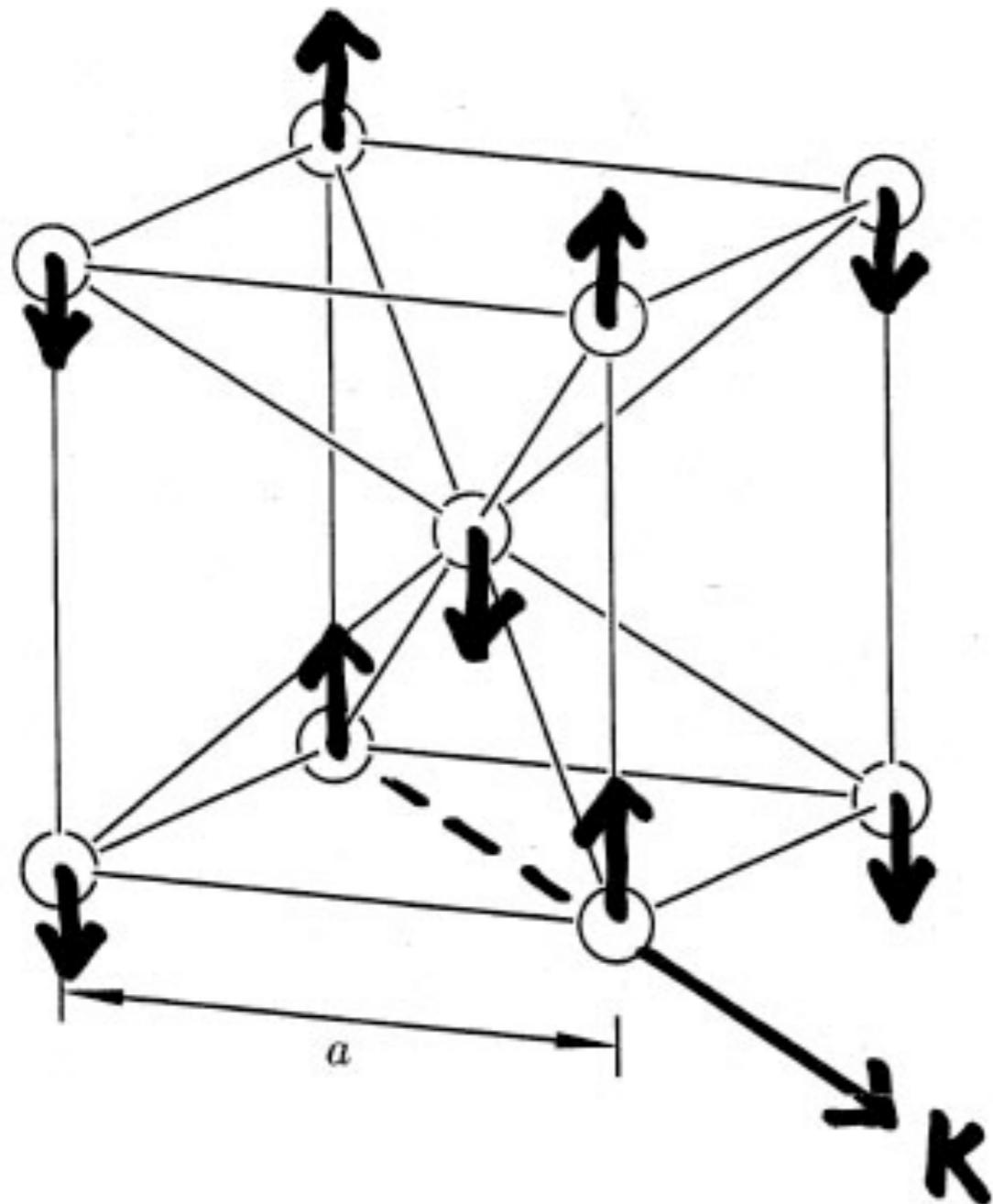






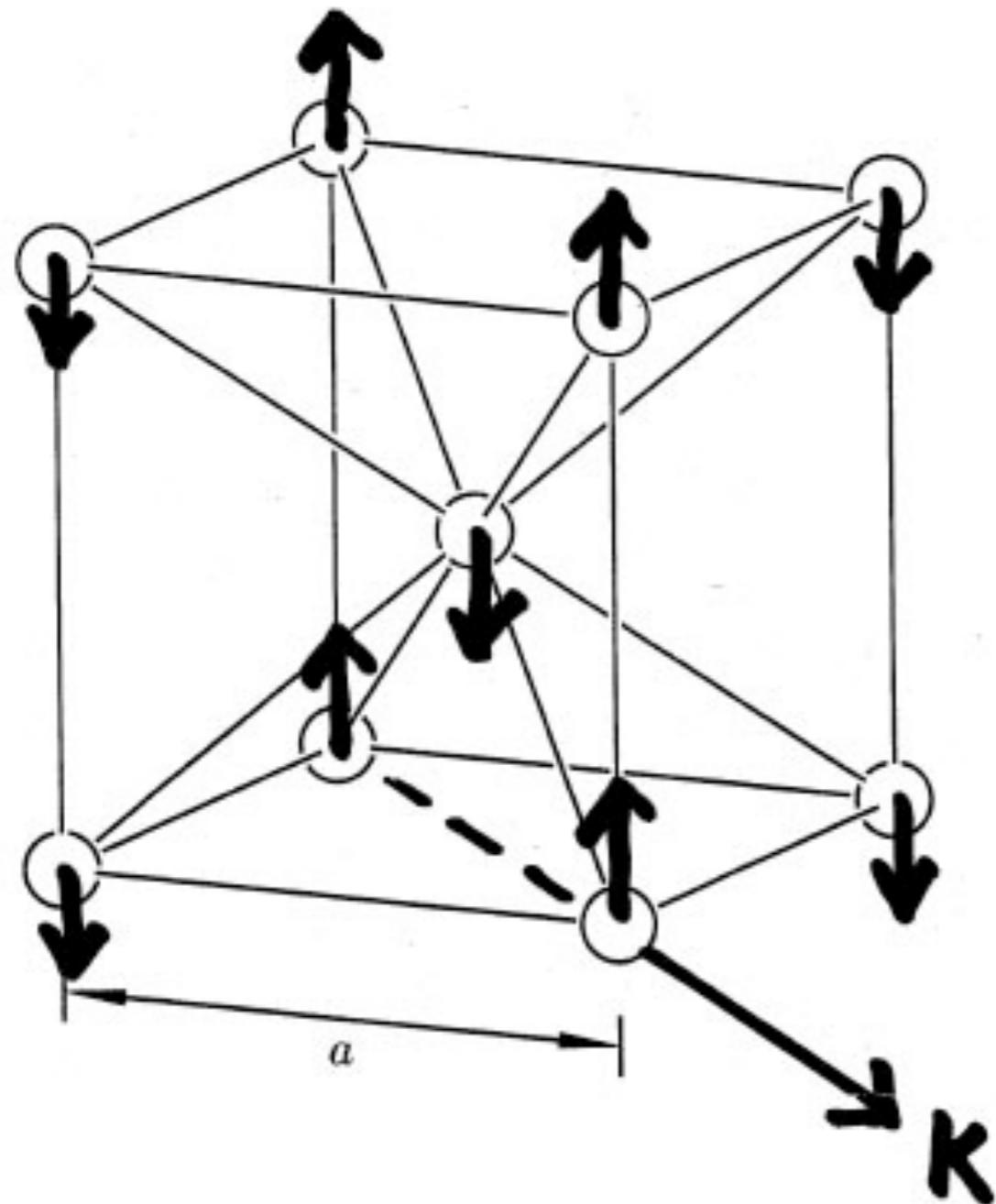
Question #19

What is the wavelength of this phonon?



- A) $2a$
- B) $\sqrt{2}a$
- C) $\frac{\sqrt{2}}{2}a$
- D) $4a$
- E) $8a$

Question #20



What is the wavevector for this phonon?

A)

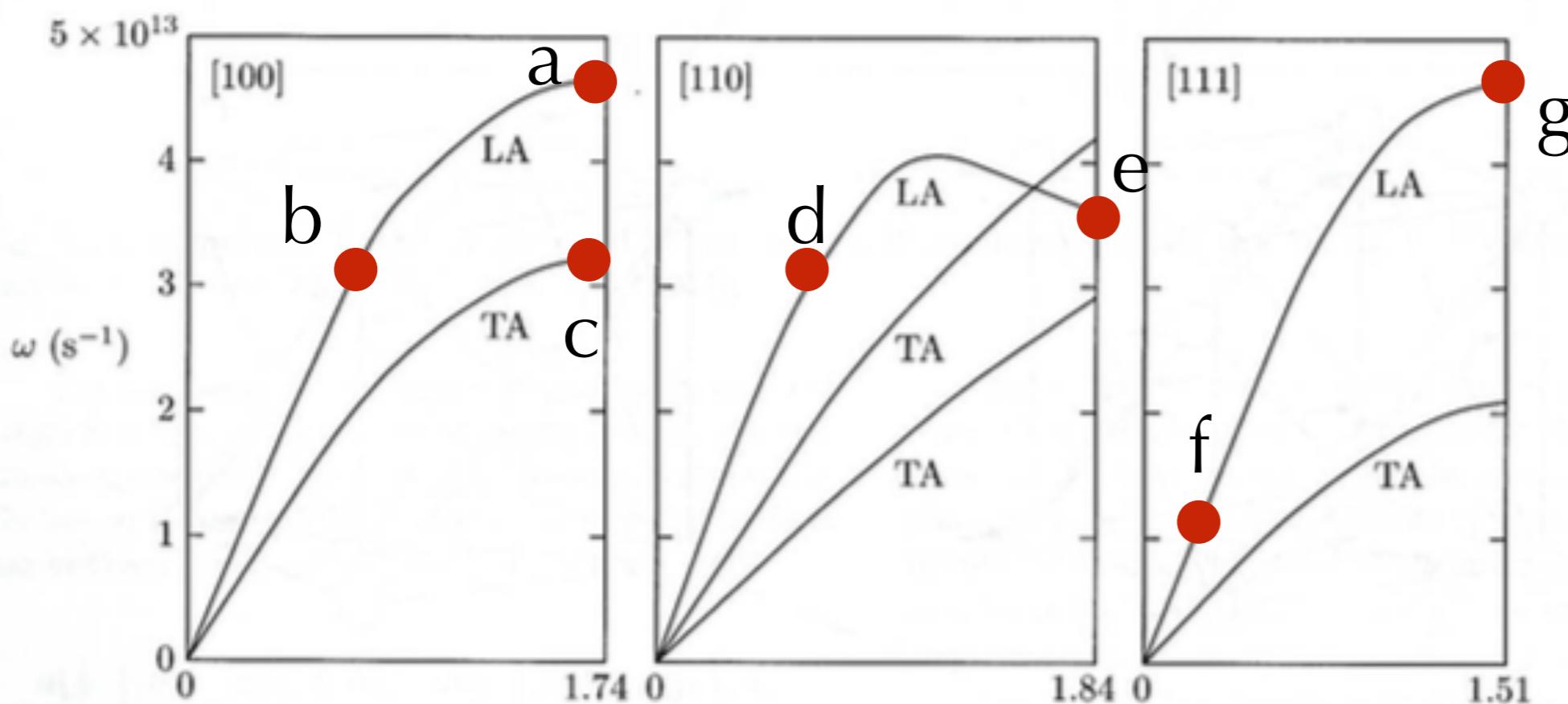
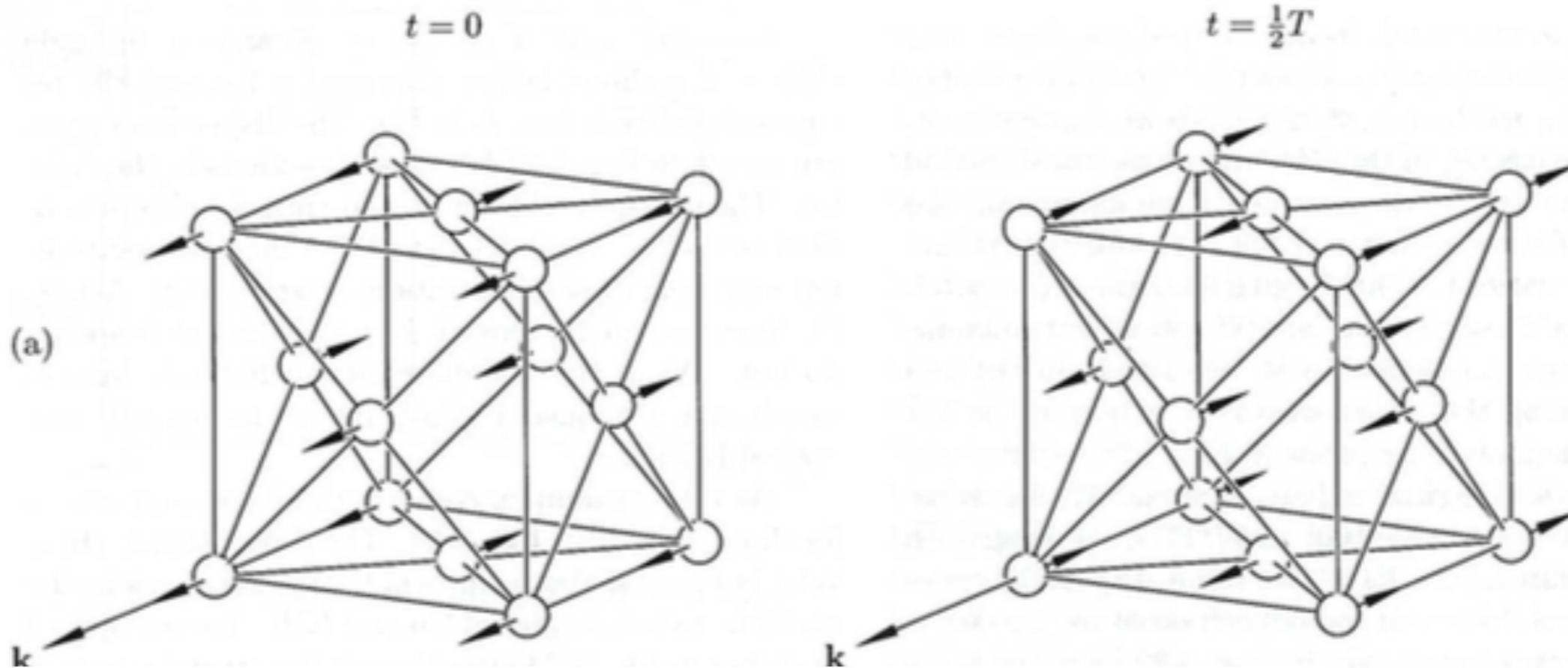
$$B) \left(\frac{\pi}{a} \hat{i} - \frac{\pi}{a} \hat{j} \right)$$

$$C) \left(\frac{2\pi}{\sqrt{2}a} \hat{i} - \frac{2\pi}{\sqrt{2}a} \hat{j} \right)$$

$$D) \left(\frac{2\pi}{\sqrt{2}a} \hat{i} + \frac{2\pi}{\sqrt{2}a} \hat{j} \right)$$

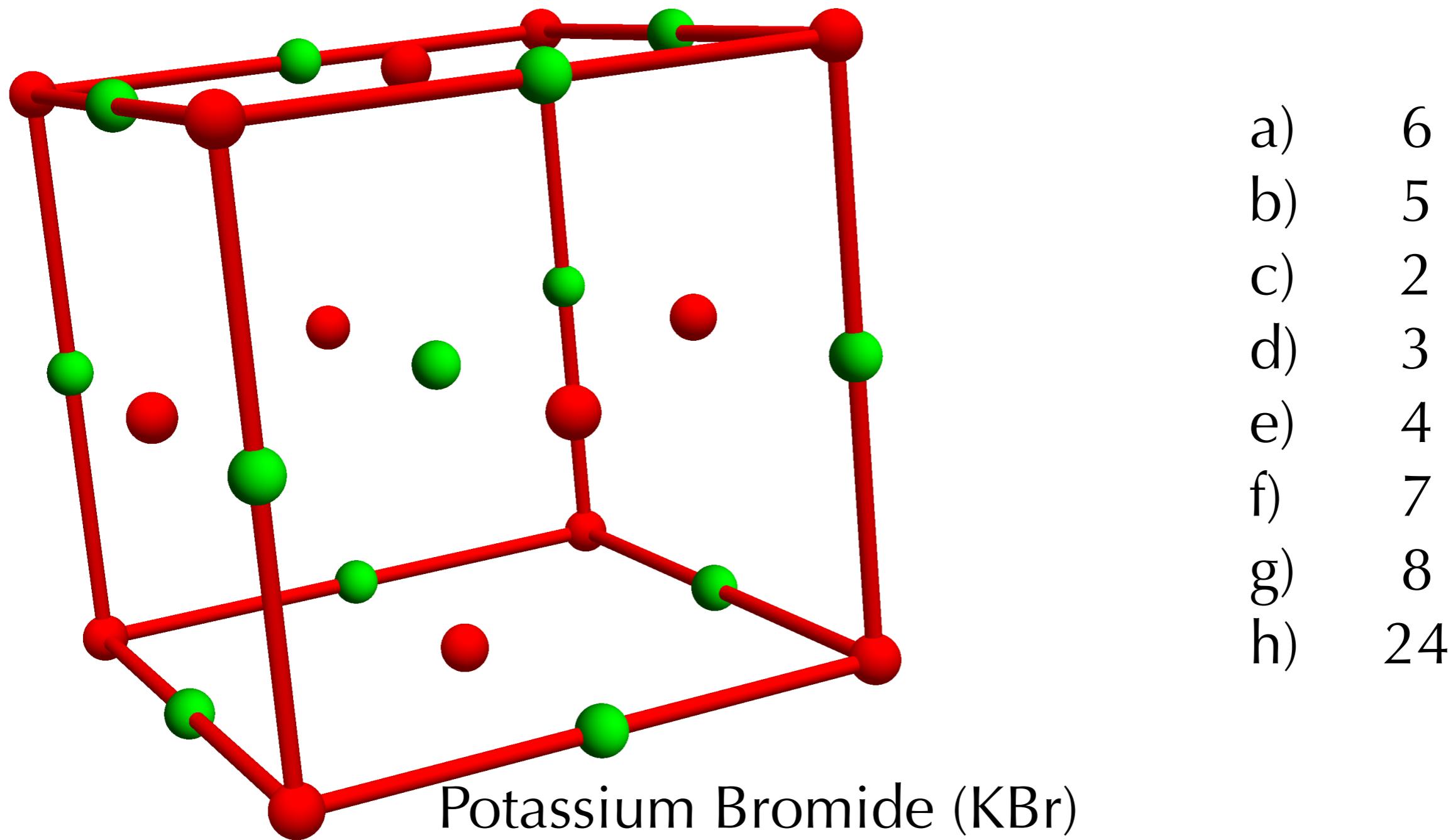
$$E) \left(\frac{\pi}{a} \hat{i} + \frac{\pi}{a} \hat{j} \right)$$

Shown are two snapshots of a lattice wave in Cu. Locate this phonon on the dispersion curves. **Question #21**



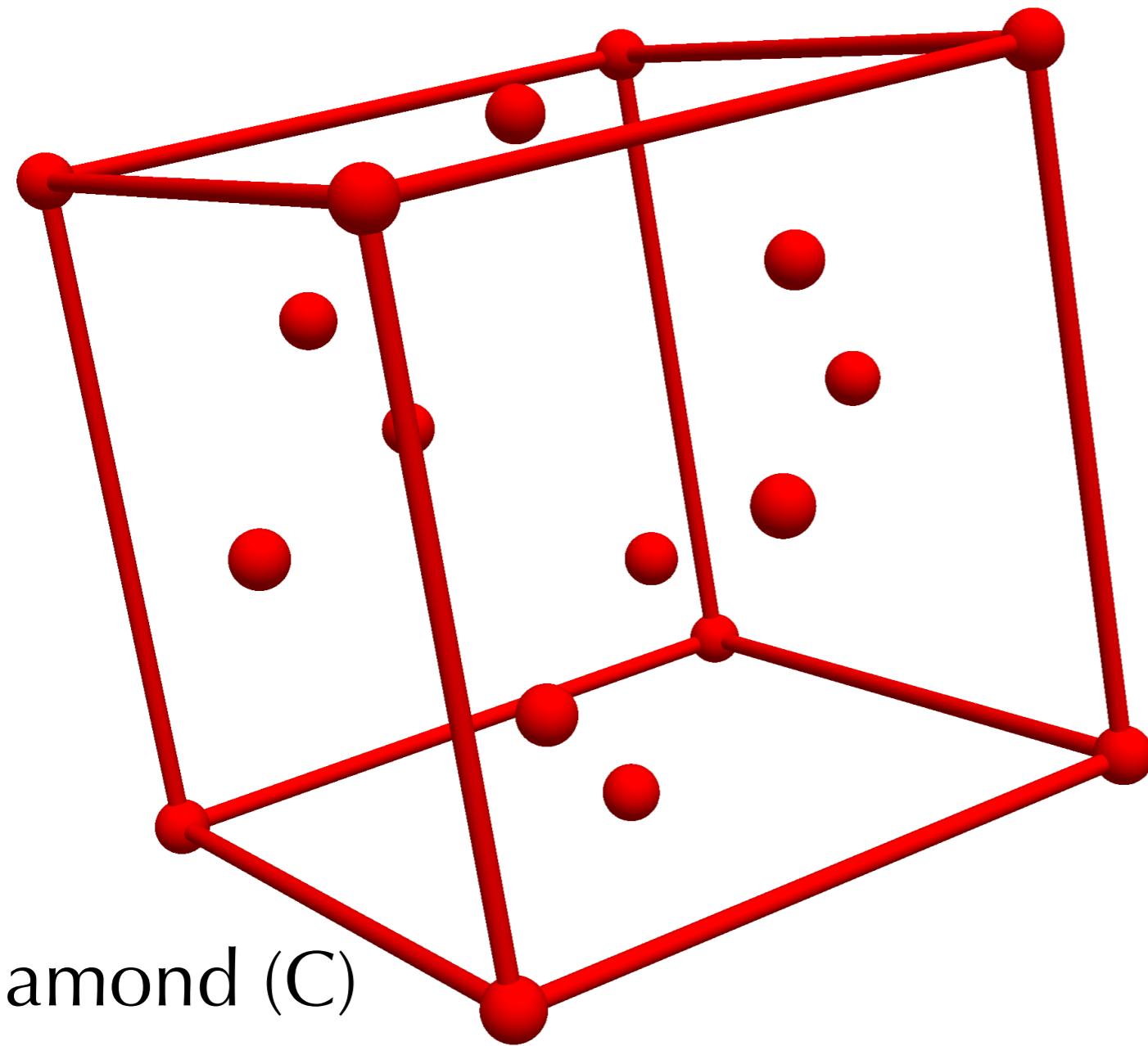
Question #5

How many dispersion curves will there be for the crystal shown?



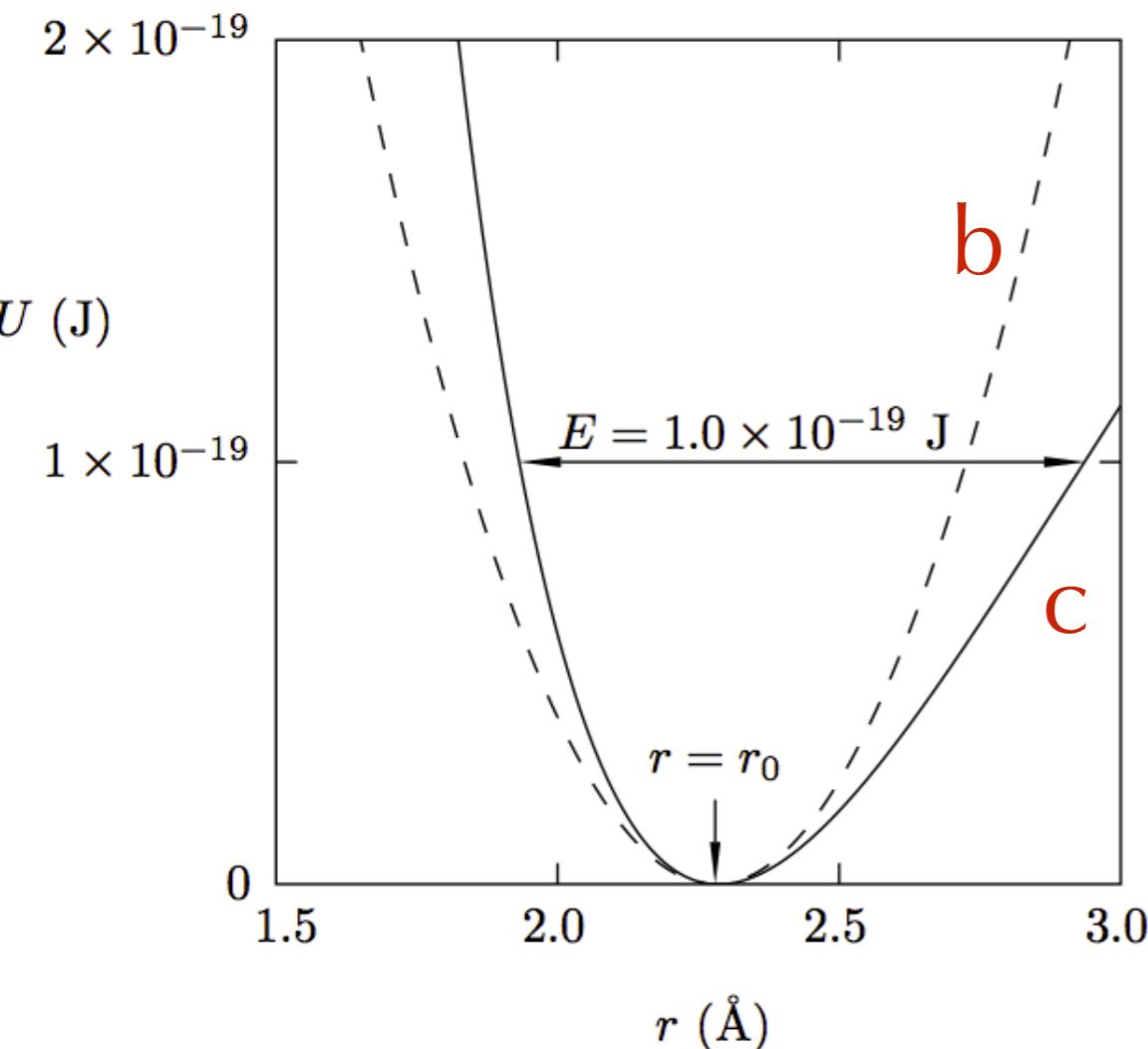
Question #6

How many dispersion curves will there be
for the crystal shown?



- a) 2
- b) 6
- c) 4
- d) 5
- e) 3
- f) 7
- g) 8
- h) 24

Question #7



Which is the anharmonic potential?

Question #8

How do lattice vibrations affect X-ray diffraction patterns?

- a) Peak locations are altered.
- b) Peak heights are diminished.
- c) Many peaks disappear.
- d) No change in the peak structure.