Condensed Matter Physics

- Dr. Baris Emre

X-ray diffraction, von Laue description

so the measured intensity is

$$I(\mathbf{K}) \propto |\int_V \rho(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} dV|^2 = |\int_V \rho(\mathbf{r}) e^{-i\mathbf{K}\cdot\mathbf{r}} dV|^2$$

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with

$$\mathbf{K} = \mathbf{k}' - \mathbf{k}$$

ρ(**r**) in
Volume V

k

k’

X-ray diffraction, von Laue description

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ρ(**r**) in
Volume V

The reciprocal lattice

for a given Bravais lattice

$$\mathbf{R} = m\mathbf{a_1} + n\mathbf{a_2} + o\mathbf{a_3}$$

the reciprocal lattice is defined as the set of vectors **G** for which

$$\mathbf{R} \cdot \mathbf{G} = 2\pi l \qquad \text{or} \qquad e^{\mathbf{iG \cdot R}} = 1$$

The reciprocal lattice is also a Bravais lattice

$$\mathbf{G} = m'\mathbf{b_1} + n'\mathbf{b_2} + o'\mathbf{b_3}$$

The reciprocal lattice

construction of the reciprocal lattice

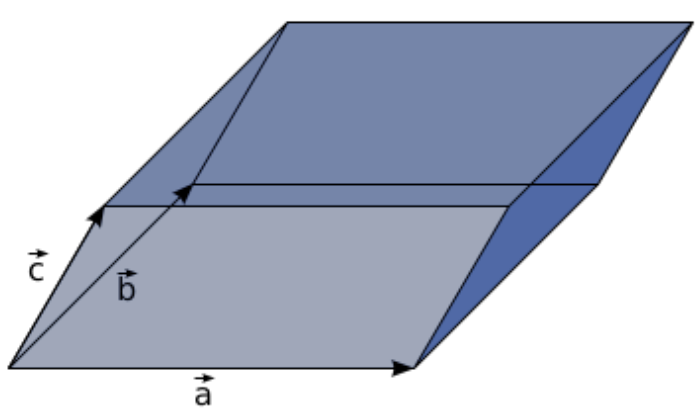
$$\mathbf{R} = m\mathbf{a_1} + n\mathbf{a_2} + o\mathbf{a_3}$$

$$\mathbf{G} = m'\mathbf{b_1} + n'\mathbf{b_2} + o'\mathbf{b_3}$$

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

a useful relation is

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$$



with this it is easy to see why

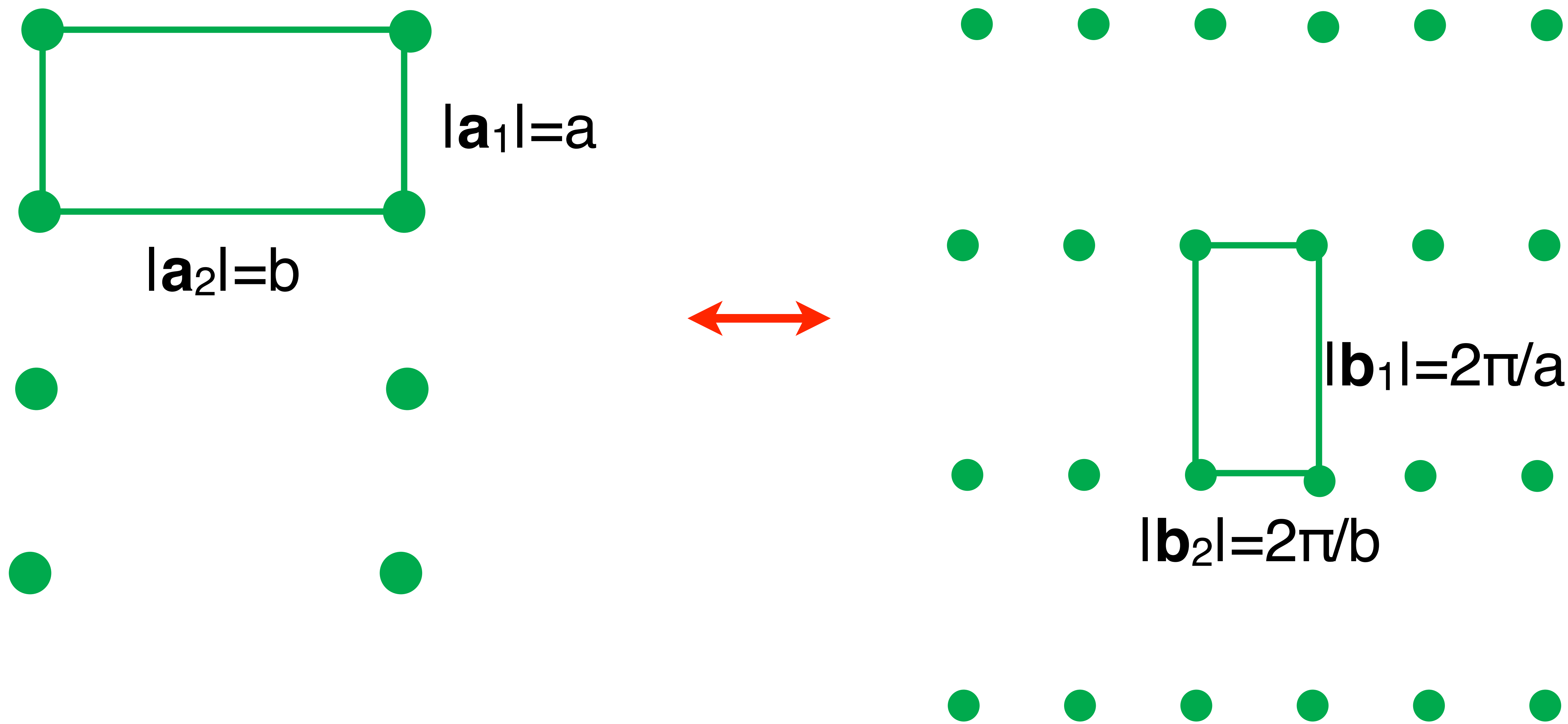
$$\mathbf{R} \cdot \mathbf{G} = 2\pi l$$

The reciprocal lattice

example 1: in two dimensions

$$\mathbf{R} = m\mathbf{a_1} + n\mathbf{a_2}$$

$$\mathbf{G} = m\mathbf{b_1} + n\mathbf{b_2} \qquad \mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$$



The reciprocal lattice

if we have

$$\mathbf{R} \cdot \mathbf{G} = 2\pi l \qquad e^{\mathbf{iG} \cdot \mathbf{R}} = 1$$

then we can write

$$e^{i\mathbf{G}\cdot\mathbf{r}} = e^{i\mathbf{G}\cdot\mathbf{r}} e^{i\mathbf{G}\cdot\mathbf{R}} = e^{i\mathbf{G}\cdot(\mathbf{r}+\mathbf{R})}$$

The vectors **G** of the reciprocal lattice give plane waves with the periodicity of the lattice. In this case **G** is the wave vector and 2π/|**G**| the wavelength.

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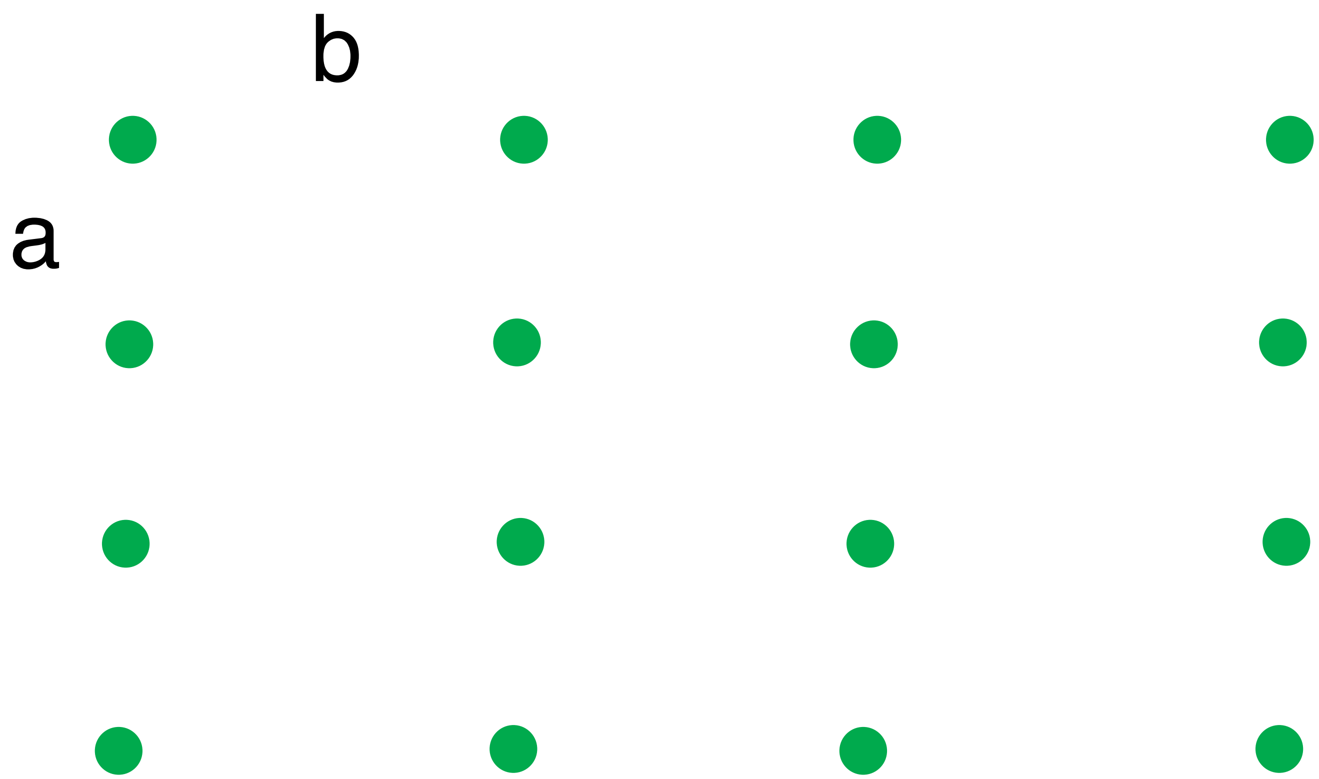
Volume
V

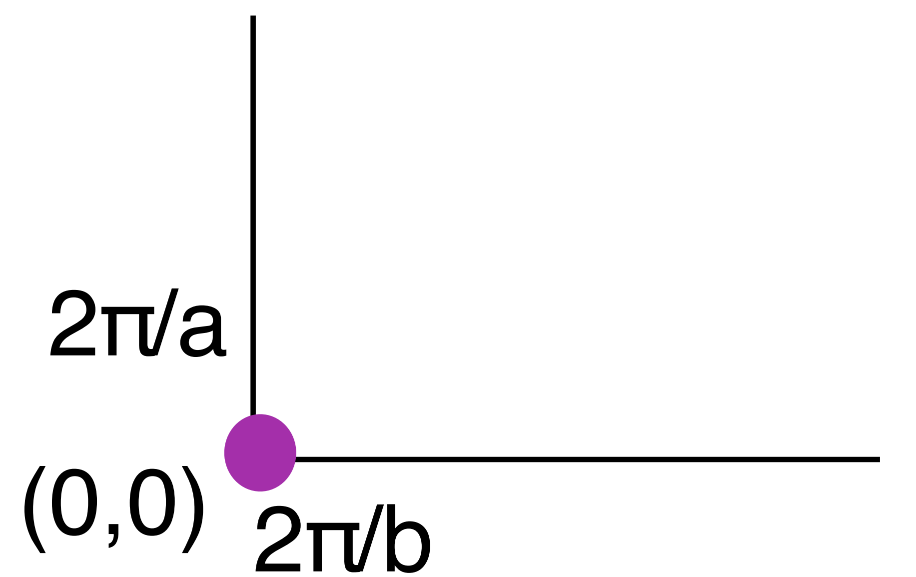
K=G

Lattice waves

real space



reciprocal space



$$e^{i\mathbf{Gr}} = e^{i\mathbf{Gr}}e^{i\mathbf{GR}} = e^{i\mathbf{G}(\mathbf{r}+\mathbf{R})}$$

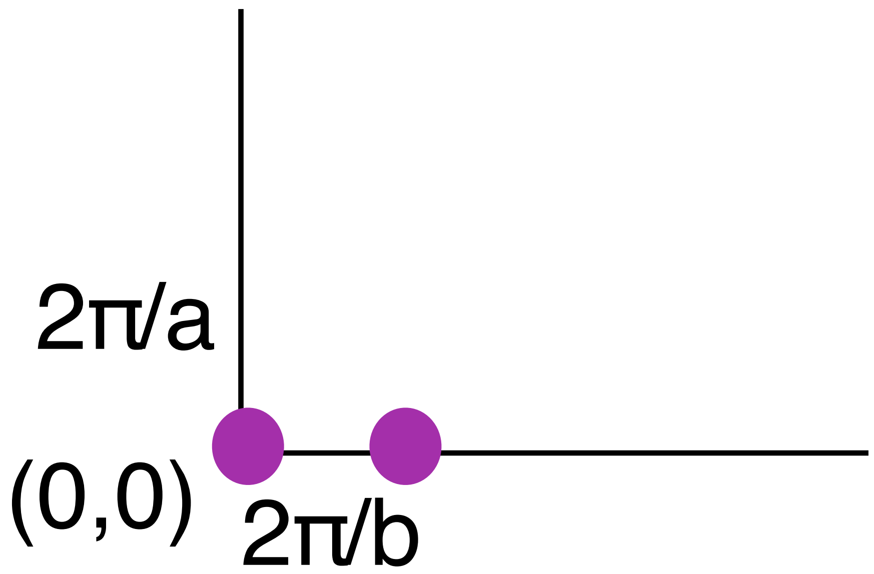
Lattice waves

real space

reciprocal space

b

a



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Lattice waves

real space

b

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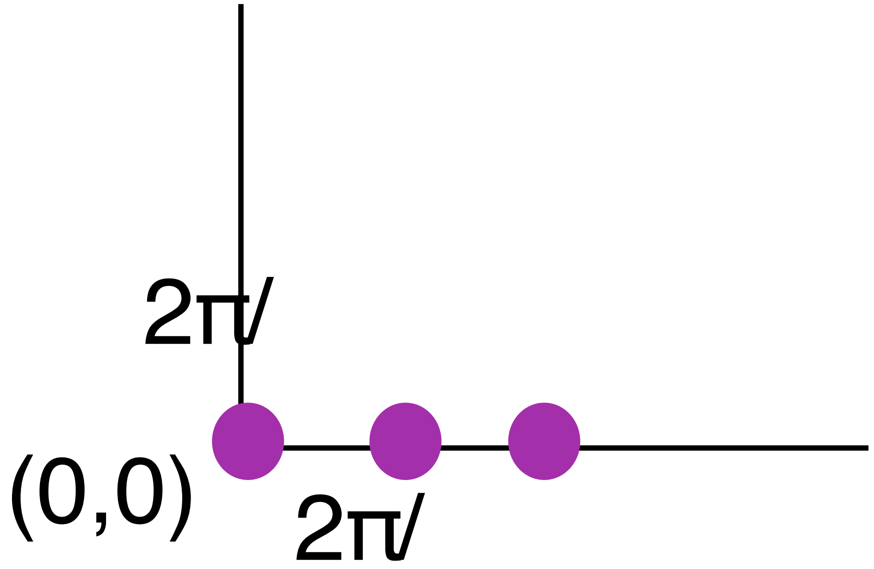
reciprocal space



$$e^{i\mathbf{G}\mathbf{r}} = e^{i\mathbf{G}\mathbf{r}}e^{i\mathbf{G}\mathbf{R}} = e^{i\mathbf{G}(\mathbf{r}+\mathbf{R})}$$

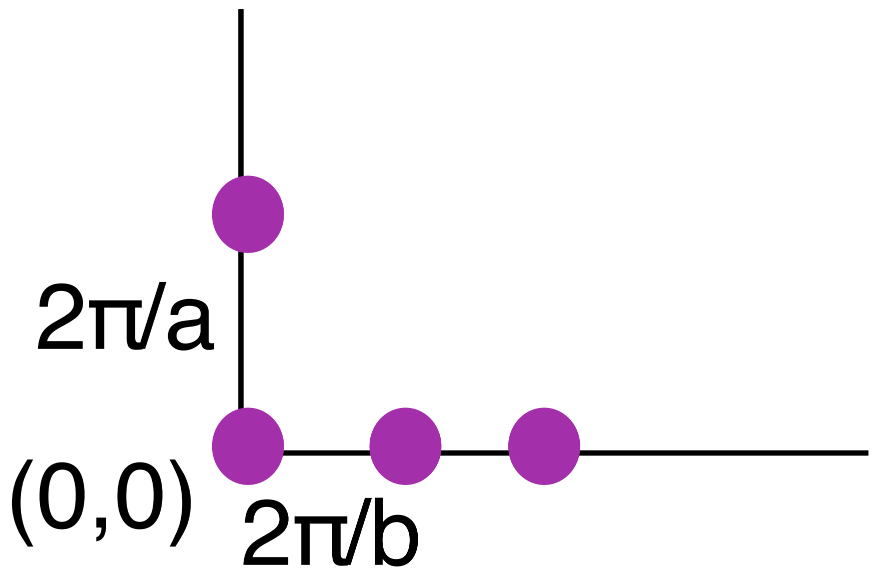
Lattice waves

real space

reciprocal space

b

a



$$e^{i\mathbf{G}\mathbf{r}} = e^{i\mathbf{G}\mathbf{r}} e^{i\mathbf{G}\mathbf{R}} = e^{i\mathbf{G}(\mathbf{r}+\mathbf{R})}$$

Lattice waves

real space

reciprocal space

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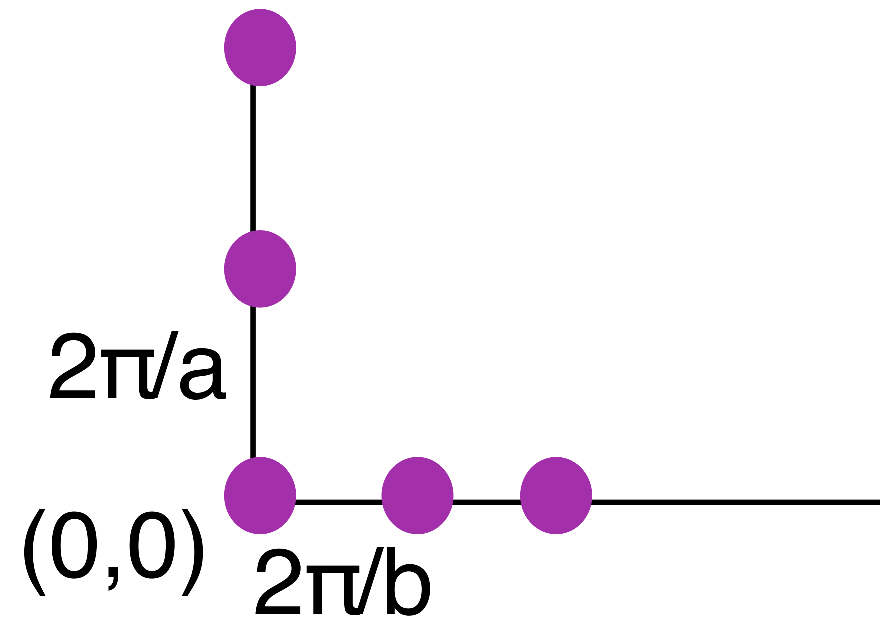

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Lattice waves

real space

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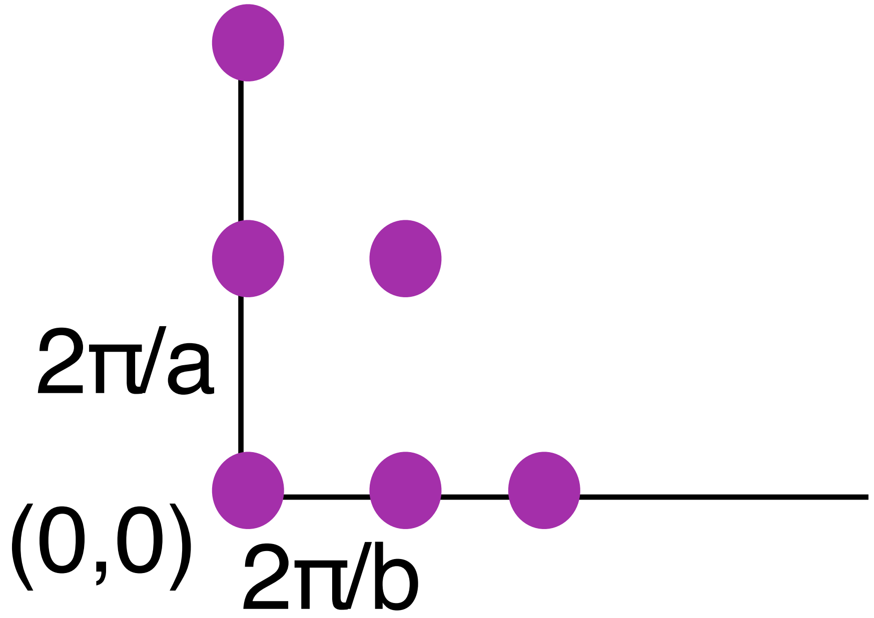
reciprocal space



$$e^{i\mathbf{G}\mathbf{r}} = e^{i\mathbf{G}\mathbf{r}} e^{i\mathbf{G}\mathbf{R}} = e^{i\mathbf{G}(\mathbf{r}+\mathbf{R})}$$

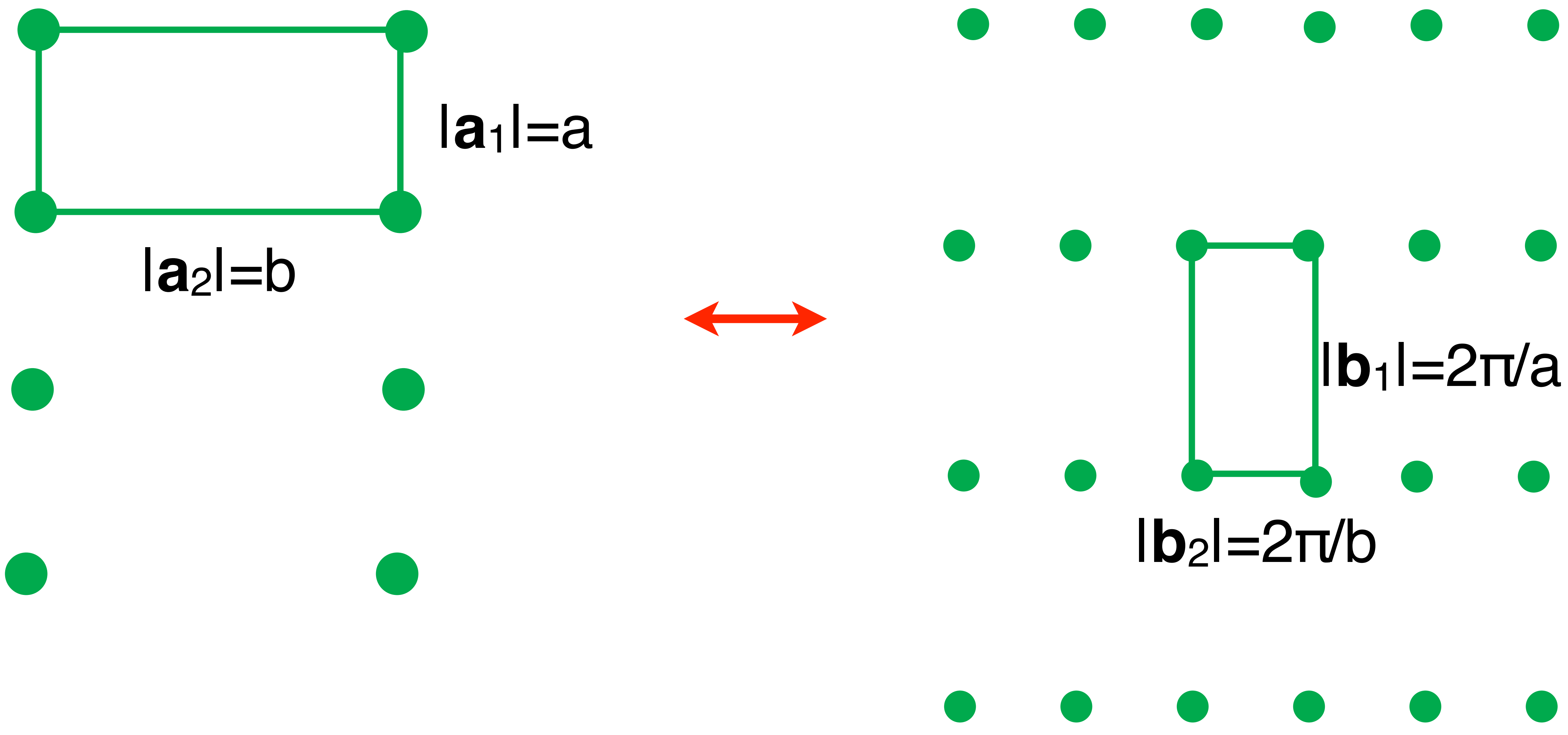
The reciprocal of the reciprocal lattice

is again the real lattice

$$\mathbf{R} = m\mathbf{a_1} + n\mathbf{a_2}$$

$$\mathbf{G} = m\mathbf{b_1} + n\mathbf{b_2}$$

$$\mathbf{a}_i\mathbf{b}_j = 2\pi\delta_{ij}.$$



The reciprocal lattice in 3D

example 2: in three dimensions bcc and fcc lattice

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

The fcc lattice is the reciprocal of the bcc lattice and vice versa.