Basic Crystallography

- Presented by
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An unspeakable horror seized me. There was a darkness; then a dizzy, sickening sensation of sight that was not like seeing; I saw a line that was no line; space that was not space.......
I shrieked aloud in agony, " Either this is madness or it is Hell."

"It is neither," calmly replied the voice of the Sphere, "it is Knowledge; it is Three Dimensions: open your eye once again and try to look steadily........

"Distress not yourself if you cannot at first understand the deeper mysteries of Spaceland. By degrees they will dawn upon you."

On the occasion of the Square's first encounter with three dimensions, from
E. A. Abbott's Flatland, (1884).

Repetition = Symmetry

Types of repetition:

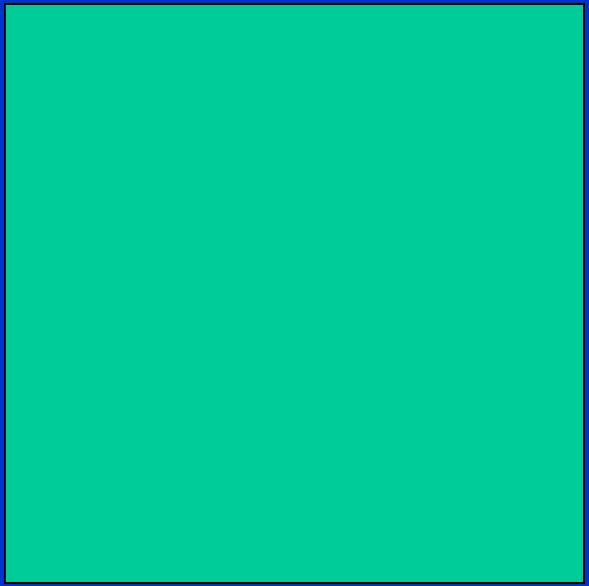
Rotation

Translation

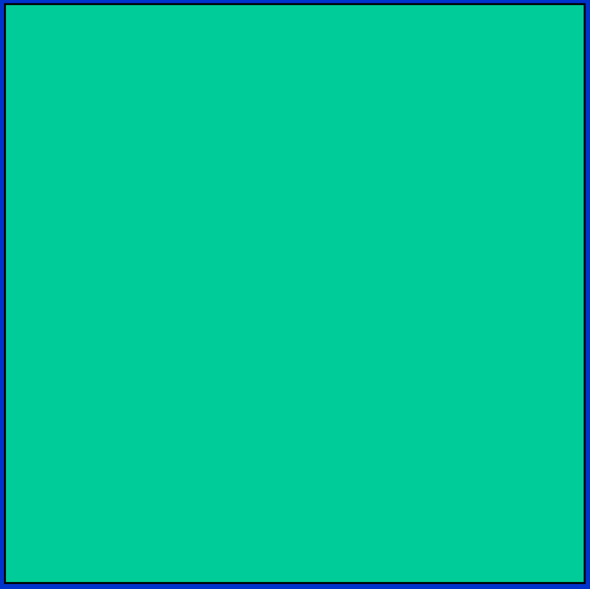
Rotation

What is rotational symmetry?

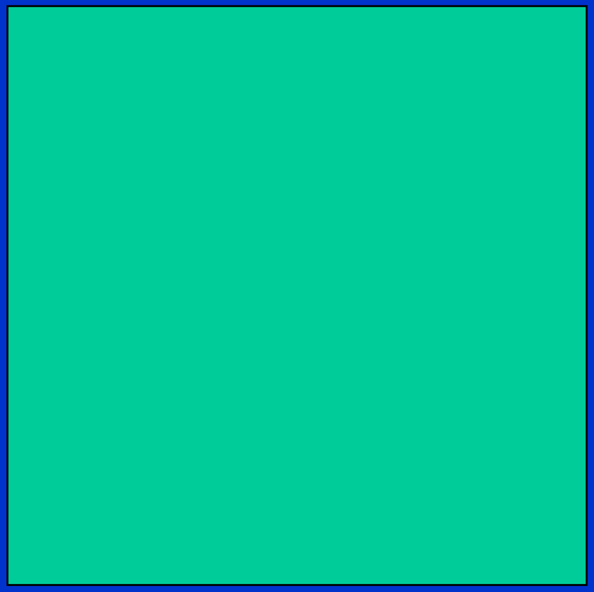
Imagine that this object will be rotated (maybe)



Was it?

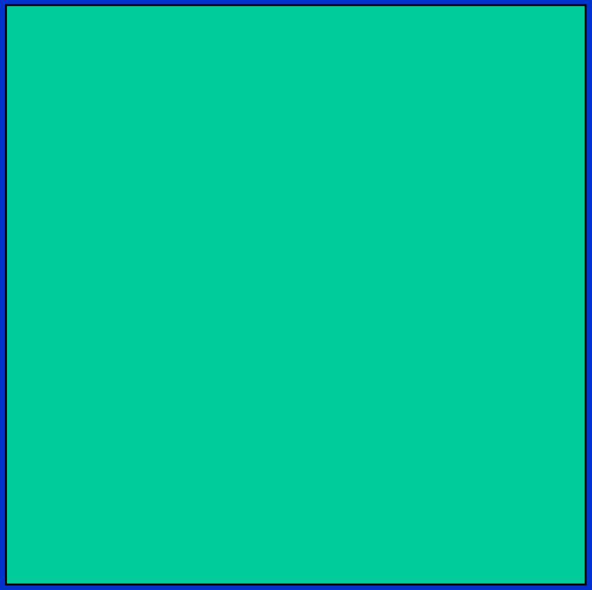


The object is obviously symmetric…it has symmetry



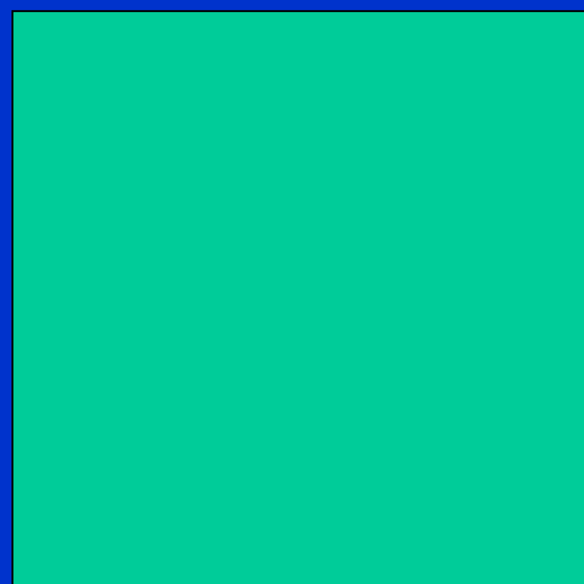
The object is obviously symmetric…it has symmetry

Can be rotated 90° w/o detection

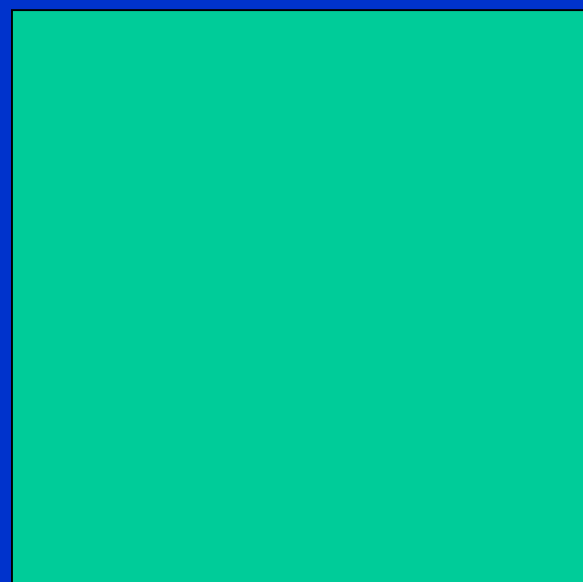


…………so symmetry is really

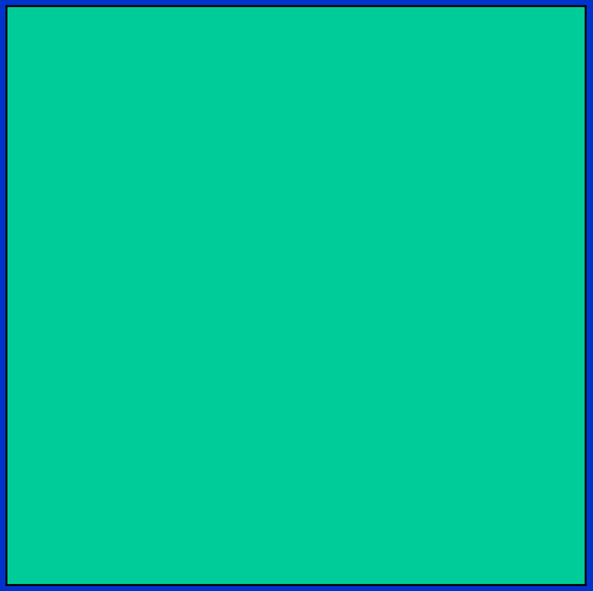
doing nothing



Symmetry is doing nothing - or at least doing something so that it looks like nothing was done!



What kind of symmetry does this object have?



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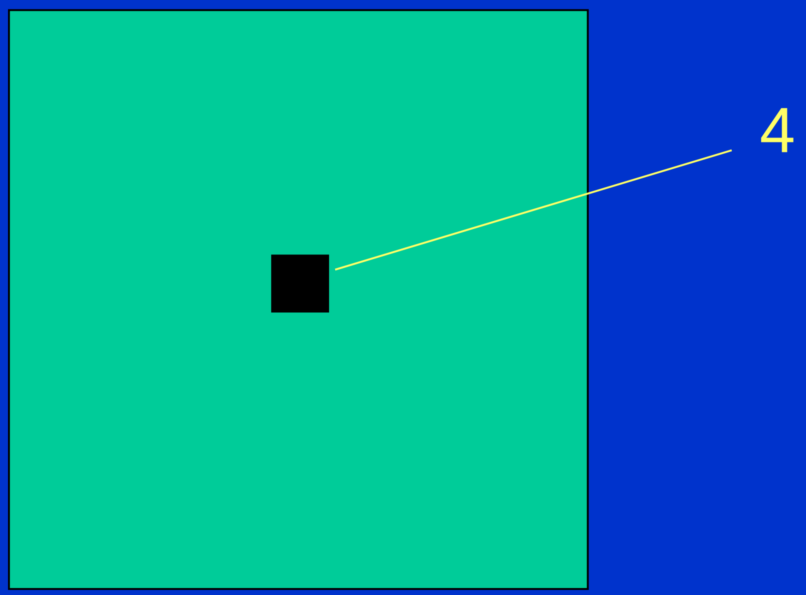

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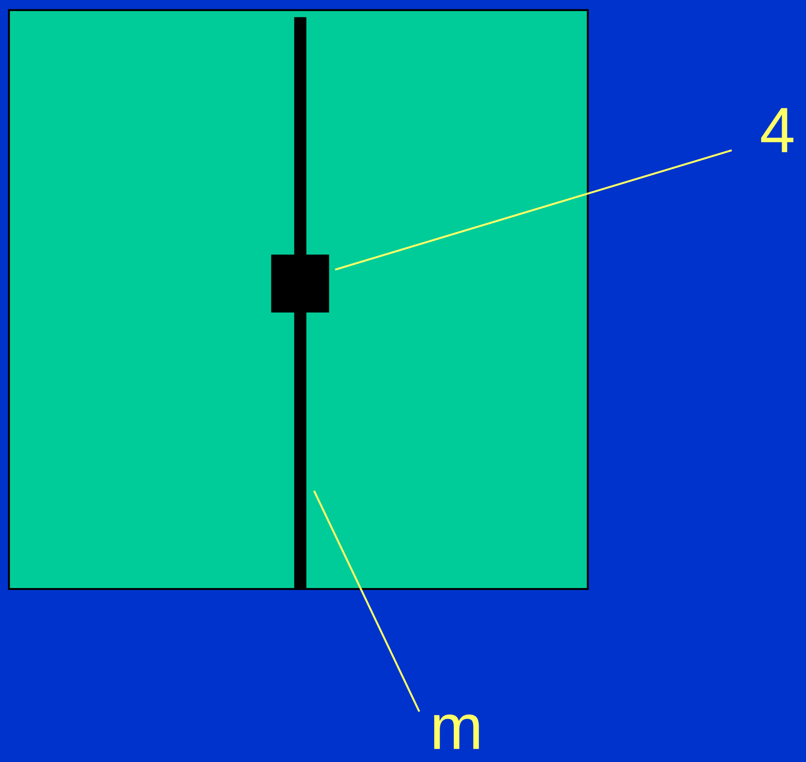

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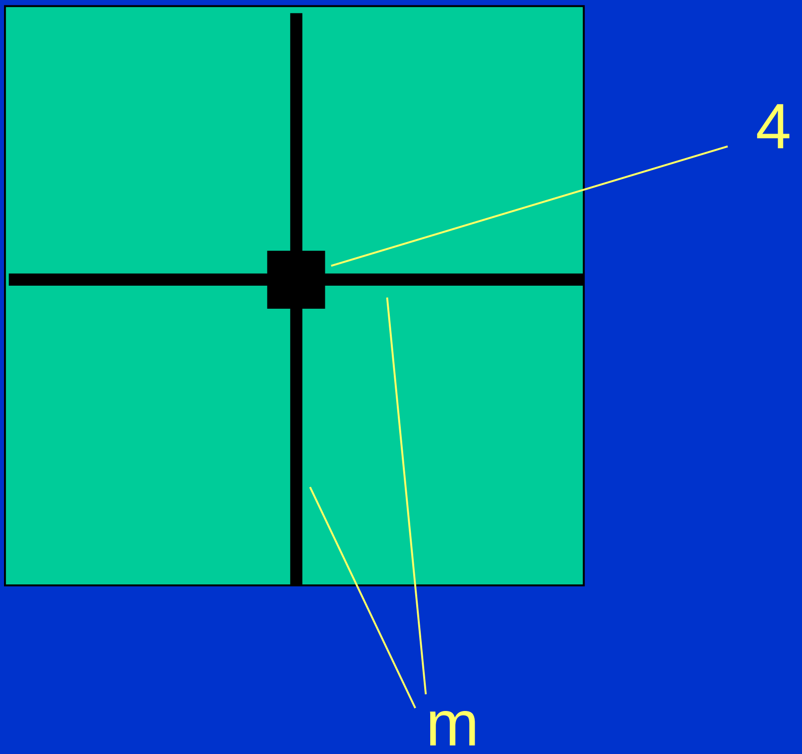

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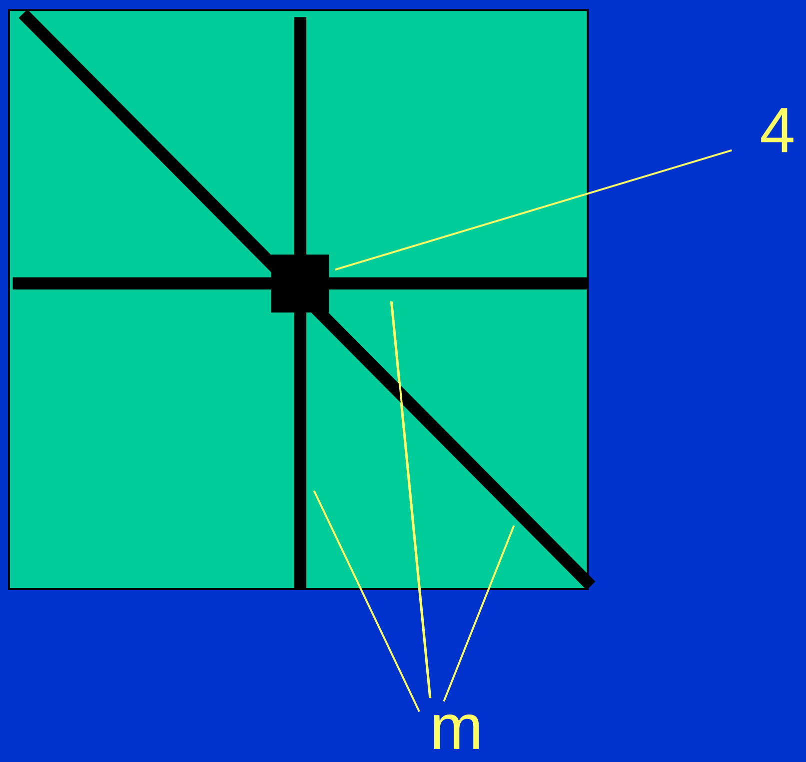

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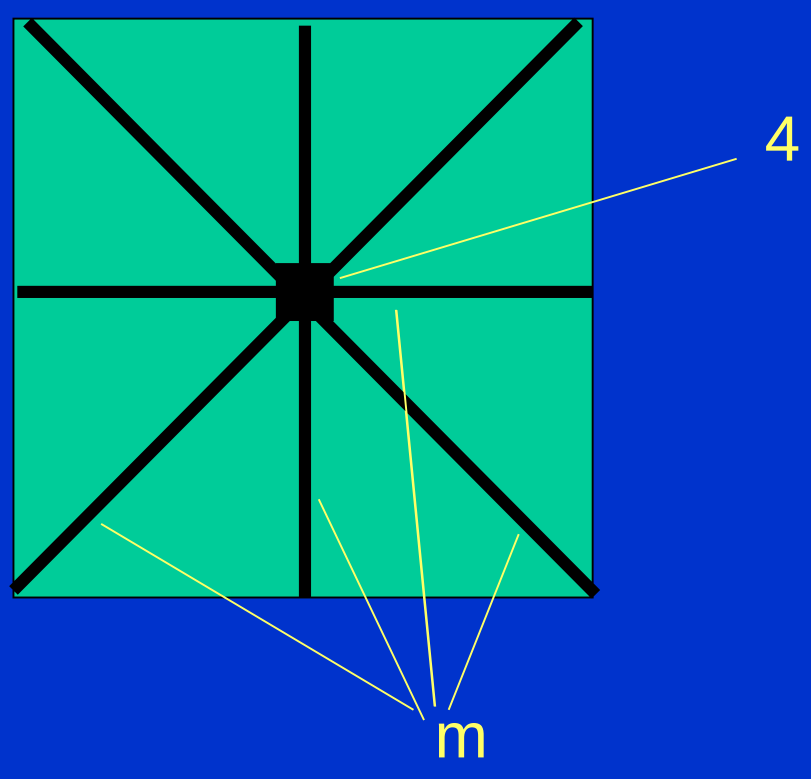
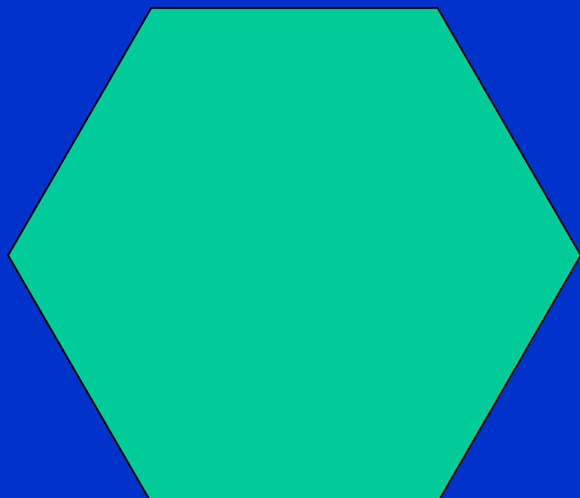
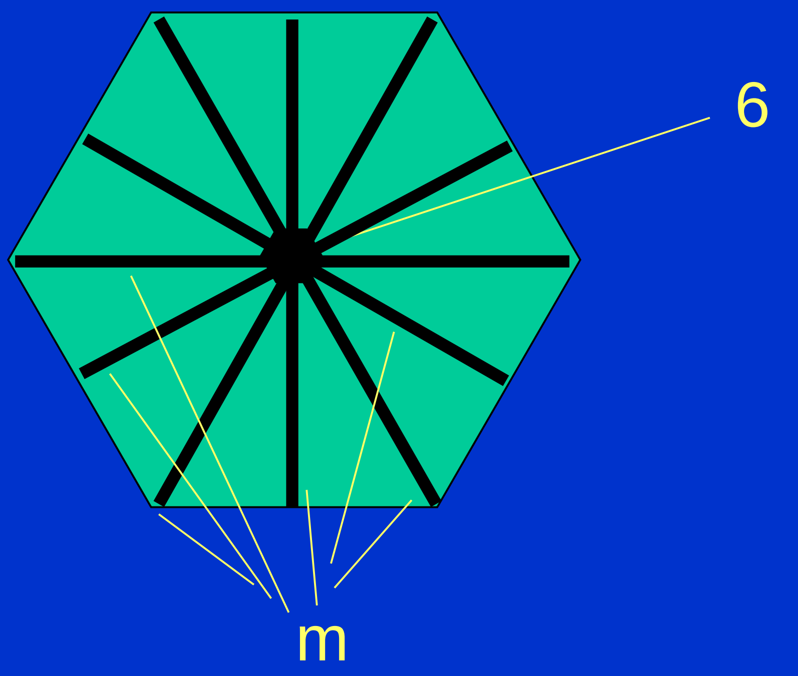


4mm

Another example:



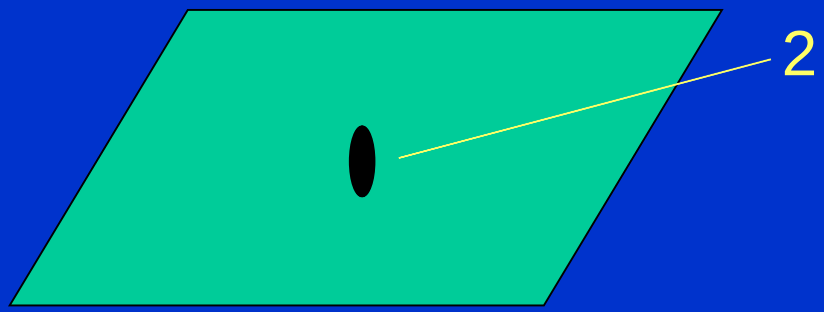
Another example:



6mm

And another:

And another:



2

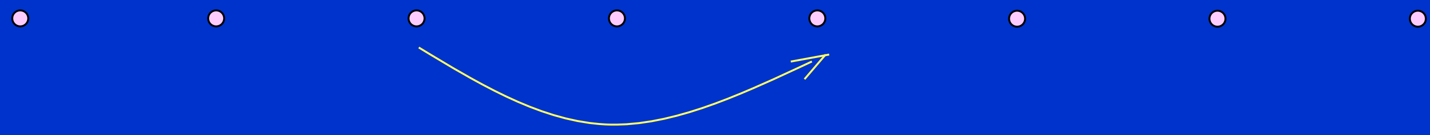
What about translation?

Same as rotation

What about translation?

Same as rotation

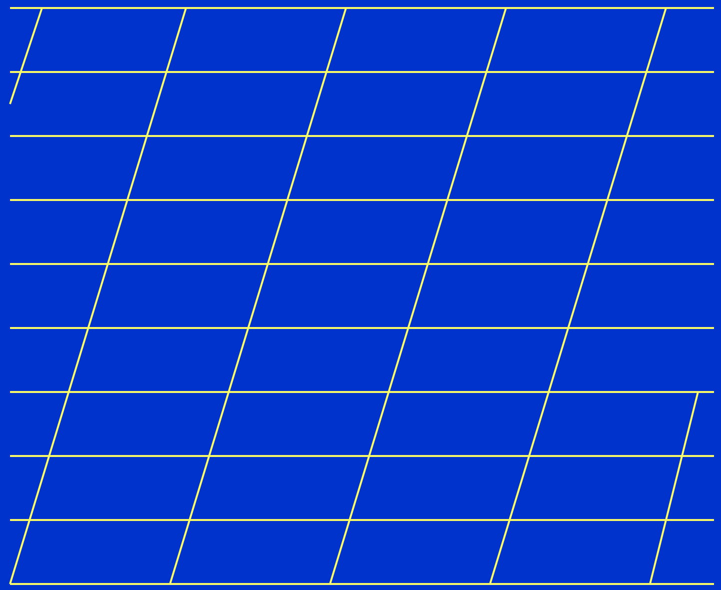
Ex: one dimensional array of points



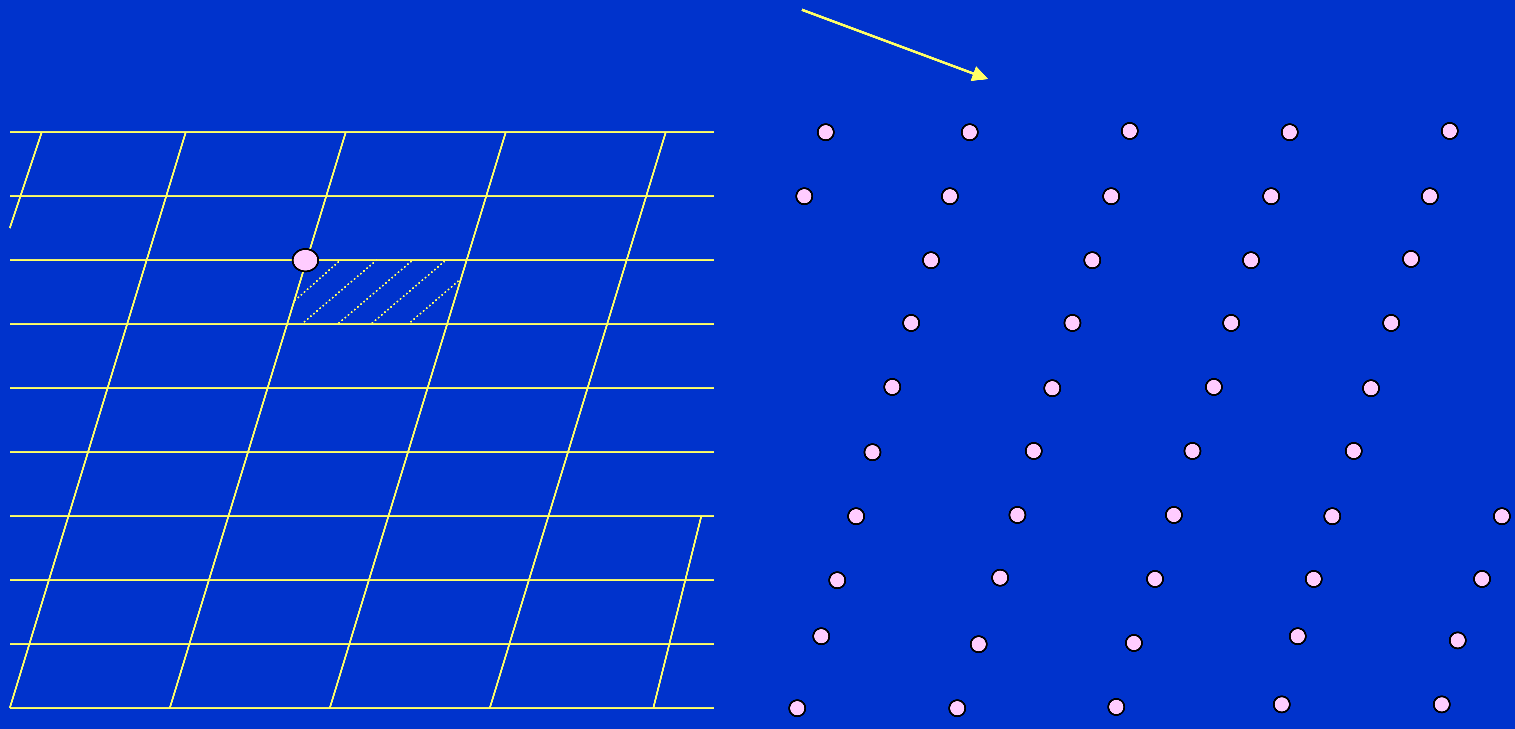
Translations are restricted to only certain values to get symmetry (periodicity)

2D translations

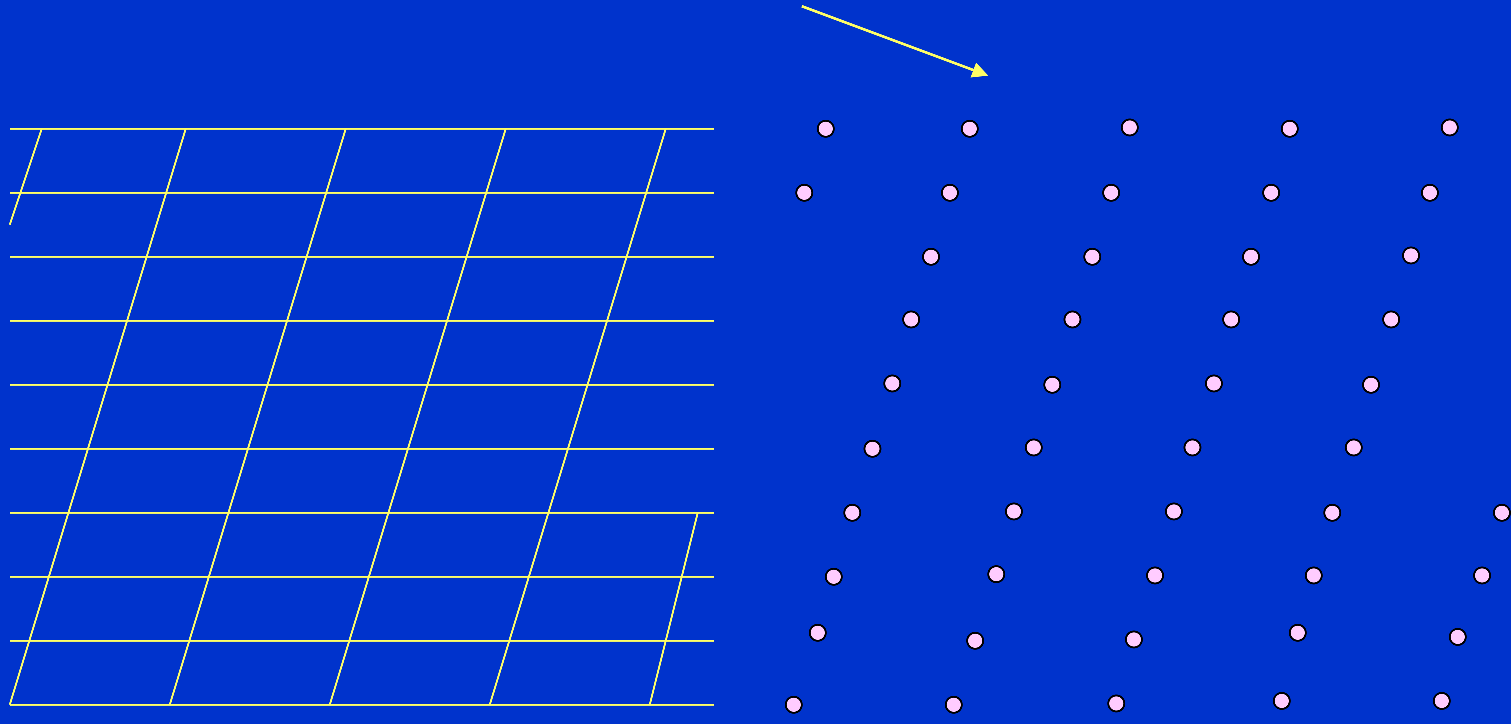
Lots of common examples



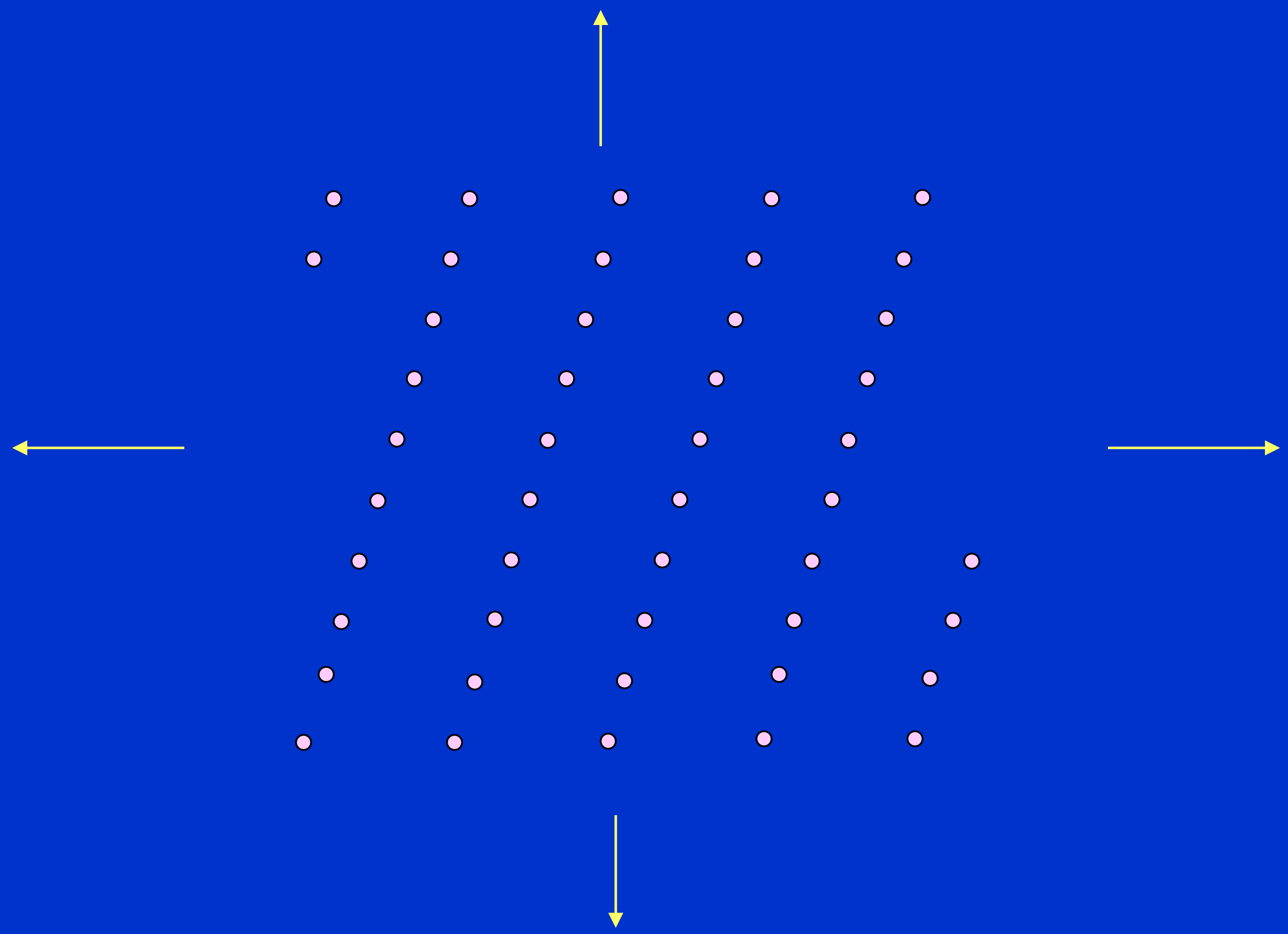
Each block is represented by a point



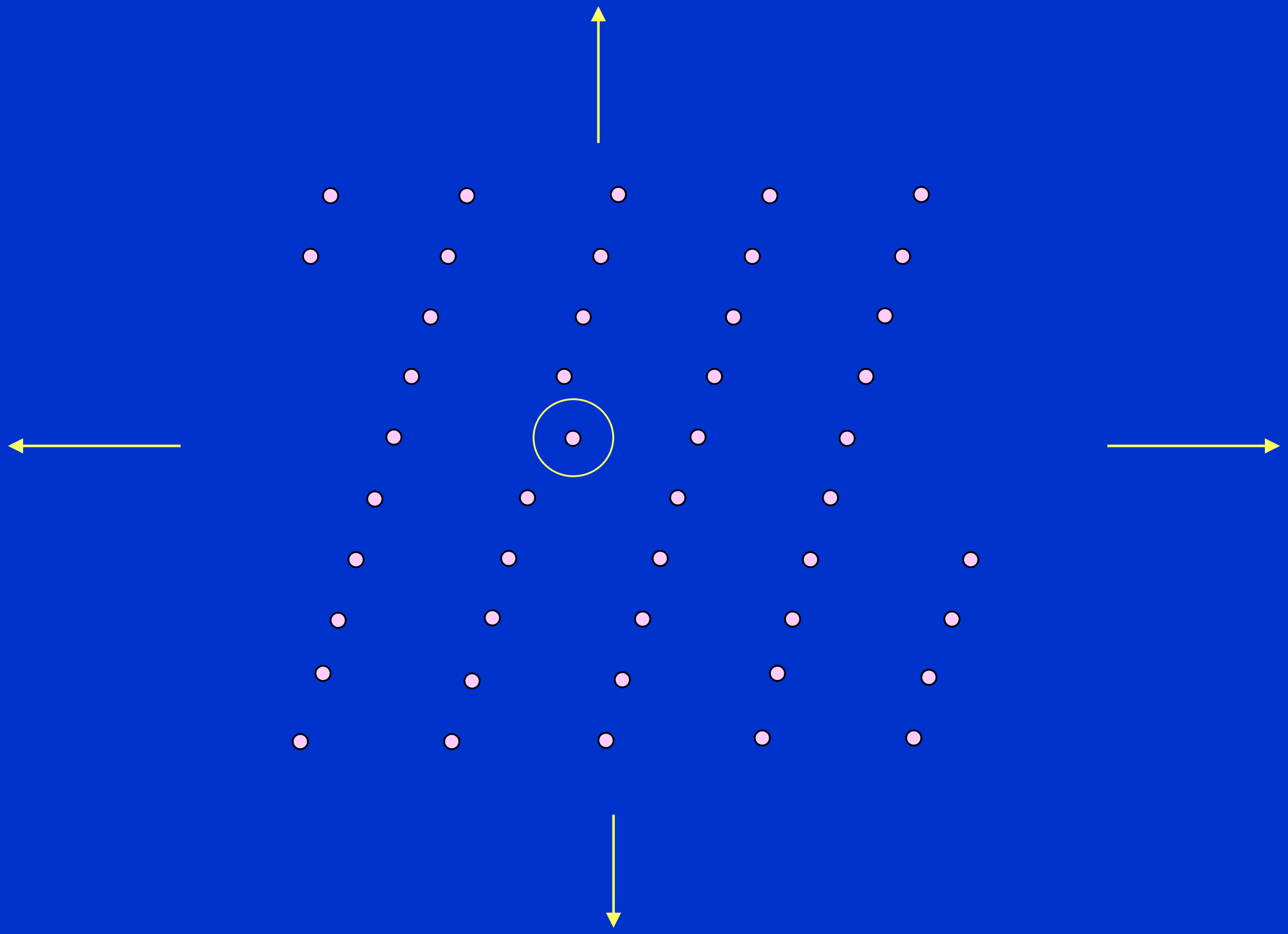
This array of points is a LATTICE



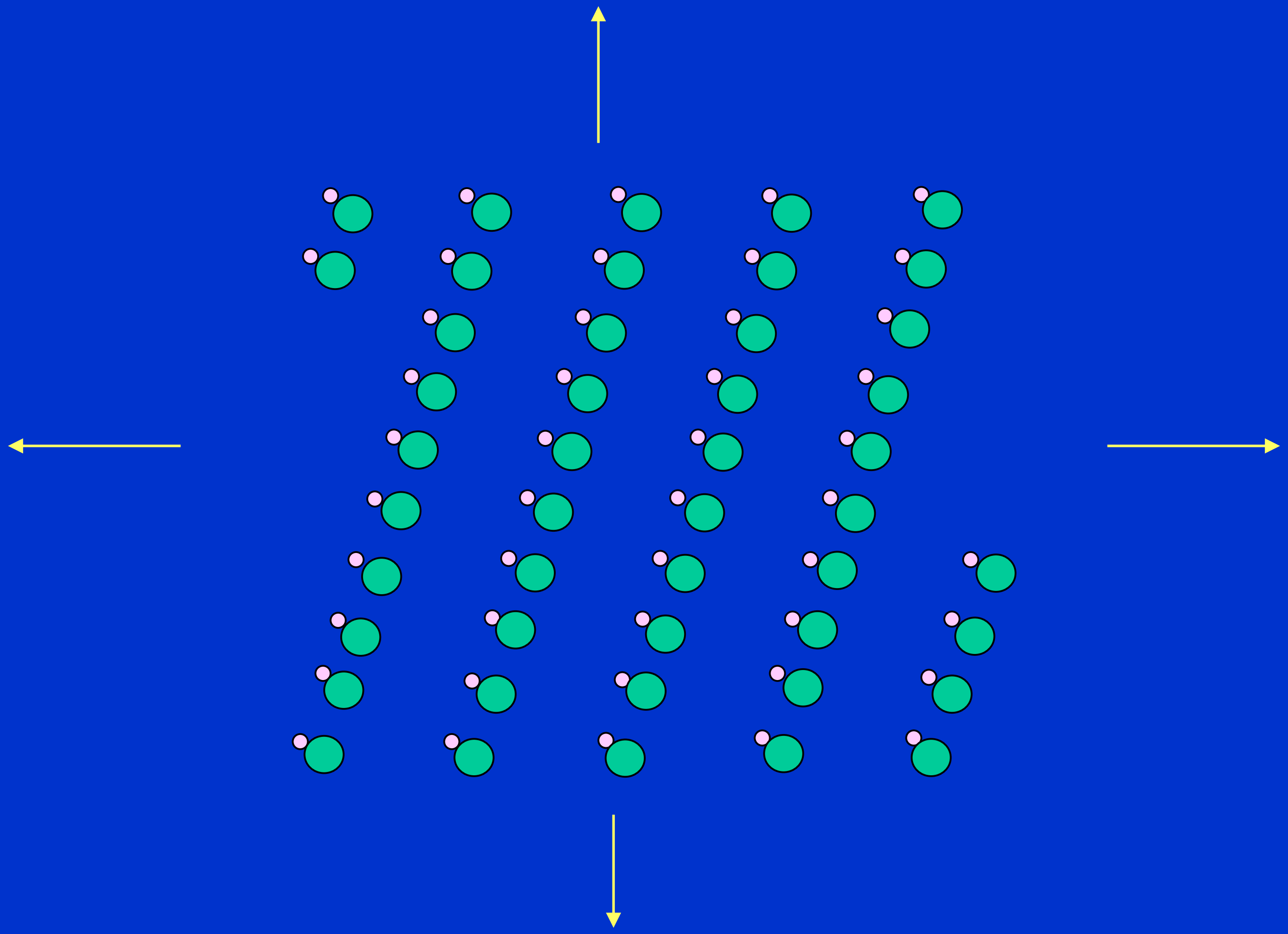
Lattice - **infinite, perfectly periodic** array of **points** in a space



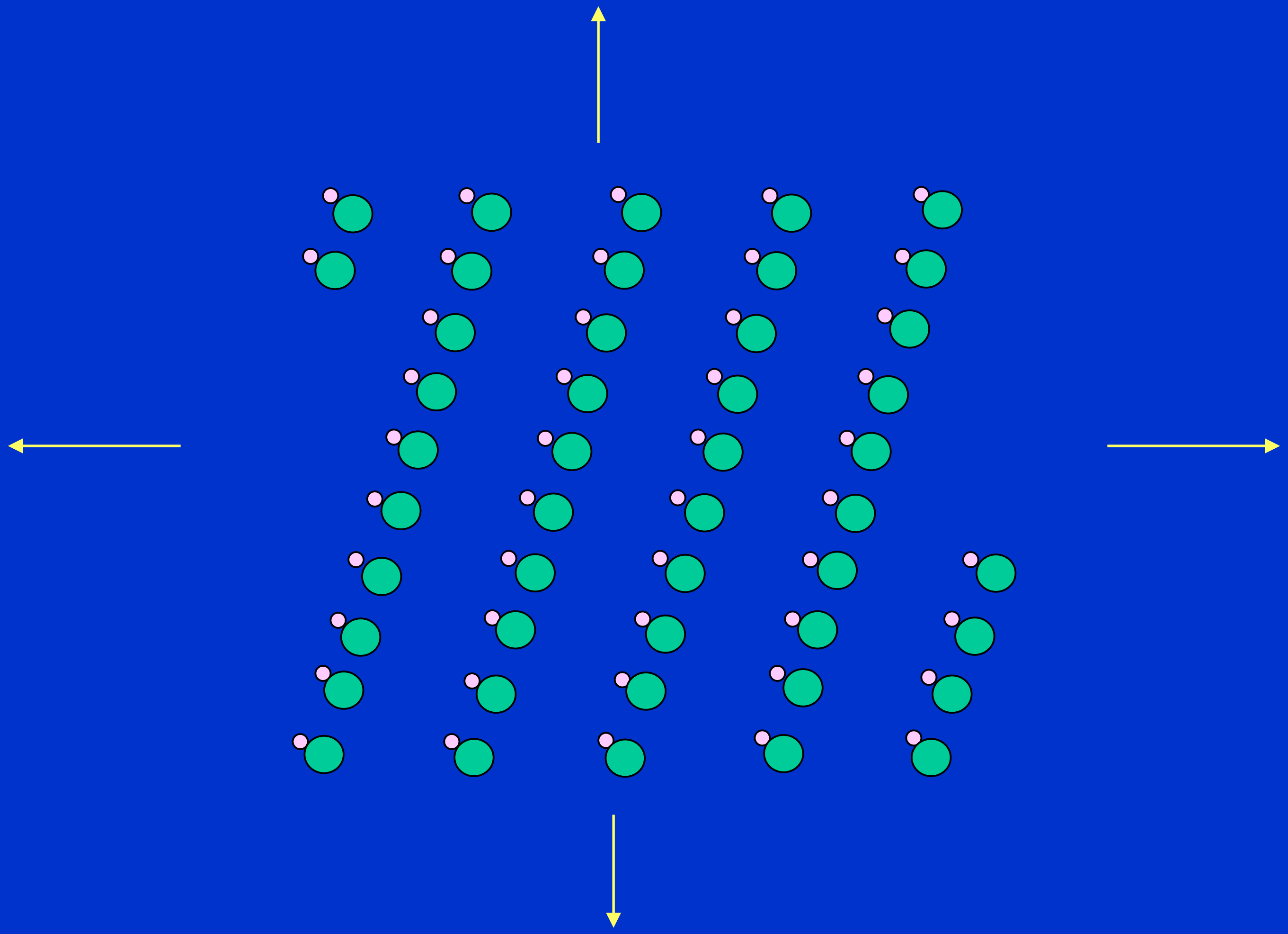
Not a lattice:



Not a lattice:

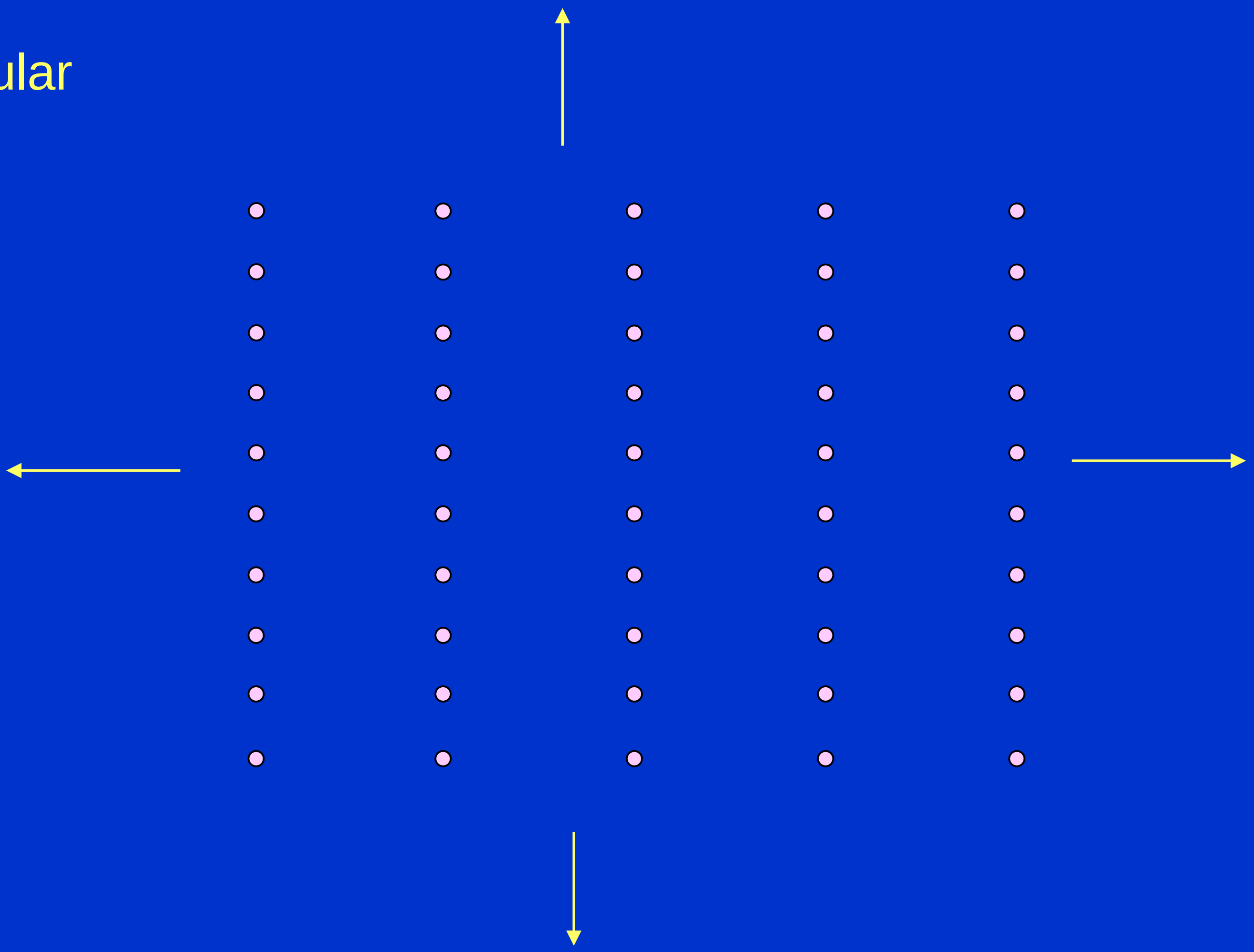


Not a lattice - ….some kind of STRUCTURE becuz not just points



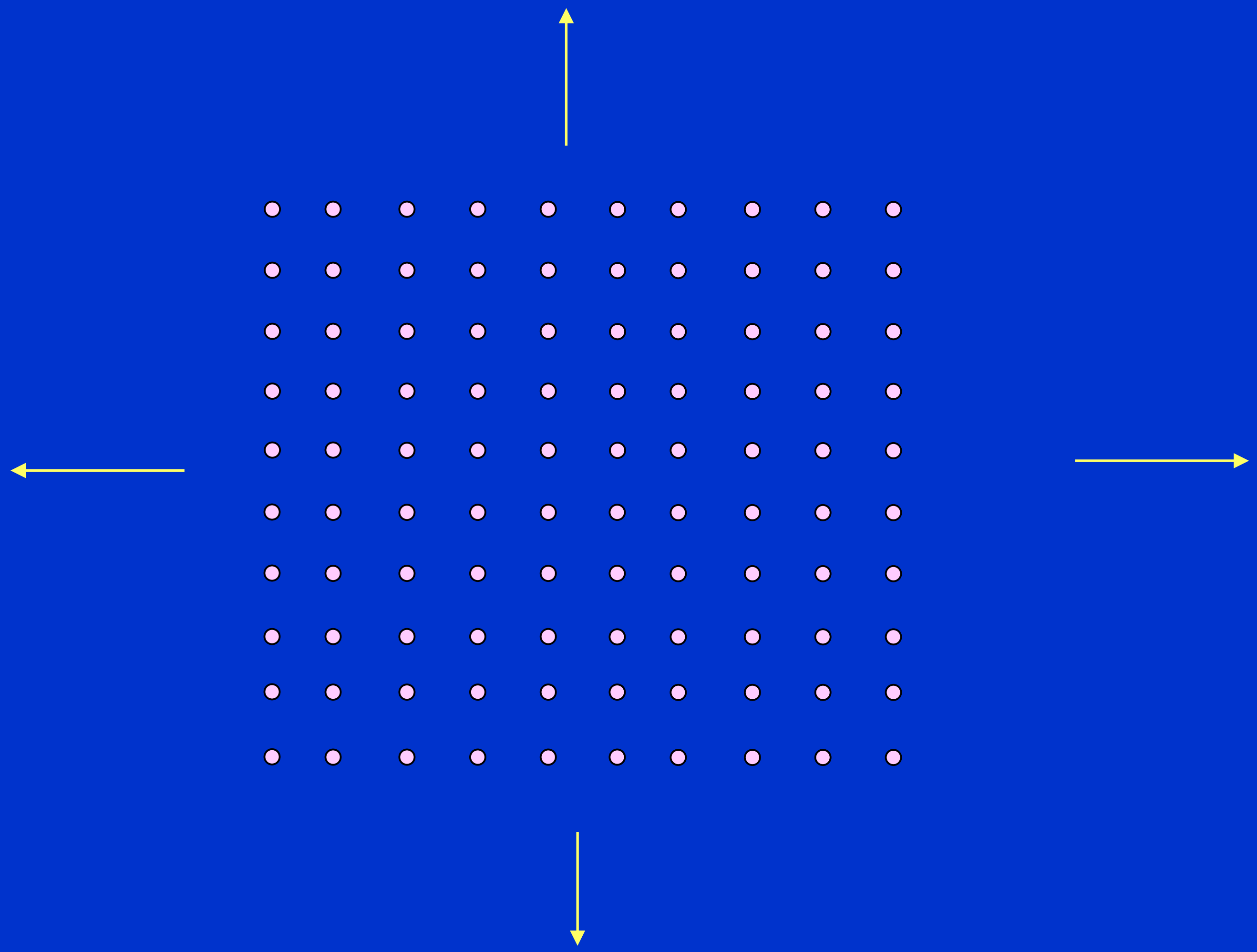
Another type of lattice - with a different symmetry

rectangular



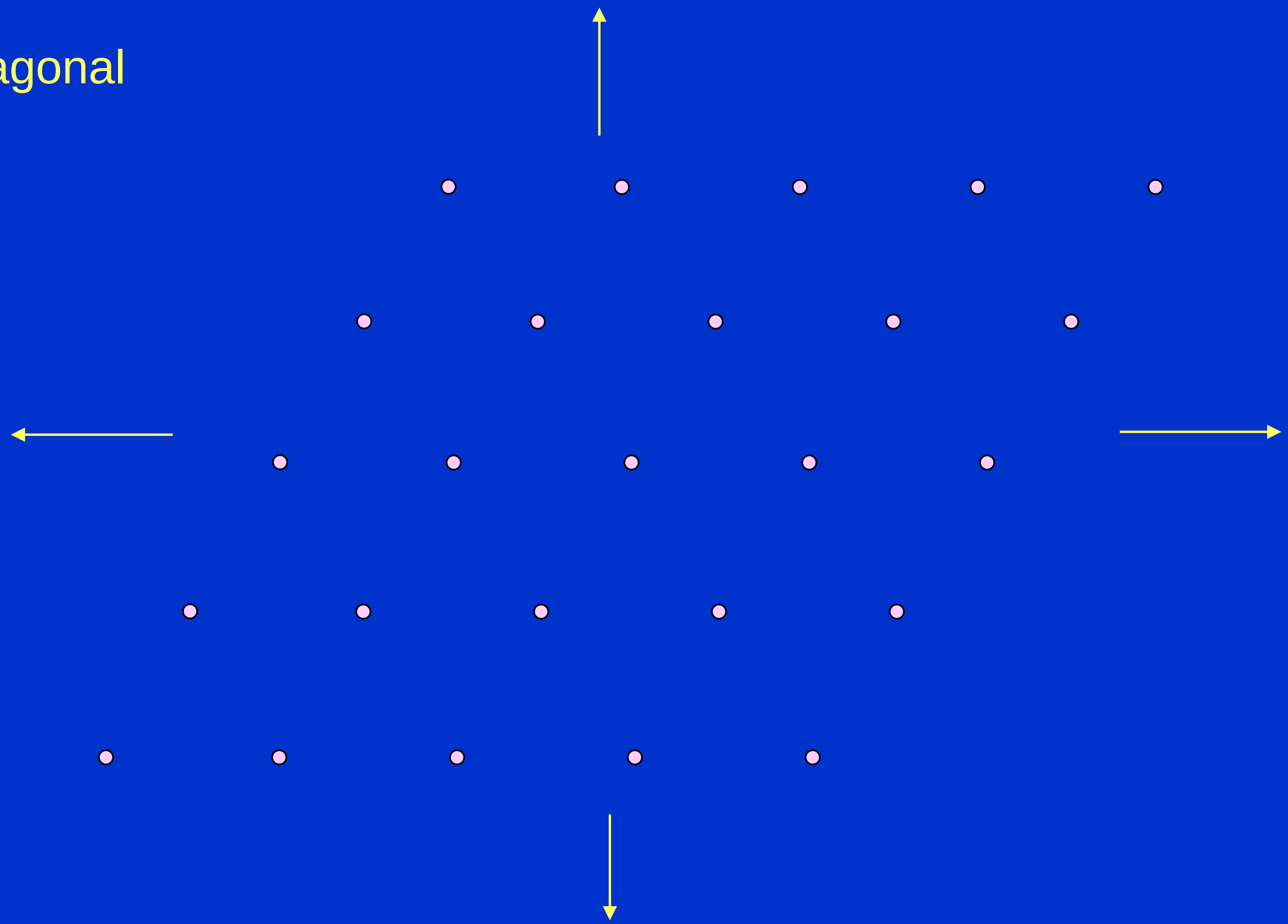
Another type of lattice - with a different symmetry

square

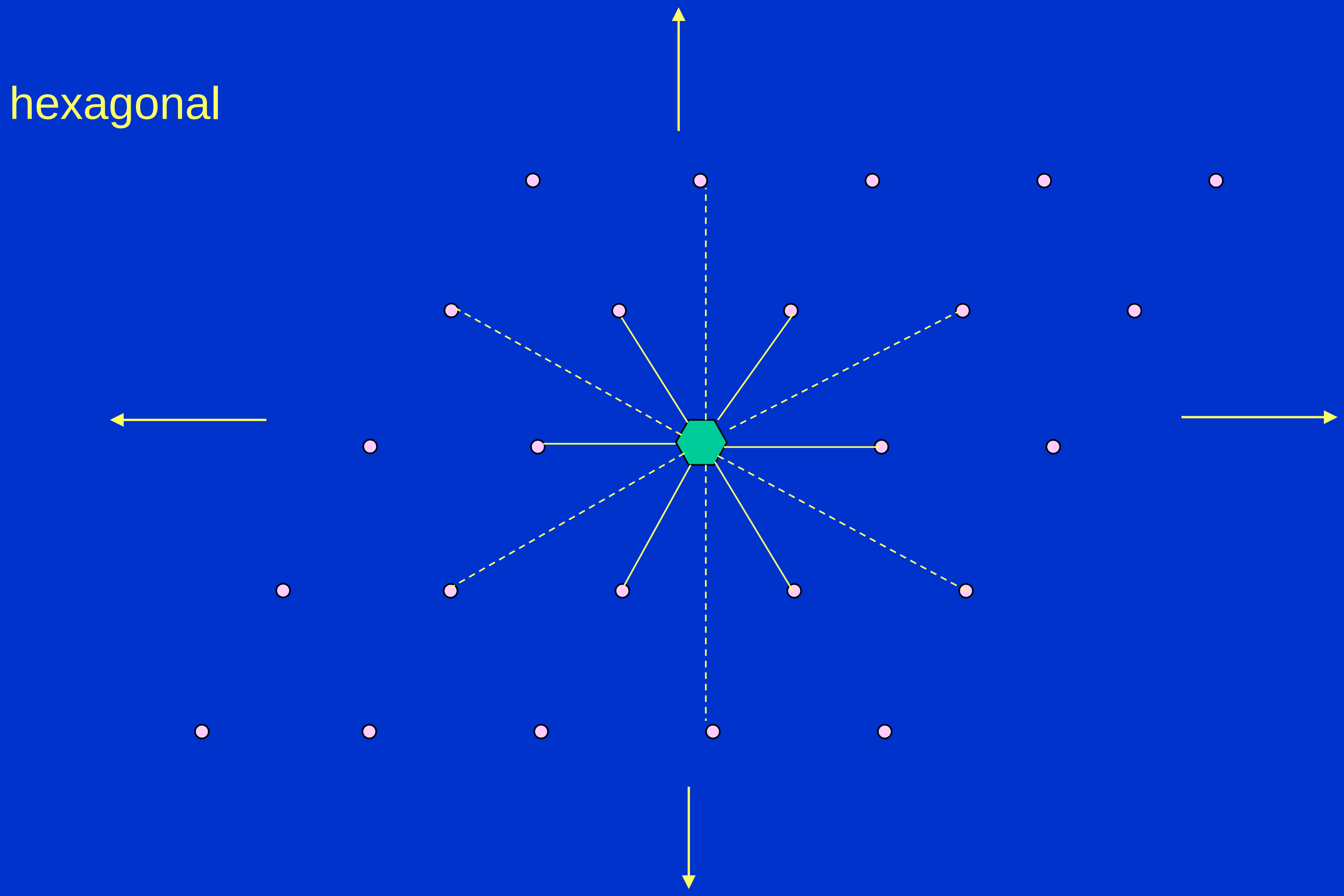


Another type of lattice - with a different symmetry

hexagonal



Back to rotation -
This lattice exhibits 6-fold symmetry

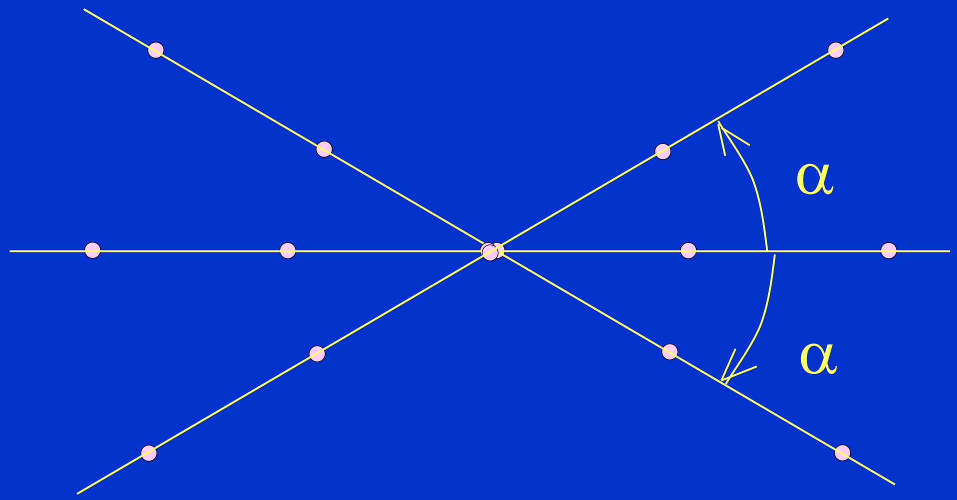


Periodicity and rotational symmetry

What types of rotational symmetry allowed?

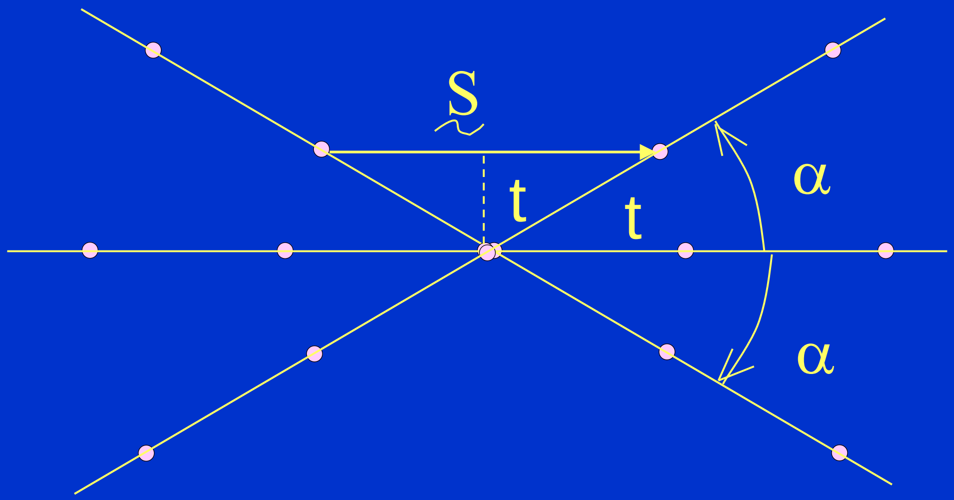
Periodicity and rotational symmetry

Suppose periodic row of points is rotated through $\pm\,\alpha$:

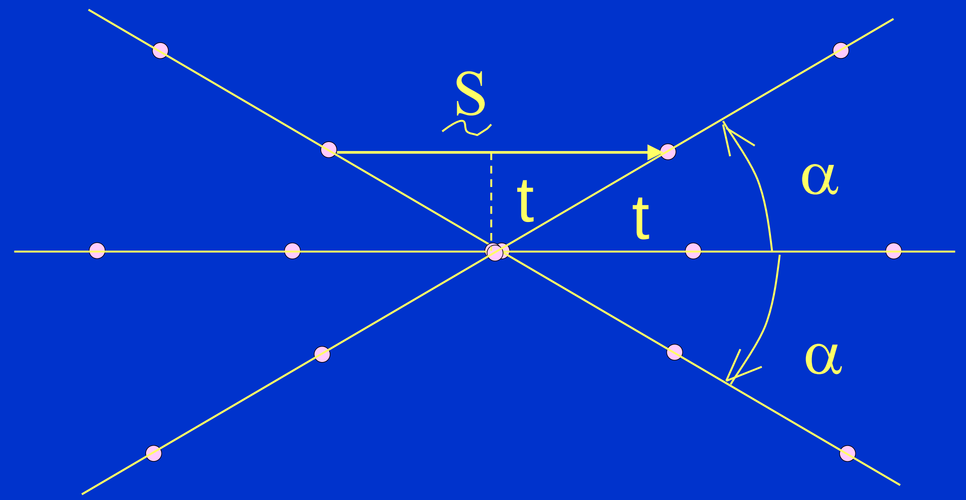


Periodicity and rotational symmetry

To maintain periodicity,



vector S = an integer x basis translation t



vector S = an integer x basis translation t

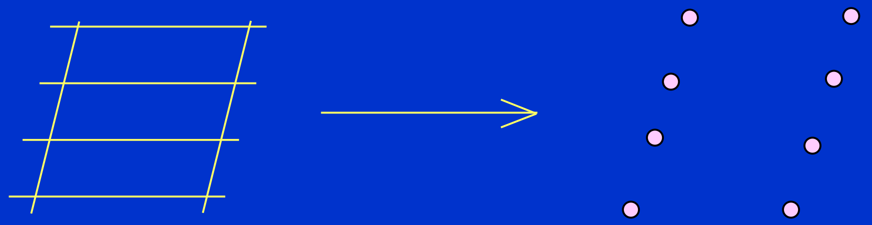
$t \cos \alpha = S/2 = mt/2$

m	cos α	α	axis
2	1	0 2 π	1
1	1/2	π/3 5π/3	6
0	0	π/2 3π/2	4
-1	-1/2	2π/3 4π/3	3
-2	-1	- π π	2

m	cos α	α	axis
2	1	0 $\quad\pi$	1
1	1/2	$\pi/3$ $\quad 5\pi/3$	6
0	0	$\pi/2$ $\quad 3\pi/2$	4
-1	-1/2	$2\pi/3$ $\quad 4\pi/3$	3
-2	-1	$-\pi$ $\quad -\pi$	2

Only rotation axes consistent with lattice periodicity in 2-D or 3-D

We abstracted points from the shape:



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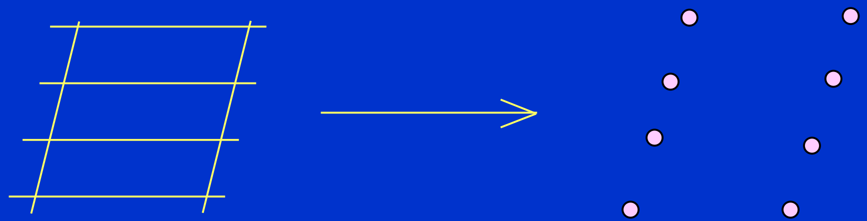
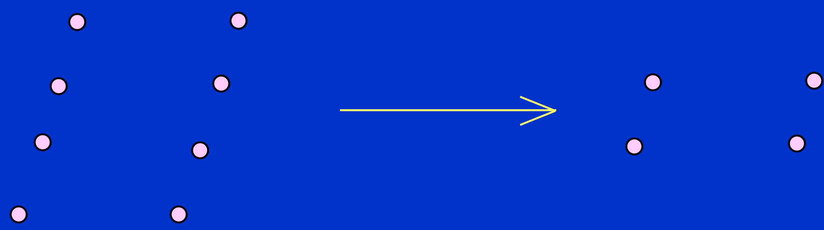


Now we abstract further:



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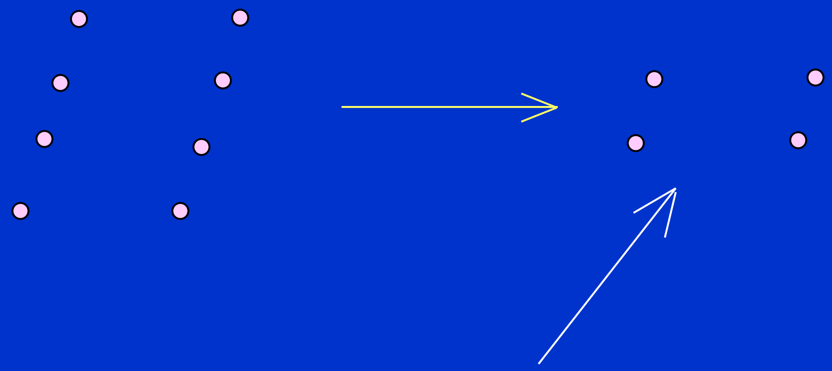
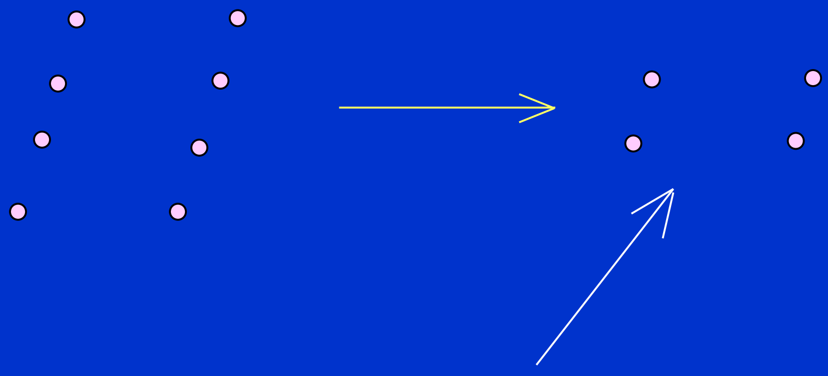


This is a UNIT CELL

Now we abstract further:

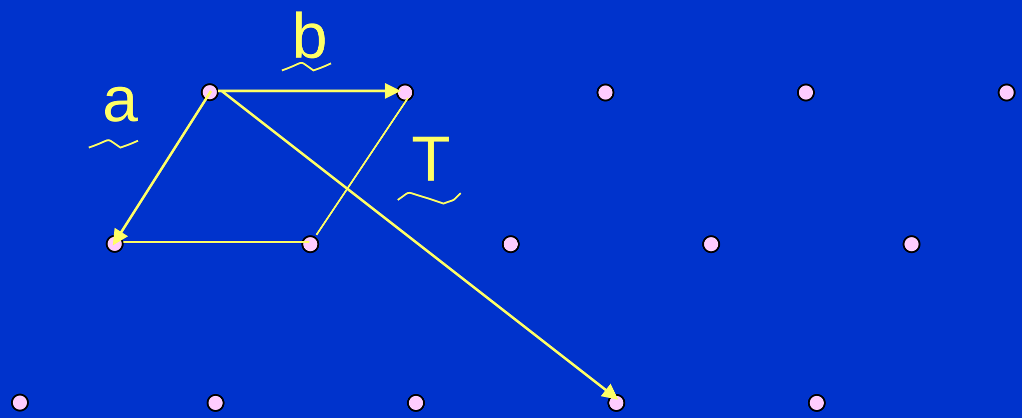


This is a UNIT CELL

Represented by two lengths and an angle

…….or, alternatively, by two vectors

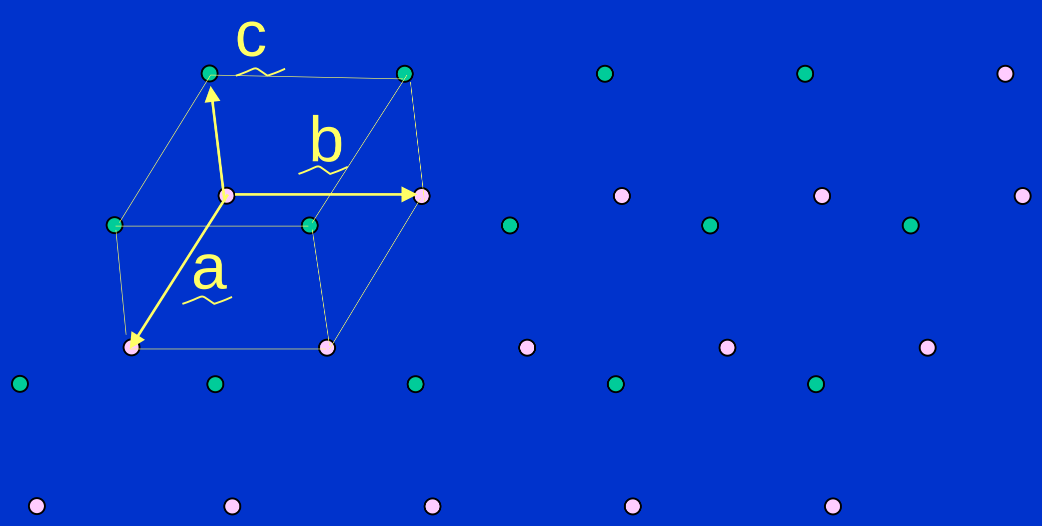
Basis vectors and unit cells



$$\underset{\sim}{T} = t_a \underset{\sim}{a} + t_b \underset{\sim}{b}$$

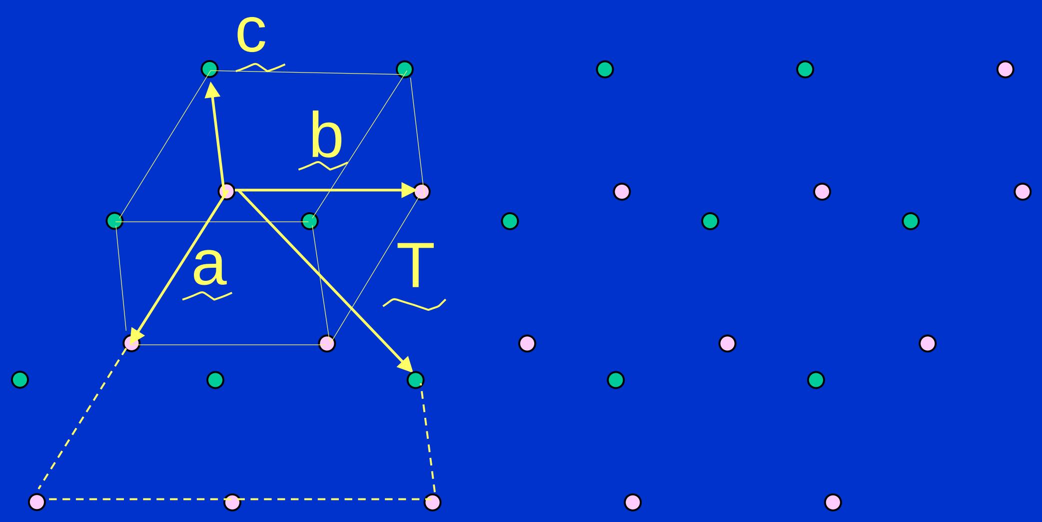
$\underset{\sim}{a}$ and $\underset{\sim}{b}$ are the basis vectors for the lattice

In 3-D:



a, b, and c are the basis vectors for the lattice

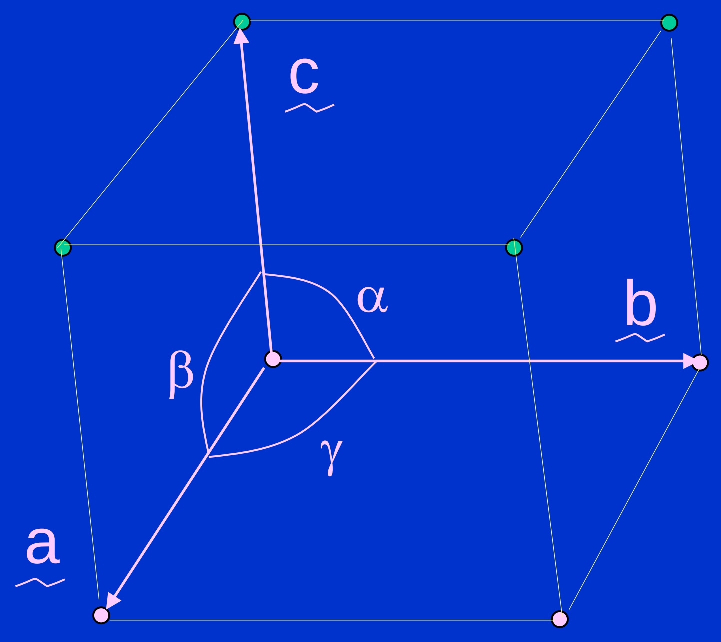
In 3-D:



$$\underset{\sim}{T} = t_a \underset{\sim}{a} + t_b \underset{\sim}{b} + t_c \underset{\sim}{c}$$

$\underset{\sim}{a}$, $\underset{\sim}{b}$, and $\underset{\sim}{c}$ are the basis vectors for the lattice

Lattice parameters:



The many thousands of lattices classified into

crystal systems

System	Interaxial Angles	Axes
Triclinic	$\alpha \neq \beta \neq \gamma \neq 90°$	$a \neq b \neq c$
Monoclinic	$\alpha = \gamma = 90° \neq \beta$	$a \neq b \neq c$
Orthorhombic	$\alpha = \beta = \gamma = 90°$	$a \neq b \neq c$
Tetragonal	$\alpha = \beta = \gamma = 90°$	$a = b \neq c$
Cubic	$\alpha = \beta = \gamma = 90°$	$a = b = c$
Hexagonal	$\alpha = \beta = 90°, \gamma = 120°$	$a = b \neq c$
Trigonal	$\alpha = \beta = 90°, \gamma = 120°$	$a = b \neq c$

The many thousands of lattices classified into

crystal systems

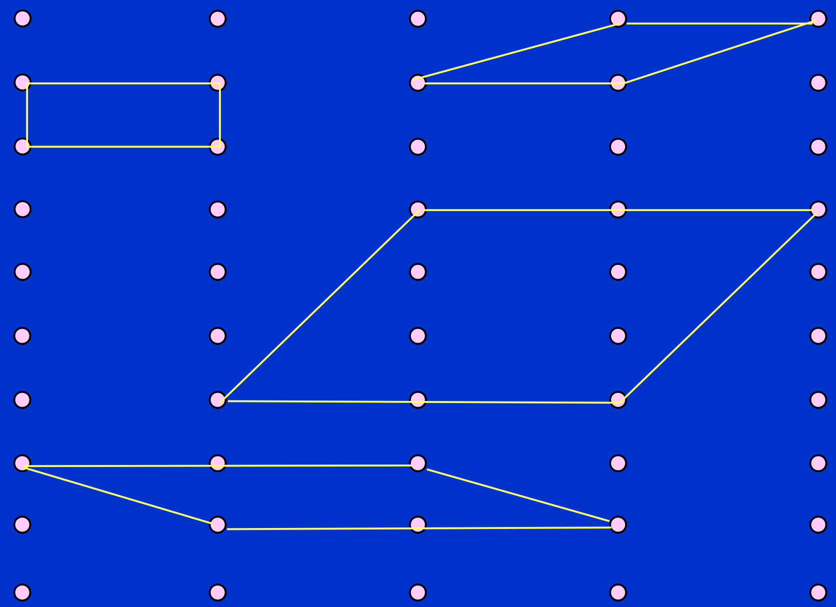
System	Minimum symmetry
Triclinic	1 or $\bar{1}$
Monoclinic	2 or $\bar{2}$
Orthorhombic	three 2s or $\bar{2}$s
Tetragonal	4 or $\bar{4}$
Cubic	four 3s or $\bar{3}$s
Hexagonal	6 or $\bar{6}$
Trigonal	3 or $\bar{3}$

Within each crystal system, different types of centering consistent with symmetry

System	Allowed centering
Triclinic	P (primitive)
Monoclinic	P, I (innerzentiert)
Orthorhombic	P, I, F (flächenzentiert), A (end centered)
Tetragonal	P, I
Cubic	P, I, F
Hexagonal	P
Trigonal	P, R (rhombohedral centered)

The 14 Bravais lattices

For given lattice, infinite number of unit cells possible:



When choosing unit cell, pick:

Simplest, smallest
Right angles, if possible
Cell shape consistent with symmetry