Order parameter spaces, homotopy theory & classification of defects in LCs

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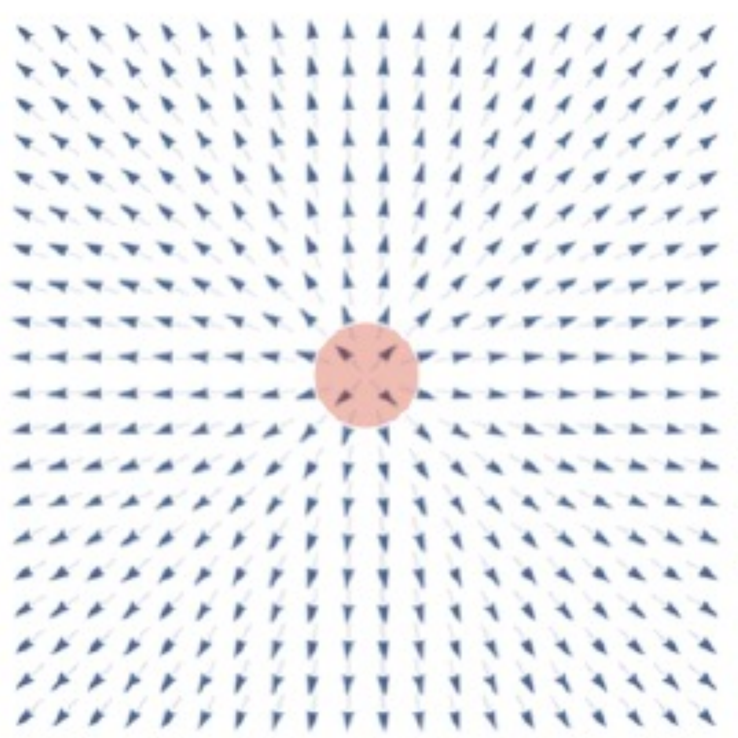
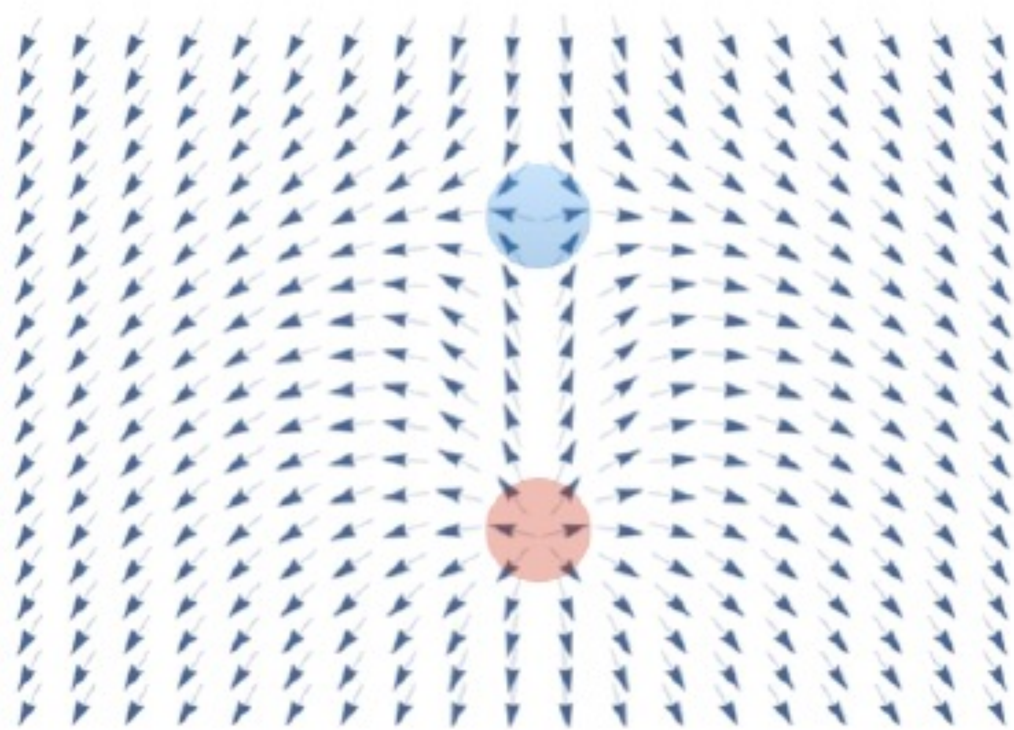
Tutorial, Part 2

Topological defect mediated phase transitions

- Kosterlitz & Thouless Nobel Prize
- Un-binding of defects by thermal energy
- A different type of phase transition!





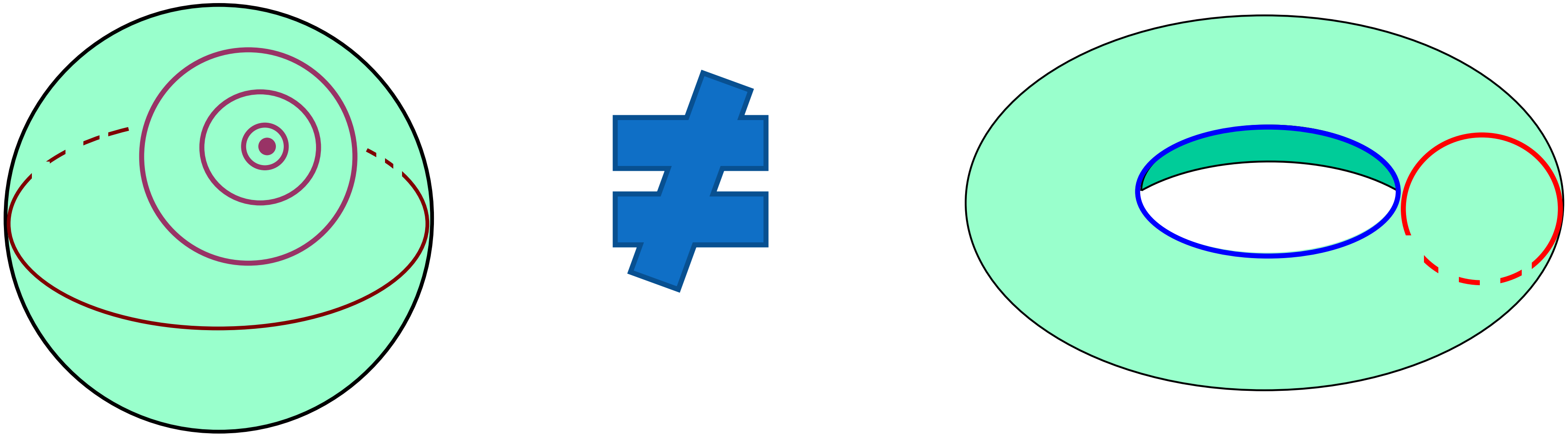
Poincare Theorem

J. Henri Poincaré (1854–1912)

Every closed simply connected (no holes) 2D surface is homeomorphic to a sphere

Simply connected surfaces (no holes)

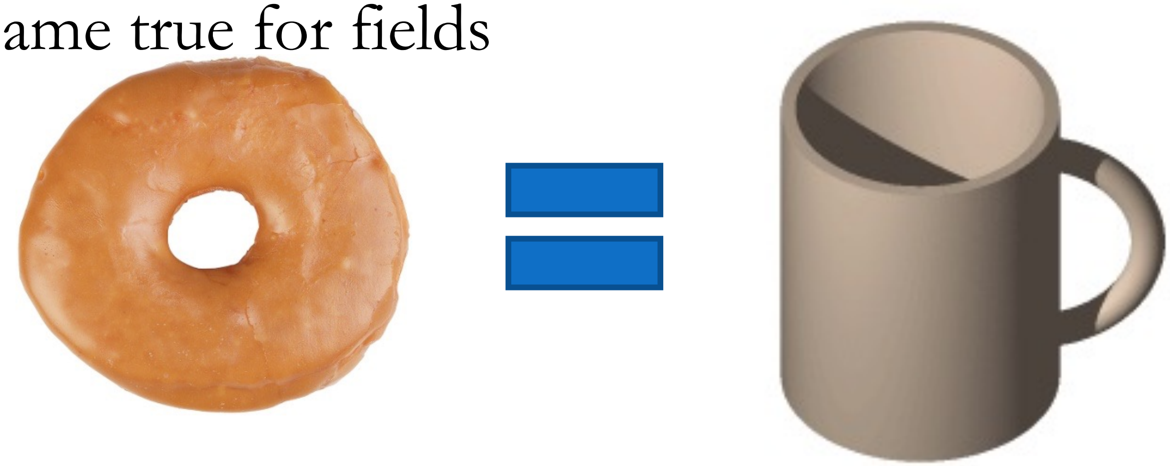
Not simply connected



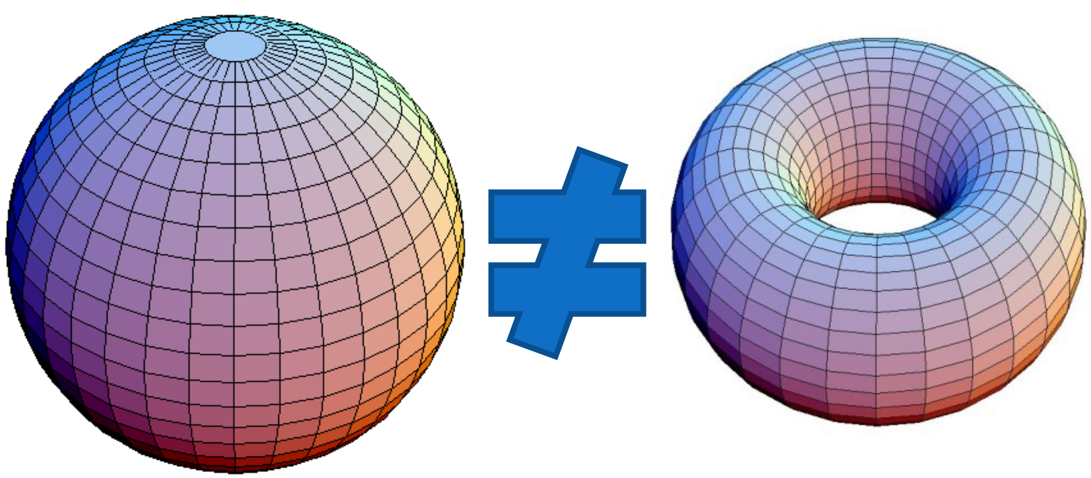
Goals & Motivation

- field theories (1D-3D ferromagnets, ferroelectrics, LCs; scalar, vector & tensorial fields...)
- Can the ground state or metastable solutions in field theories have different topology?
- Distinct topologically –cannot be morphed one to another
- Examples of surfaces – same true for fields

homeomorphic



But,



Fields we cannot morph smoothly one to another?

Topology & topological soliton

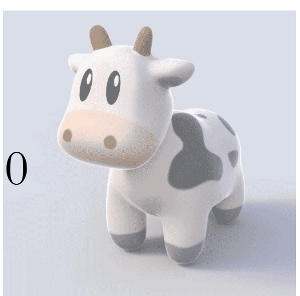
- Topology – properties preserved under **continuous** deformations.

Surfaces

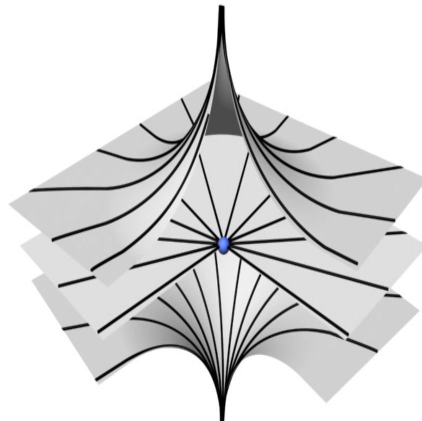
genus 1

≠

genus 0



https://en.wikipedia.org/wiki/Topology



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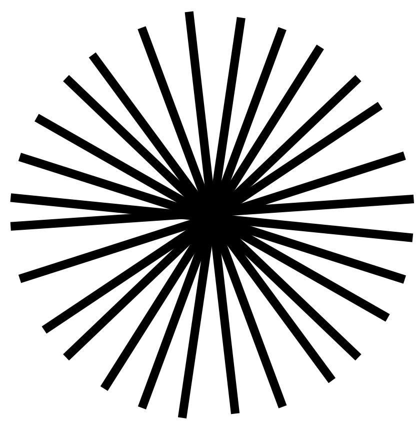
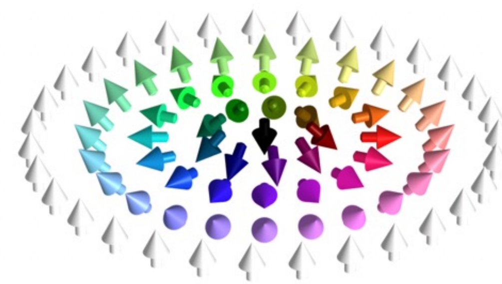
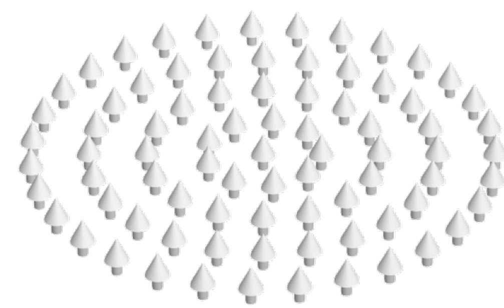


Nonsingular fields



$N_{\mathrm{sk}} = 1$

≠



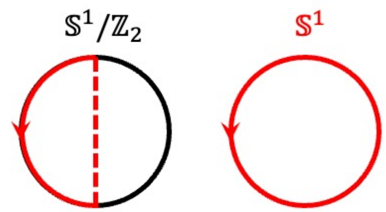
$N_{\mathrm{sk}} = 0$

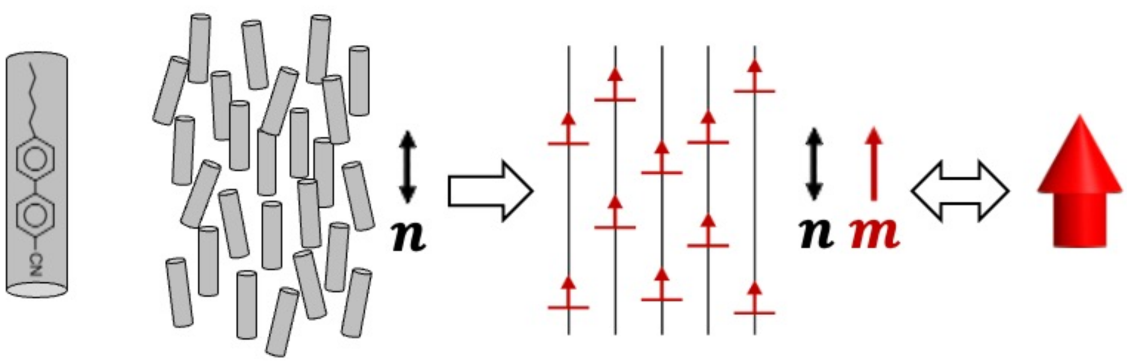
Sphere-sphere maps are well understood

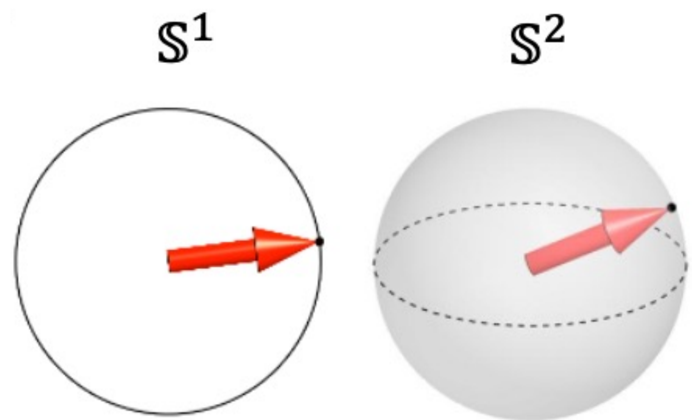
	π_1	π_2	π_3	π_4	π_5
S^0	0	0	0	0	0
S^1	Z	0	0	0	0
S^2	0	Z	Z	Z_2	Z_2
S^3	0	0	Z	Z_2	Z_2
S^4	0	0	0	Z	Z_2
S^5	0	0	0	0	Z

two maps connected by continuous path are said to be homotopic

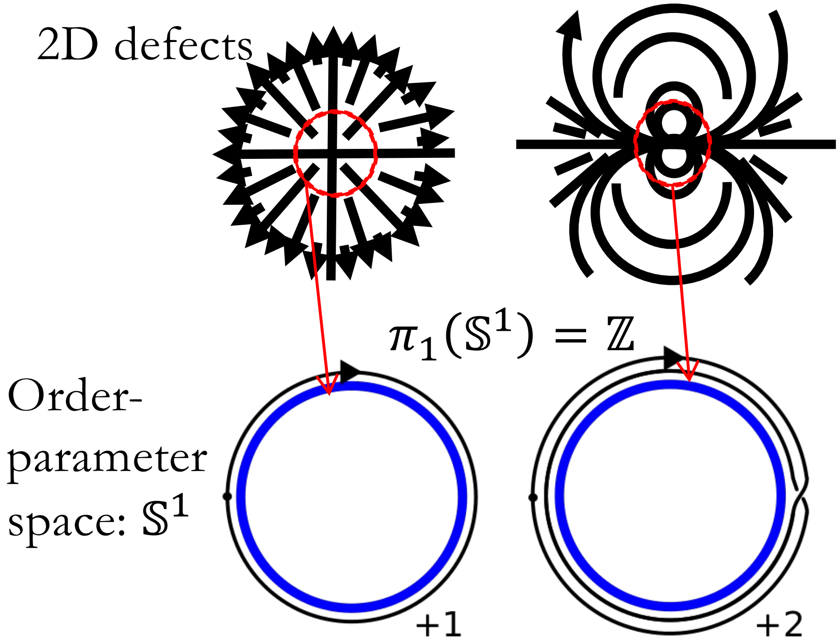
- Spheres as OP Spaces and defect-surrounding surfaces
- i-th homotopy group $\pi_i(S^n)$ – ways the i-dimensional sphere S^i can be mapped into n-dimensional sphere S^n



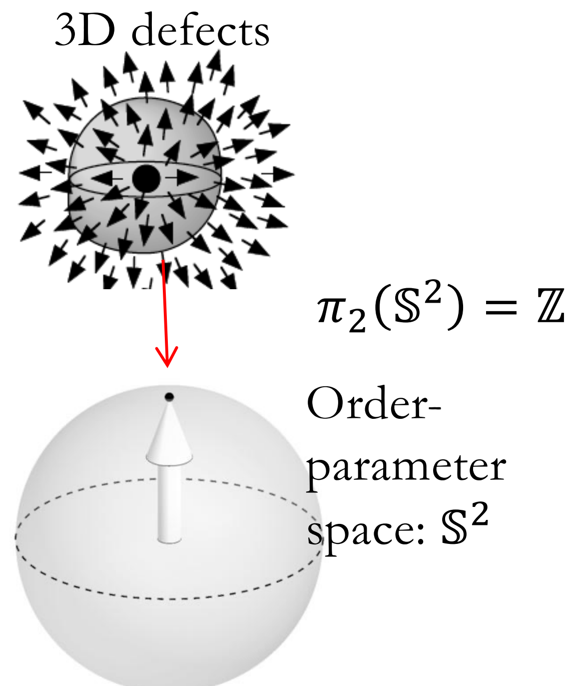




Homotopy theory (sphere-sphere maps) of singular defects



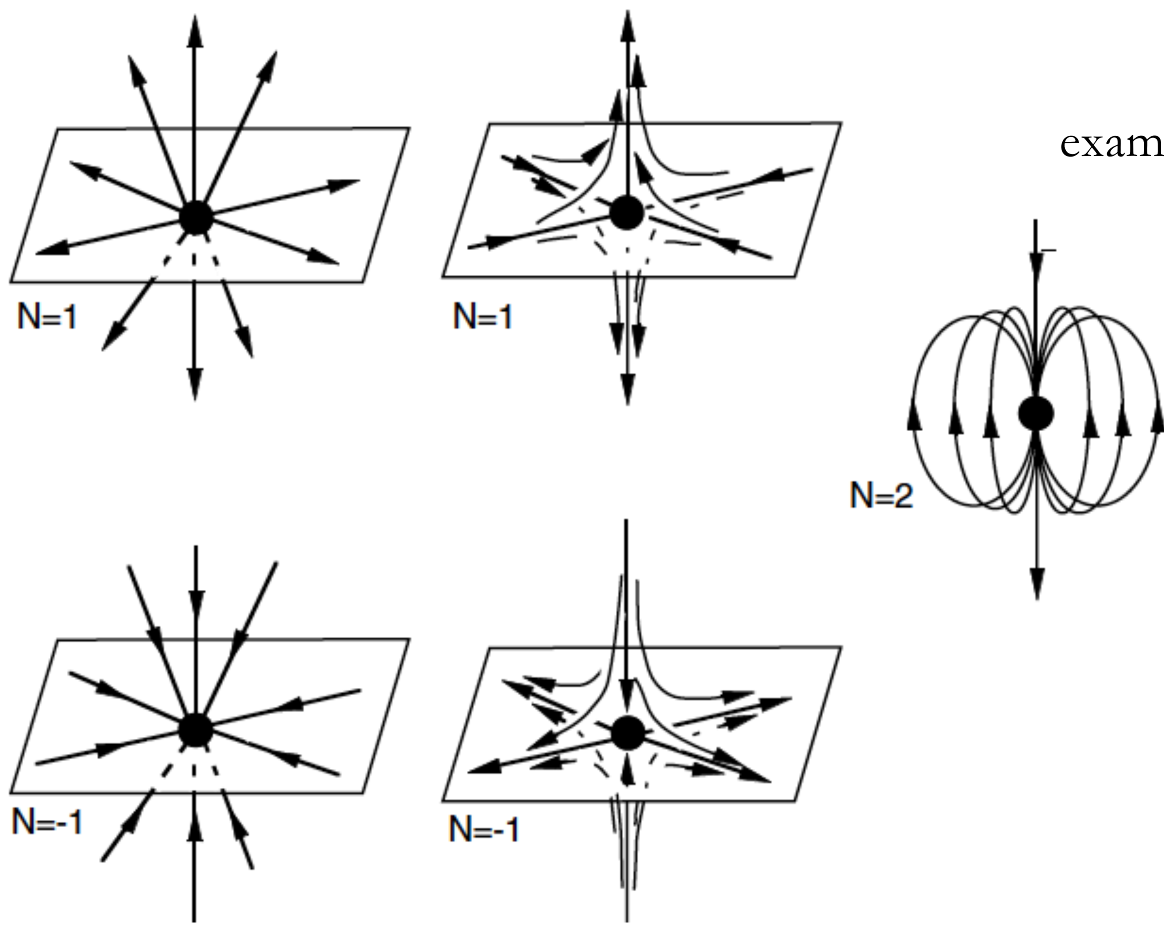
	π_1	π_2	π_3
$\mathbb{S}^0$	0	0	0
$\mathbb{S}^1$	$\mathbb{Z}$	0	0
$\mathbb{S}^2$	0	$\mathbb{Z}$	$\mathbb{Z}$
$\mathbb{S}^3$	0	0	$\mathbb{Z}$



→Spheres as order-parameter Spaces and defect-surrounding surfaces
→i-th homotopy group $\pi_i(S^n)$ – ways the field on S^i can be mapped to S^n

Procedure

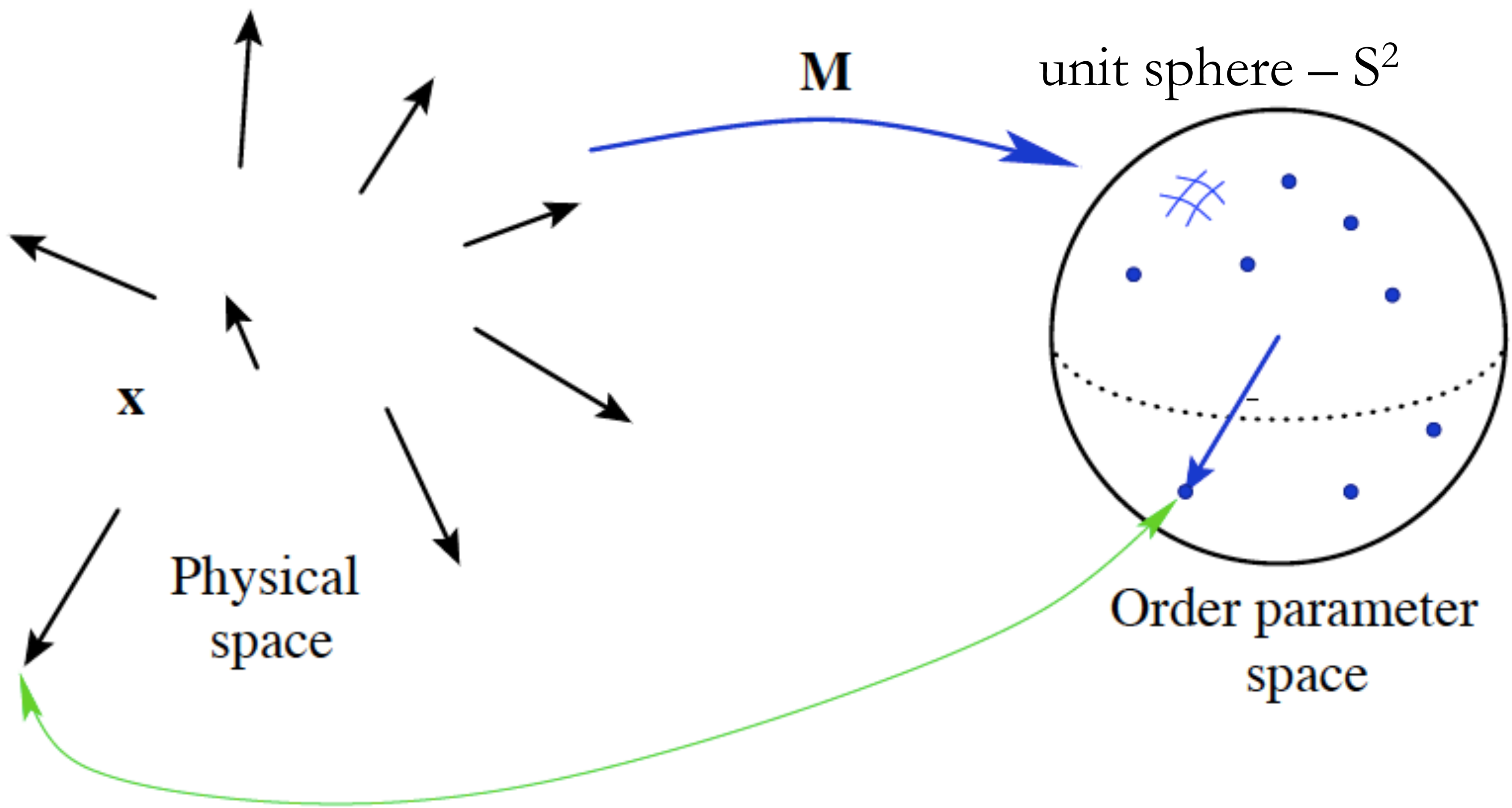
- Identify the ground state manyfold (degeneracy of order parameter) – the order parameter space
- Map the order parameter from the sample to the OP space
- Identify topology of the OP maps
- Topologically similar maps - homotopic



examples of point defects

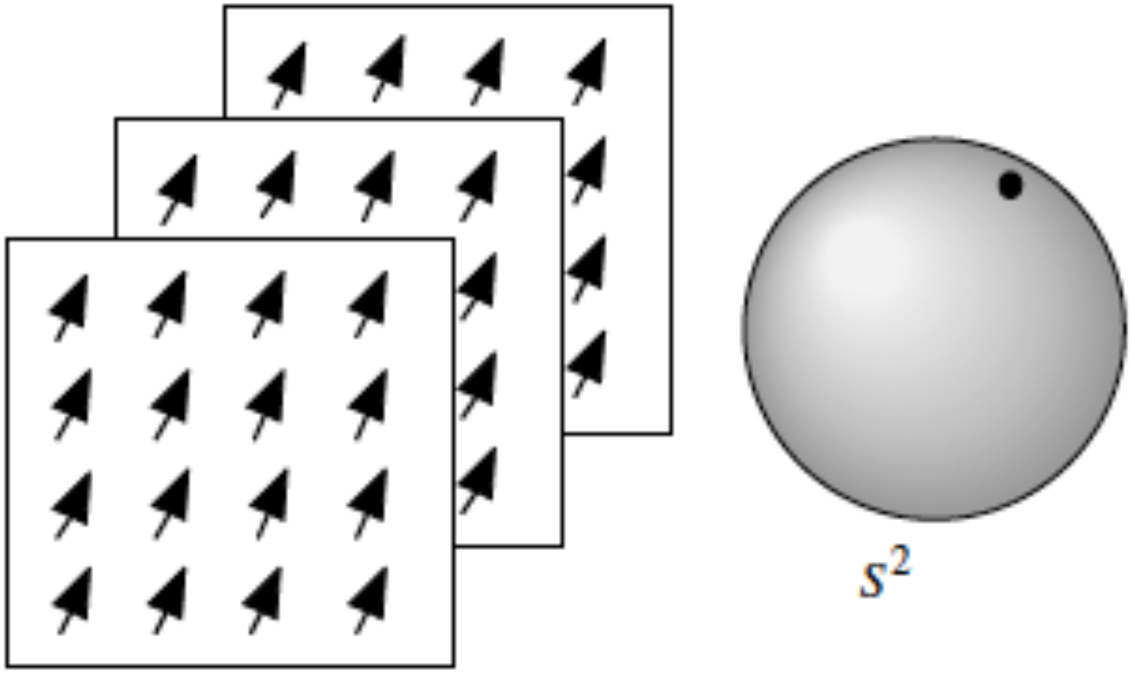
Order Parameter Spaces (ground state manyfolds)

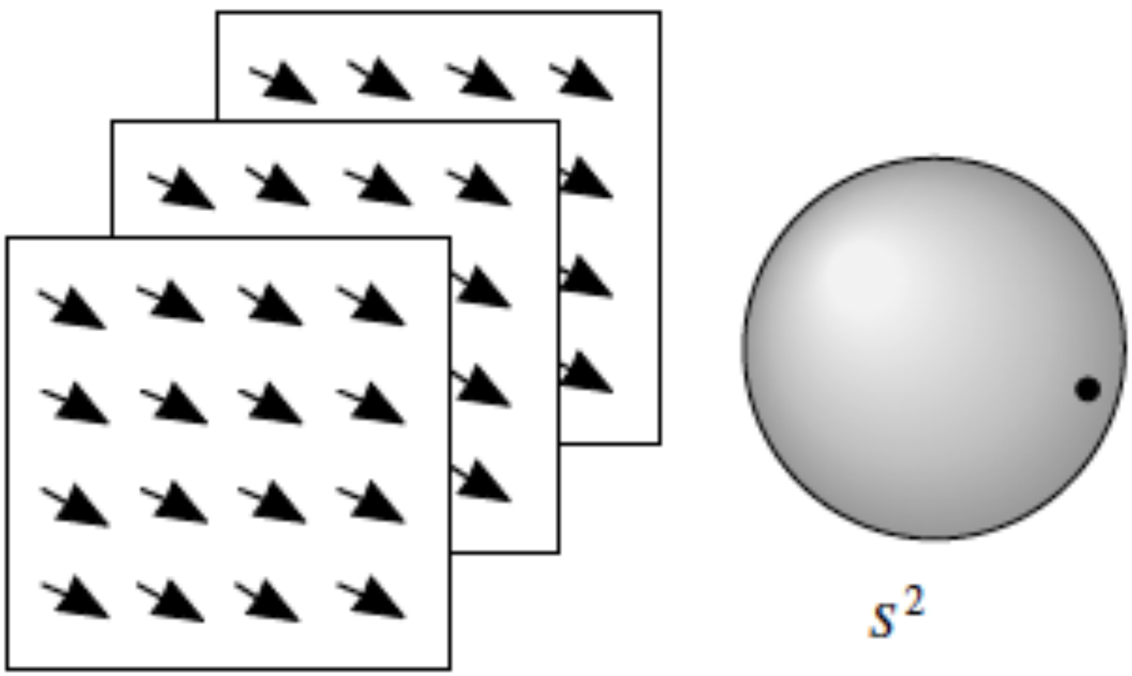
- 3D ferromagnet as an example – Magnetization **M**;
- Maps from real to order parameter space – space of all allowed values of unit vector **m**=**M**/M



How about 3D ferroelectrics? Also S^2

Order Parameter Space: 3D Ferromagnet





Different directions of the magnetization vector M correspond to the different points on the order parameter space S^2

1D, 2D Ferromagnets & Ferroelectrics

- Imagine a ferromagnetic or ferroelectric solids for which **M** or **P** are confined to a 2D plane (only in-plane orientations).
- What is the OP space?

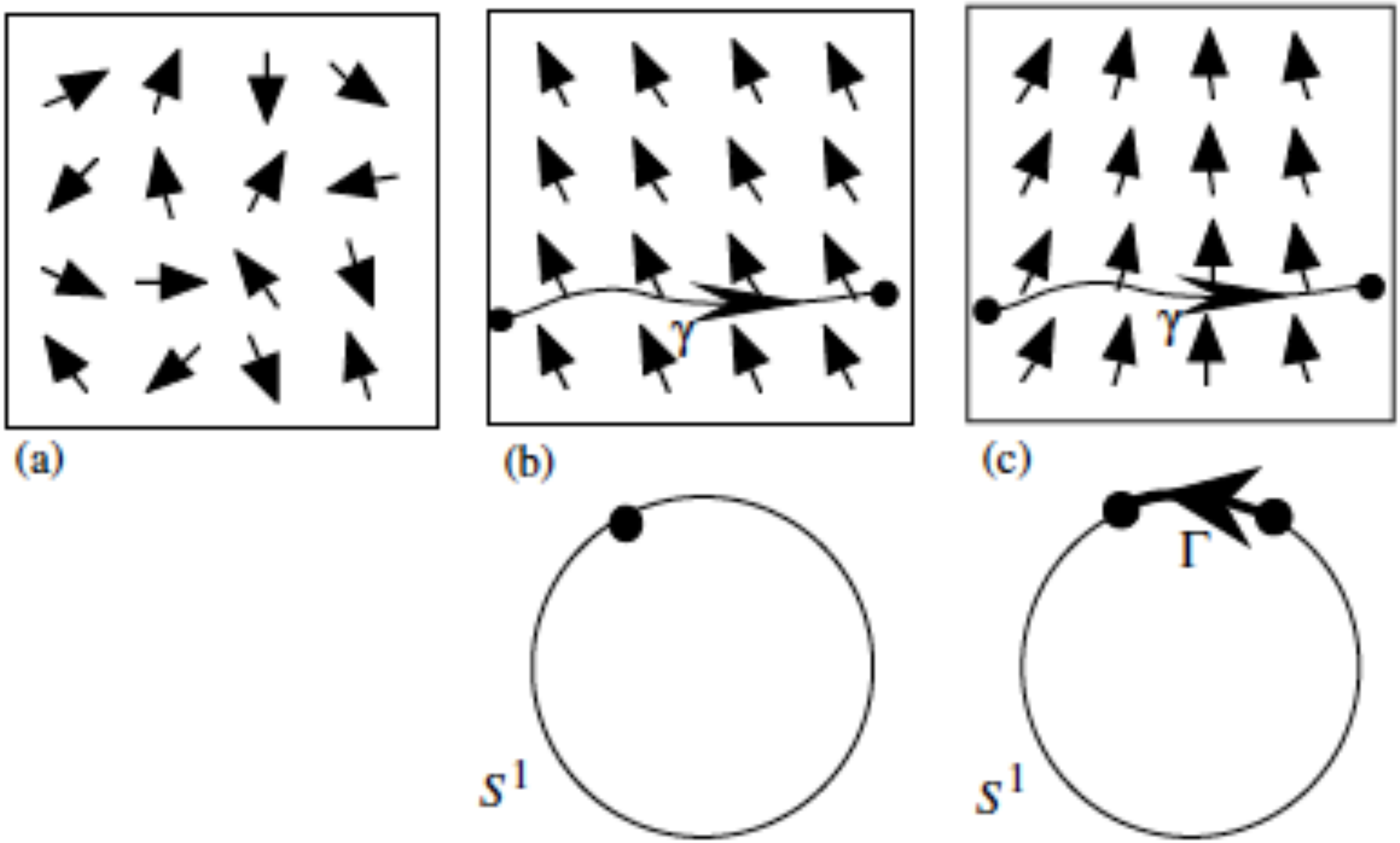
S^1 – a 1D sphere (circle)

- Ising ferromagnet (up-down **M**) – what is the OP space?

S^0 – a 0D sphere (2 points equidistant from center) – Note that the dimension refers to the location of points equidistant from the center of origin

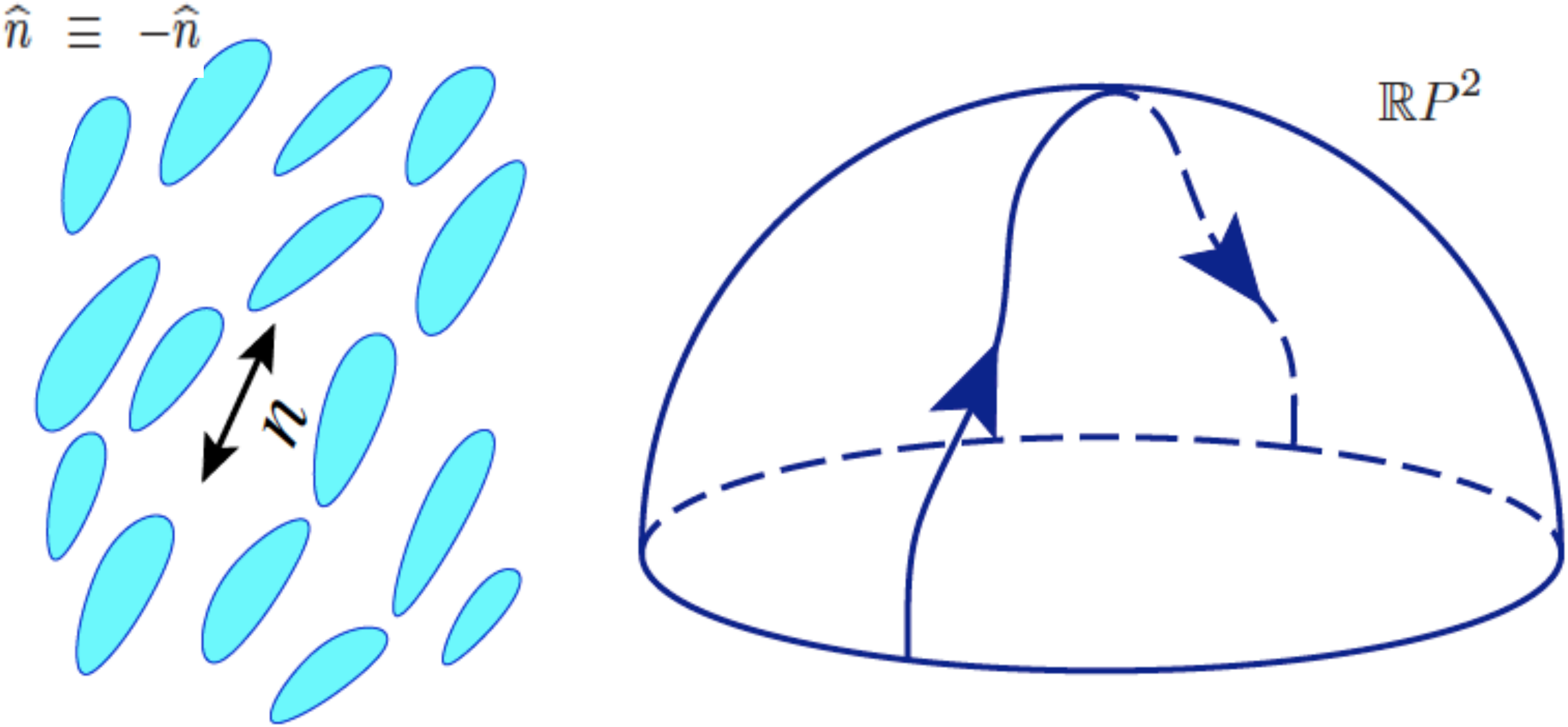
Another example: order parameter space for superconductors & superfluids is a circle $\mathbf{S^1}$

Order Parameter Space: 2D Ferromagnet



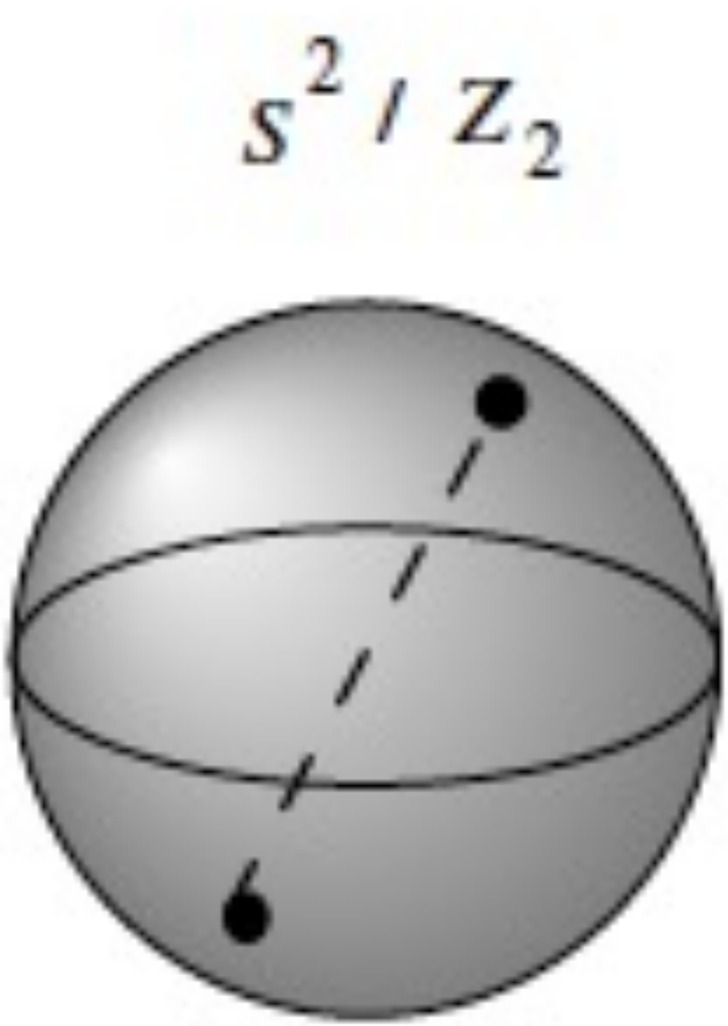
The path γ in the ferromagnet is mapped into a single point in the order parameter space $\mathbf{S}^1$, when the state is uniform and into a path when the state is nonuniform (topologically trivial here).

Nematic LCs with orientational order only



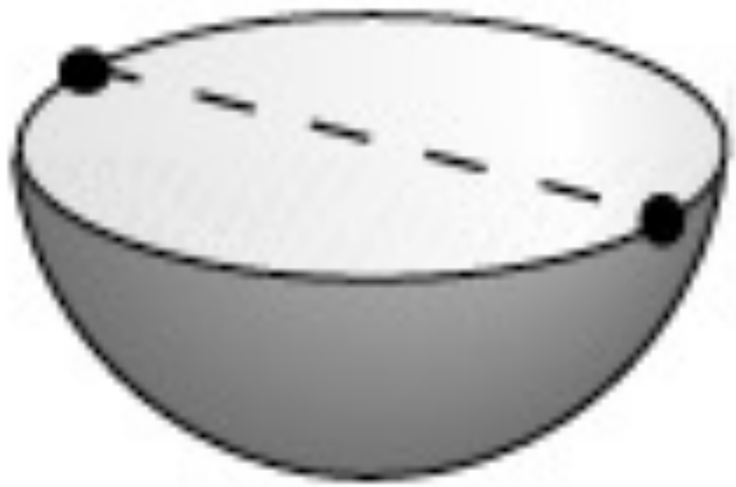
- Nonpolar director – opposite orientations cannot be distinguished
- OP space is a sphere with diametrically opposite points identified (S^2/Z_2), topologically equivalent to the projectile plane ($\mathbf{R}P^2$)

Order parameter space for the uniaxial nematic



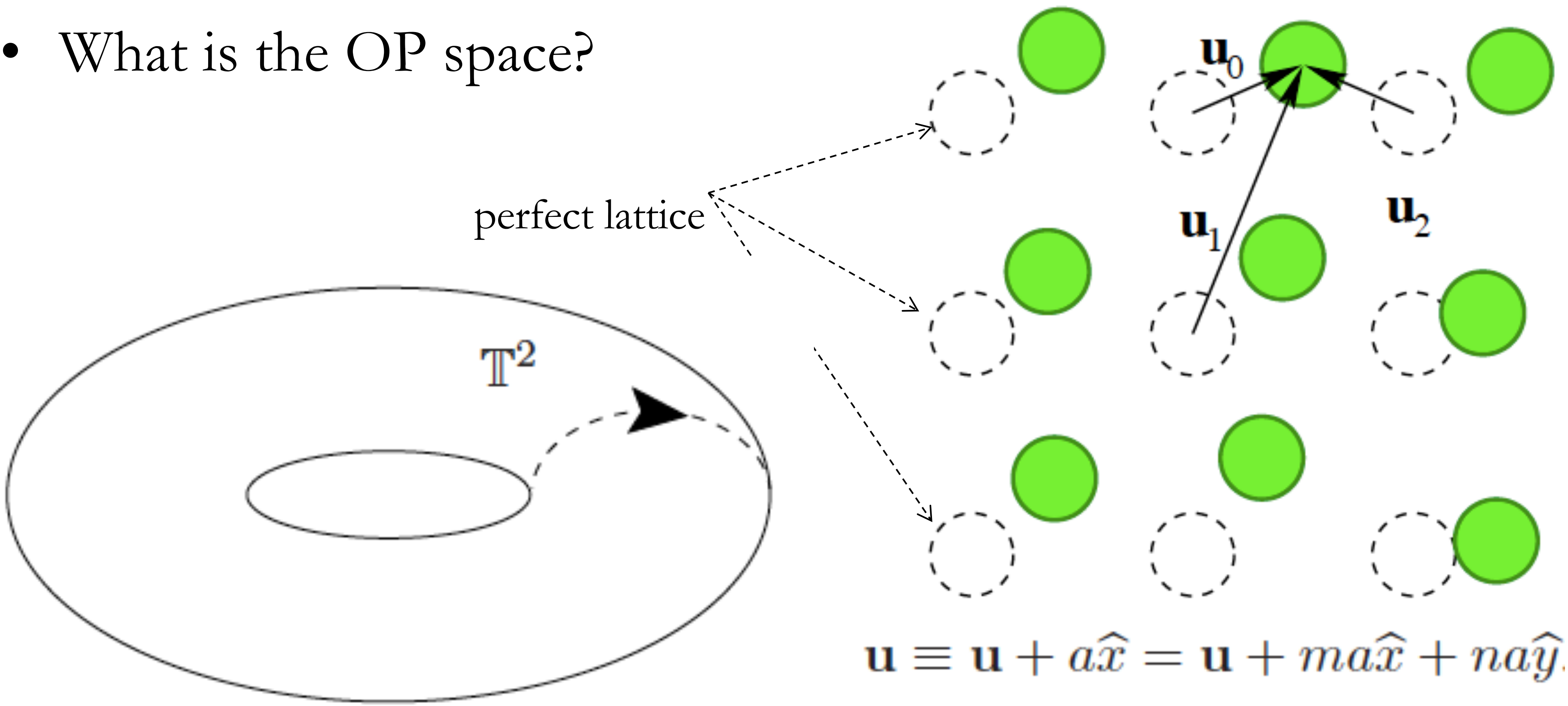
The $\mathbf{S}^2$ sphere is twice too large, because each realization of the nematic phase is represented by two opposite points; the sphere with pairs of antipodal points identified is noted $\mathbf{S}^2/\mathbf{Z}^2$

Half-sphere and opposite points identified (also topology of a projective plane RP^2):



Crystals with translational order

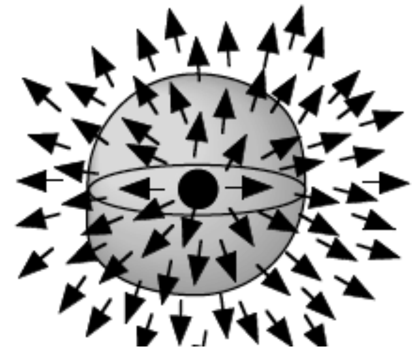
- A crystal – OP is a displacement U
- What is the OP space?



- OP at a point is that translation which aligns a perfect square grid to the deformed grid at that point
- OP space is a torus- square with periodic boundary conditions

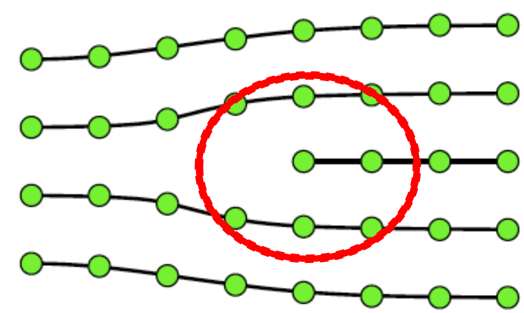
Singular Defects: classification based on order discontinuity & topology

- Point defects

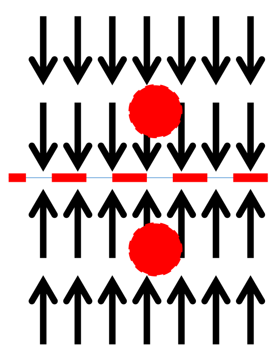


surround by S^2

- Line Defects (disclinations, dislocations), e.g the dislocation perpendicular to screen



- Wall defects;



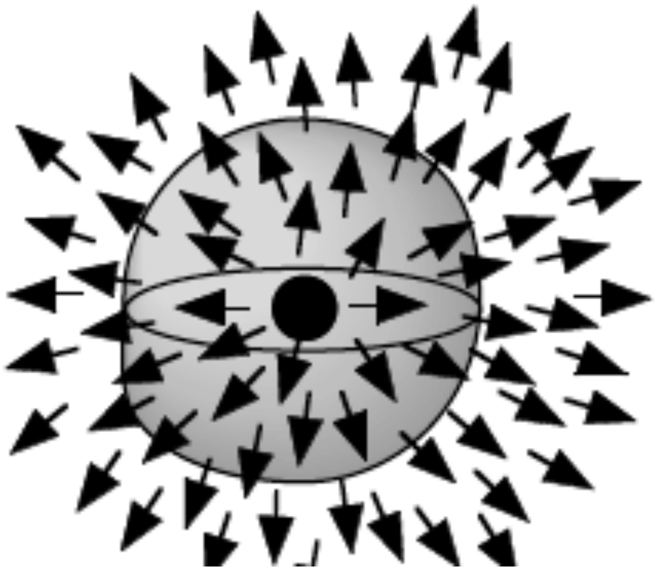
surround by S^0

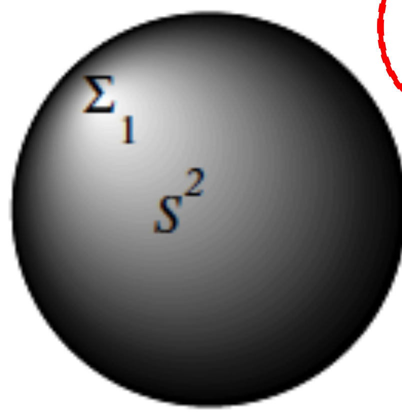
surround by S^1

- Order not defined on a point, along a line, or a wall

What happens with the OP around the defect?

Homotopy theory: analyze defects based on maps





$\Pi_2(\mathbb{S}^2) = \mathbb{Z}$

defect Surrounded by S^2 – 2nd homotopy group

- Example – a point defect in a ferromagnet
- map from S^2 surrounding it to the S^2 OP space
- Labeled $\Pi_2(S^2)=Z$ or $\pi_2(S^2)=Z$
- Meaning – can cover OP sphere integer number of times (Z=1 in this case, but can be other integers)

Sphere-sphere maps are well understood

	π_1	π_2	π_3	π_4	π_5
S^0	0	0	0	0	0
S^1	Z	0	0	0	0
S^2	0	Z	Z	Z_2	Z_2
S^3	0	0	Z	Z_2	Z_2
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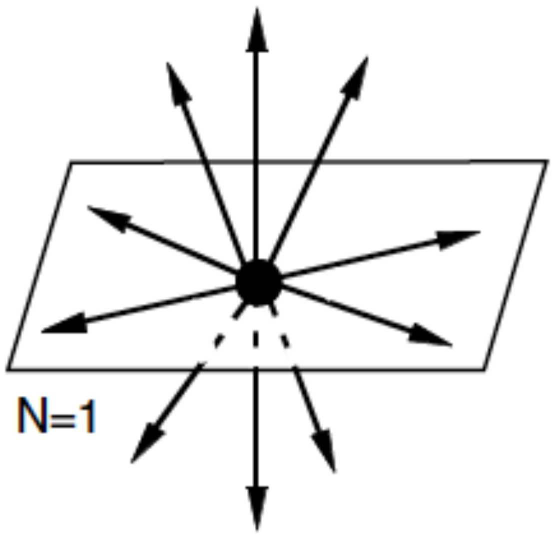
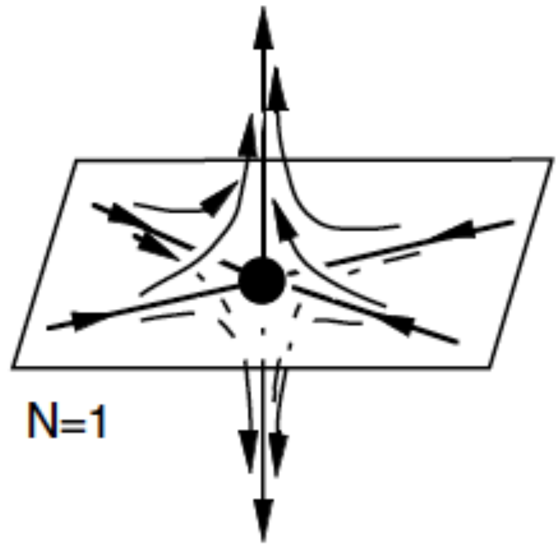
S^5	0	0	0	0	Z

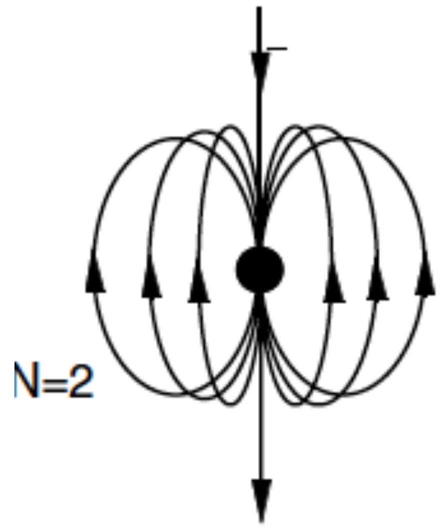
two maps connected by continuous path are said to be homotopic

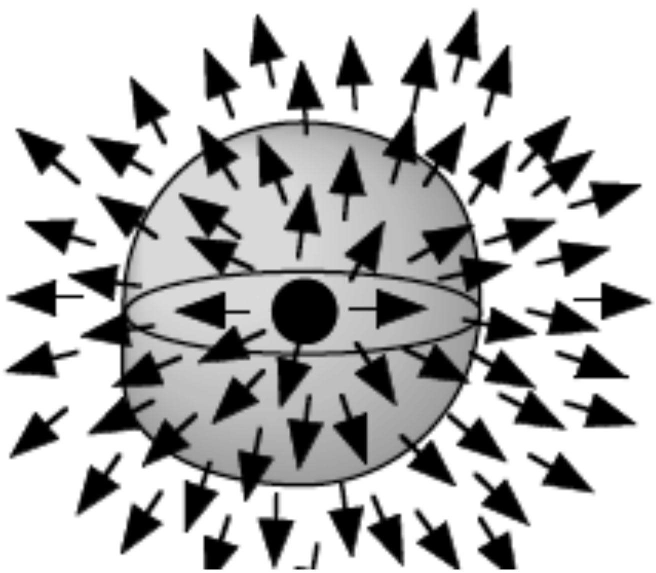
- Spheres as OP Spaces and defect-surrounding surfaces
- i-th homotopy group $\pi_i(S^n)$ – ways the i-dimensional sphere S^i can be mapped into n-dimensional sphere S^n

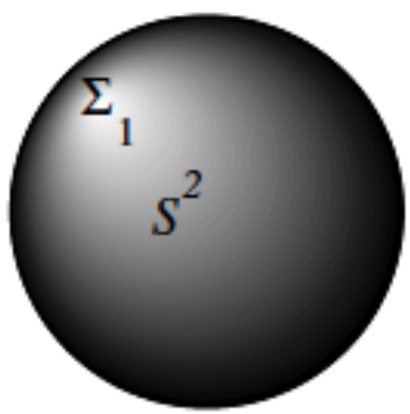
Point defects in a 3D vector field







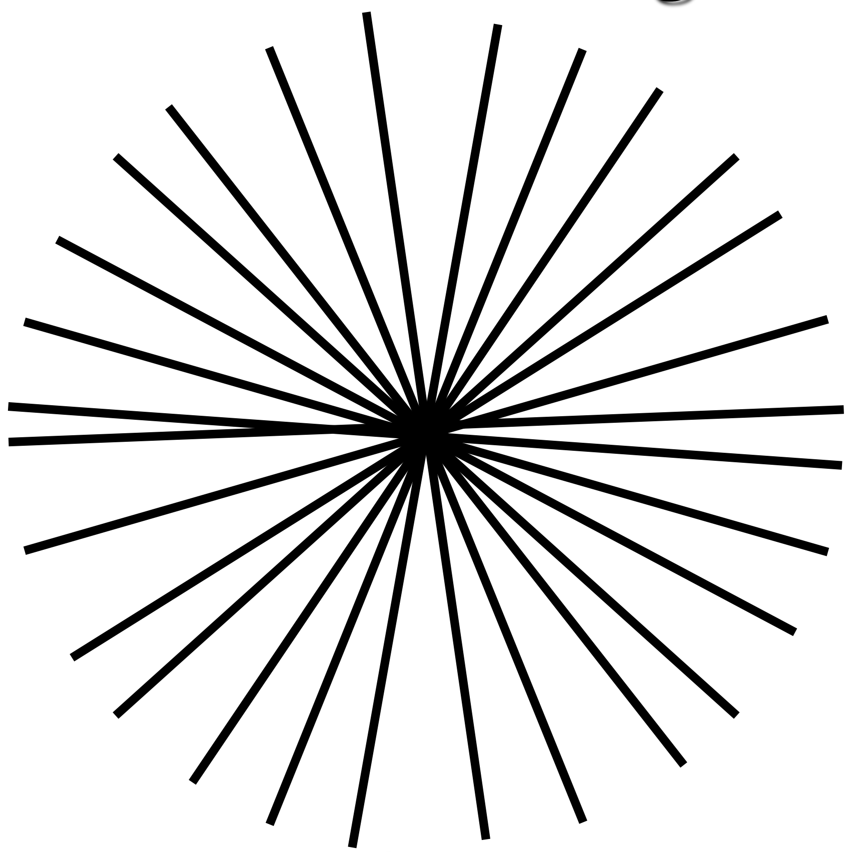




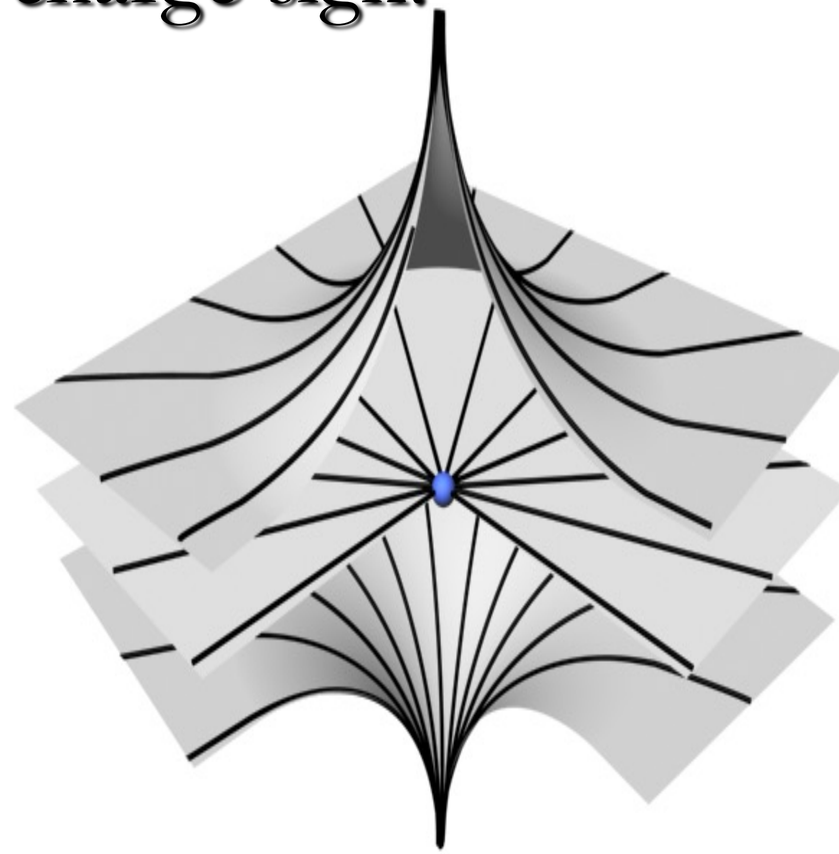
How many times they cover the S^2 order parameter space?

Point Defects

- Nonpolar director field;
- Conventional assignment of charge sign:



$$\mathbf{n} = (x, y, z)/\sqrt{x^2 + y^2 + z^2}$$



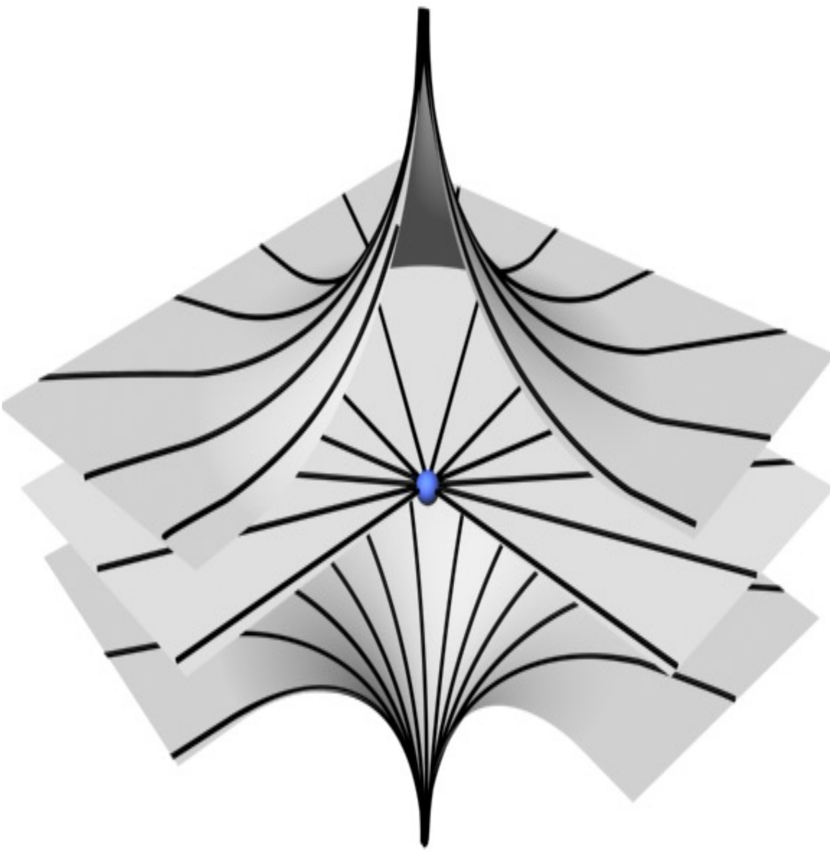
$$\mathbf{n} = (-x, -y, z)/\sqrt{x^2 + y^2 + z^2}$$

- Hedgehog
- Hyperbolic Hedgehog

- How do we find topological charge of a point defect?

Point Defects

- How do we find topological charge of a point defect?



Charge – number of times the director around the defect covers the OPS

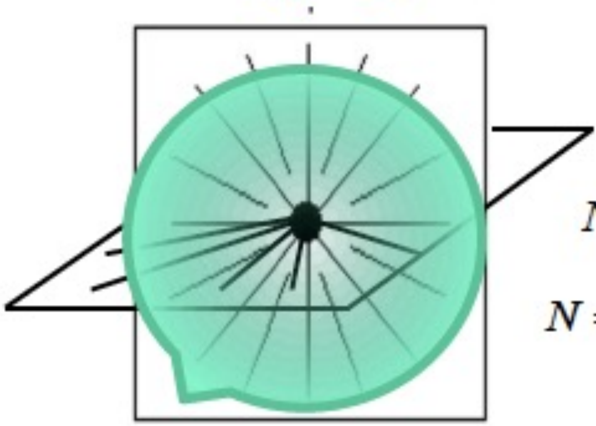
- Hedgehog

Point Defects

Hedgehogs (point defects) in uniaxial N

$$\pi_2\left(S^2/Z_2\right) = N = 0, \pm 1, \pm 2, \ldots$$

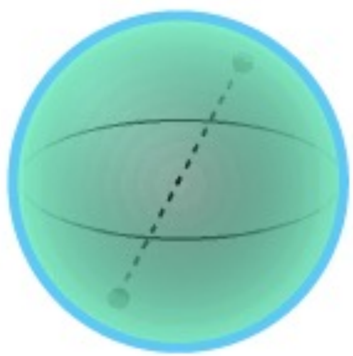
Radial hedgehog

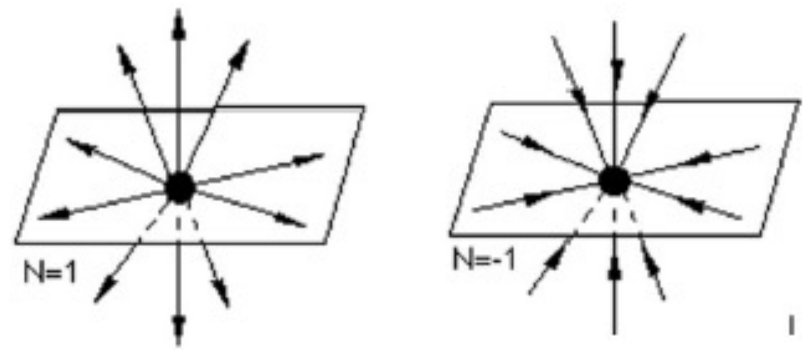


$N = 1?$

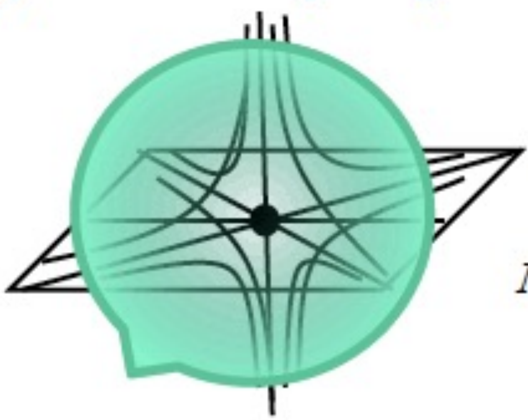
$N = -1?$

S^2/Z_2



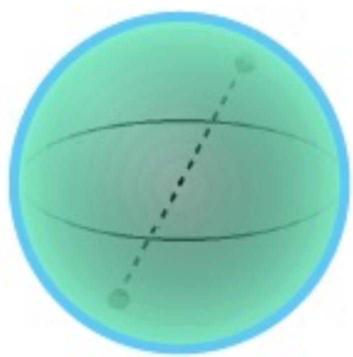


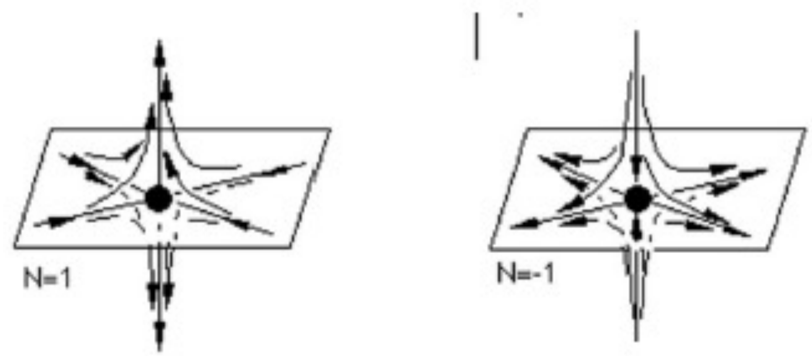
Hyperbolic hedgehog



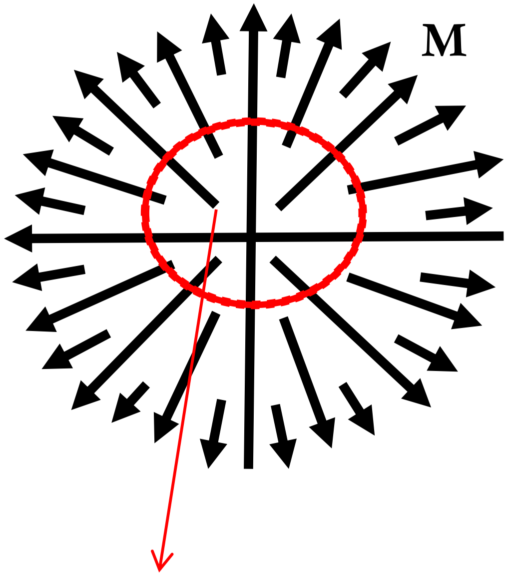
$N = 1?$

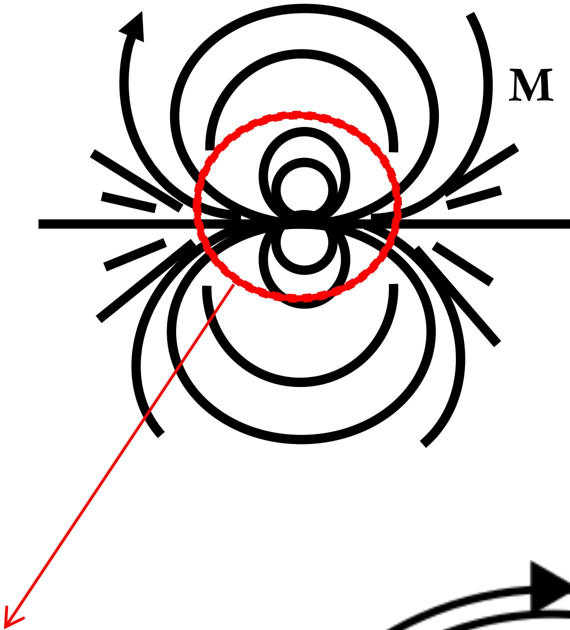
$N = -1?$



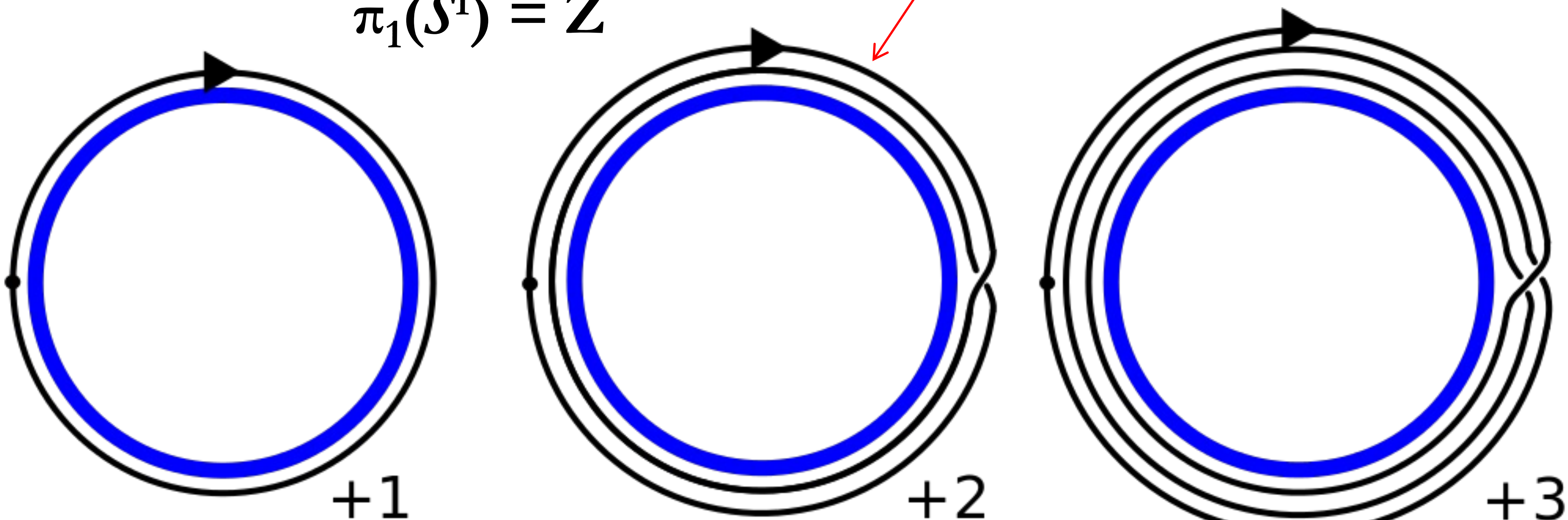


Defects in 2D ferromagnet: $\pi_1(S^1)=Z$





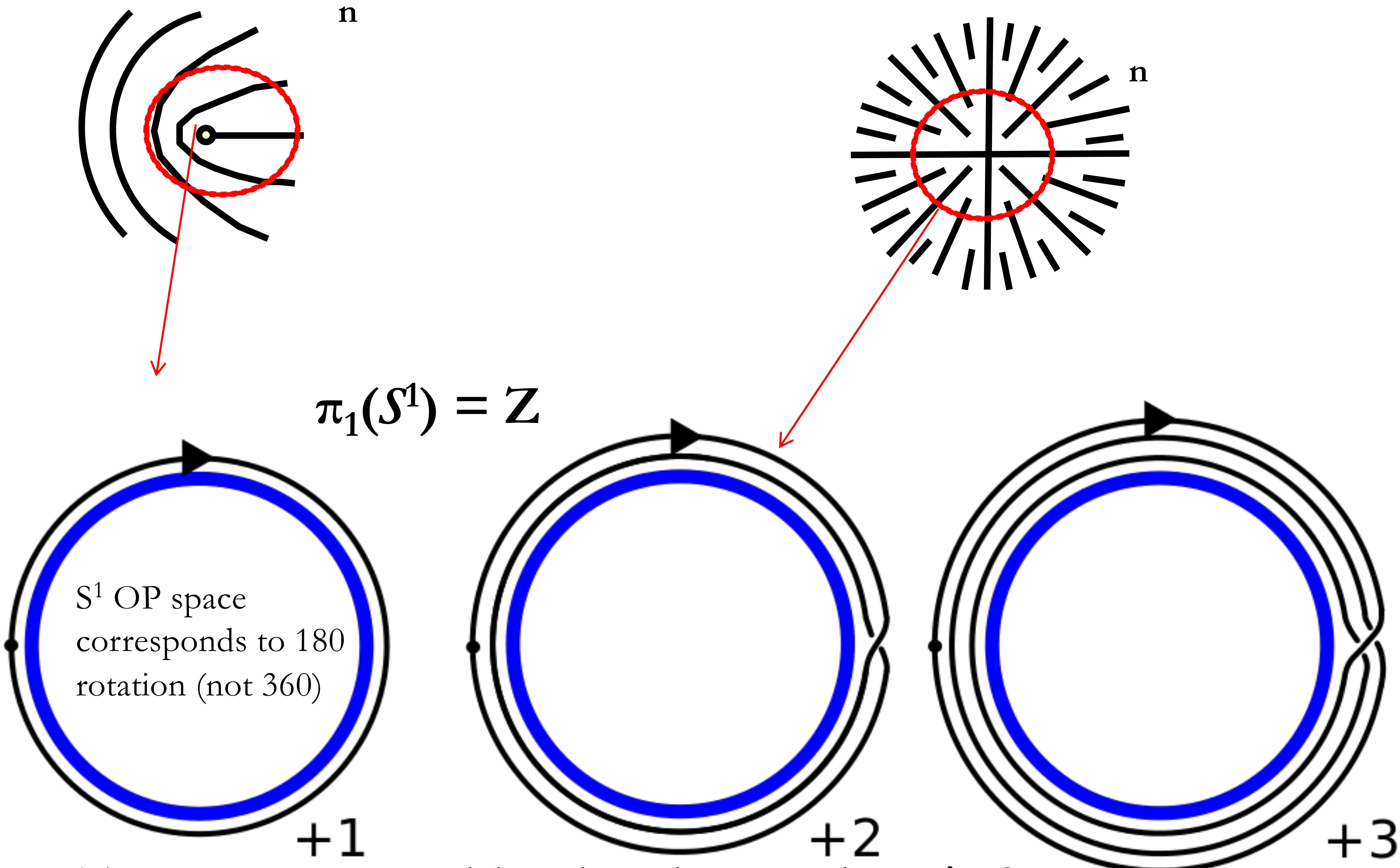
$\pi_1(S^1) = Z$



like wrapping a rubber band around one's finger

How about the 2D nematic? What is OP and what defects allowed

Defects in 2D nematic: $\pi_1(S^1)=Z$



like wrapping a rubber band around one's finger

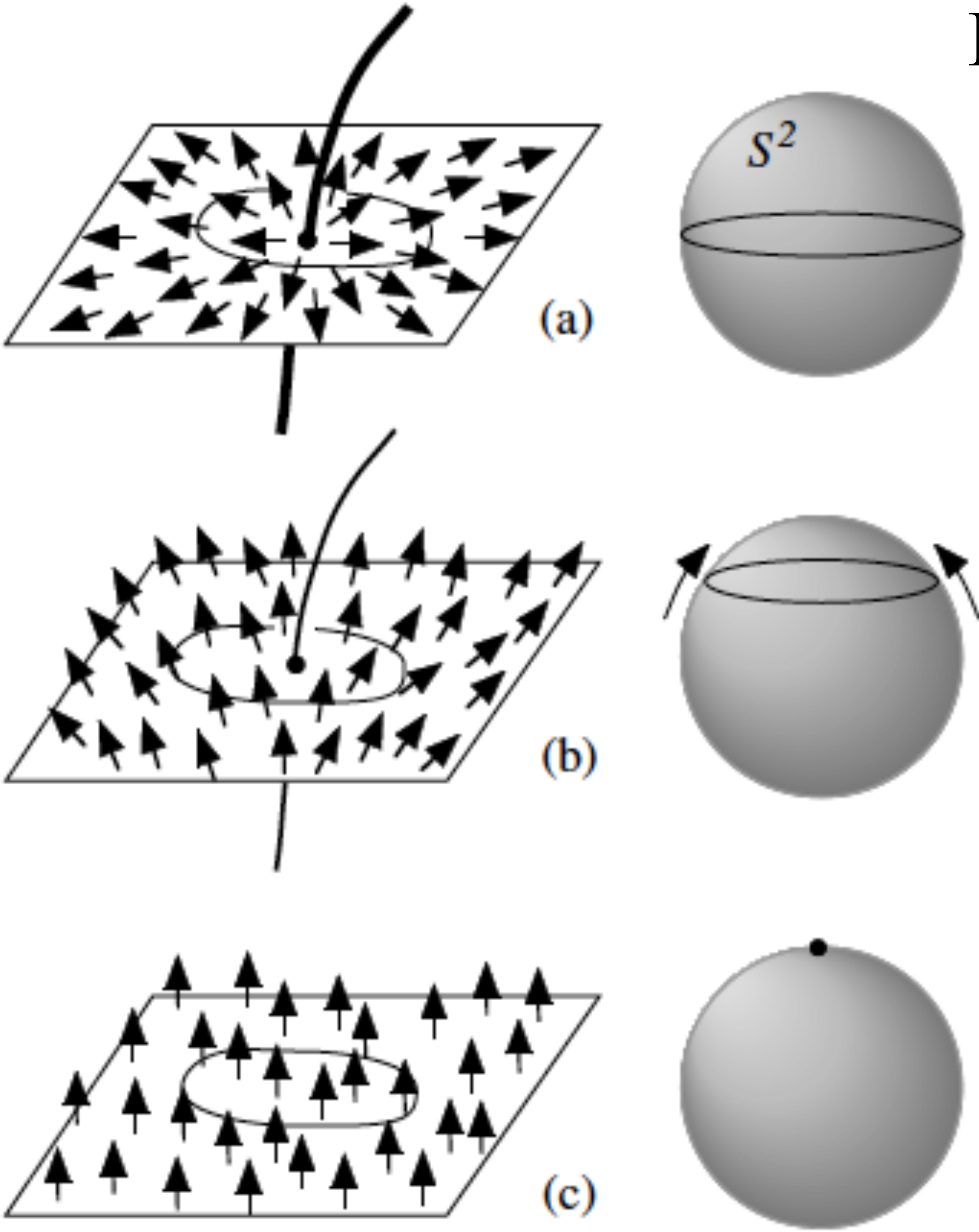
Same homotopy group but subtle details are different!

No line defects in 3D ferromagnets, $\pi_1(S^2) = 0$

What happens in a real space as we shrink the loop?

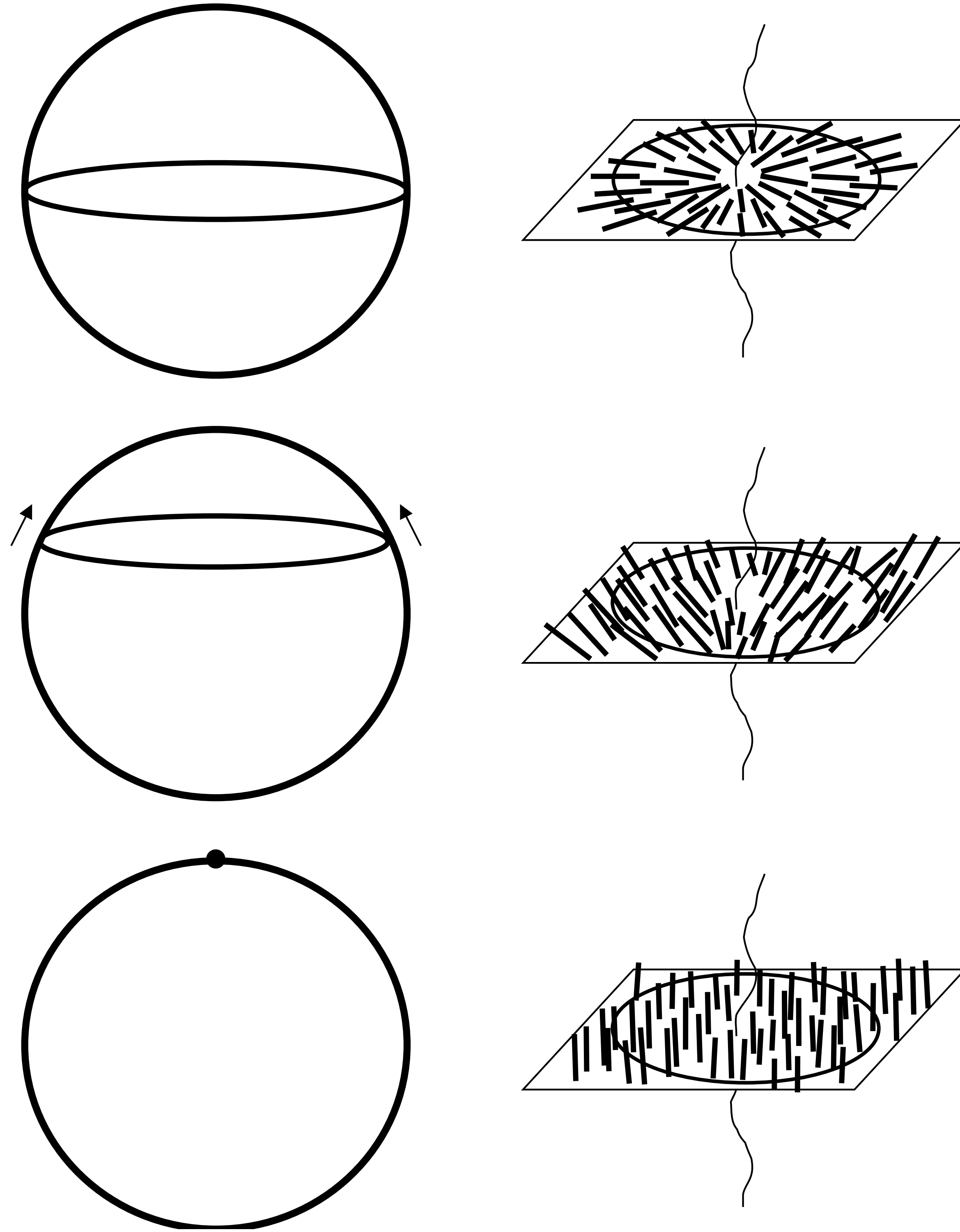
- Any continuous mapping from a circle to an ordinary sphere can be continuously deformed to a one-point mapping, and so its homotopy class is trivial
- All mappings from a lower-dimensional sphere into a sphere of higher dimension are similarly trivial

Escape in a 3D ferromagnet



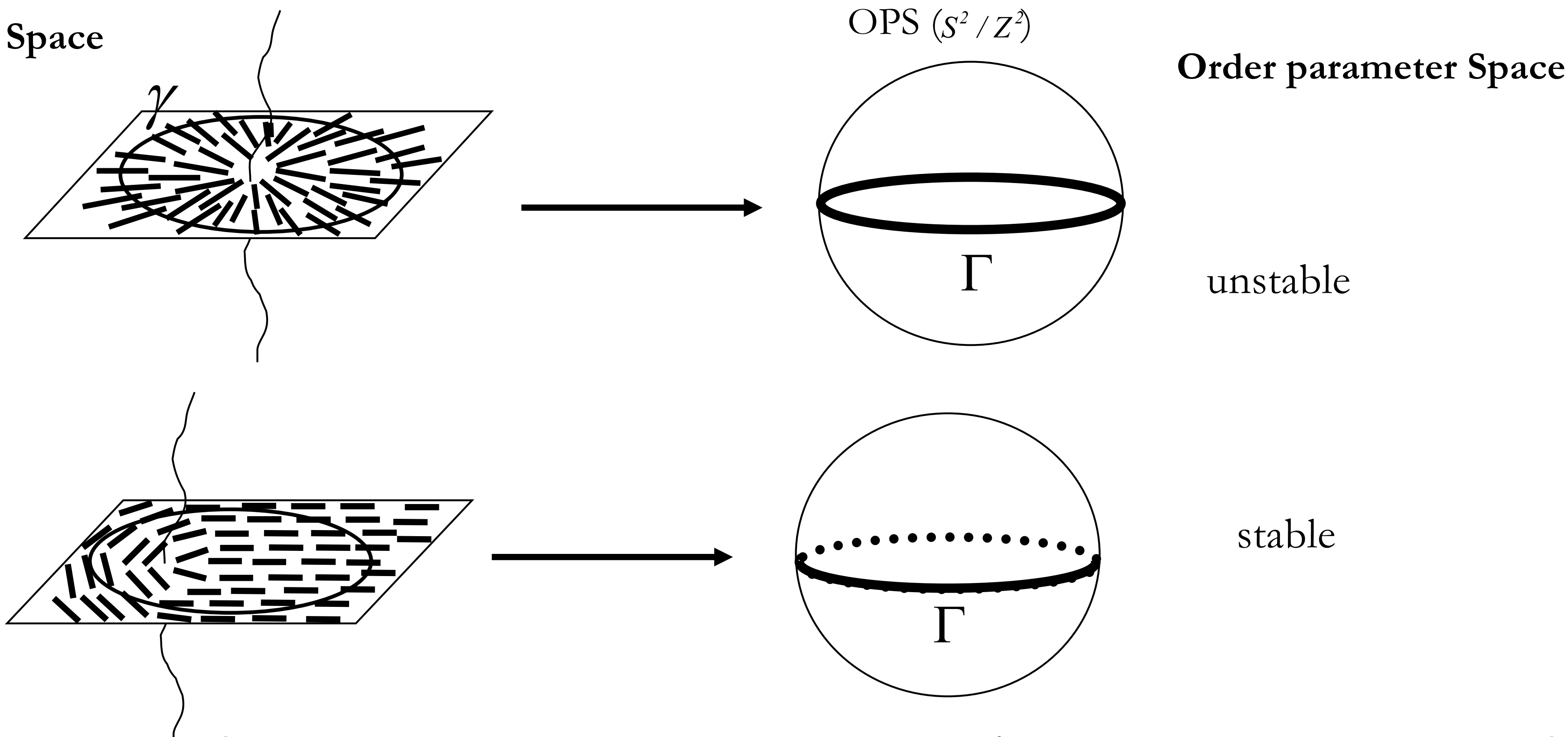
Continuous transformation of a disclination s = 1 (a) into a uniform state s = 0 (c) in a 3D ferromagnetic phase (left); corresponding contraction of a loop in the order parameter space (right).

Escape in a nematic LC



also
unstable

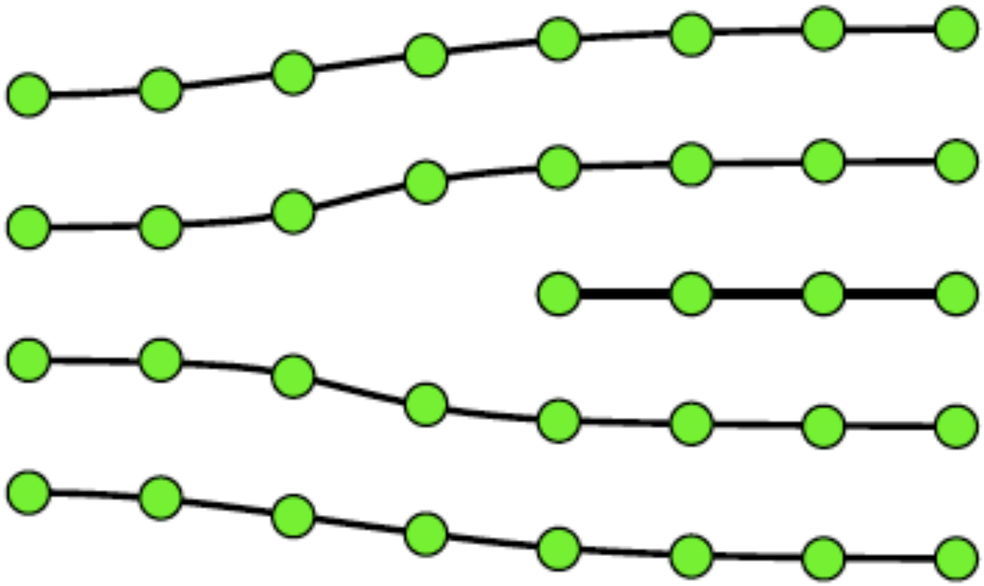
Mappings from the real space to the order parameter space



Mappings from the real space to the order parameter space for two different director fields:

1. The contour completes the great circle on S^2/Z^2
2. The contour connects the diametrically opposite points.

Dislocations in a solid crystal

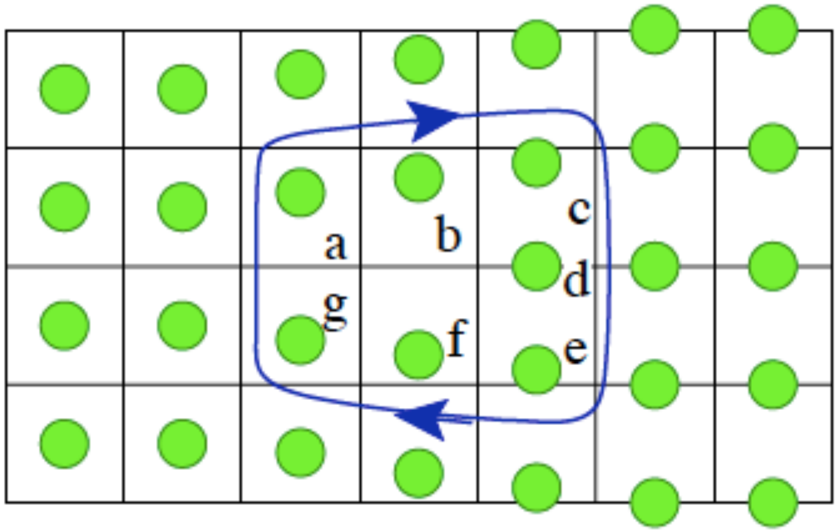


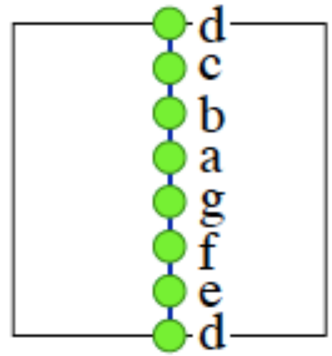
Recall characterization based on the Burgers vector

Singularity in the order parameter – how to understand based on the topology of the order parameter space?

Homotopy theory analysis?

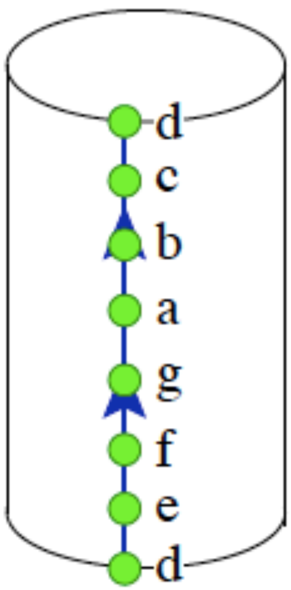
Dislocations in a solid crystal

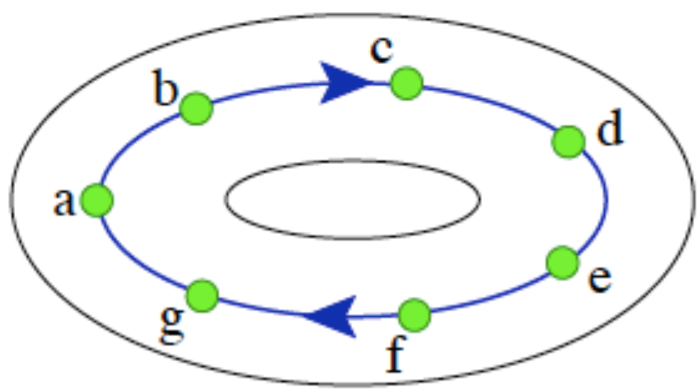




$$\Pi_1(\mathbb{T}^2) = \mathbb{Z} \times \mathbb{Z},$$

defect surrounded by S^1 – first homotopy group

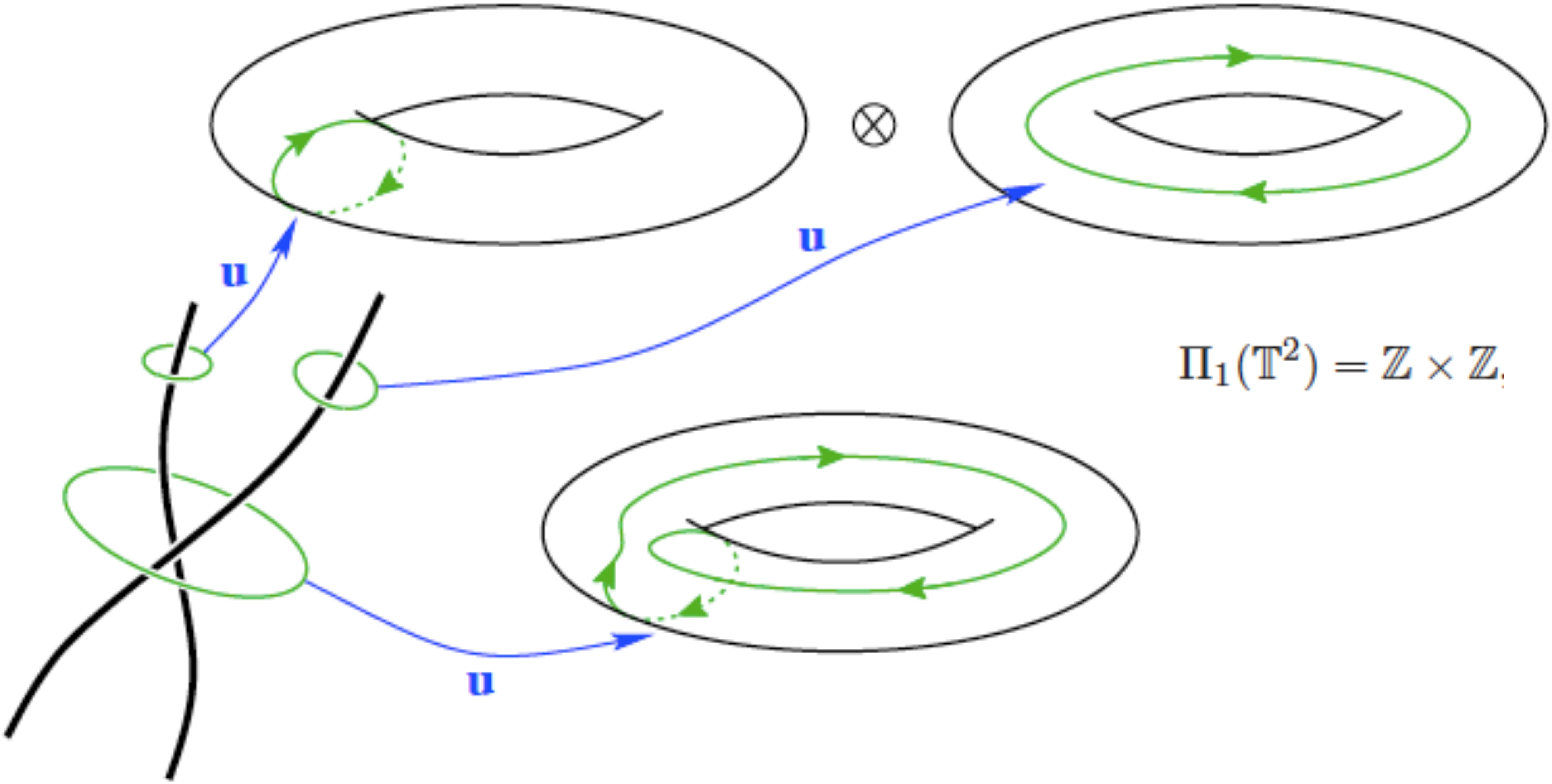




Mapping from the Burgers circuit onto the OP space – T^2

Two integers – characterize the pathway on the torus

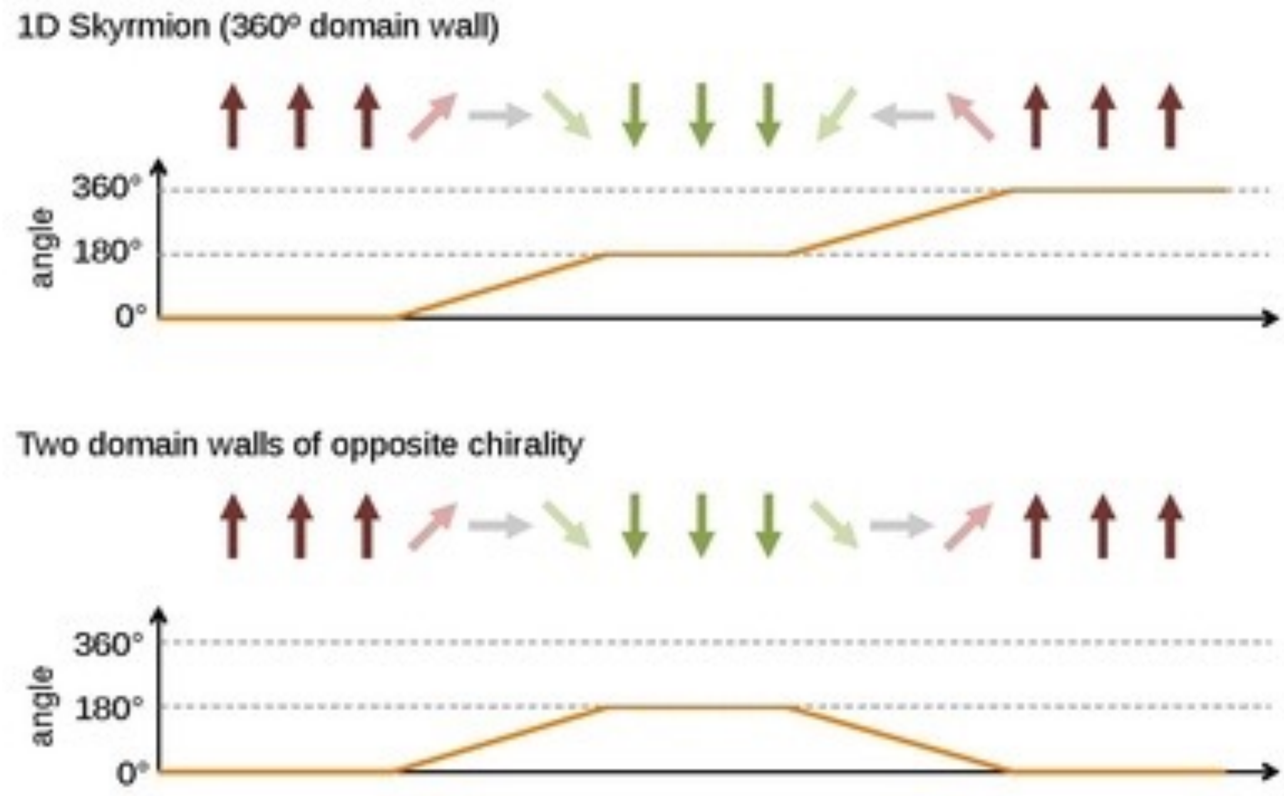
Dislocations in a solid crystal with defects in rows & columns



(m, n) represent the number of extra rows & extra columns of atoms

Topological solitons – continuous but topologically nontrivial field configurations

Example – 1D soliton in a ferromagnet

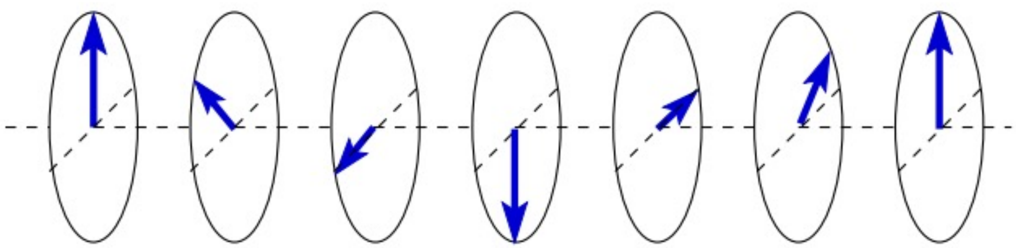


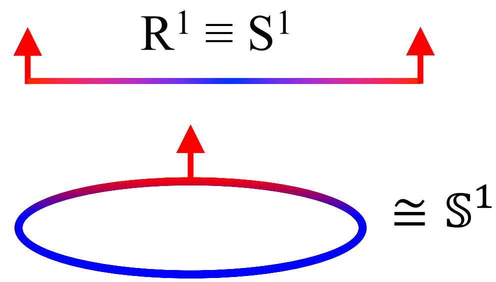
Homotopy maps
$\pi_1(S^1) = Z$

- **Mapping the field along x into S^1 fully covers it!**
- **equivalent to the S^1 surrounding space when the far-field is uniform!**

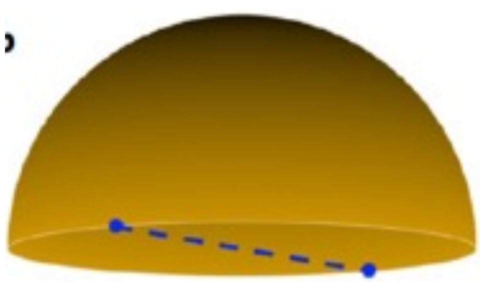
Directors versus vectors & twist walls as topological 1D solitons

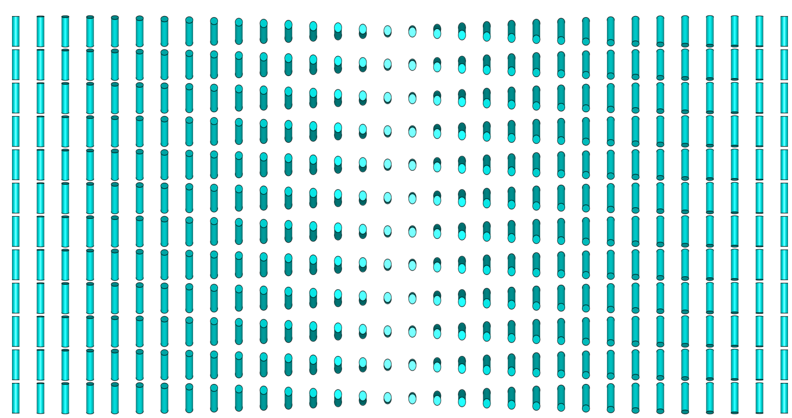
Vector field

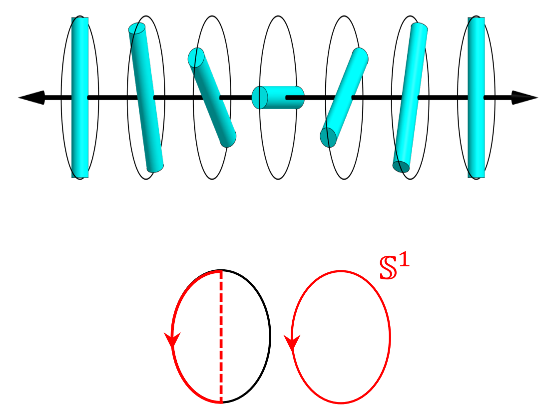




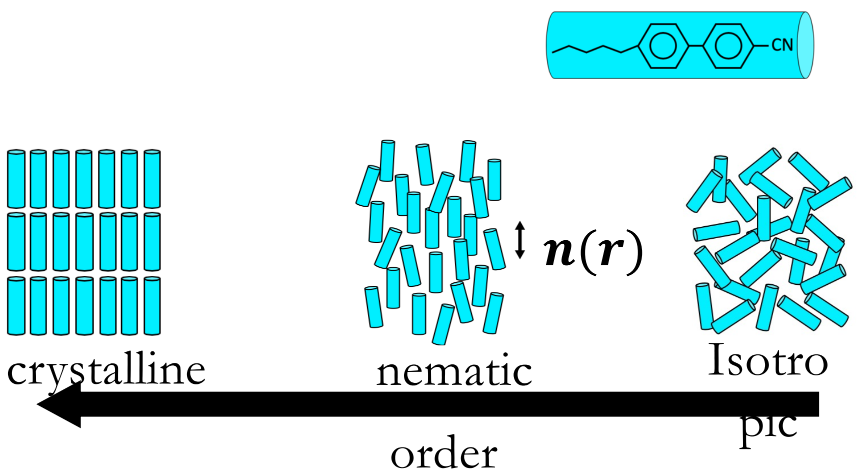
Director field (nonpolar)





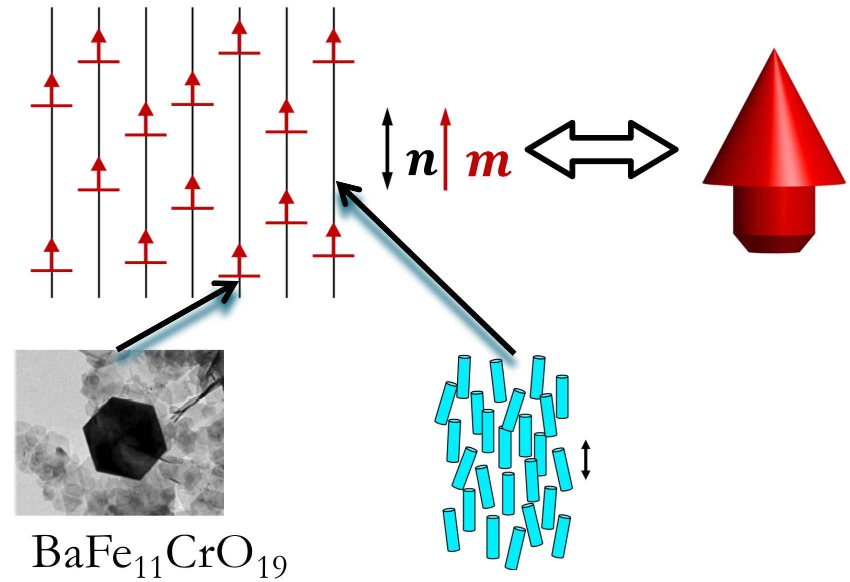


Magnetic Colloidal Liquid crystals



- Ordered fluid with long-range orientational order
- Director $\boldsymbol{n}(\boldsymbol{r})$

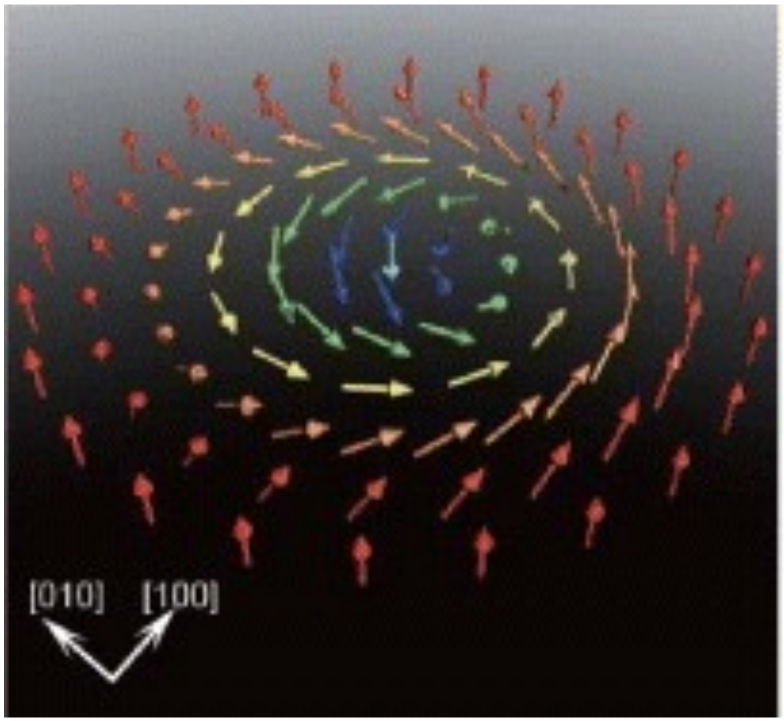
- LC ferromagnets

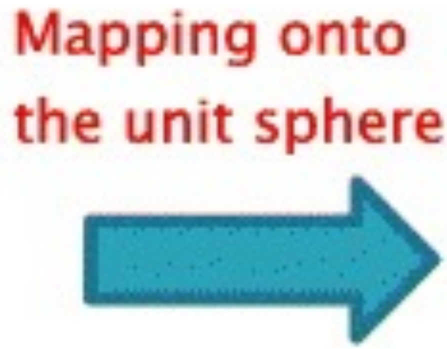


- Vector $\boldsymbol{m}(\boldsymbol{r})$
- Polar switching by weak fields

2D soliton example – "Baby Skyrmion"

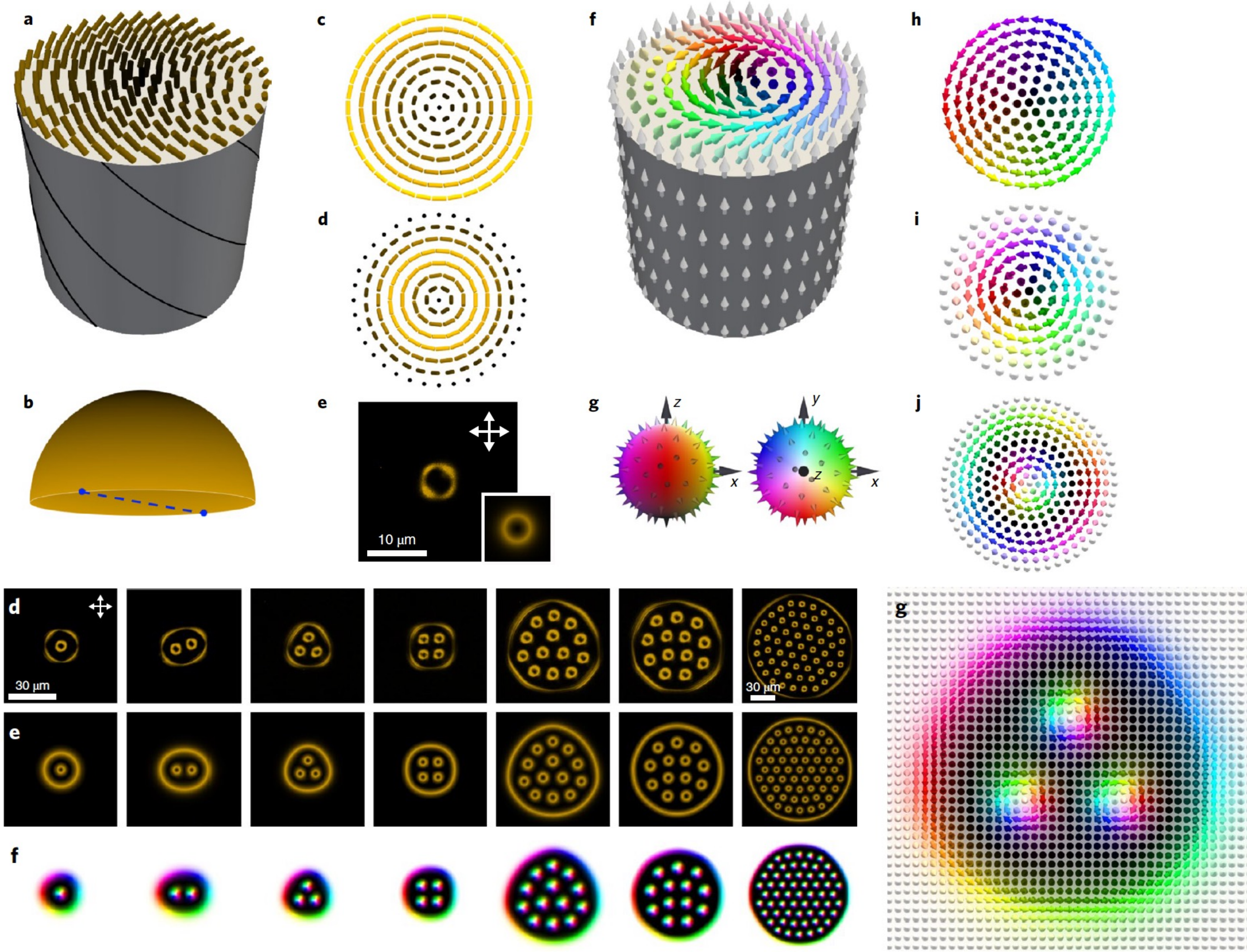
2D soliton in a 3D ferromagnet, $\pi_2(S^2) = Z$





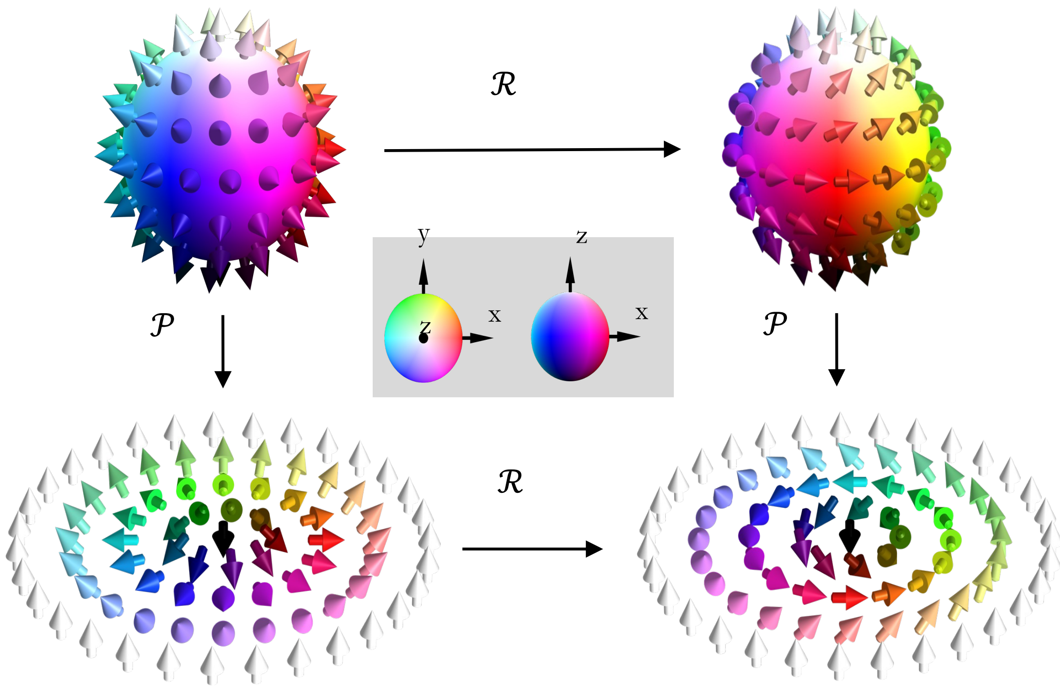
- **Mapping of the field from a 2D plane into a unit sphere fully covers it!**
- **2D plane & sphere are equivalent when the far-field is uniform!**

High-degree 2D Skyrmions

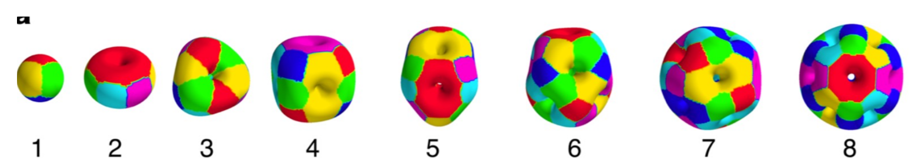


2D solitons, stereographic projection

S^2 in 2 and 3 Dimensions



	π_1	π_2	π_3	π_4	π_5
$\mathbb{S}^0$	0	0	0	0	0
$\mathbb{S}^1$	$\mathbb{Z}$	0	0	0	0
$\mathbb{S}^2$	0	$\mathbb{Z}$	$\mathbb{Z}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$
$\mathbb{S}^3$	0	0	$\mathbb{Z}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$
$\mathbb{S}^4$	0	0	0	$\mathbb{Z}$	$\mathbb{Z}_2$
$\mathbb{S}^5$	0	0	0	0	0



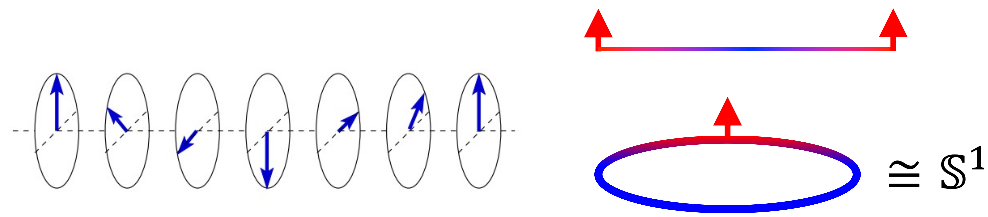
2D Soliton: baby Skyrmions

3D solitons?

Homotopy theory and topological solitons

$\boldsymbol{m}(\boldsymbol{r})$: $\boldsymbol{r} \in$ configuration space $\longrightarrow \boldsymbol{m} \in$ order-parameter space

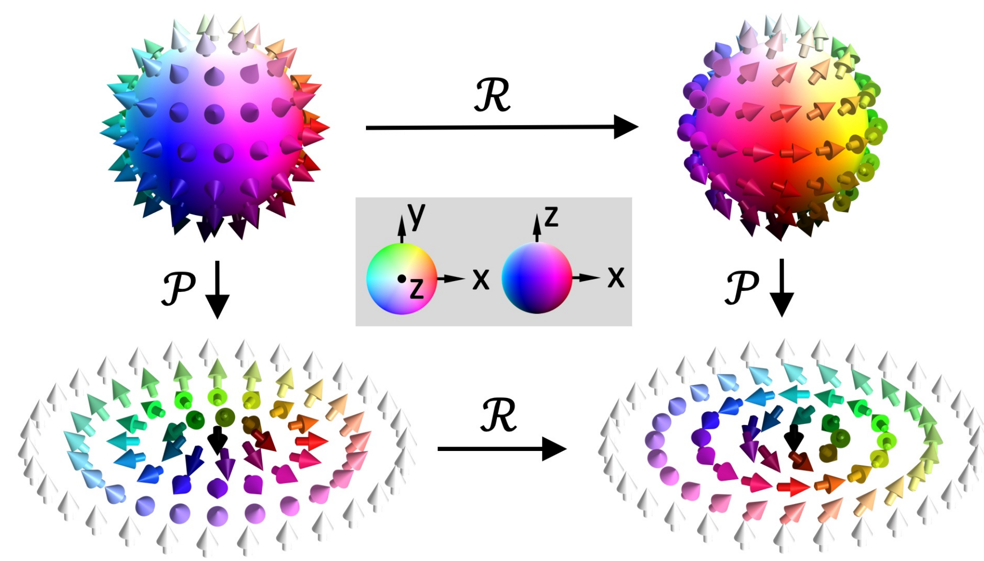
- 1D kink or wall ($\pi_1(\mathbb{S}^1) = \mathbb{Z}$)
  - Configuration space $\mathbb{R}^1$
  - $\mathbb{R}^1 \cong \mathbb{S}^1$ if far-field uniform
  - Examples: domain walls in ferromagnets with ***M*** constrained in a plane ($\mathbb{S}^1$)



http://iht.univ.kiev.ua/Kolezhuk

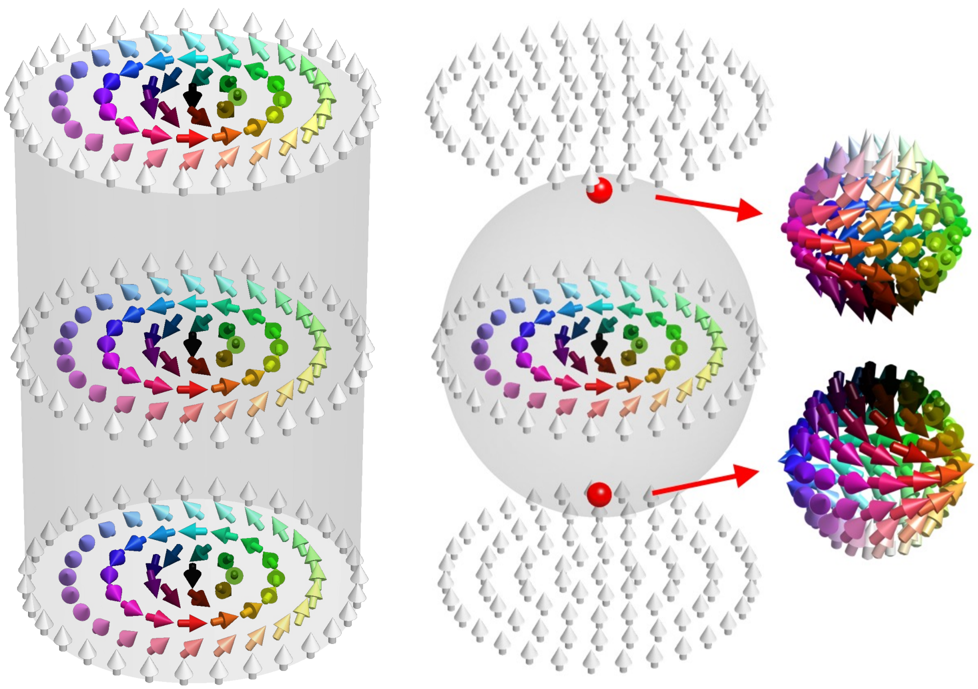
- 2D skyrmion ($\pi_2(\mathbb{S}^2) = \mathbb{Z}$)
  - $\mathbb{R}^2 \cong \mathbb{S}^2$ when the far-field is uniform
  - 2D soliton in a ferromagnet with ***M*** taking all possible orientations on $\mathbb{S}^2$

$$N_{\mathrm{sk}} = \frac{1}{4\pi}\int dxdy\boldsymbol{m}(\boldsymbol{r}) \cdot \left(\partial_x \boldsymbol{m}(\boldsymbol{r}) \times \partial_y \boldsymbol{m}(\boldsymbol{r})\right)$$

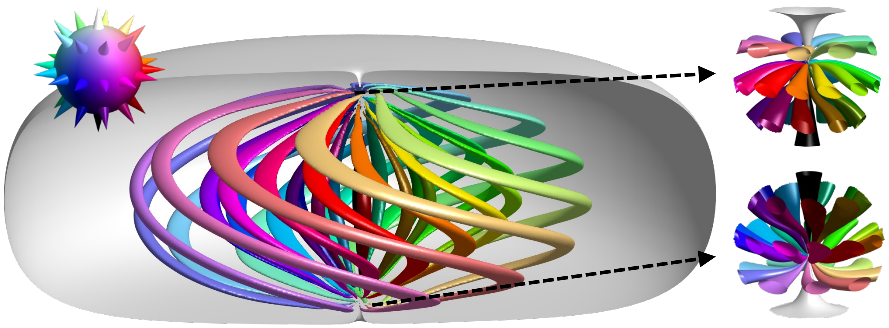


2D skyrmions ($\pi_2(\mathbb{S}^2) = \mathbb{Z}$) in LCs

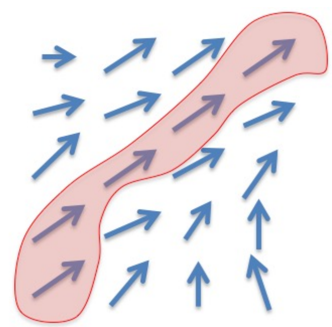
- 2D skyrmion & Toron

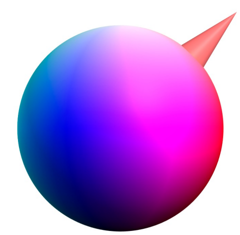


- Preimages



Preimage (inverse image) of $\boldsymbol{m}(\boldsymbol{r})$: $\boldsymbol{r} \longrightarrow \boldsymbol{m}$ map
Region of a constant $\boldsymbol{m}$

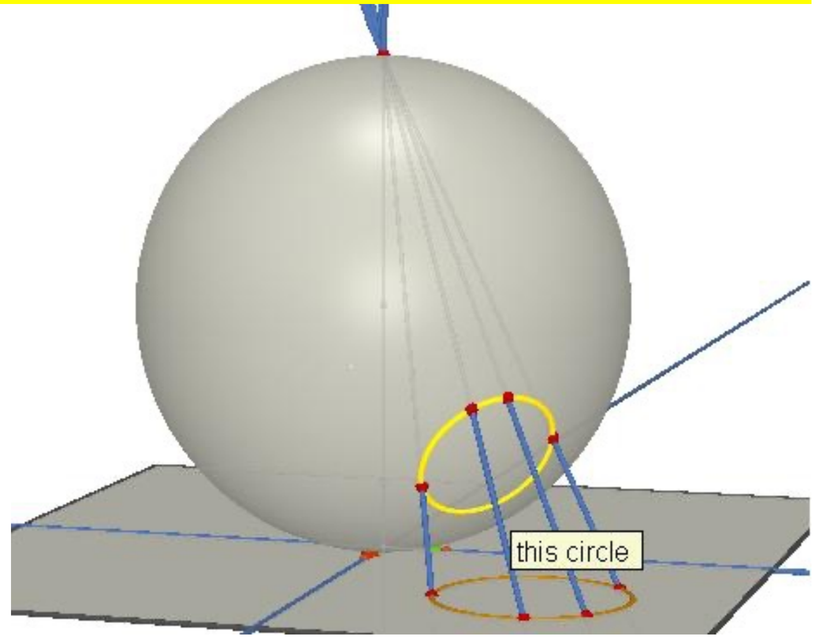


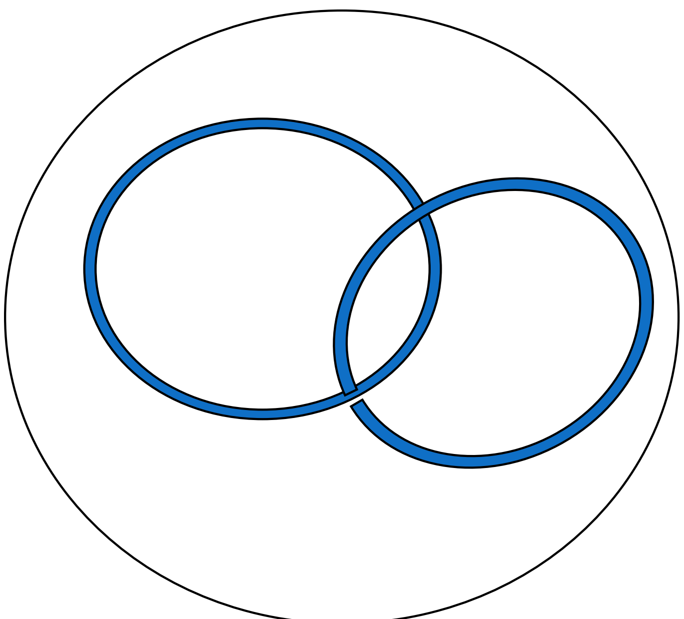


Stereographic projection

- Stereographic Projection of S^2 in 3D onto a 2D plane

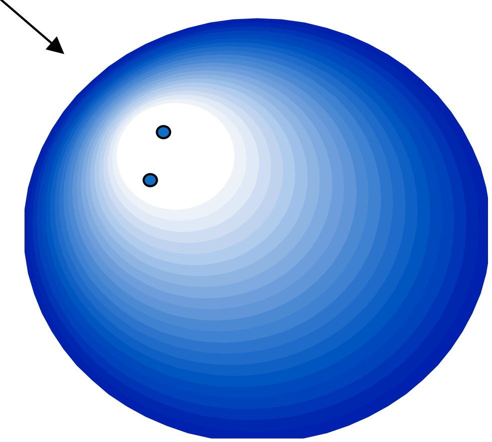
- Stereographic Projection of S^3 in 4D into the 3D space





S^3

each point of S^2 corresponds to a distinct circle of S^3 & its projection

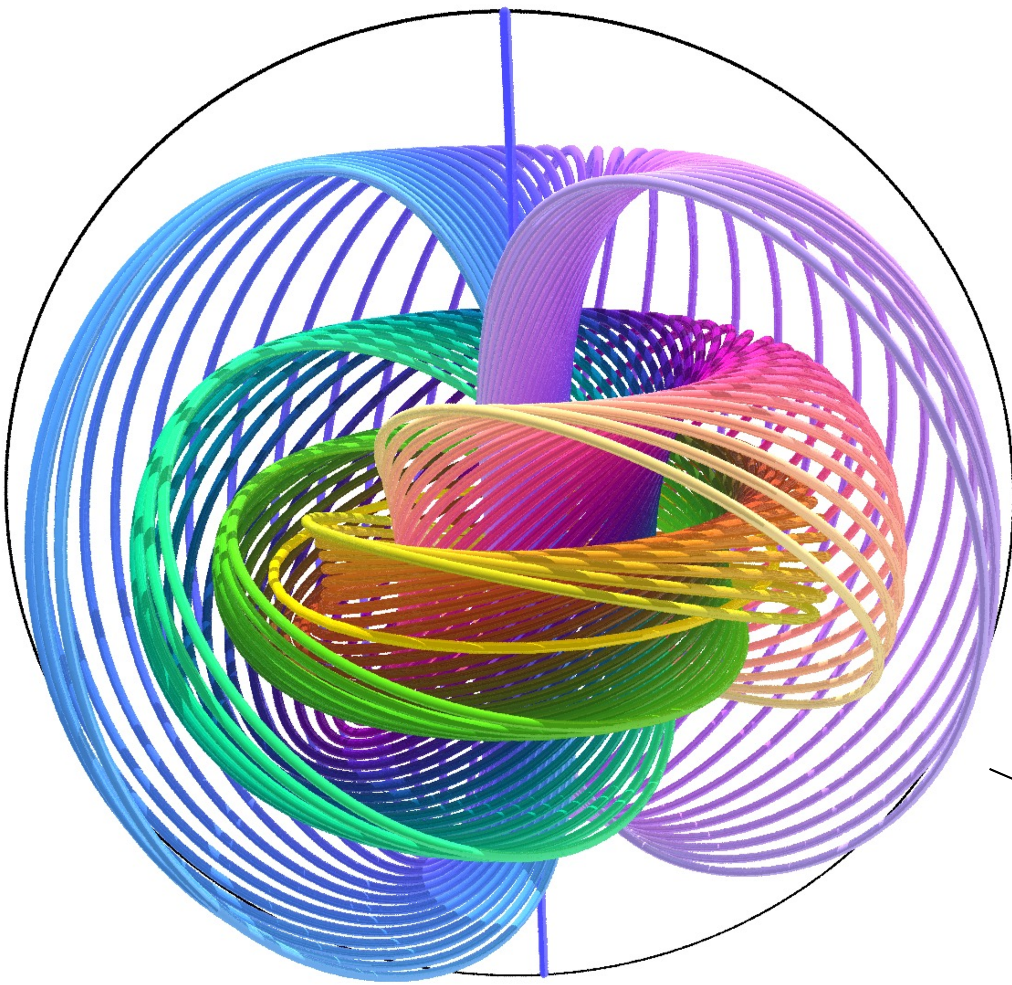


S^2

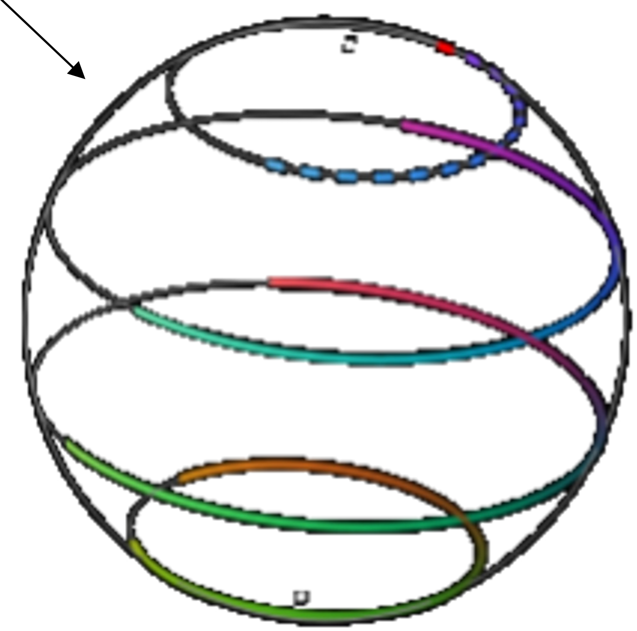
Circles are linked!

Hopf fibration

S^3 in terms of S^1 circles projected to 3D space & points on S^2



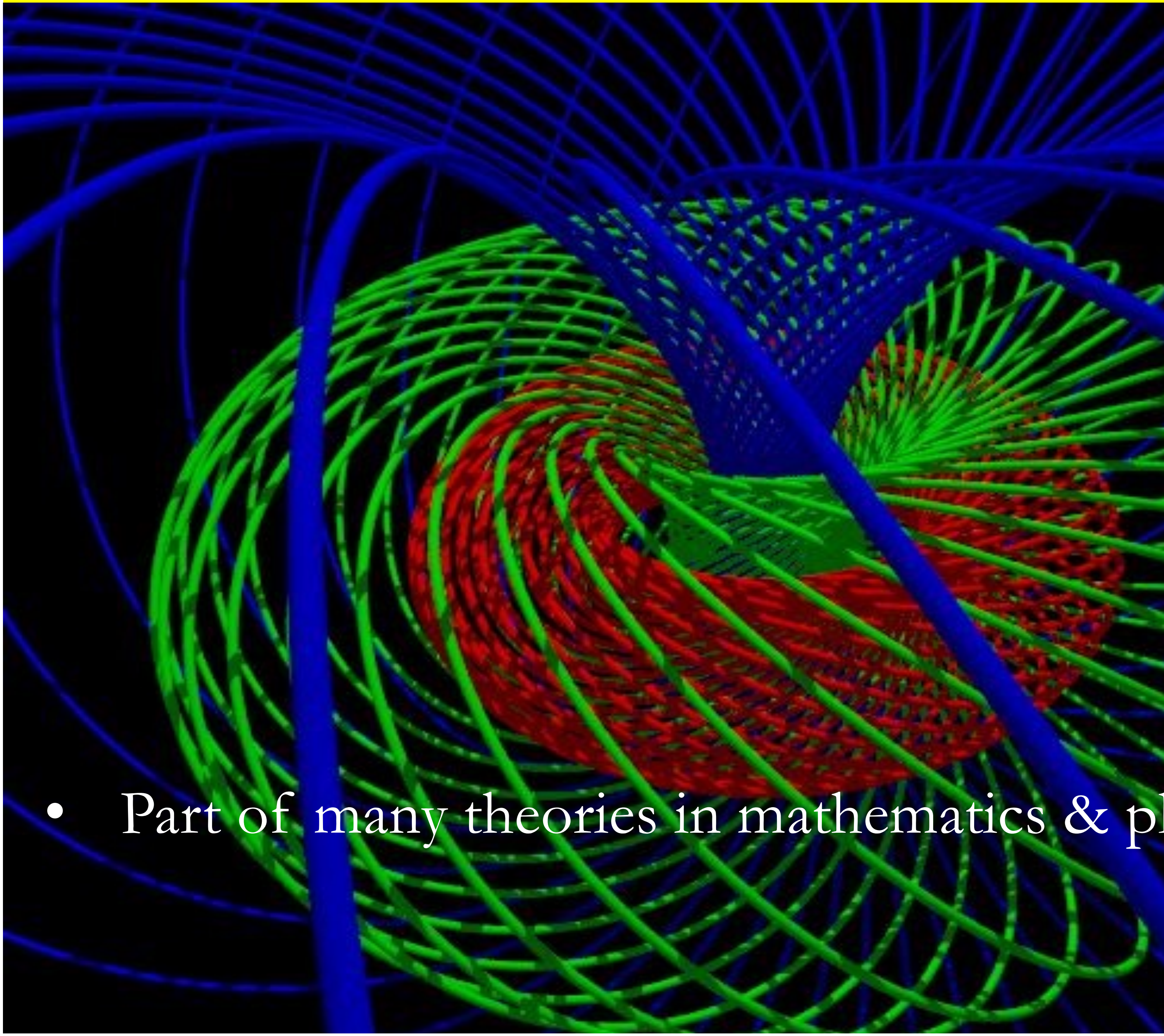
S^3



S^2

Topologically nontrivial!

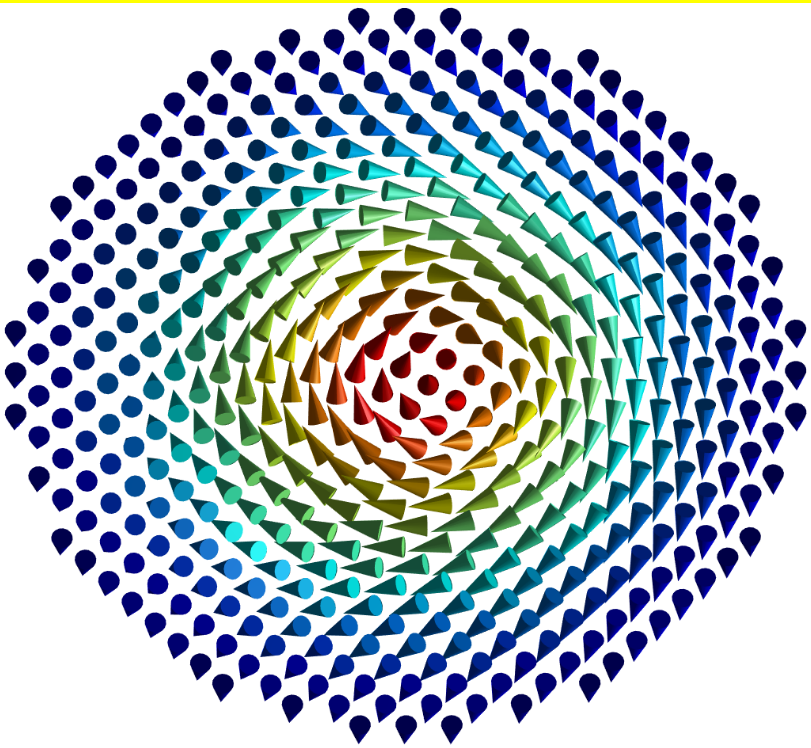
Hopf fibration

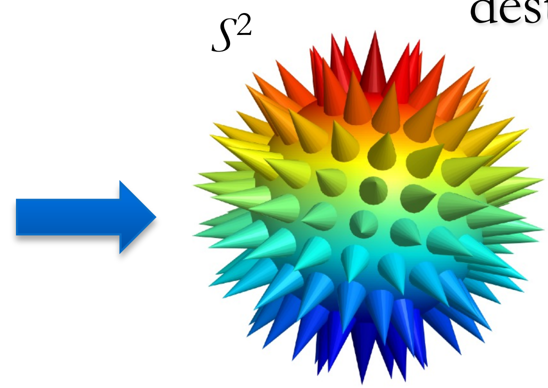


Heinz Hopf (1894-1971)

- Part of many theories in mathematics & physics

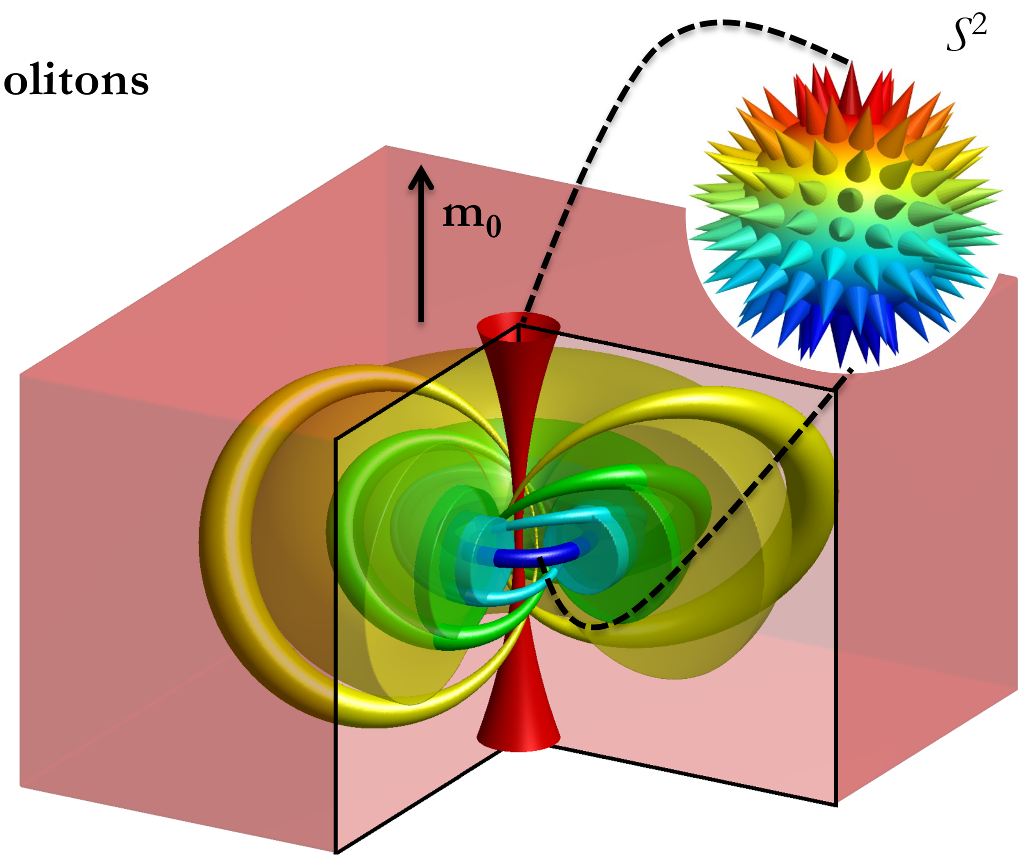
2D versus 3D topological solitons





- Cannot be eliminated without destroying the order

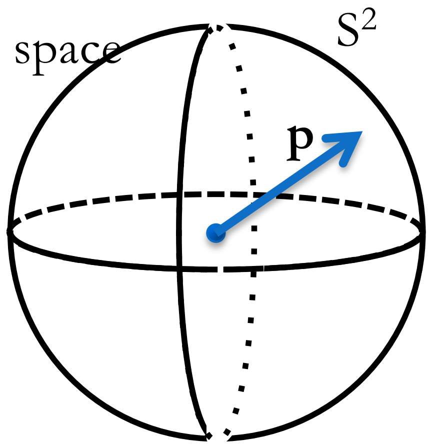
3D solitons

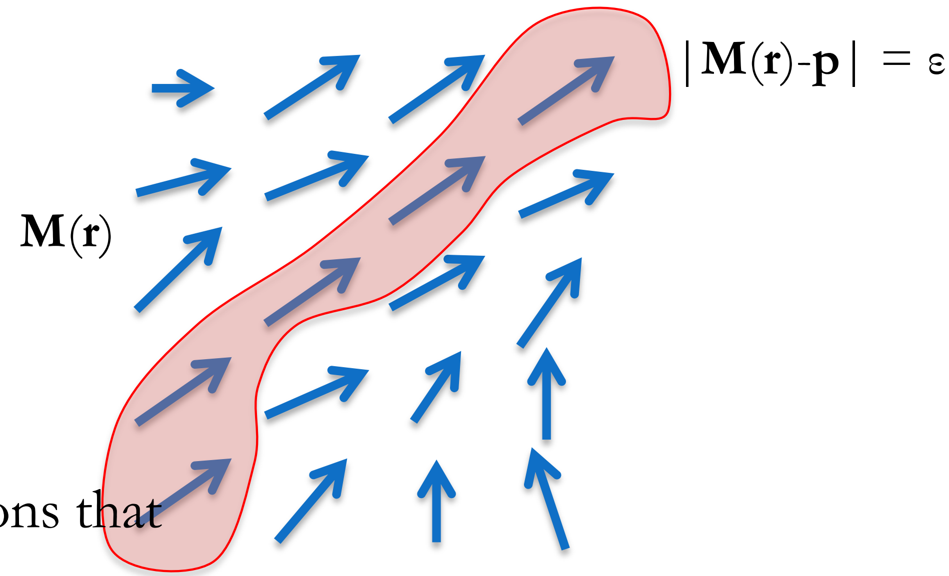


- Continuous, nonsingular, but topologically nontrivial
- Knots/links in continuous fields embedded in a uniform background

3D topological solitons & *preimages*

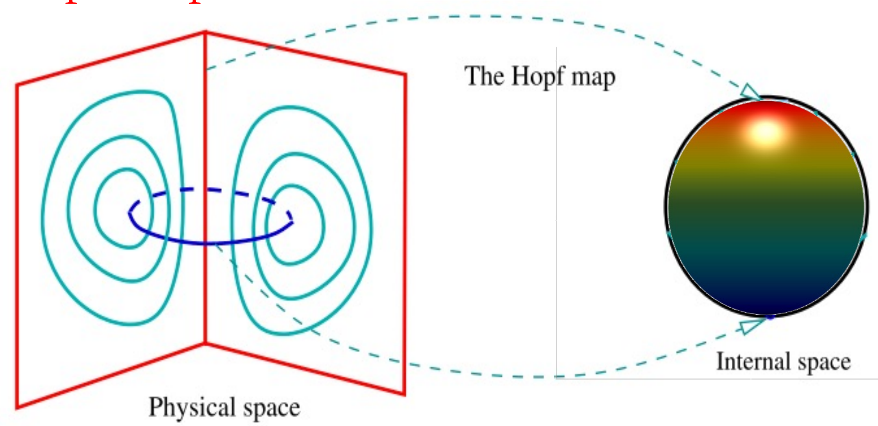
Order parameter space for $\mathbf{M}(\mathbf{r})$





Preimage of unit vector **p** on S^2 : sample regions that have the same $\mathbf{M}(\mathbf{r})$-orientation

Hopf map from 3D to S^2



→Choose **M**-orientation on S^2

→Find regions within the soliton with this $\mathbf{M}(\mathbf{r})$ orientation

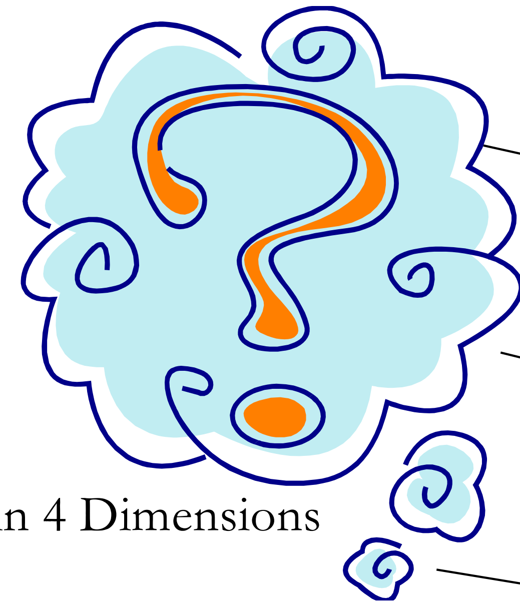
→Do this for all points on S^2

→**Look for preimages that are linked circles!!!**

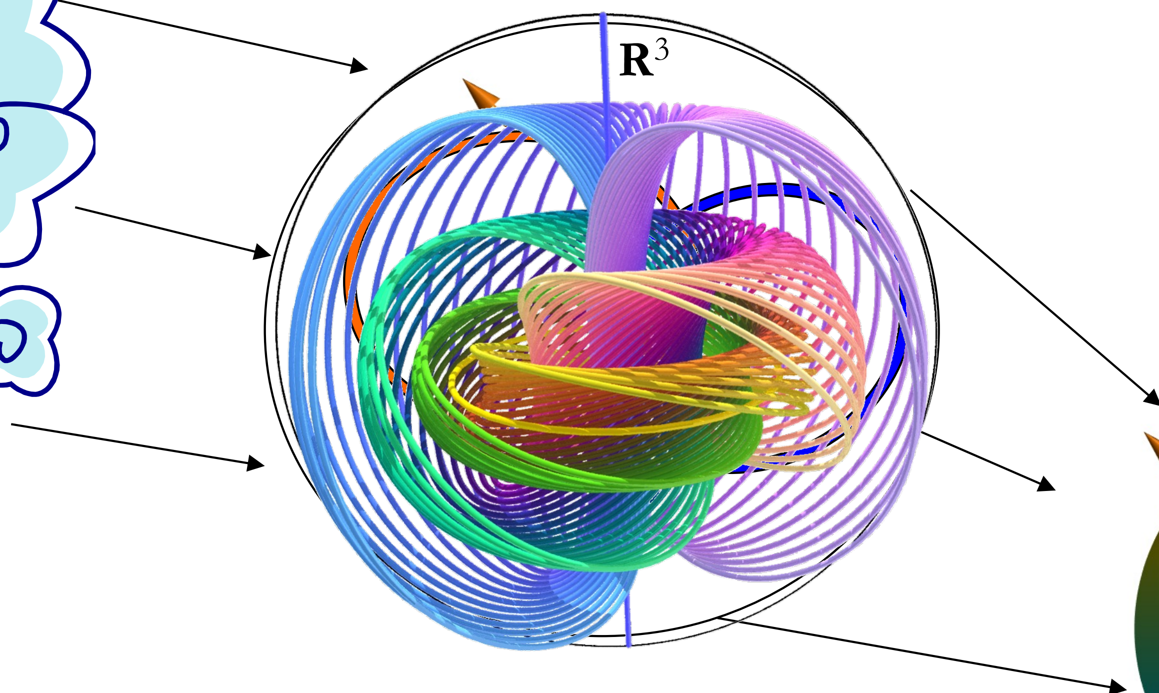
3D solitons, stereographic projection from S^3

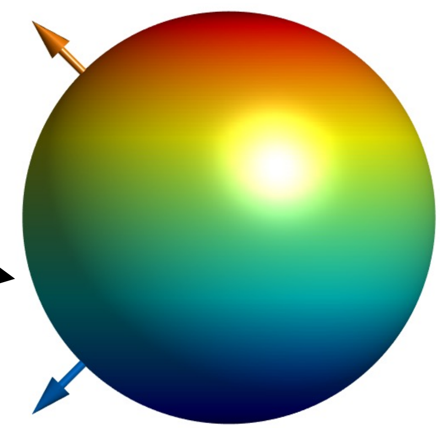
S^3 can represent a soliton in the 3D space ($\mathbf{R}^3$) for the uniform far-field background

each point of S^2 corresponds to a distinct circle of S^3 & its projection



S3 in 4 Dimensions

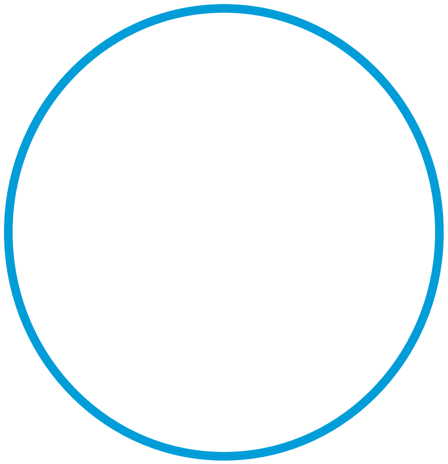




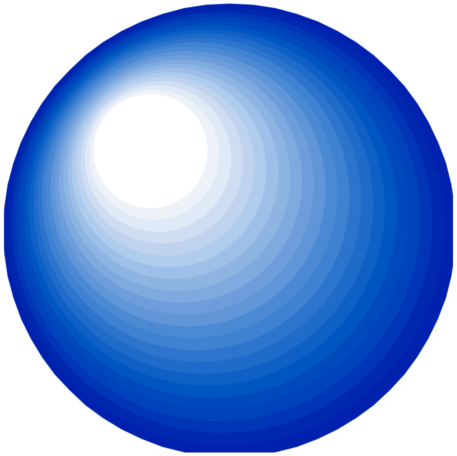
- Each point on S^2 corresponds to a closed loop (circle) of spatial positions within the solitons
- $\pi_3(S^2)$ solitons in $\mathbf{M}(\mathbf{r})$ & $\pi_3(RP^2)$ in $\mathbf{n}(\mathbf{r})$

Spheres

S^1 in 2 Dimensions



S^2 in 3 Dimensions



S^3 in 4 Dimensions

S^2 - all points in 3D space at distance 1 from the origin.

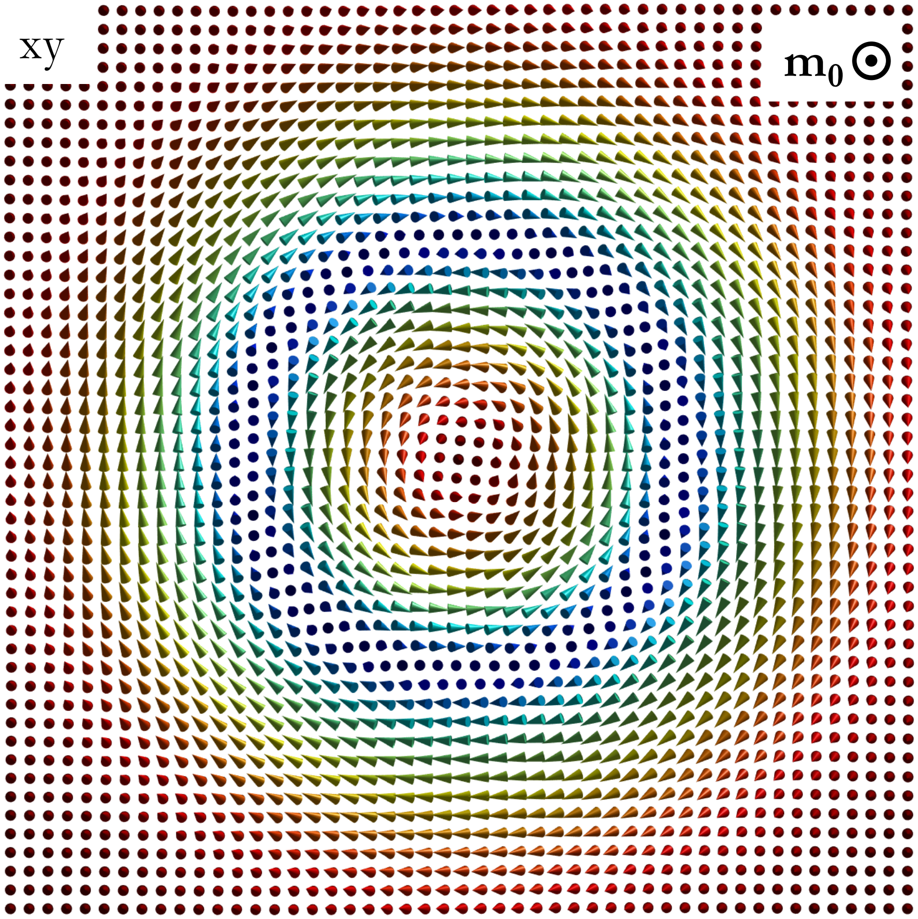
$$\sqrt{x^2 + y^2 + z^2} = 1$$

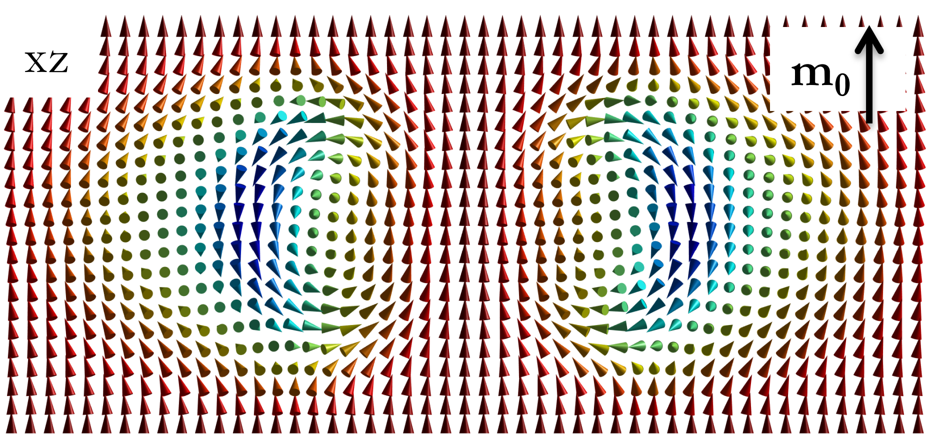
S^3 – all points (x,y,z,w) in 4D space at distance 1 from the origin.

$$\sqrt{x^2 + y^2 + z^2 + w^2} = 1$$

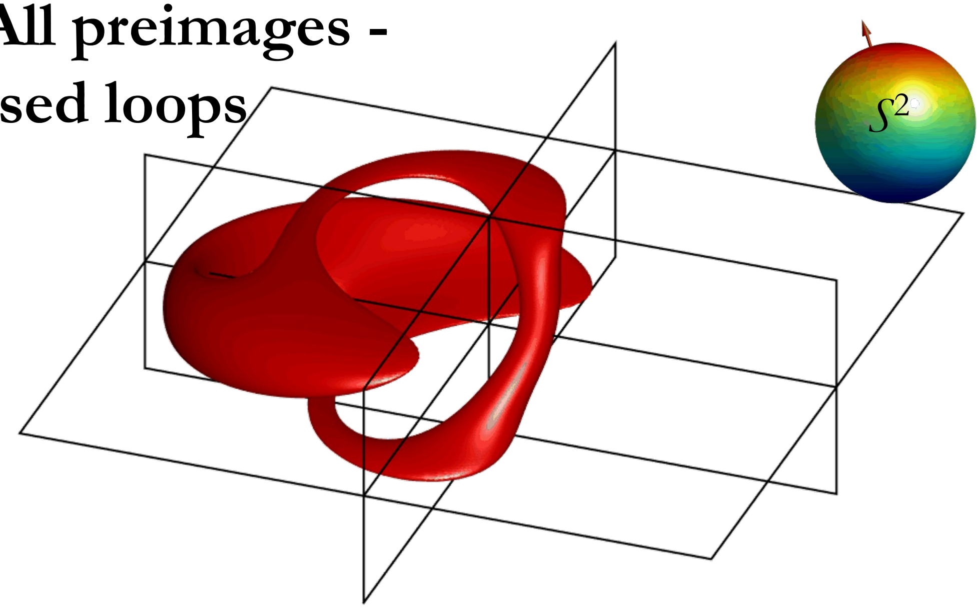
Can we see the high-dimensional spheres?

3D solitons, Numerical Modeling & Analysis

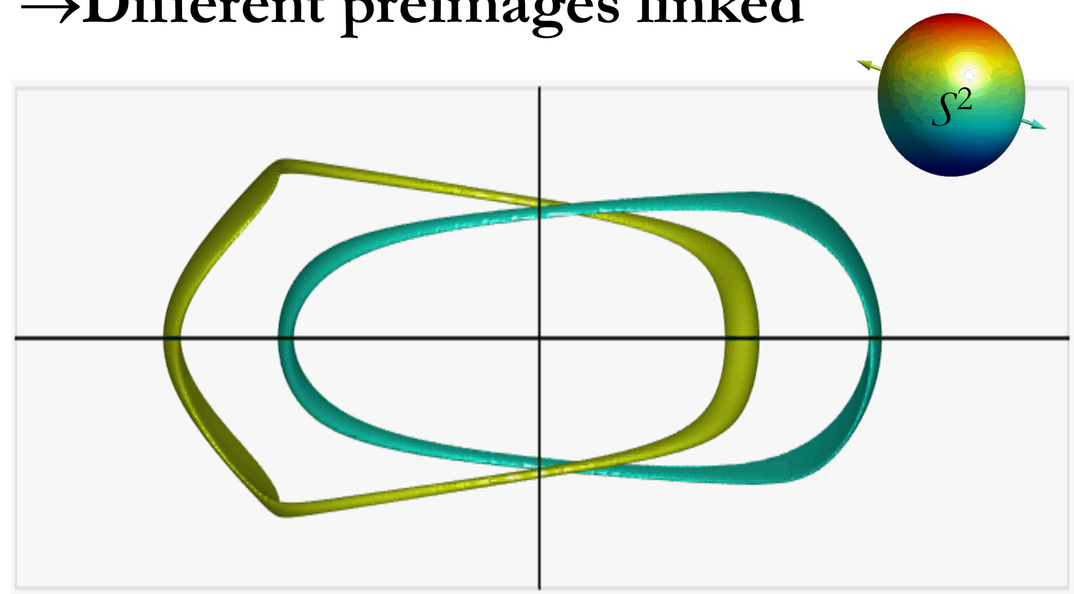




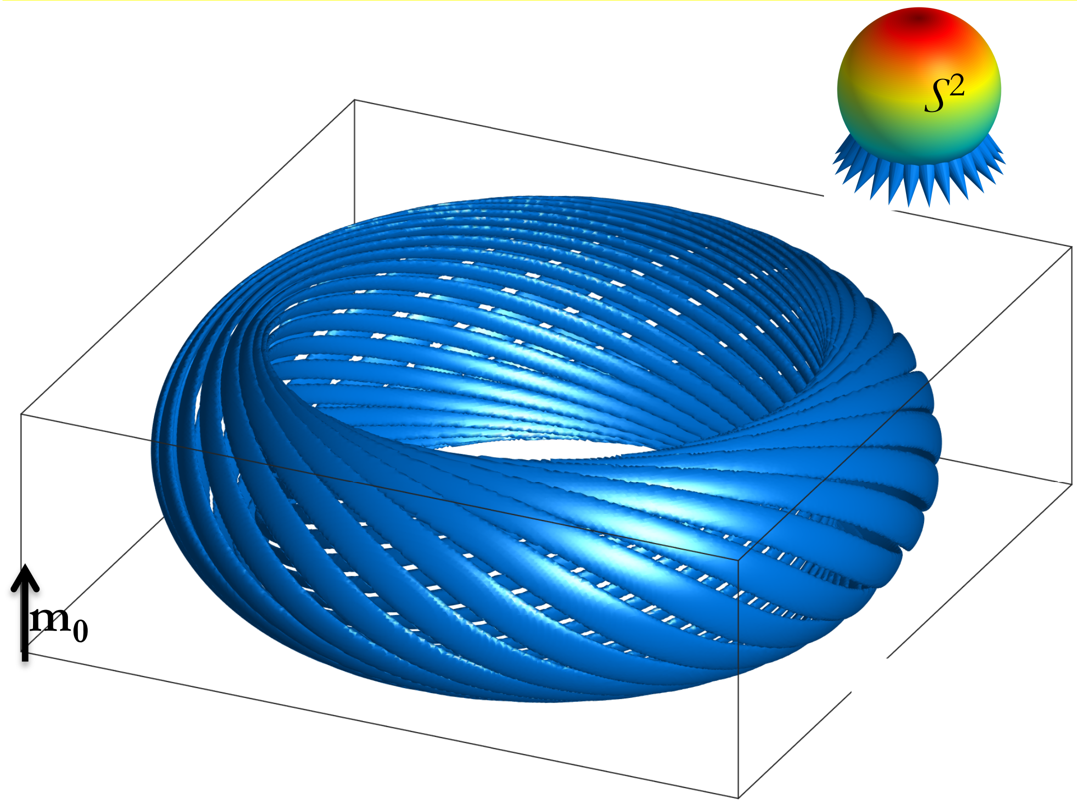
→All preimages - closed loops



→Different preimages linked

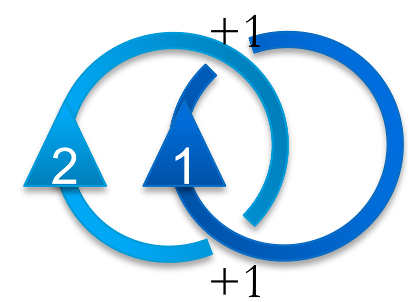


Topological solitons with Hopf index *Q*=1

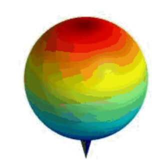


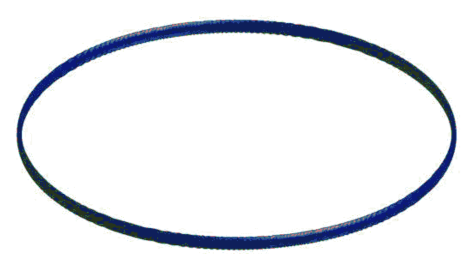
→crossings- linking number

→Hopf index $Q = \Sigma C/2 = 1$



→Filling localized space with all preimages:

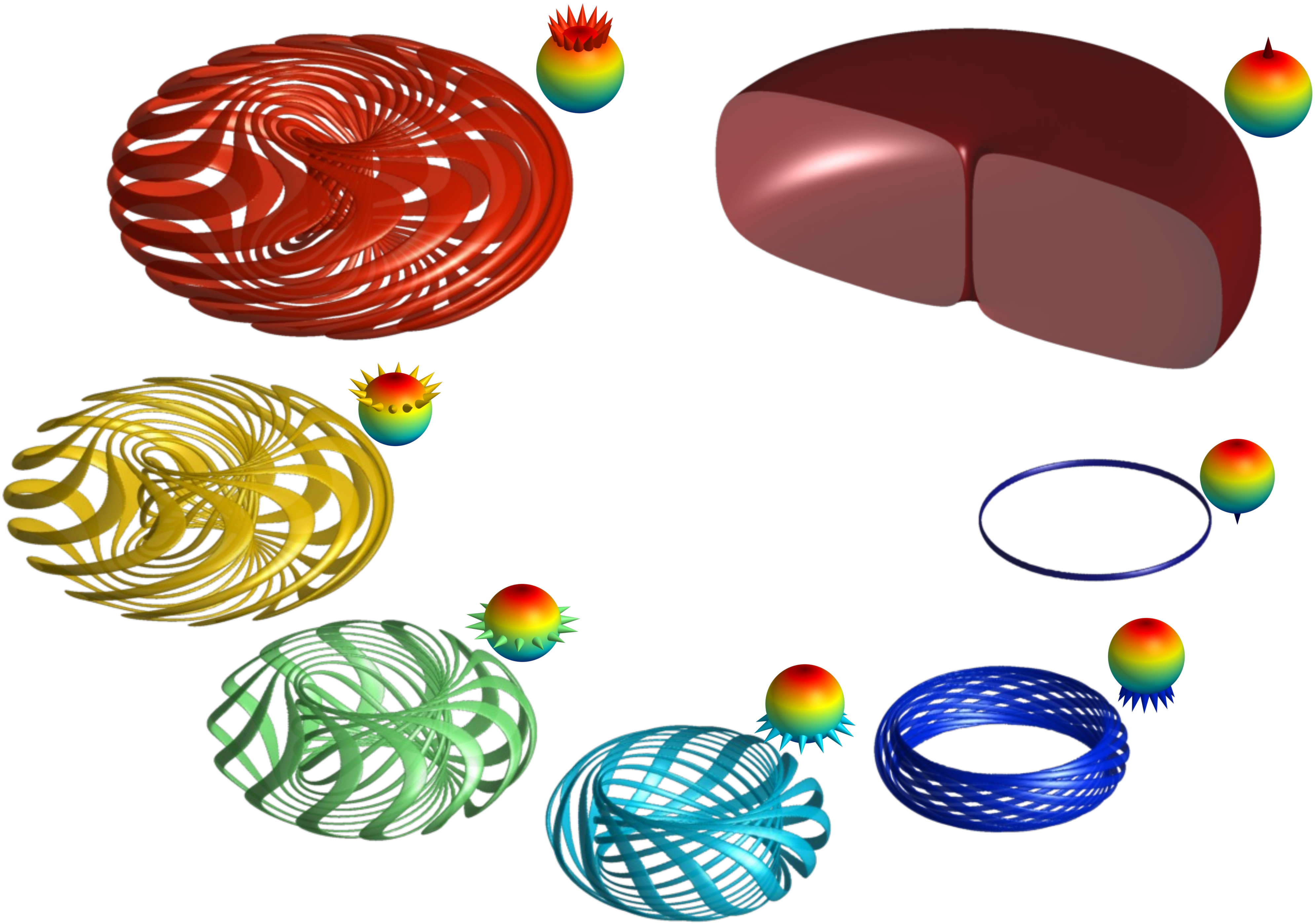




→Preimages of points with the same polar angle tile into tori

→Nested tori fill the 3D space

Nested tori of linked preimages

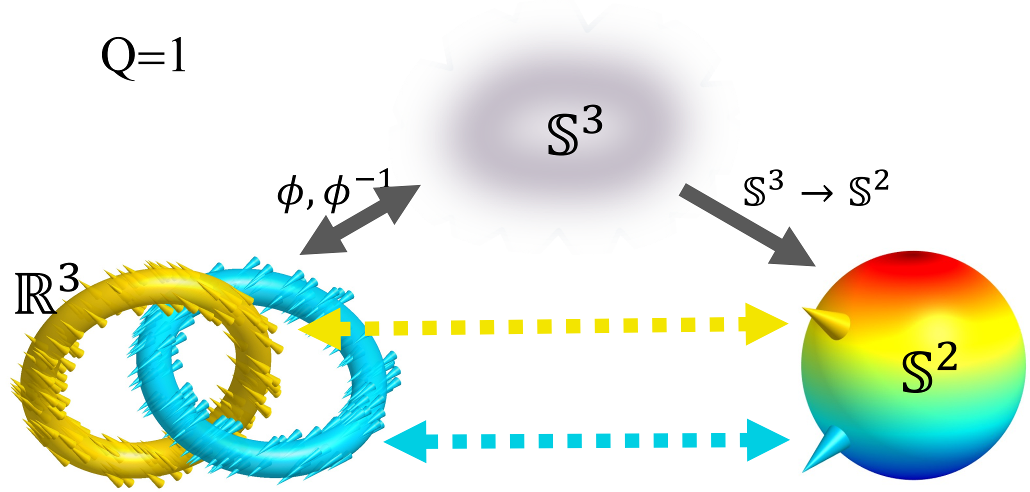


Sphere-sphere maps homotopy theory

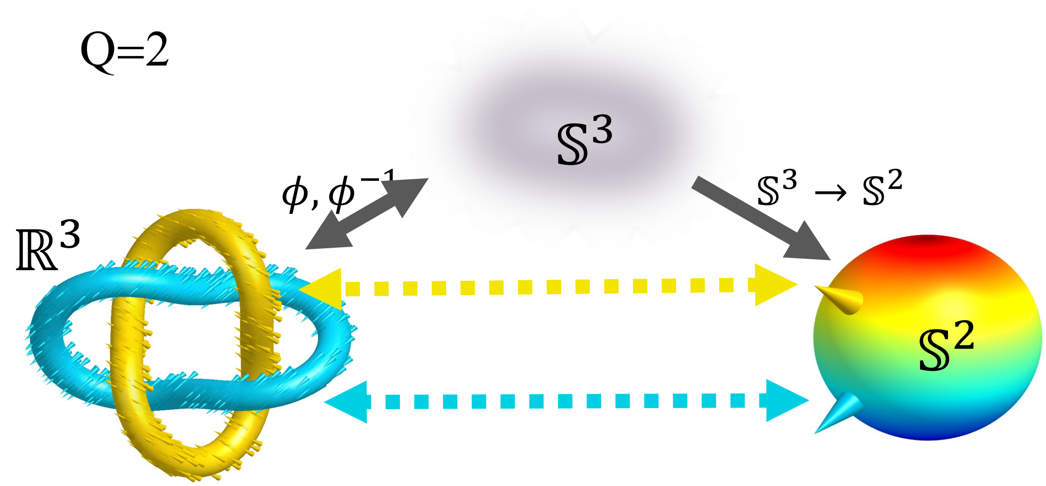
	π_1	π_2	π_3	π_4	π_5
S^0	0	0	0	0	0
S^1	Z	0	0	0	0
S^2	0	Z	Z	Z_2	Z_2
S^3	0	0	Z	Z_2	Z_2
S^4	0	0	0	Z	Z_2
S^5	0	0	0	0	Z

$Q=\pi_3(S^2)=Z$ solitons

Q=1



Q=2



- i-th homotopy group $\pi_i(S^n)$ – ways the i-dimensional sphere S^i can be mapped into n-dimensional sphere S^n