



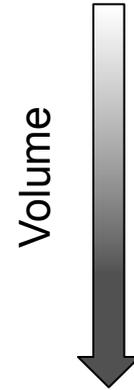
# HOMOGENEOUS VACUUM

very long time ago



slightly less long ago

small



larger

After  $10^{-37}$  seconds: **Grand Unification Transition**

HOMOGENEOUS VACUUM

very long time ago

small

Time

Volume

slightly less long ago

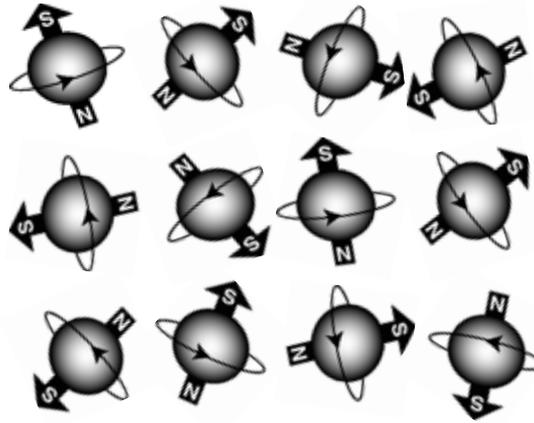
larger

LOWER SYMMETRY VACUUM



# Symmetry lowering phase transition in a ferromagnet

high temperature

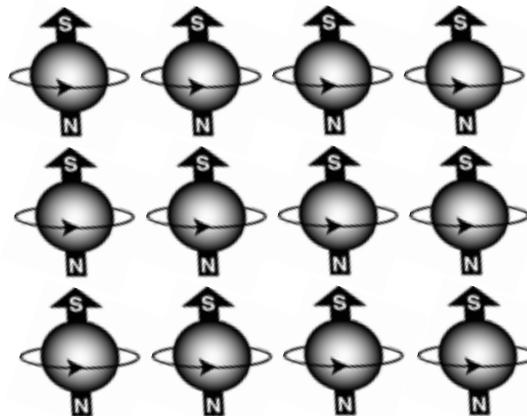


high symmetry

Transition (Curie) temperature,  $T_c$

---

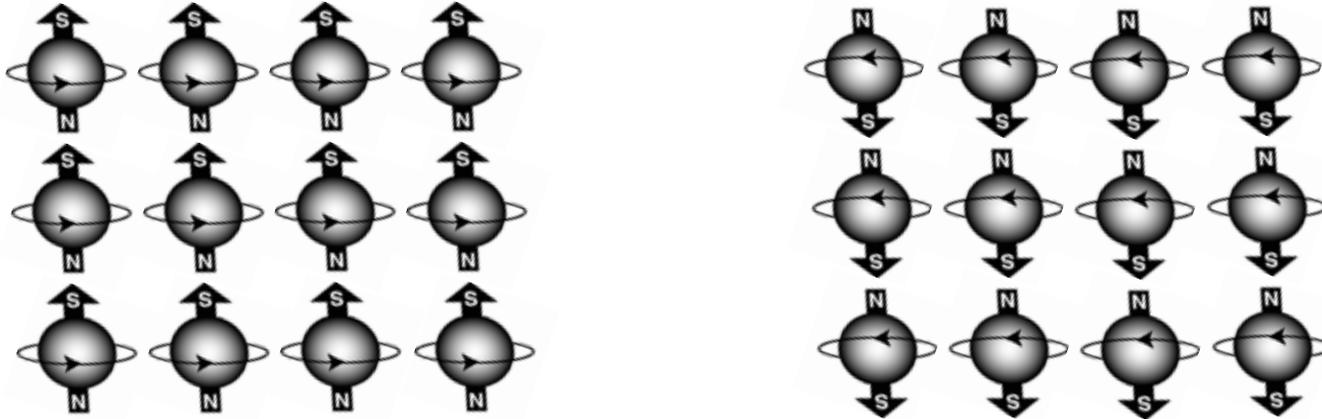
low temperature



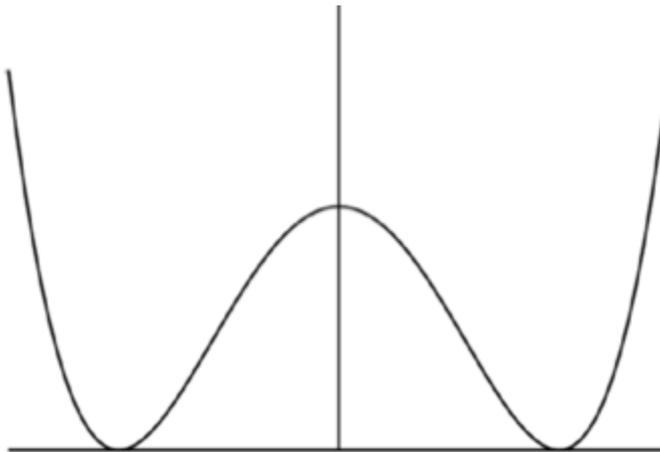
low symmetry

# If the ferromagnet is uniaxial...

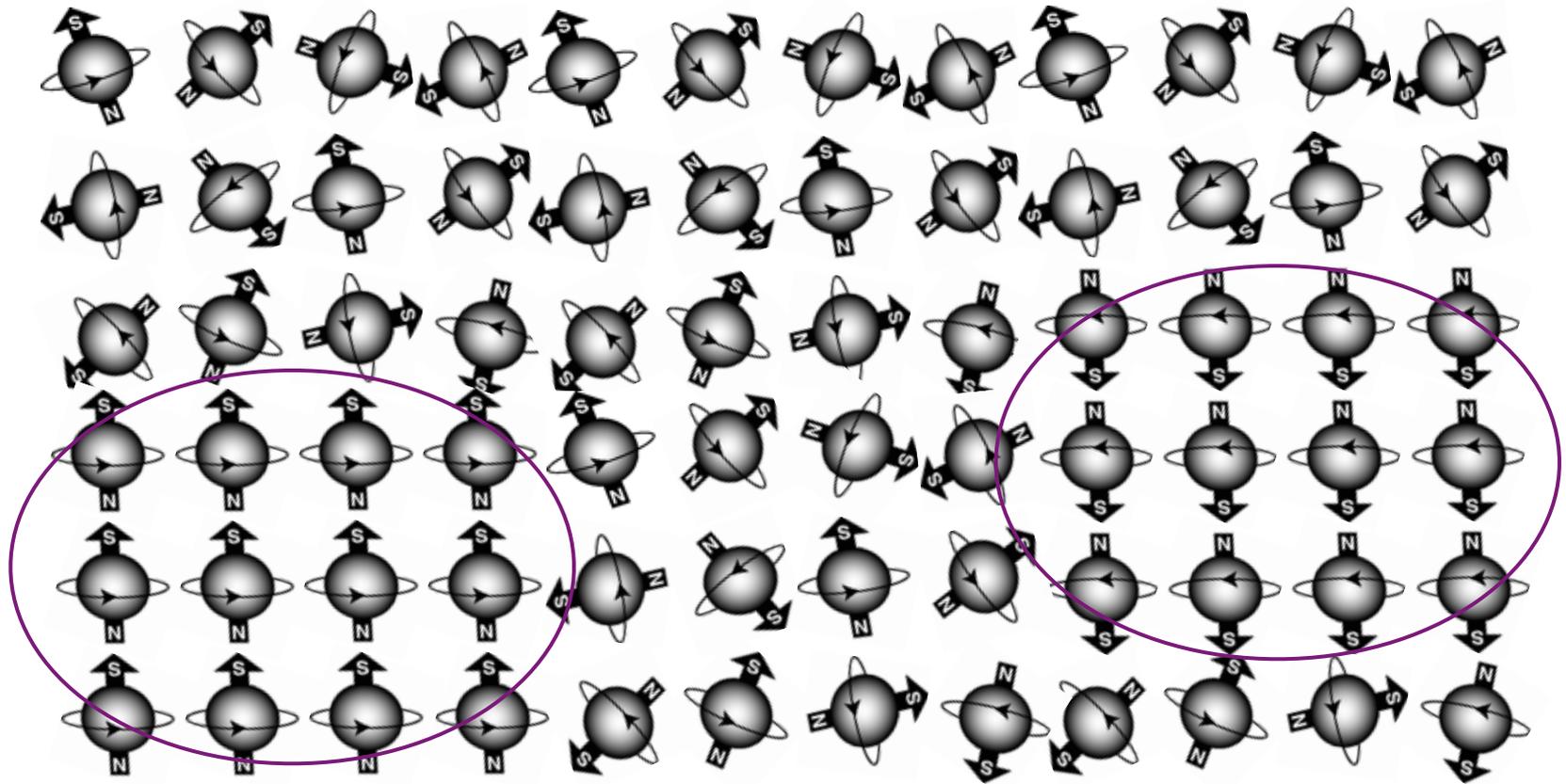
... then there are two equivalent low symmetry states



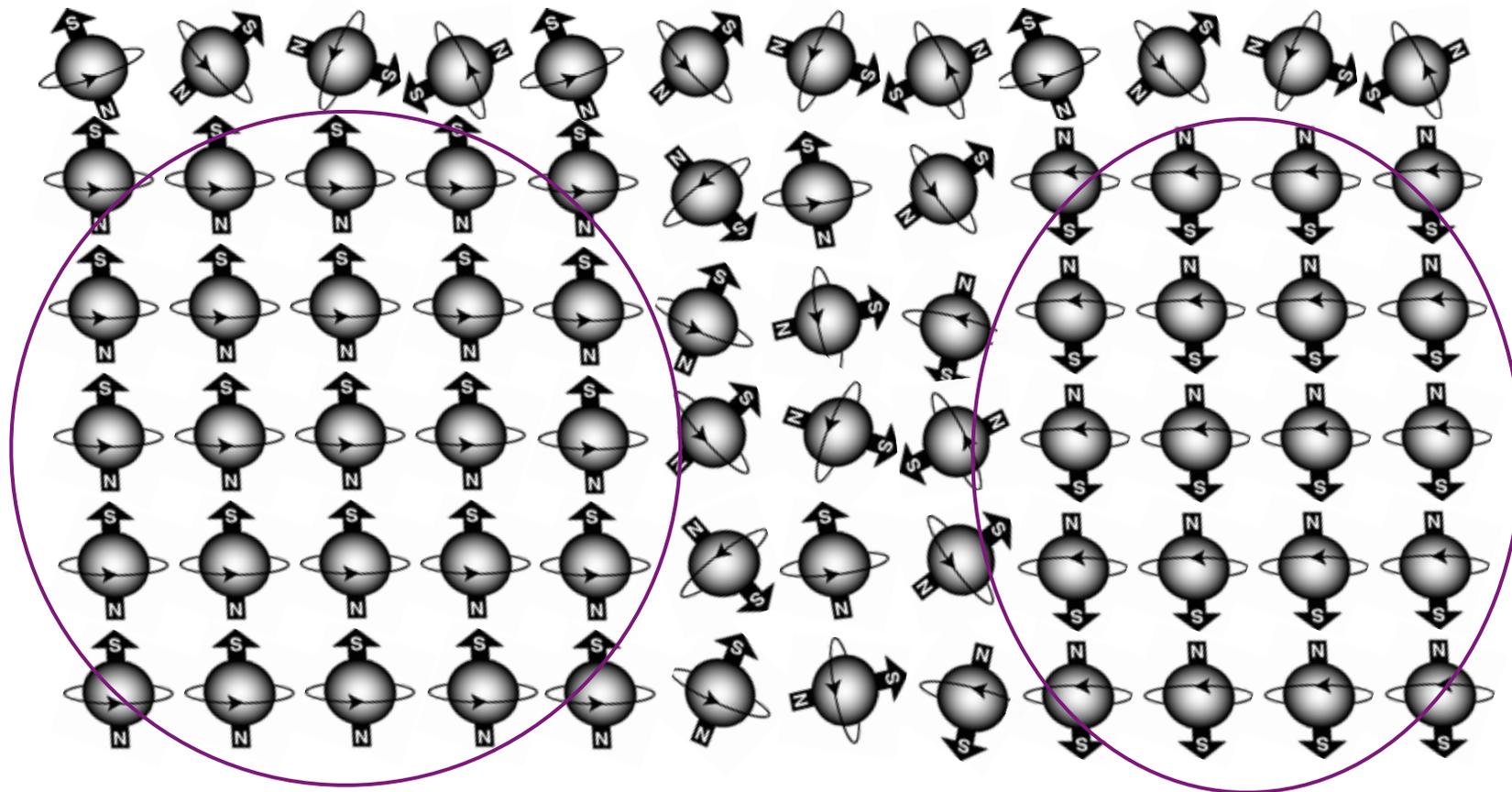
and the symmetry-lowering phase transition is described by a double well potential:



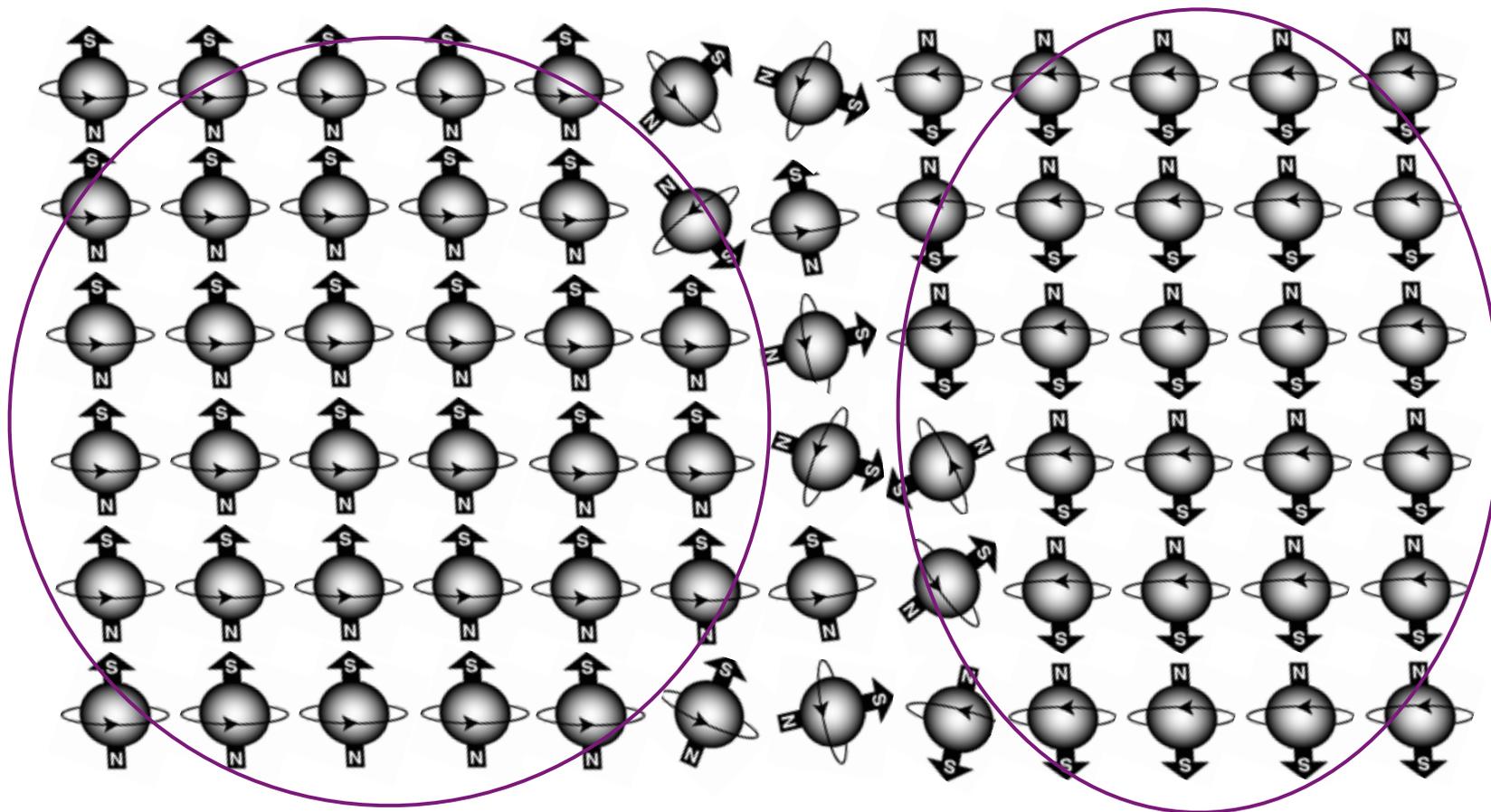
# Defect formation at symmetry-lowering phase transitions



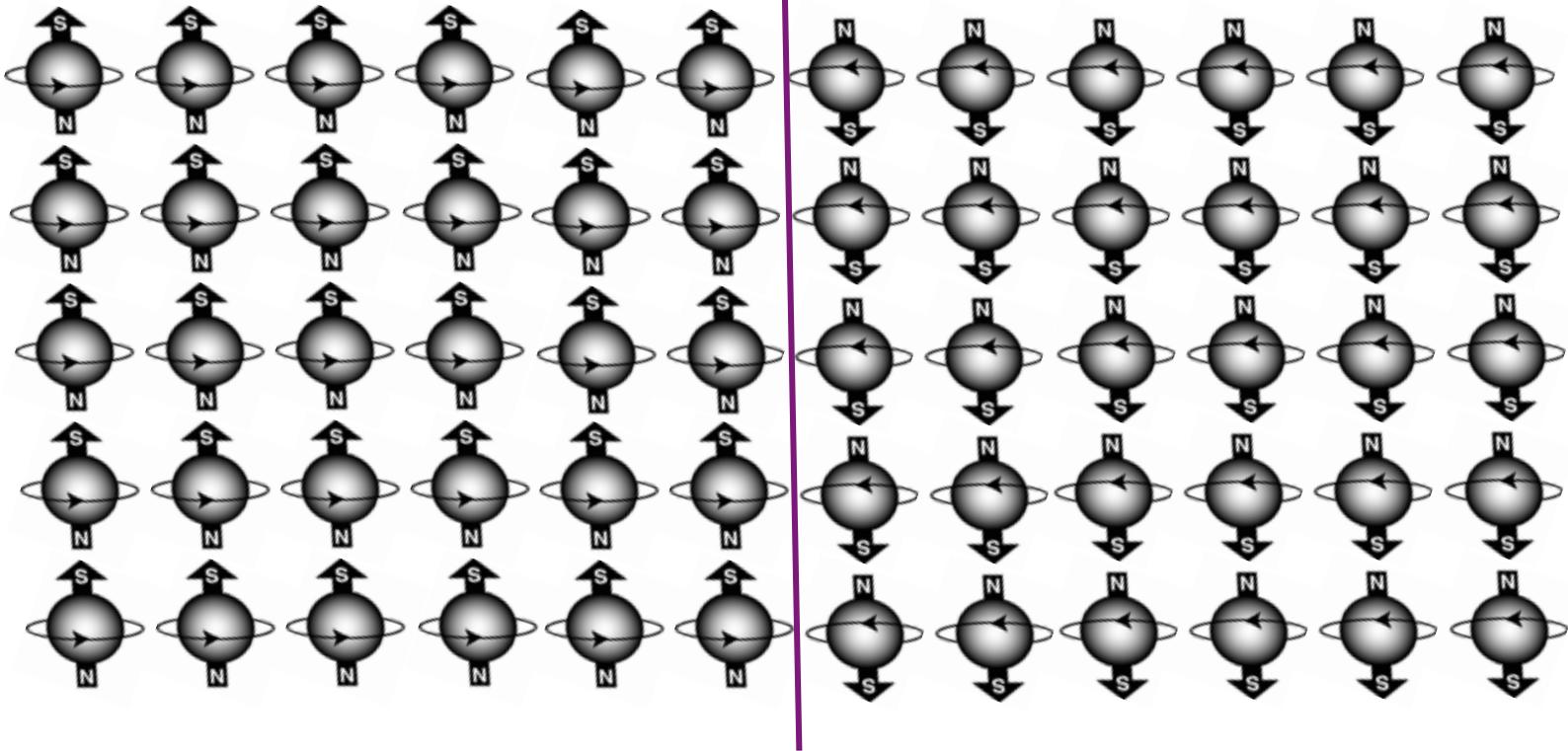
# Defect formation at symmetry-lowering phase transitions



# Defect formation at symmetry-lowering phase transitions

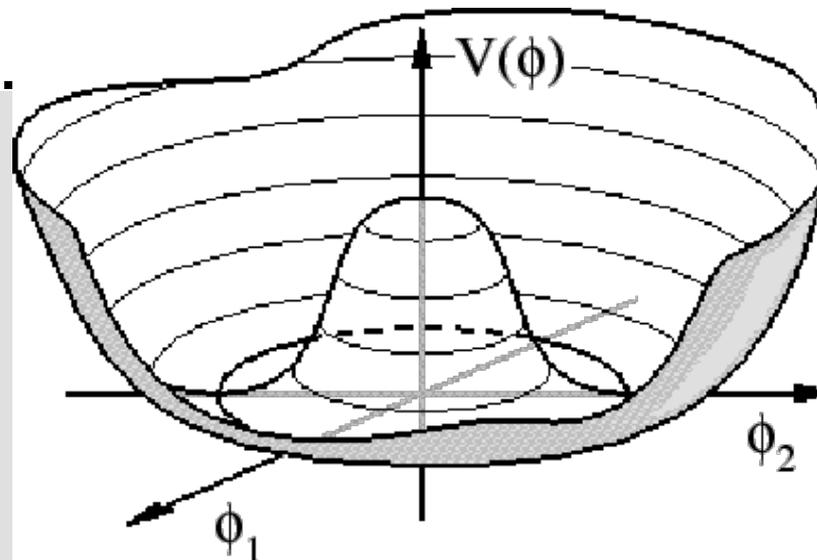


# Defect formation at symmetry-lowering phase transitions



# Symmetry lowering at the Grand Unification Transition

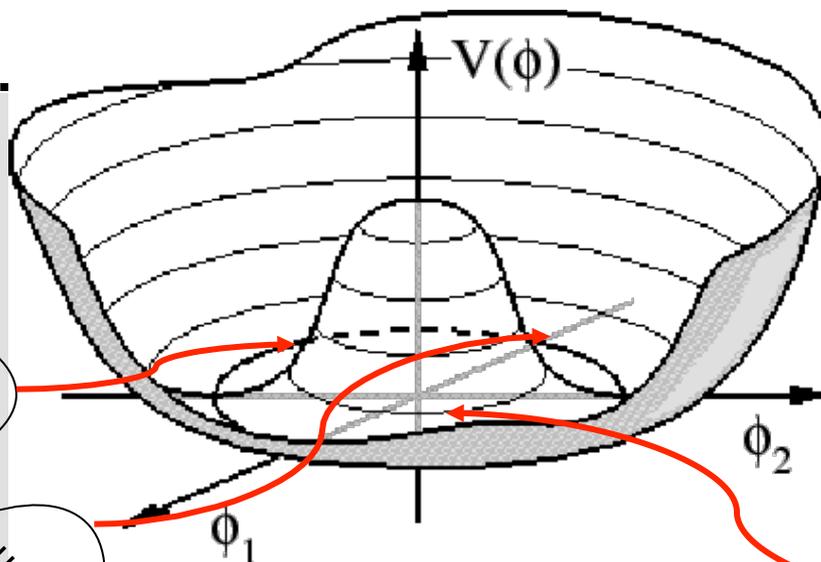
HOMOGENEOUS VACUUM



LOWER SYMMETRY VACUUM

# Symmetry lowering at the Grand Unification Transition

HOMOGENEOUS VACUUM



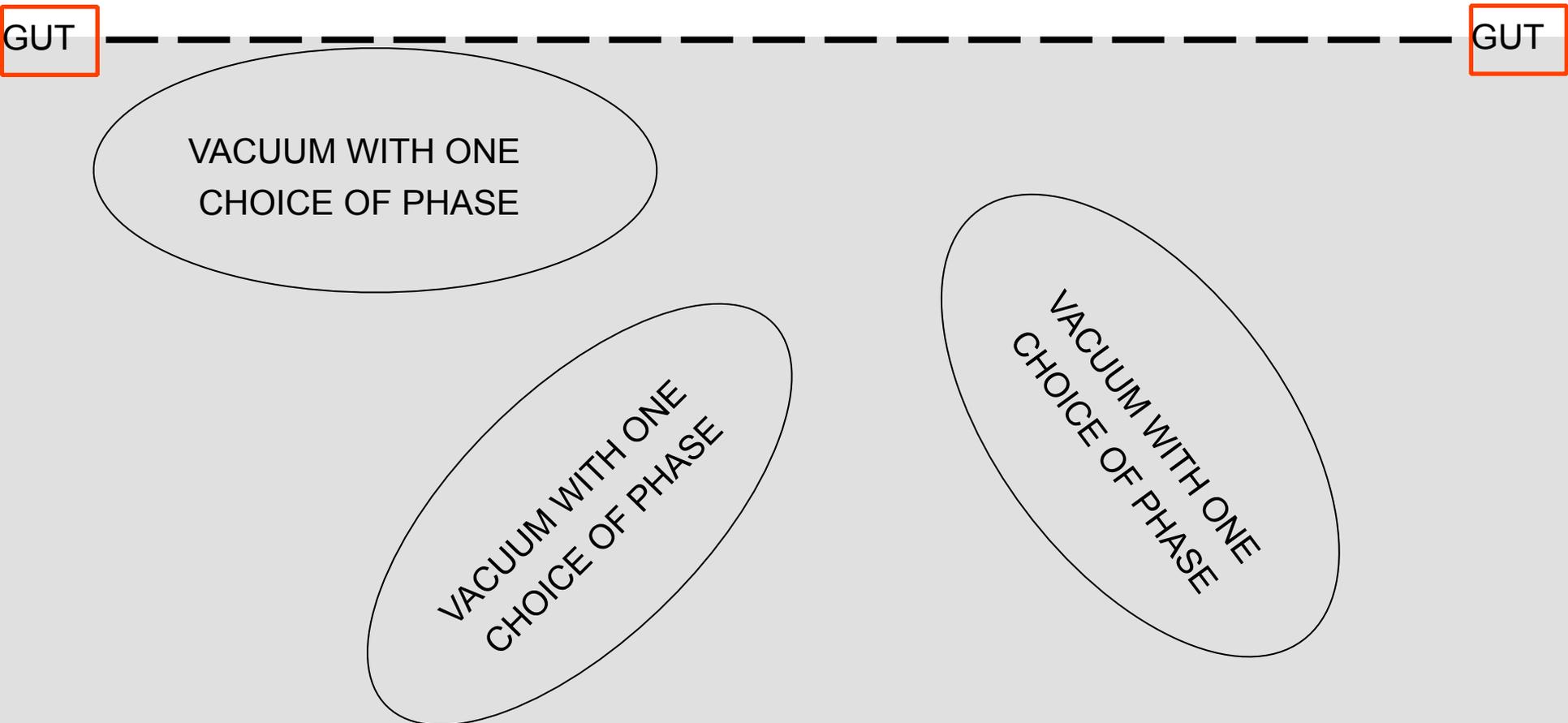
VACUUM WITH ONE  
CHOICE OF PHASE

VACUUM WITH ONE  
CHOICE OF PHASE

LOWER SYMMETRY VACUUM

VACUUM WITH ONE  
CHOICE OF PHASE

As the universe expands through the transition, the low symmetry regions grow...



and grow...

GUT

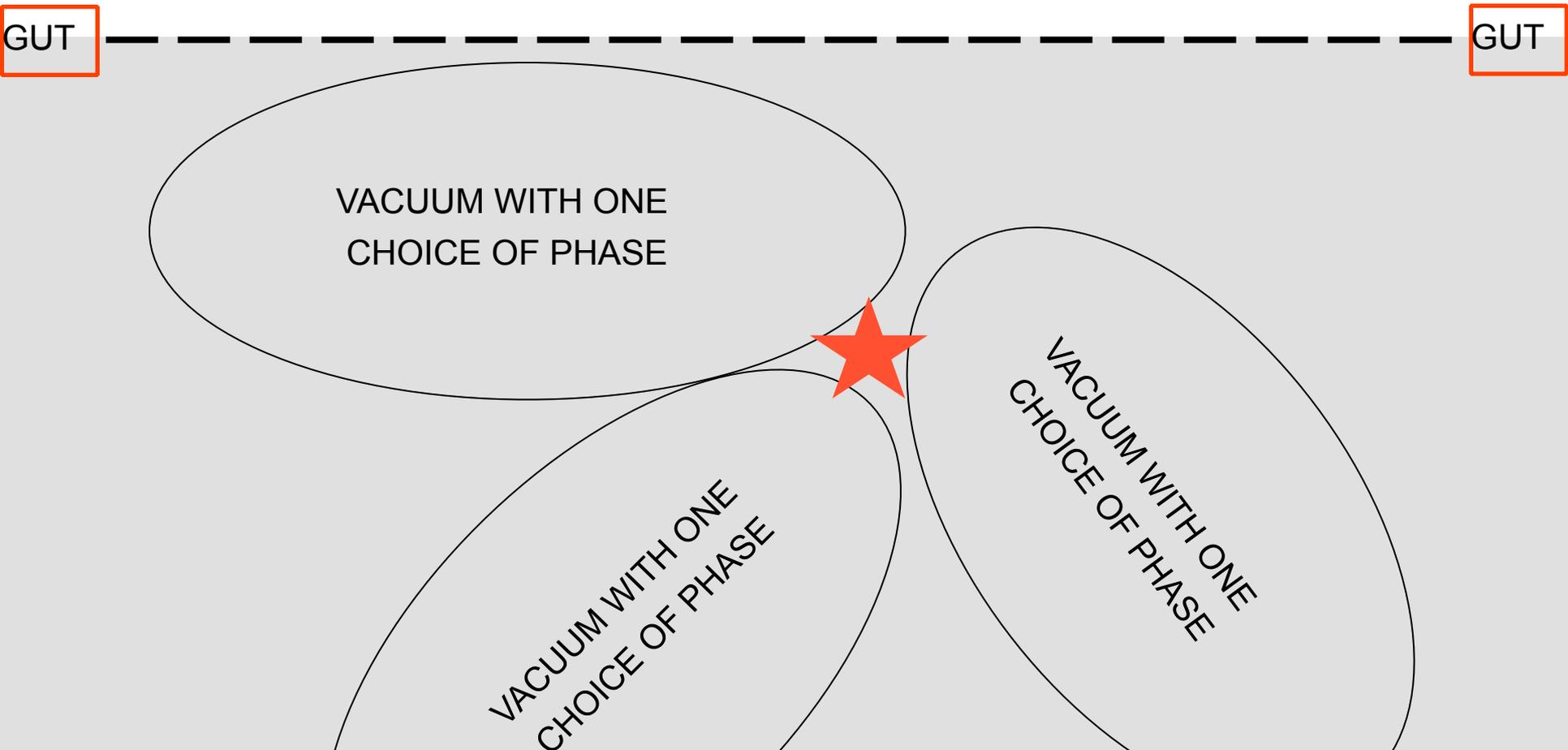
GUT

VACUUM WITH ONE  
CHOICE OF PHASE

VACUUM WITH ONE  
CHOICE OF PHASE

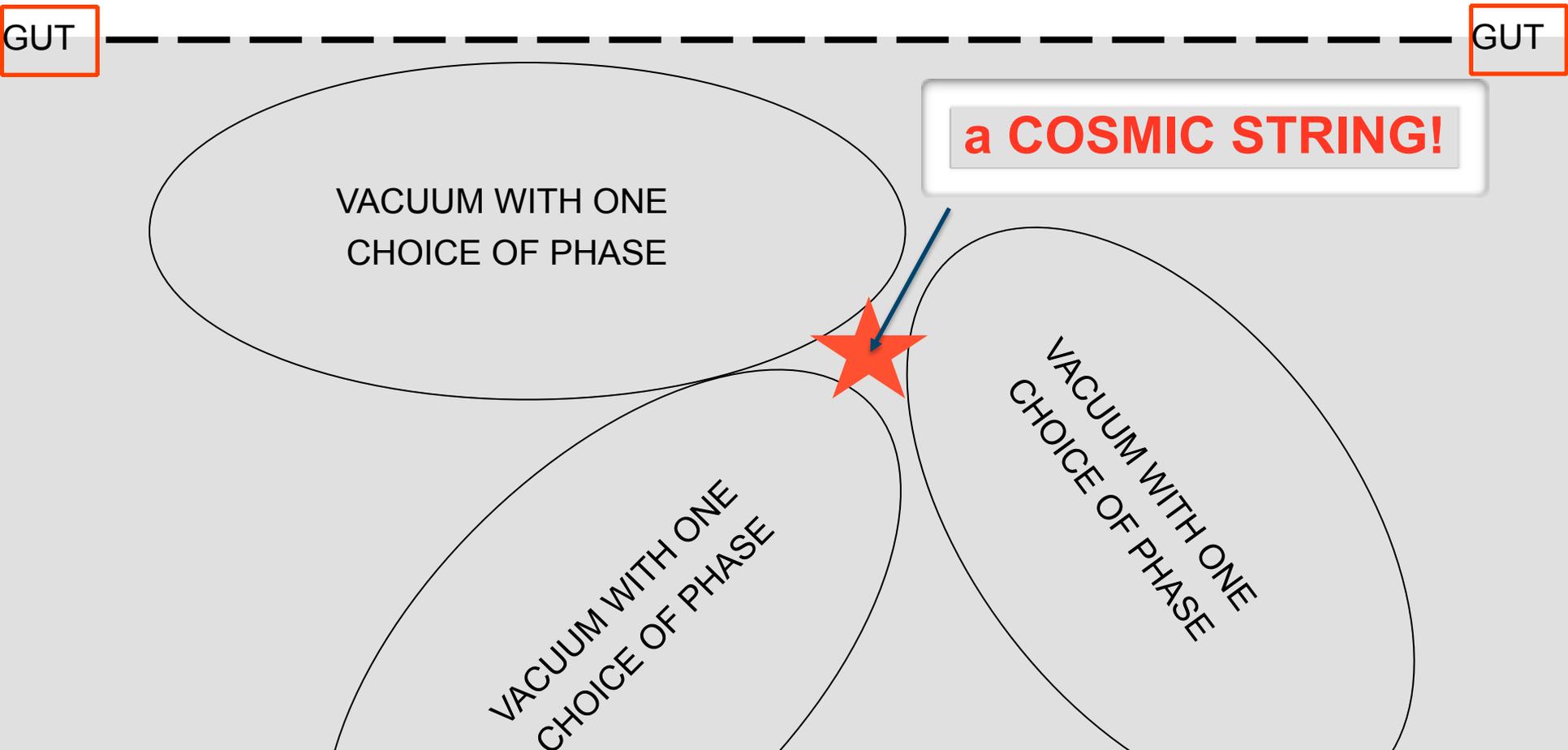
VACUUM WITH ONE  
CHOICE OF PHASE

and eventually meet!



$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = H \Psi(\mathbf{r}, t)$$
$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = H \Psi(\mathbf{r}, t)$$
$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = H \Psi(\mathbf{r}, t)$$

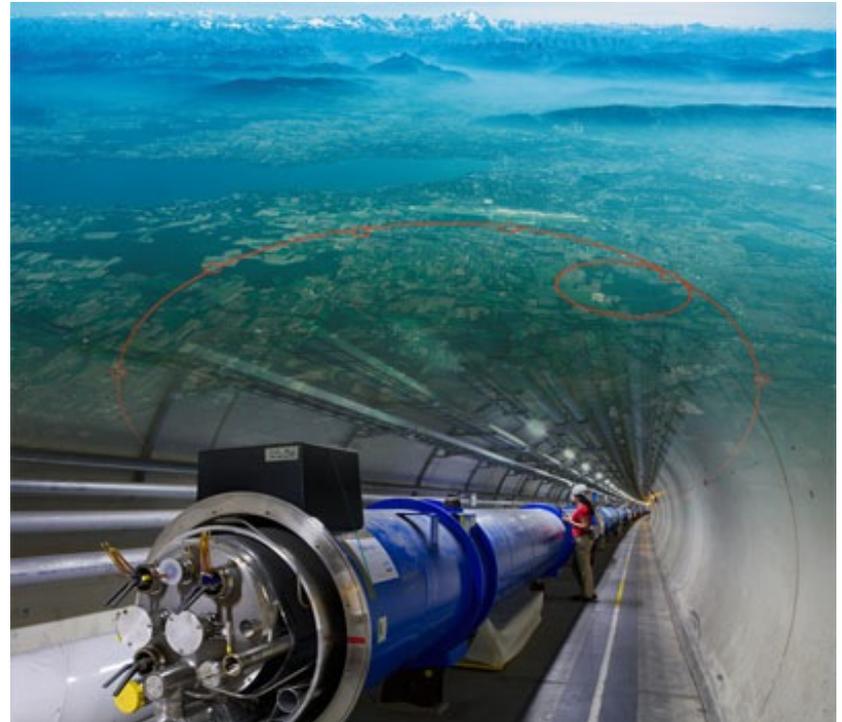
The phase mismatch in the vacuum is a *topologically protected defect* with energy and mass



# Do cosmic strings exist? How can we study them?

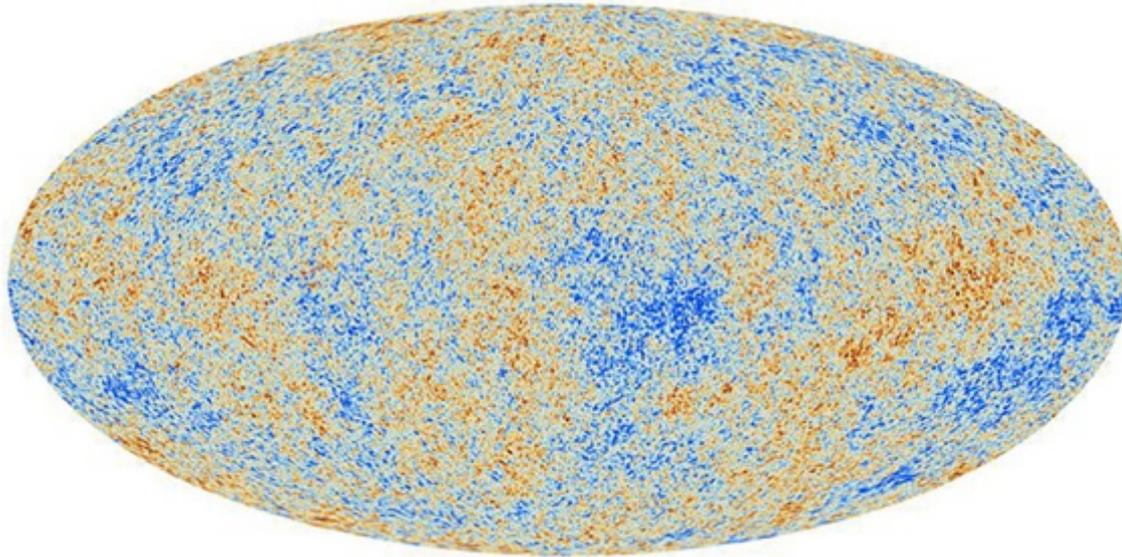
For direct study we need a probe with a similar energy,  $\sim 10^{15}$  GeV

Our highest energy probes, the largest hadronic colliders reach  $\sim 1$  GeV

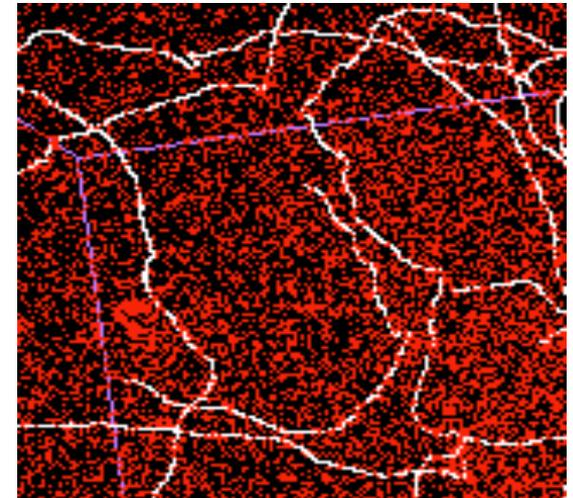


# How is Cosmic String Formation at the Grand Unification Transition studied?

Analyzing the Cosmic Microwave Background



Computer Simulation



$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = H \Psi(\mathbf{r}, t)$$

**Instead we will study cosmic string formation in the lab.**

What are the laboratory equivalent of cosmic strings?

Defects formed as a result of symmetry-lowering phase transitions

## Plan for studying early universe processes in the lab.

First will identify a material with a symmetry-lowering phase transition described by the same mathematics as that proposed for the GUT

spontaneous symmetry breaking *described by a non-trivial homotopy group*

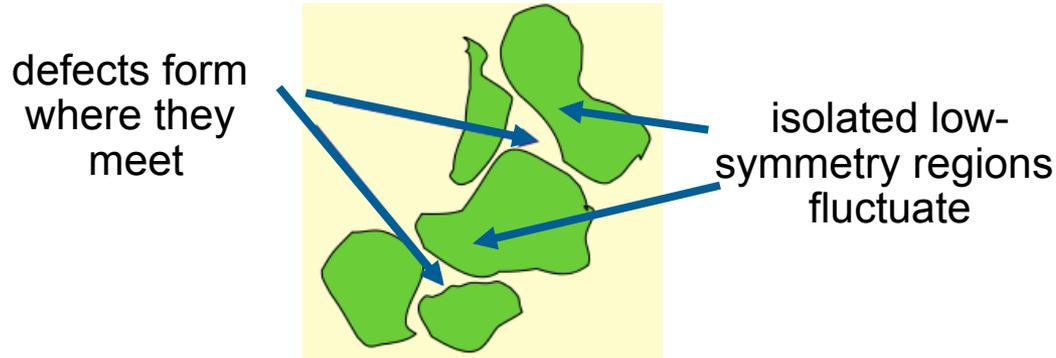
Results in formation of *topologically-protected defects* (Kibble)

Then we will do experiments on the material to test the behavior predicted for the GUT!

In particular the proposed *scaling laws* – the number of topologically-protected defects formed as a function of cooling rate

Kibble-Zurek scenario

## Physics of a “GUT-like” transition (Zurek scaling):



### Size of the resulting domains set by competition between:

- Speed of information propagation
- Rate of cooling through the transition

**Cool slowly:** Different regions can communicate their choice of phase

- **Large regions of the same choice**
- **Low density of defects**

**Cool quickly:** Not much time to communicate choice of phase

- **Many smaller regions with different choice of phase**
- **High density of defects**



# Kibble-Zurek scaling law for defect formation

domain size (for linear quench)

defined as  $T_c$  / cooling rate

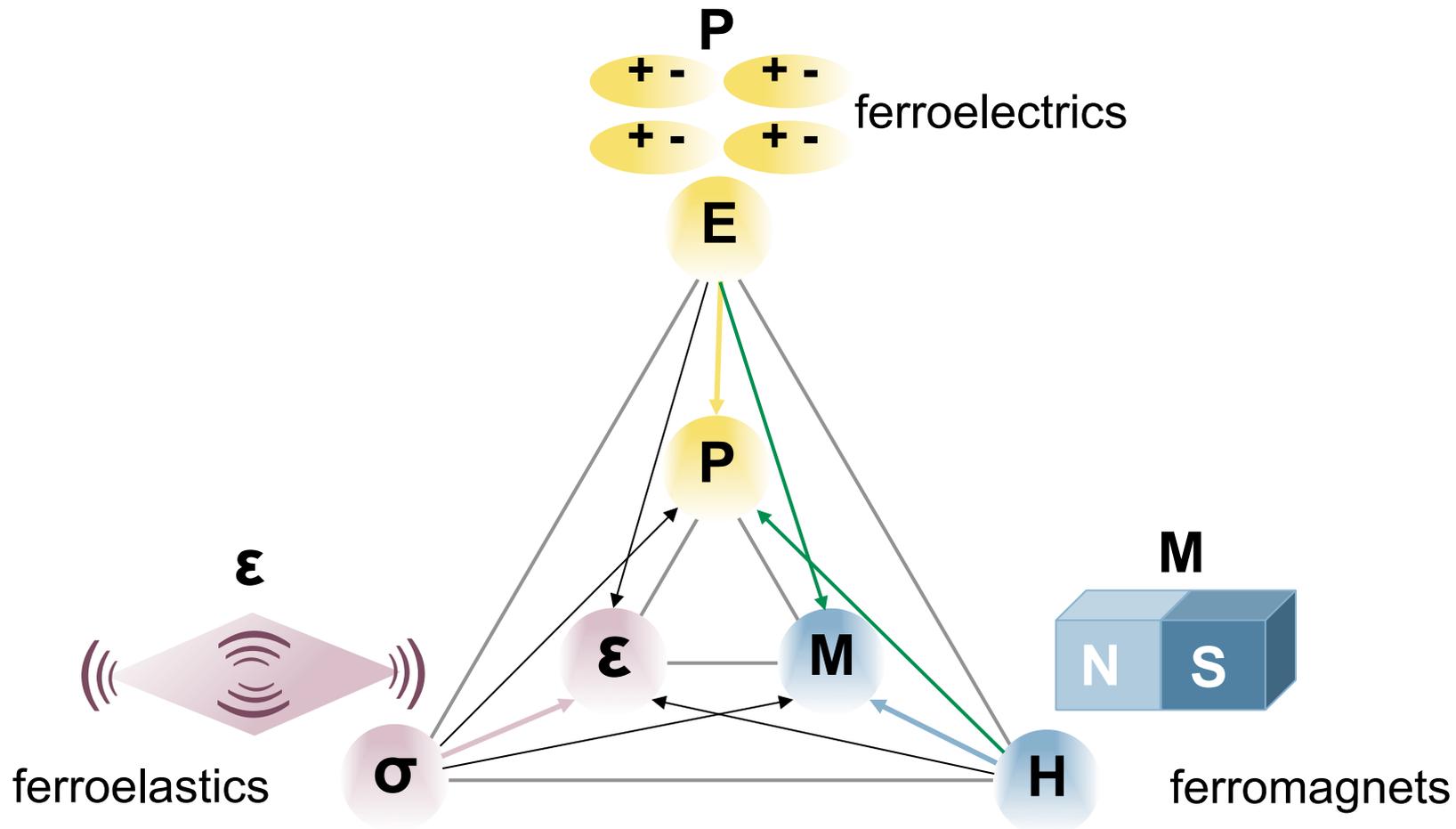
$$d = \xi_0 \left( \frac{\tau_q}{\tau_0} \right)^{\frac{\nu}{1+\mu}}$$

Critical exponents

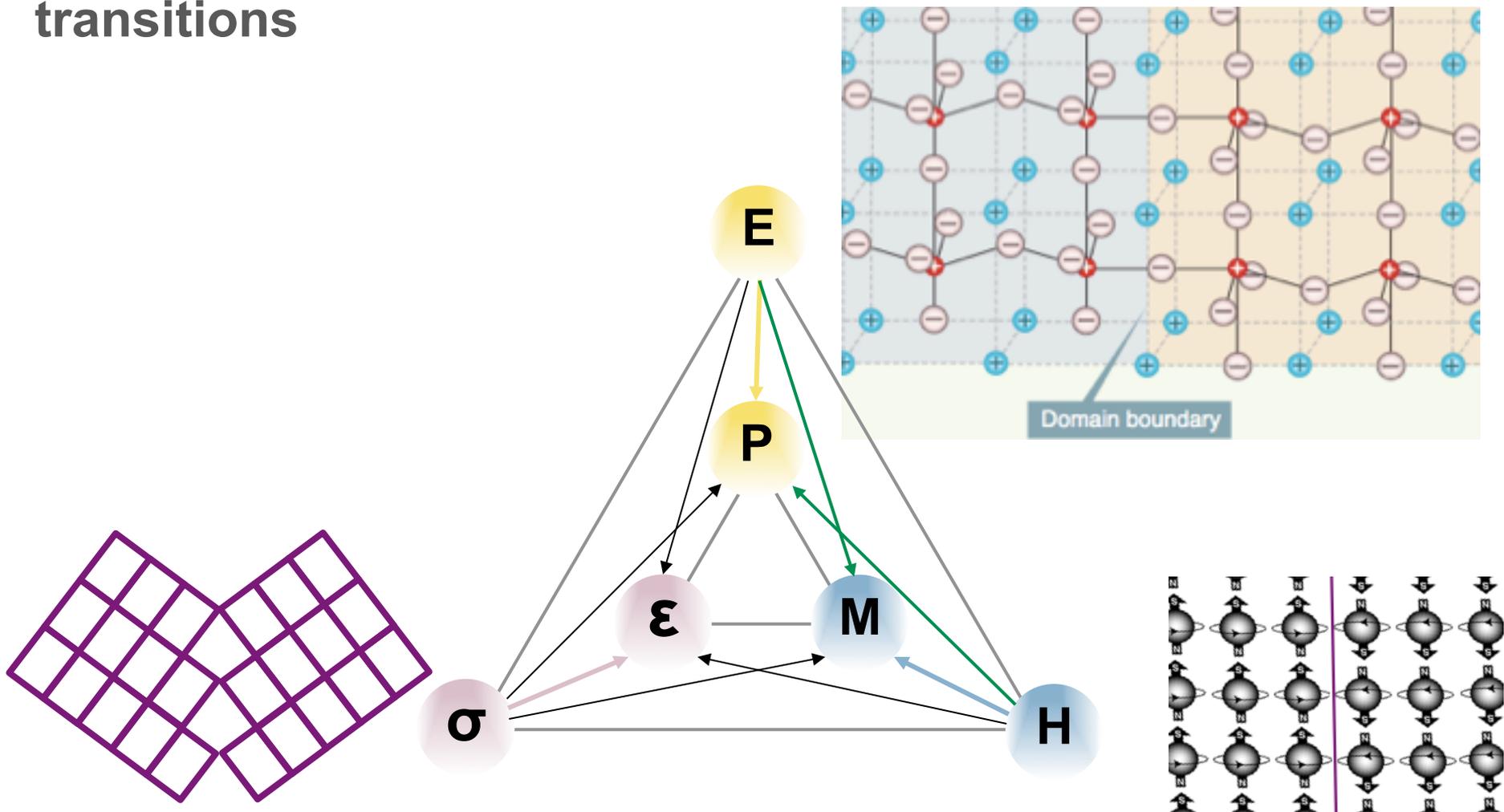
zero-temperature correlation length

zero-temperature relaxation time =  
 $\xi_0$  / speed of information transfer

# Multiferroics: Multiple ferroic orders...

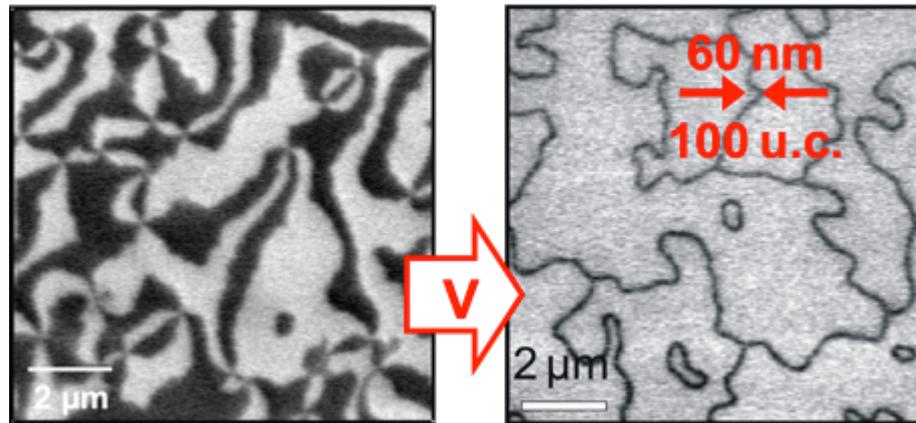


# ...and multiple defects from spontaneous symmetry-lowering transitions



## Our candidate multiferroic: $\text{YMnO}_3$

The ferroelectric domain intersections are somehow “protected”:



Perhaps they are mathematically topologically protected too?

# Outline

Use electronic structure calculations to understand the phase transition in  $\text{YMnO}_3$

Check mathematically whether it meets the Kibble requirements

Use electronic structure calculations to calculate how many topologically protected defects should be formed as a function of cooling rate

Measure how many topologically protected defects are formed as a function of cooling rate

Does a system that is described by the same physics and symmetry as the GUT exhibit the predicted Kibble-Zurek behavior?!

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = H \Psi(\mathbf{r}, t)$$
$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = H \Psi(\mathbf{r}, t)$$
$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = H \Psi(\mathbf{r}, t)$$

## The Materials Theory group at ETH

Yu Kumagai



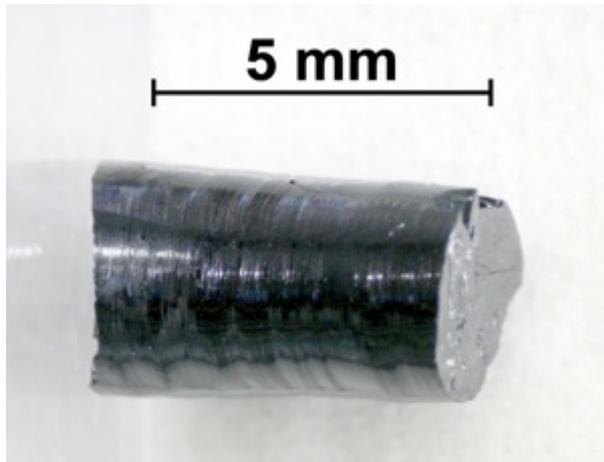
Sinead Griffin

## The Multifunctional Ferroic Materials group at ETH

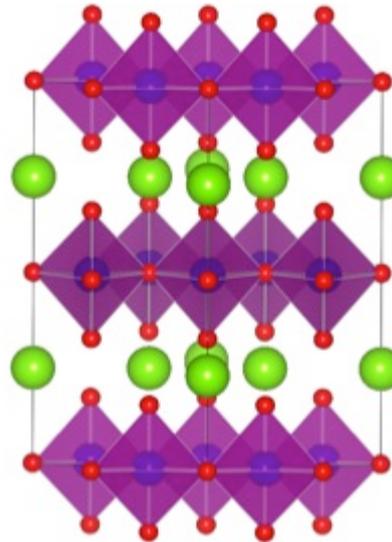
Manfred Fiebig and Martin Lilienblum



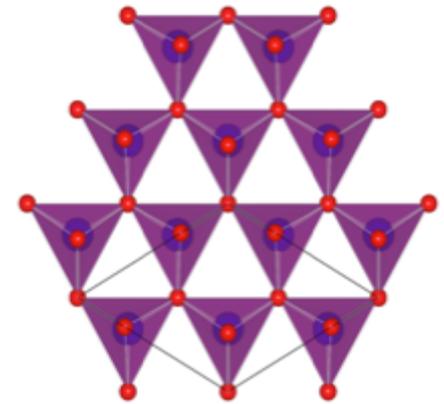
# Our material: Multiferroic $\text{YMnO}_3$



Side view



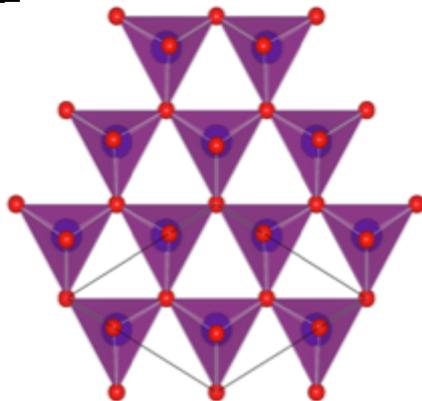
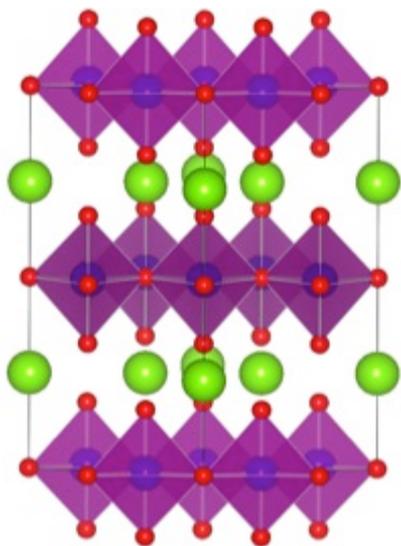
Top view



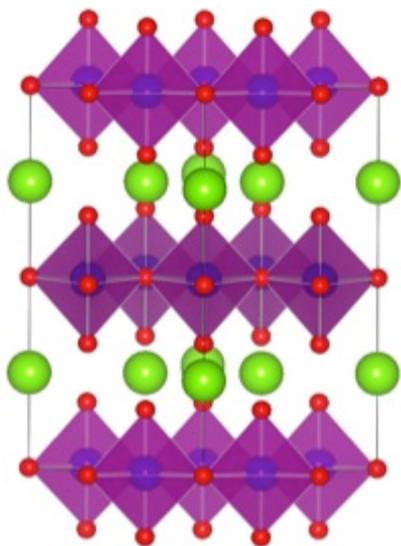
# Structural phase transition in $\text{YMnO}_3$

High temperature

$P6_3/mmc$

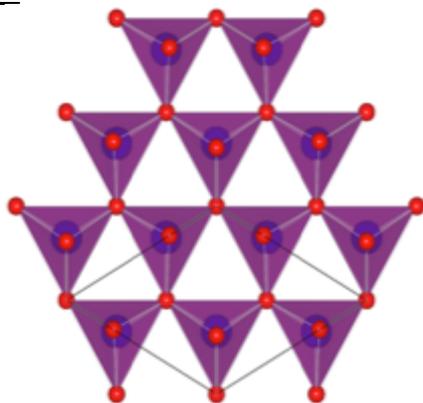
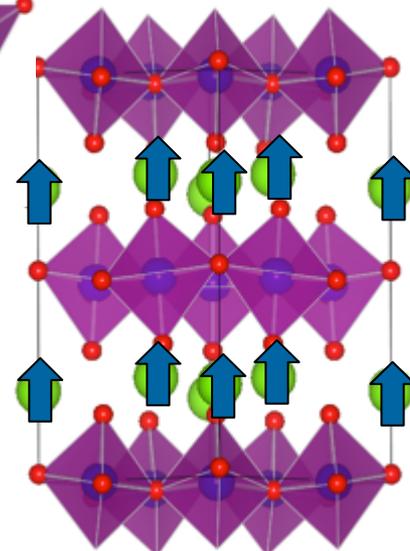


paraelectric

Structural phase transition in  $\text{YMnO}_3$ High temperature $P6_3/mmc$ 

paraelectric

~1000K

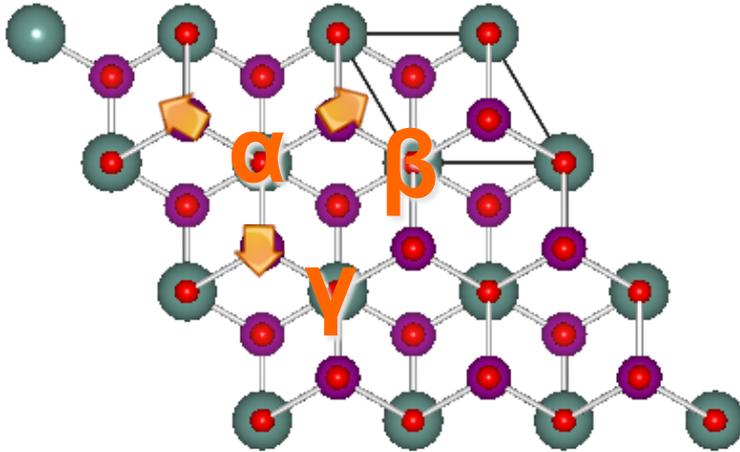
Low temperature $P6_3cm$ 

ferroelectric

Polarization ( $5.6 \mu\text{C}/\text{cm}^2$ )

Look at these distortions in more detail:

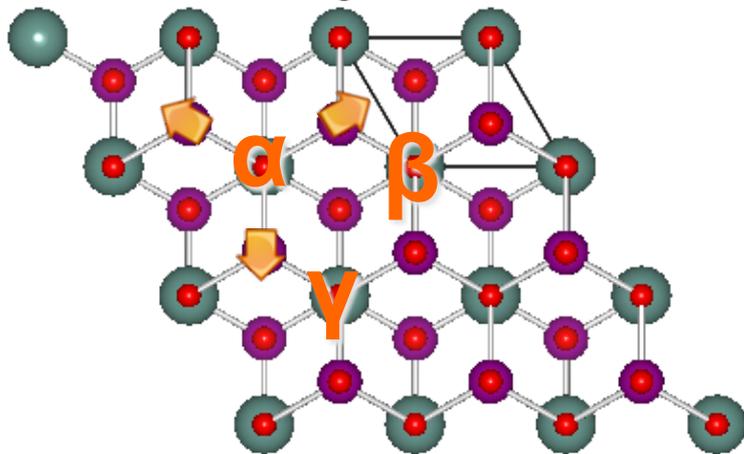
Trimerization / Tilting



Three possible origins

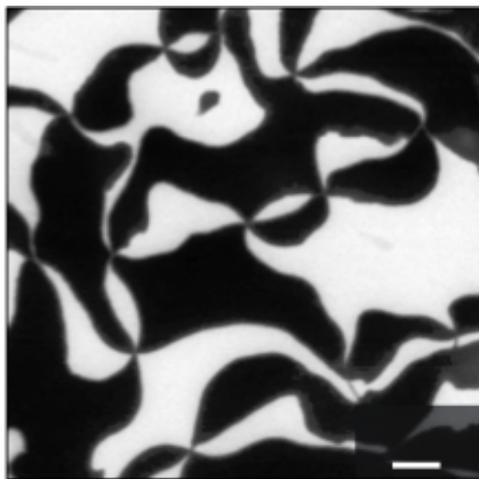
Look at these distortions in more detail:

### Trimerization / Tilting

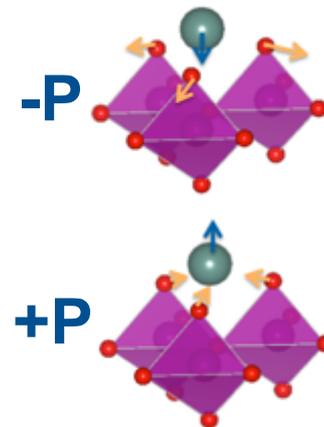


Three possible origins

Results in six domains



### Polarization



Two possible orientations

# Formalize with symmetry analysis and DFT

Landau free energy

$$f_u = \frac{a}{2}Q^2 + \frac{b}{4}Q^4 + \frac{Q^6}{6}(c + c' \cos 6\Phi) - gQ^3P_z \cos 3\Phi$$

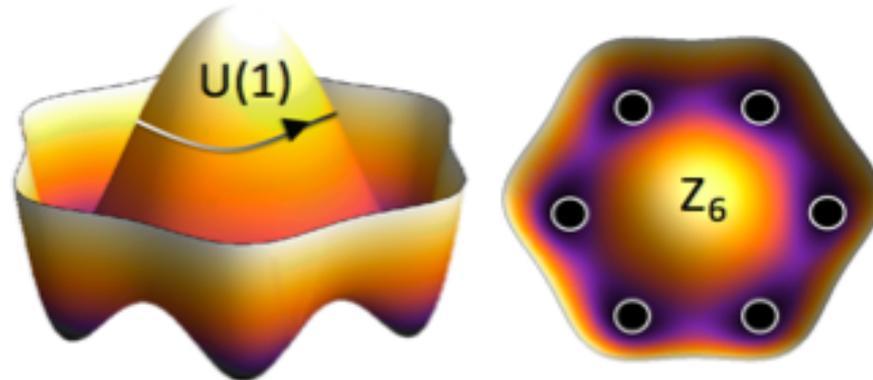
$Q$  is amplitude of trimerization mode

$\Phi$  is phase of trimerization mode

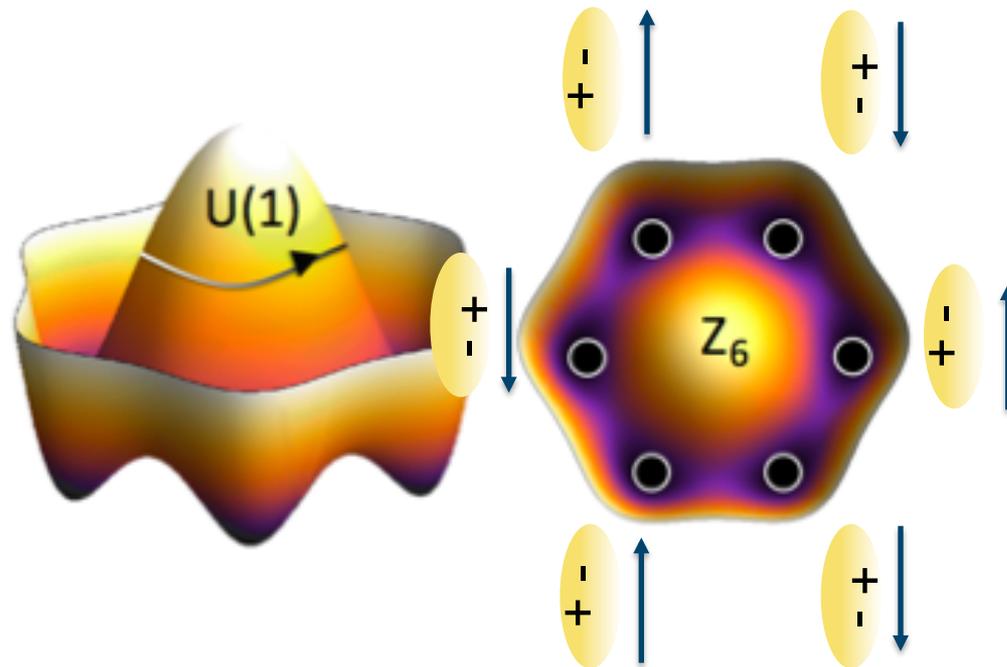
$P_z$  is polarization

The ferroelectricity is *improper*

The phase transition is described by a Mexican-hat-like potential!



And the details of our “Mexican Hat-like” potential make it easy for us to measure!

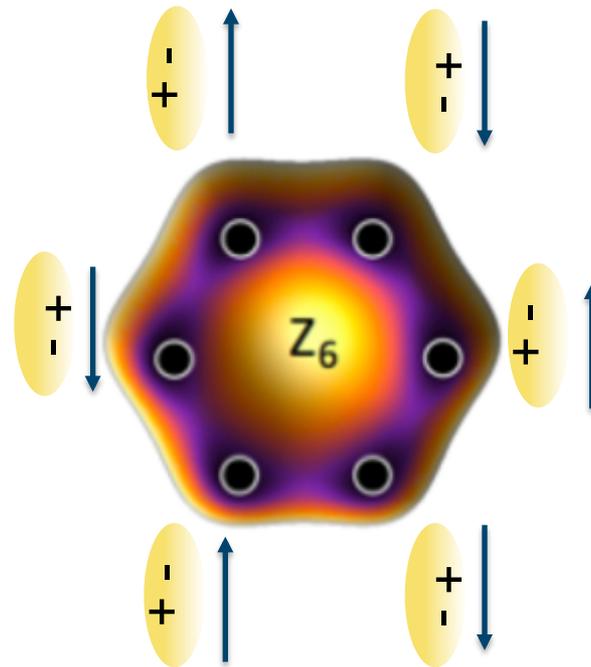
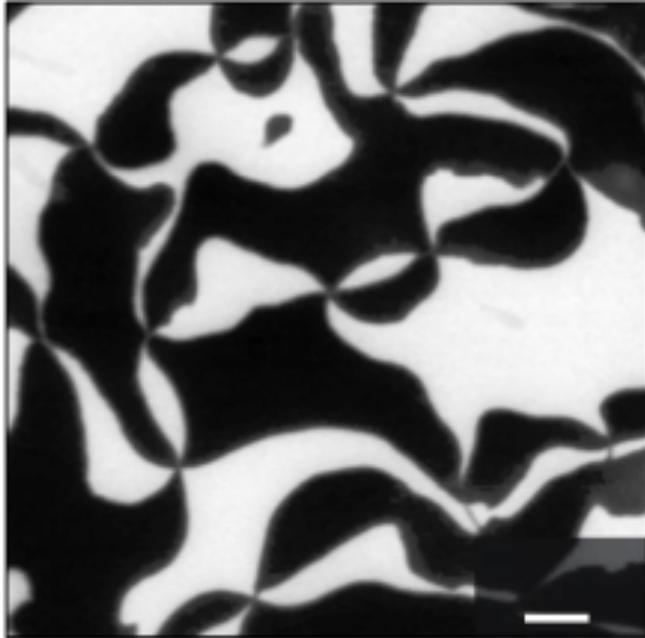


S. Artyukhin, K.T. Delaney, NAS and M. Mostovoy, *Landau theory of topological defects in multiferroic hexagonal manganites*, Nature Materials, 13, 42 (2014)

S. Griffin, M. Lilienblum, K. Delaney, Y. Kumagai, M. Fiebig and NAS, *Scaling behaviour and beyond equilibrium in the hexagonal manganites*, PRX 2, 041022 (2012)

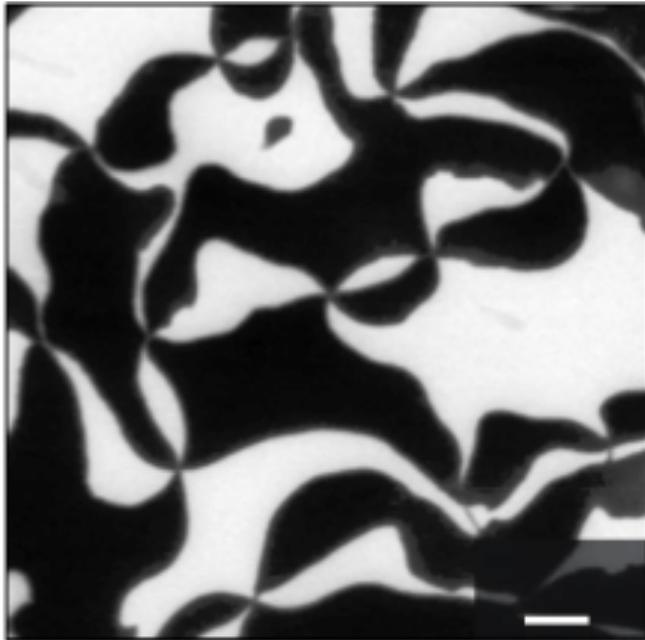
And the details of our “Mexican Hat-like” potential make it easy for us to measure!

Piezoforce Microscopy Image of  
the Defects in YMnO<sub>3</sub>

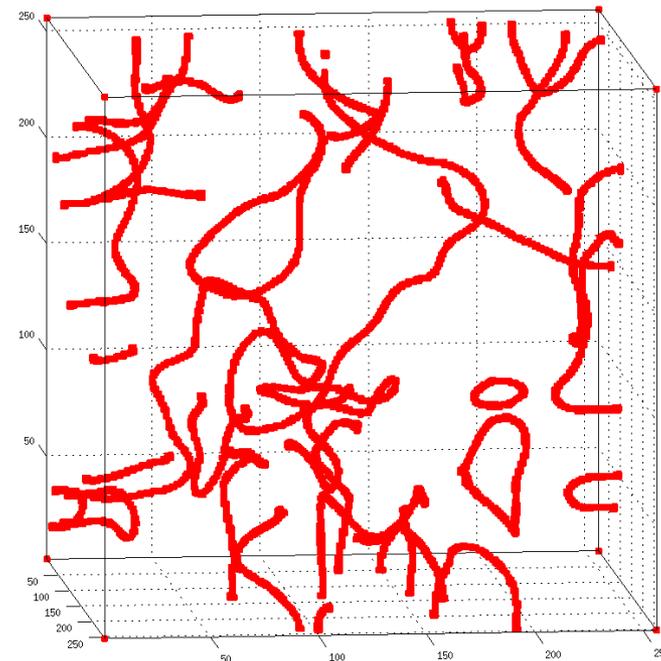


# The meeting points of the ferroelectric domains are in fact one-dimensional “strings”

Piezoforce Microscopy Image of the Defects in  $\text{YMnO}_3$



3-D Simulation



$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = H \Psi(\mathbf{r}, t)$$

## One last requirement:

The phase transition must be described by a non-trivial homotopy group (for the defects to be topologically protected)

# When are two objects homotopic?

- ✓ **Allowed:** Stretch, twist, bend, pull, shrink, enlarge, squeeze
- ✗ **Not allowed:** Cutting, pasting, or volumes shrinking to zero

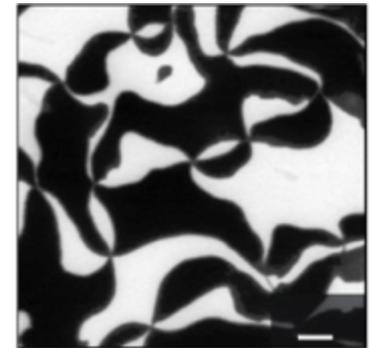
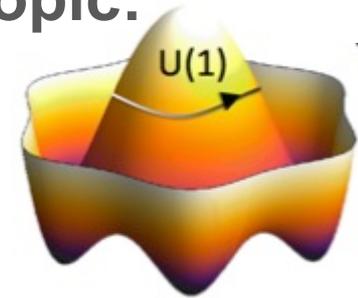


Homotopic

Not  
Homotopic

# Fortunately there exists a “recipe” for working out whether a phase transition of continuous symmetry is homotopic:

- 1) Map the symmetry characteristic of the order parameter –  $U(1)$  – onto an  $n$ -dimensional sphere: one-dimensional circle  $S^1$
- 2) Look up in a topology textbook whether the homotopy group  $\pi$  of  $S^1$  is non-trivial or not
- 3) In fact  $\pi_1(S^1)$  is non-trivial and produces 1-dimensional topologically protected singularities – these are the lines of intersection of the domains



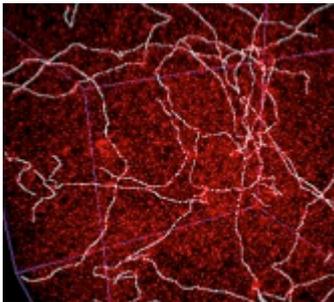
The domain intersections in  $YMnO_3$  are formally mathematically topologically protected

# The structural phase transition in multiferroic $\text{YMnO}_3$ fulfills the Kibble requirements!

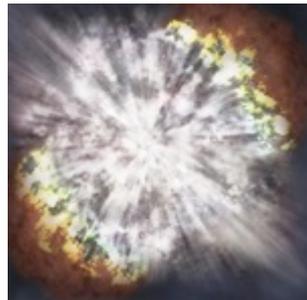
spontaneous symmetry breaking described by a non-trivial homotopy group

Results in formation of *topologically-protected defects*

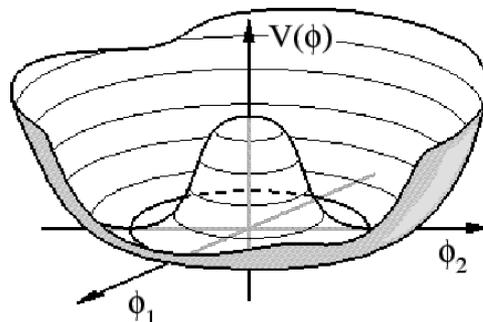
Early Universe



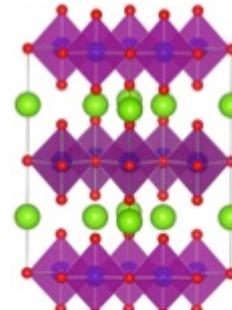
High symmetry vacuum



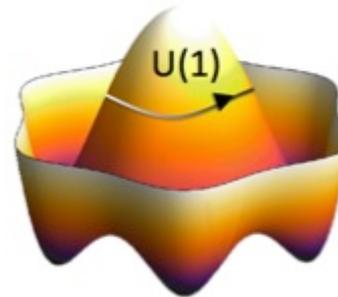
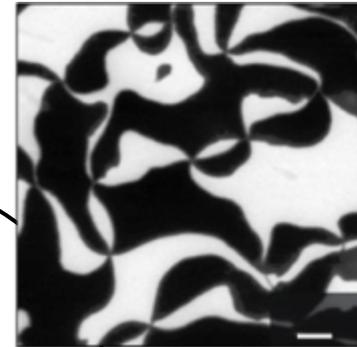
Low symmetry vacuum



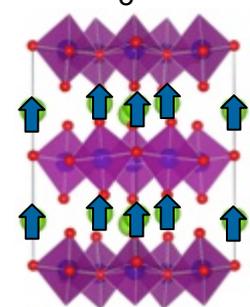
$P6_3/mmc$



$\text{YMnO}_3$



$P6_3cm$

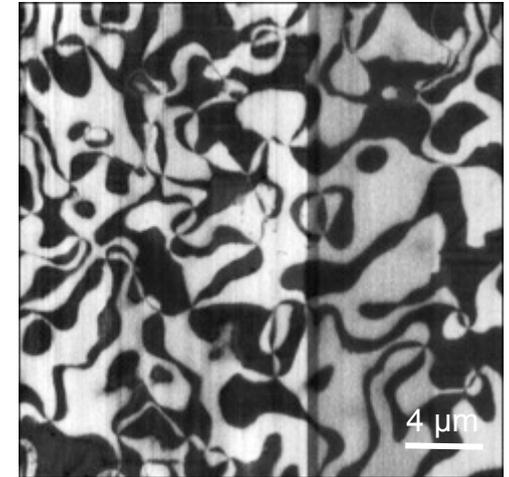
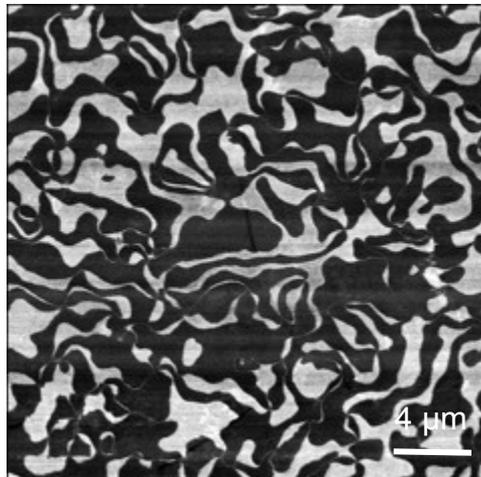
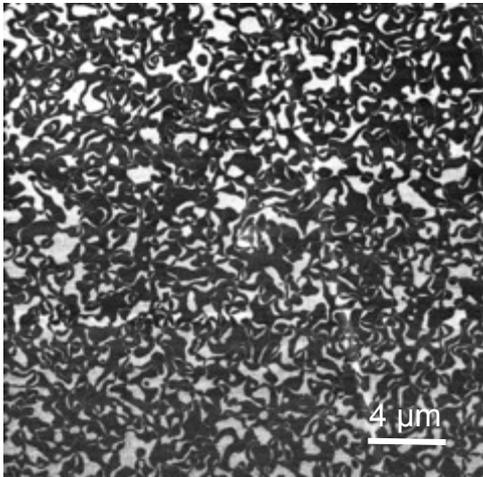


Does it behave as cosmologists predict?

# What experiment would we like to do on the early universe?

We'd like to expand it at different rates, crossing the GUT, and see how many cosmic strings form in each case

Instead we will cool  $\text{YMnO}_3$  at different rates through the structural phase transition and count how many domain intersections form



# Testing the Kibble-Zurek scaling law for defect formation

domain size,

defined as  $T_c$  (1400K) / cooling rate

$$d = \xi_0 \left( \frac{\tau_q}{\tau_0} \right)^{\frac{\nu}{1+\mu}}$$

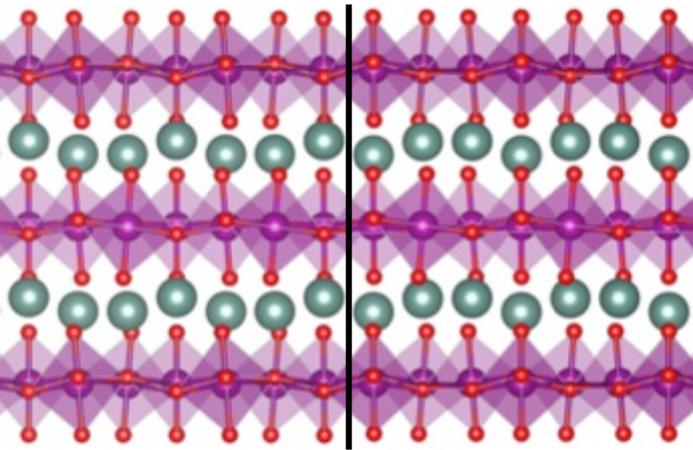
Critical exponents:  $\nu = 0.6717$

$\mu = 1.3132$

from MC simulations for 3D XY model

M. Campostrini et al., Phys. Rev. B 74, 144506 (2006)

zero-temperature correlation length  $\sim$   
domain wall width in ferroelectrics (DFT)



zero-temperature relaxation time =

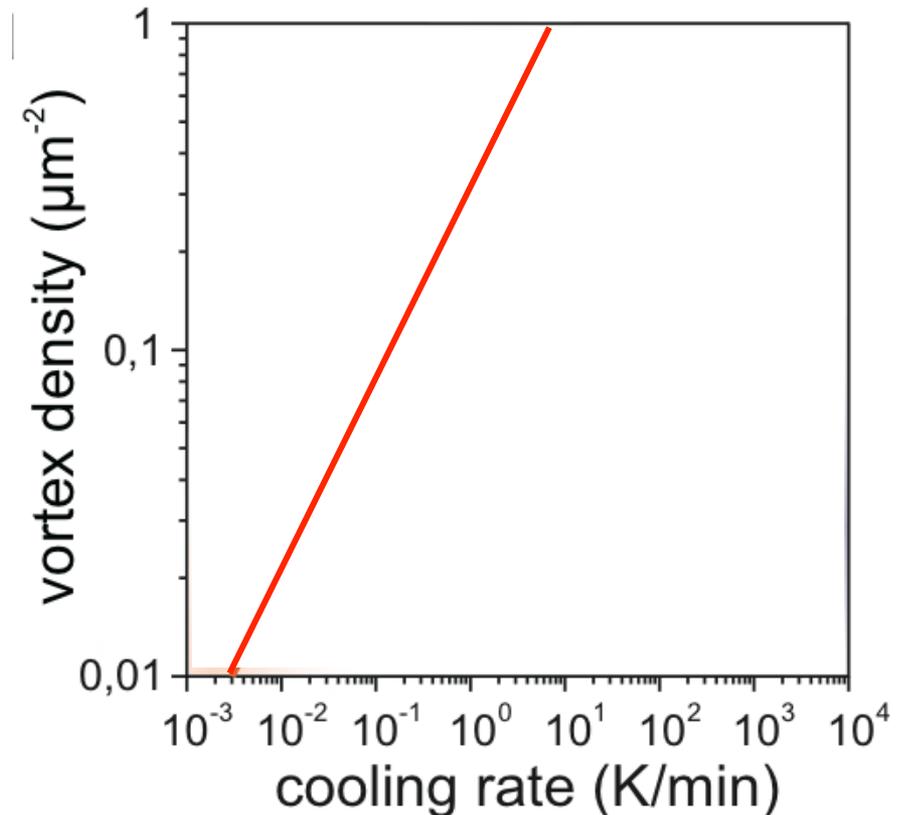
$\xi_0$  / speed of sound

speed of sound = 640 m/s (DFT)

Yu Kumagai and NAS, *Structural domain walls in polar hexagonal manganites*, Nat. Comm. 4, 1540 (2013)

# Comparison of KZ theory (DFT parameters) with experiment

Red line: our calculations  
with  $\xi_0 = 0.06 \text{ \AA}$



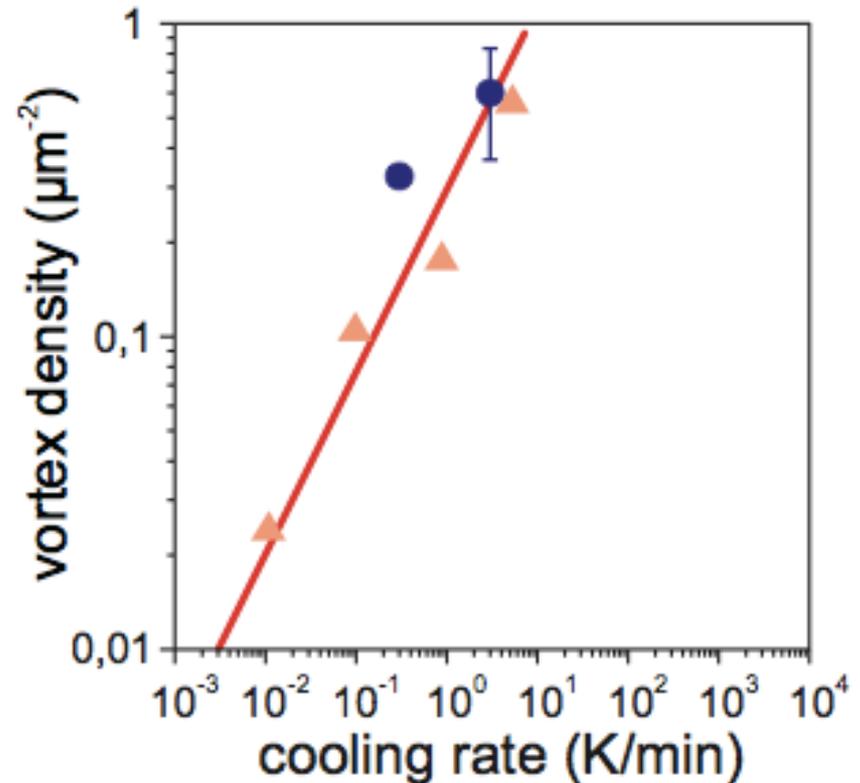
# Comparison of KZ theory (DFT parameters) with experiment

Red line: our calculations  
with  $\xi_0 = 0.06$  A

Red triangles: measured by Chae et al.

Blue circles: measured by Fiebig et al.

KIBBLE-ZUREK BEHAVIOR!



S. C.. Chae et al., *Direct observation of the proliferation of ferroelectric loop domains and vortex-antivortex pairs*, PRL **108**, 167603 (2012)

S. Griffin, M. Lilienblum, K. Delaney, Y. Kumagai, M. Fiebig and N. A. Spaldin, *Scaling behaviour and beyond equilibrium in the hexagonal manganites*, PRX **2**, 041022 (2012)

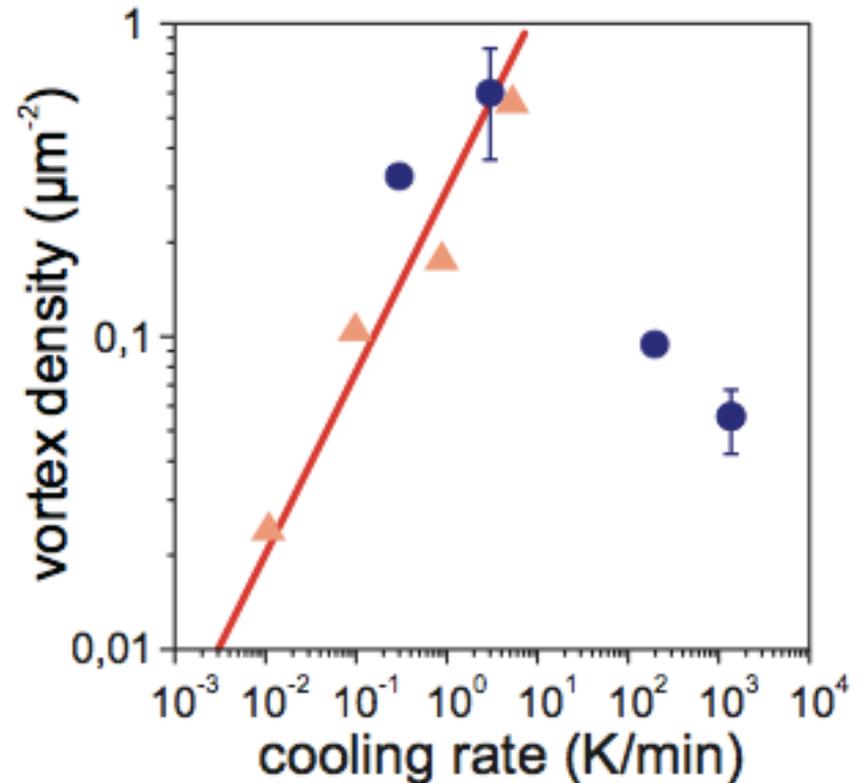
# Comparison of KZ theory (DFT parameters) with experiment

Red line: our calculations  
with  $\xi_0 = 0.06$  A

Red triangles: measured by Chae et al.

Blue circles: measured by Fiebig et al.

KIBBLE-ZUREK BEHAVIOR  
AT SLOW COOLING RATES!

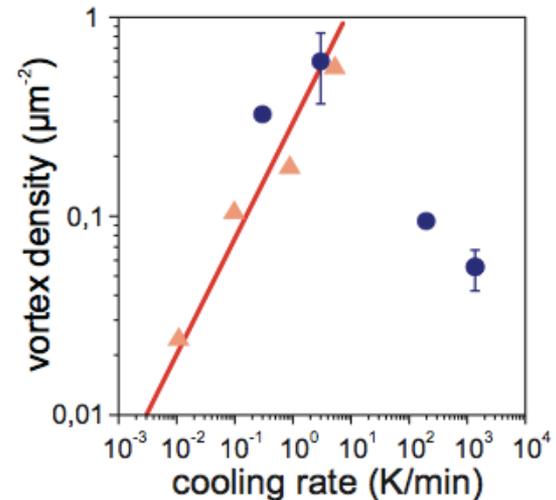


## Open questions:

Are we now able to explore the “beyond-Kibble-Zurek” regime?

If so, what is the origin of the turnaround?

Or do we not have K-Z behavior at all?

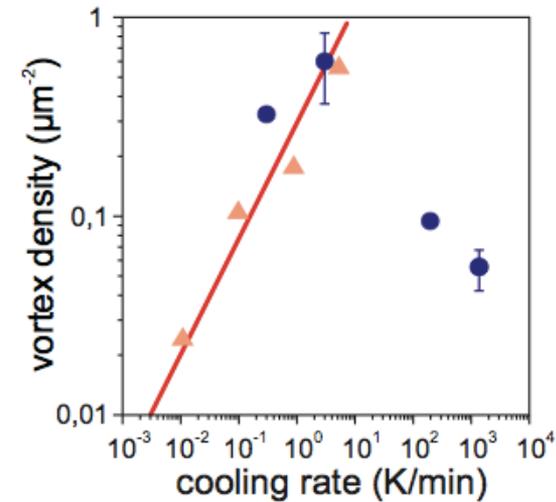


## Open questions:

Are we now able to explore the “beyond-Kibble-Zurek” regime?

If so, what is the origin of the turnaround?

Or do we not have K-Z behavior at all?



## What next?

More samples / more measurements

A room-temperature system?

Early cosmic string dynamics / evolution?

## Summary

YMnO<sub>3</sub> seems to provide the first example of Kibble-Zurek scaling in a condensed matter system

Cosmic strings formed the way cosmologists thought ;)

Use of real materials to explore questions in cosmology is a lot of fun



Table-top astrophysics

## How to build a multiverse

Small models of cosmic phenomena are shedding light on the real thing

Mar 16th 2013 | From the print edition



Whether all this ingenuity unravels any cosmic truth is uncertain. Cliff Burgess, a theorist at Perimeter Institute for Theoretical Physics in Ontario, has his doubts. But he thinks that such experiments are nevertheless worth pursuing. "Like tap-dancing snakes," he says, "the point is not that they do it well, it is that they do it at all."