

Self-organisation and phase transitions in ion Coulomb Crystals

Ramil Nigmatullin

C³ Symposium
11 December 2017



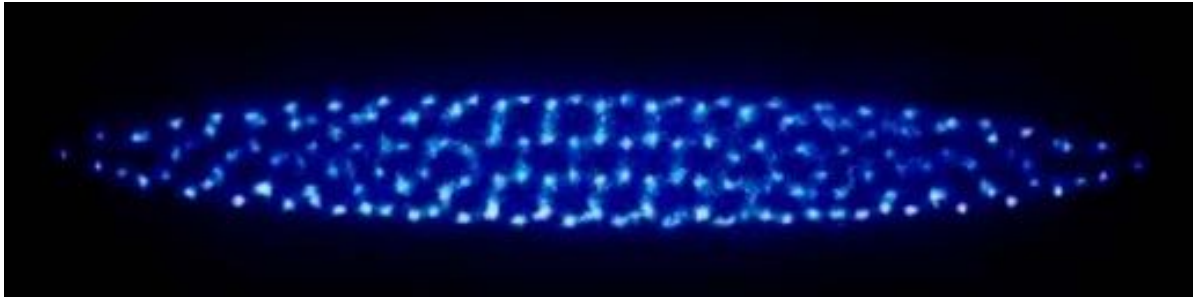
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SYDNEY

Outline

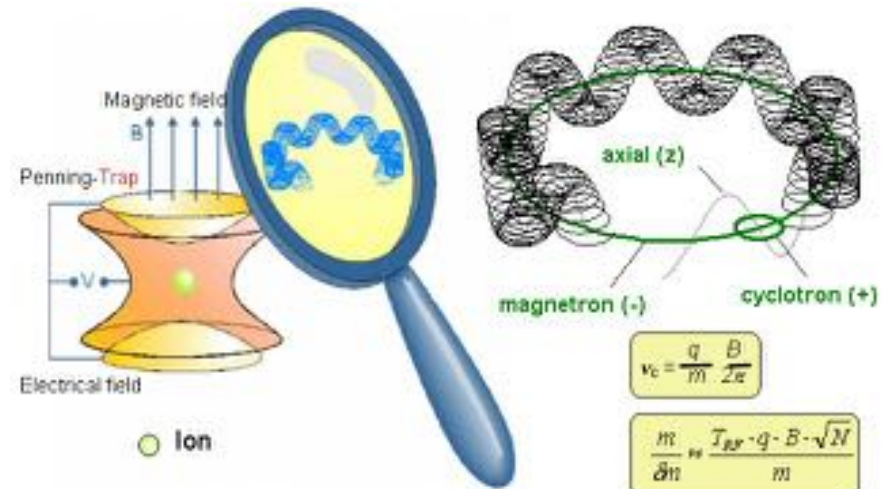
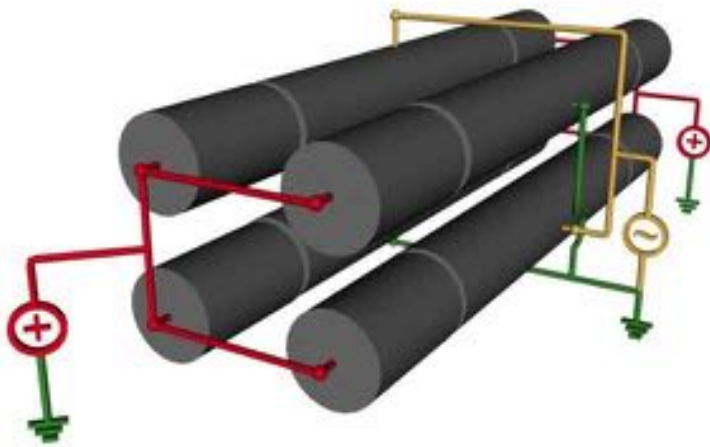
- Ion Coulomb crystals as models of collective phenomenon
- Collective Phenomenon 1 – formation of topological defects
 - Kibble-Zurek mechanism
- Collective Phenomenon 2 - pinned to sliding transition between atomic contacts
 - Aubry phase transition

Coulomb crystals

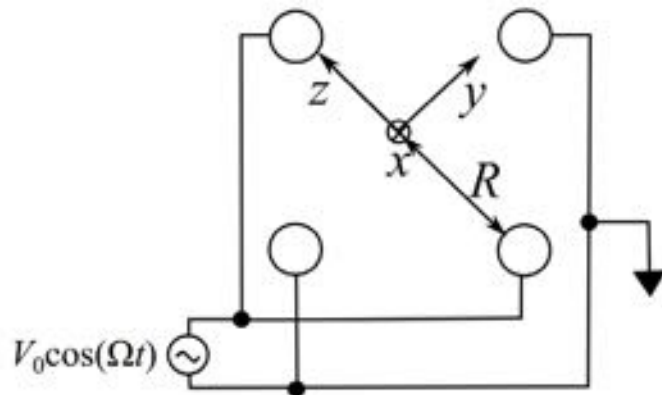
- Paul or Penning traps + Laser Cooling = ion Coulomb crystals
- Few control parameters but complex structures
- Crystals of electrons is known as Wigner crystal



Paul Trap and Penning Trap



ν_c : cyclotron frequency q : charge of the ion m : ion mass B : magnetic field strength



Equations of motion

The potential energy of N ions in a Paul or Penning trap using the pondermotive approximation is

$$V = \frac{1}{2}m \sum_i^N (\omega_x^2 x_i^2 + \omega_y^2 y_i^2 + \omega_z^2 z_i^2) + \frac{e^2}{4\pi\epsilon_0} \sum_{i \neq j}^N \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

Under the influence of laser cooling, equations of motion are approximately

$$m \frac{d^2 \mathbf{r}_j}{dt^2} + \eta \frac{d\mathbf{r}_j}{dt} + \nabla V = \xi_j(t)$$

where $\langle \xi_{\alpha j}(t) \rangle = 0$ and $\langle \xi_{\alpha j}(t) \xi_{\beta k}(t') \rangle = 2k_B T \delta_{\alpha\beta} \delta(t - t')$

Ion Coulomb crystals in Penning Traps

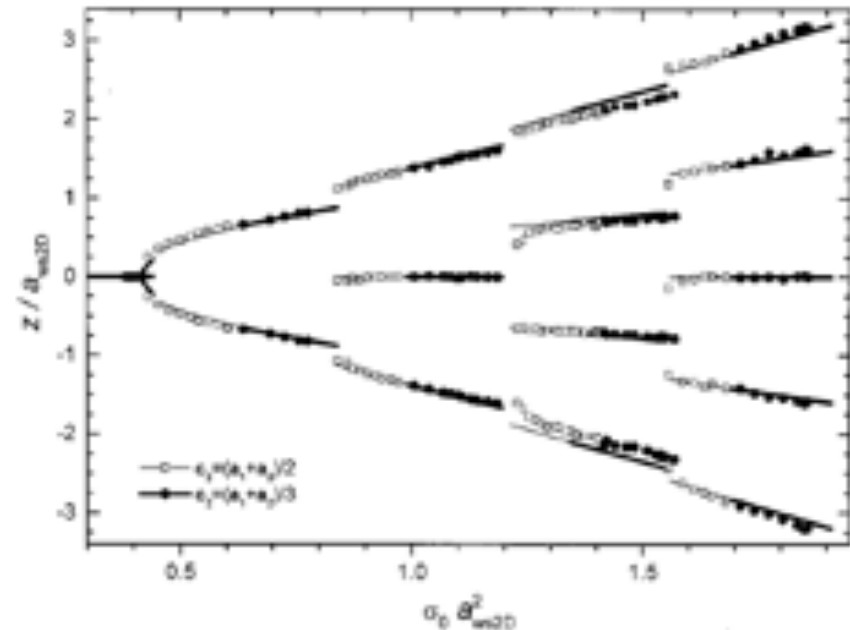
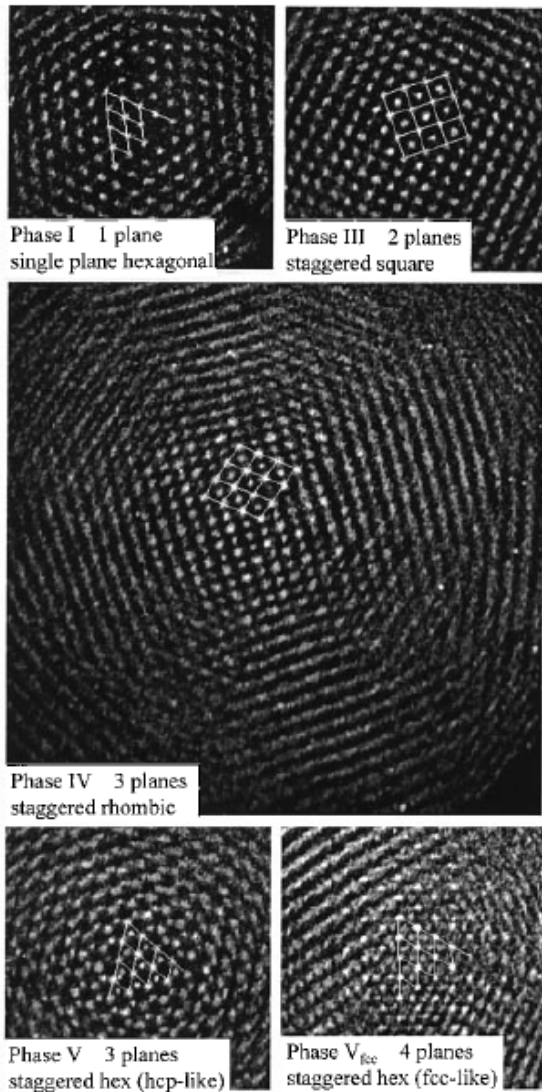
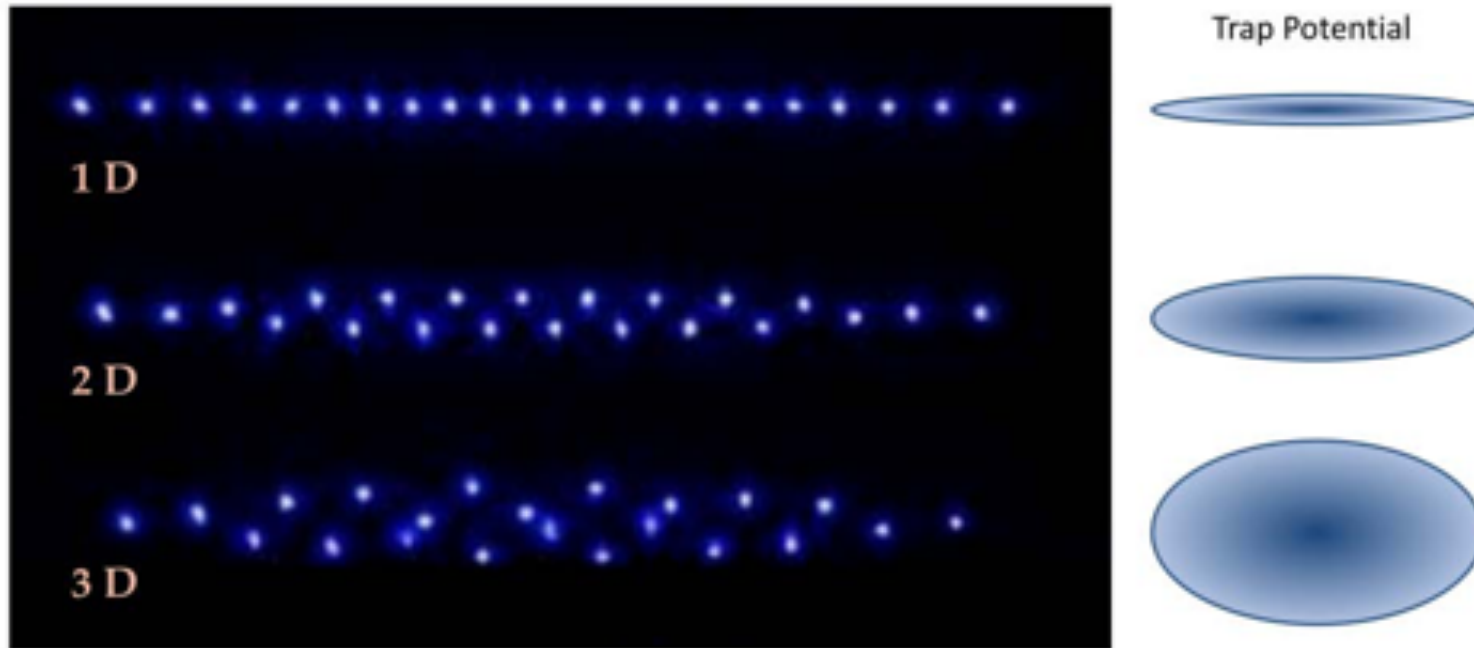


Fig. 3 (left). Interlayer structure (plane axial positions and displacement vectors) of the central region as a function of normalized central areal charge density. The lines show predictions from theory, and symbols show experimental measurements. The symbols indicate whether the lattices had an interlattice displacement vector ϵ_2 that was characteristic of the hexagonal phases (circles) or the square and rhombic phases (squares). Lengths have been normalized by $a_{ws20} = (3e^2/4\pi\epsilon_0 m\omega_z^2)^{1/3}$

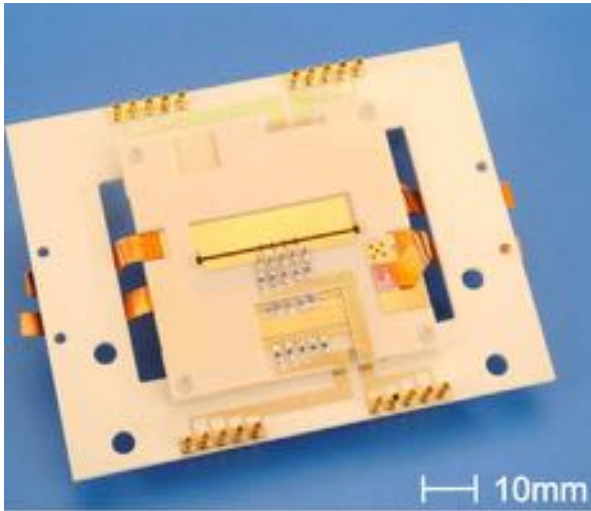
Science, 282, 1290, (1998)

Ion Coulomb crystals in Paul Traps

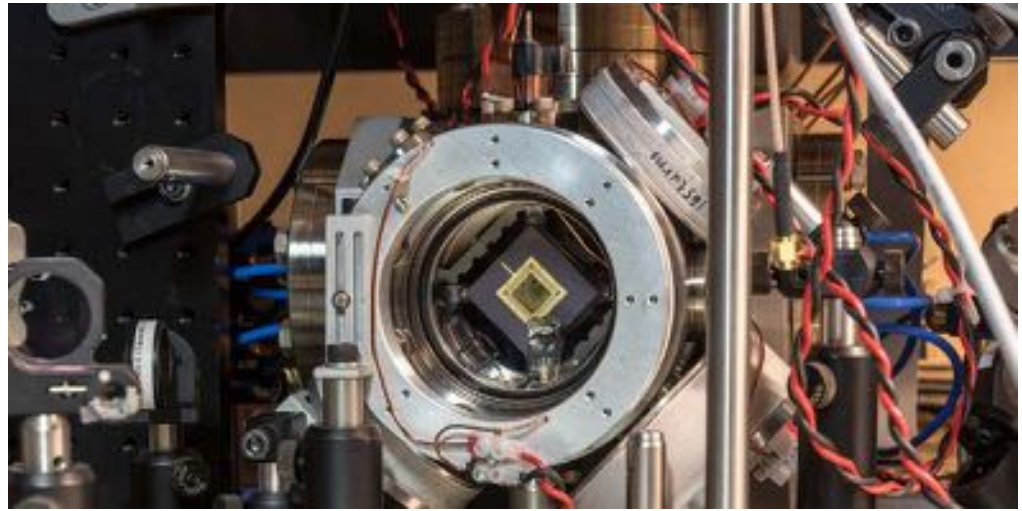


PTB

How does the trap typically look like?



Miniturized Paul trap | Credit: PTB/Karsten Pyka



Ion trap experimental setup | Credit: NQIT/Stuart Bebb

Applications

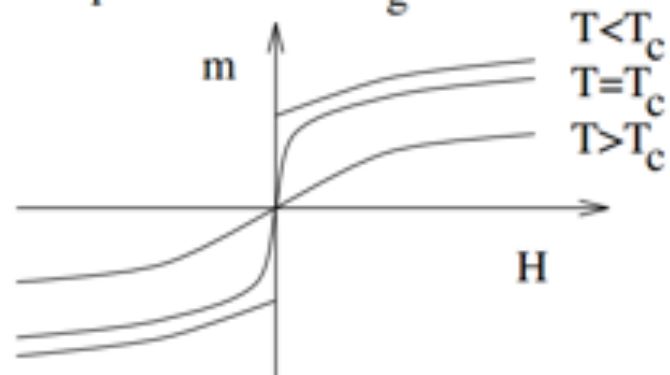
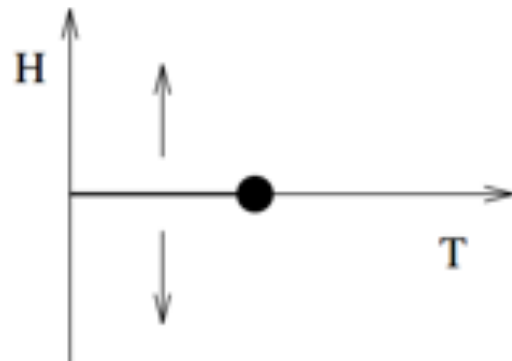
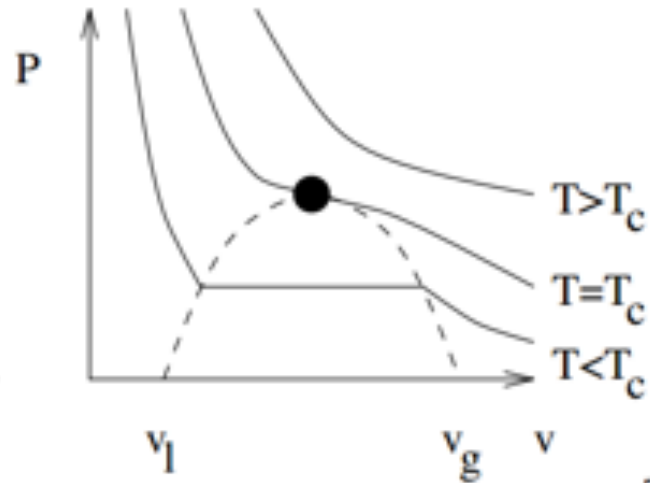
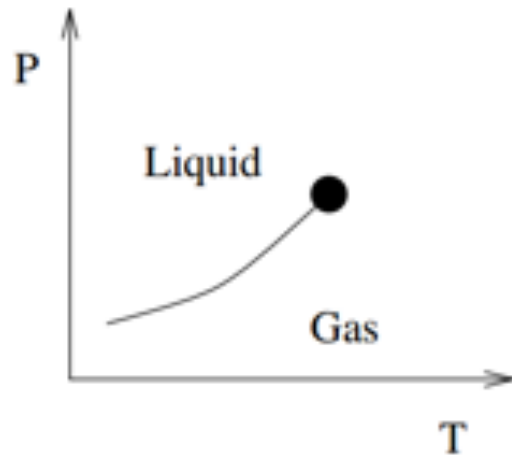
- Spectroscopy, metrology
- Quantum computing, **complexity and self-organization**

Collective phenomenon 1 – Formation of topological defects

Thermodynamic Phase Transitions

- Correspond to abrupt changes in thermodynamic quantities
- Can be first or second order
- Qualitative behavior near critical points is does not depend on microscopic details of the system

Thermodynamic Phase Transitions



Critical exponents

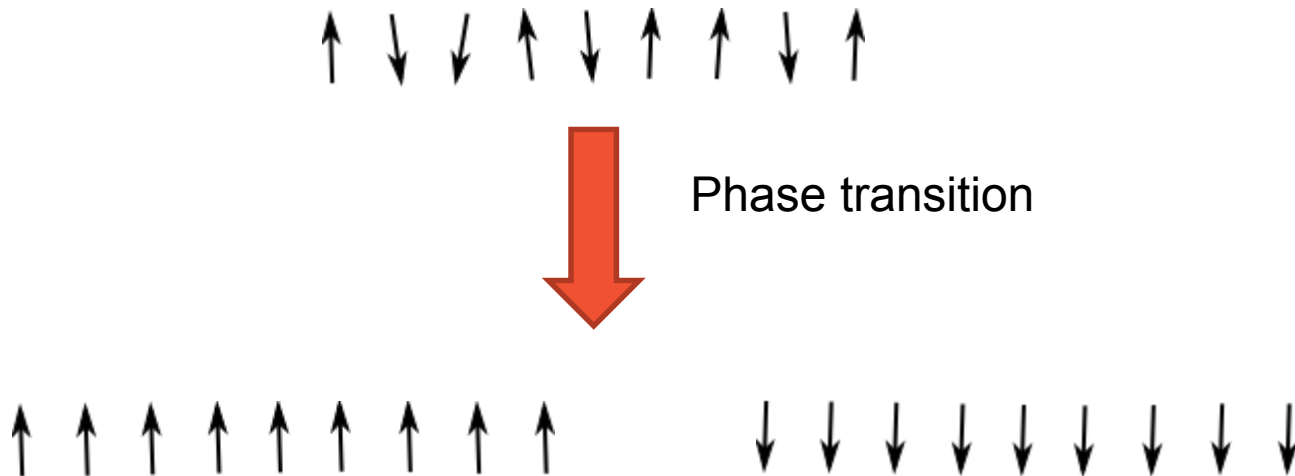
- The vicinity of the critical point of 2nd order phase transition is characterized by divergences in thermodynamic quantities, e.g. heat capacity, susceptibility, correlation length, relaxation time etc.

- Divergence of correlation length and relaxation time

$$\xi = \frac{\xi_0}{|\epsilon|^\nu} \quad \tau = \frac{\tau_0}{|\epsilon|^\mu} \quad \epsilon = \frac{T_C - T}{T_C}$$

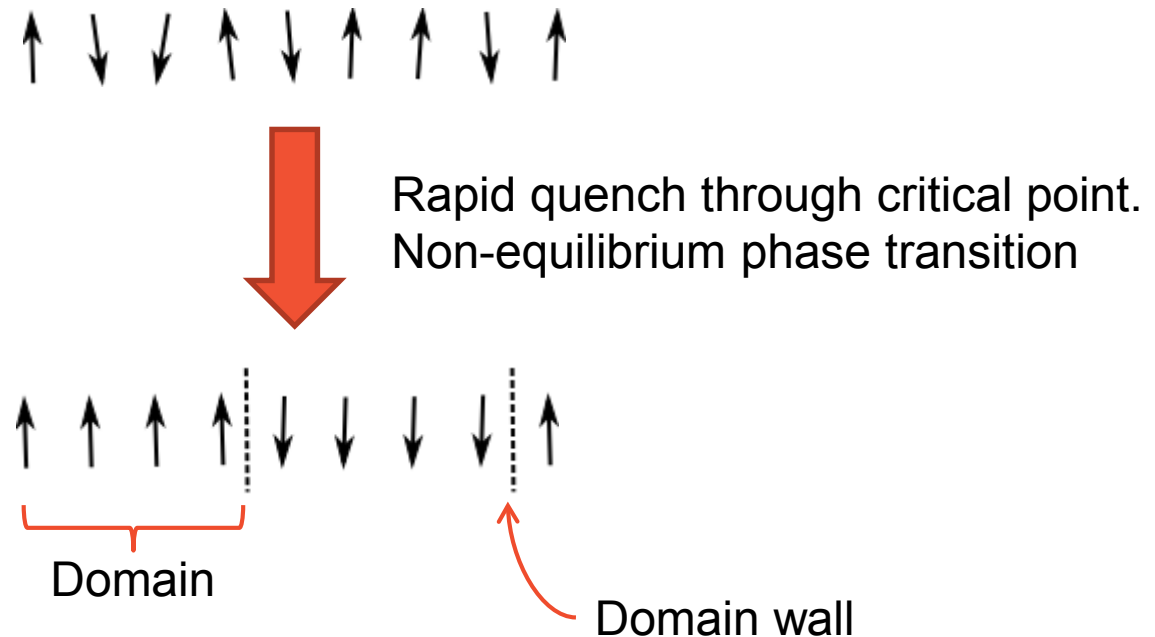
- Exponents ν and μ are **universal**

Non-equilibrium Phase Transitions

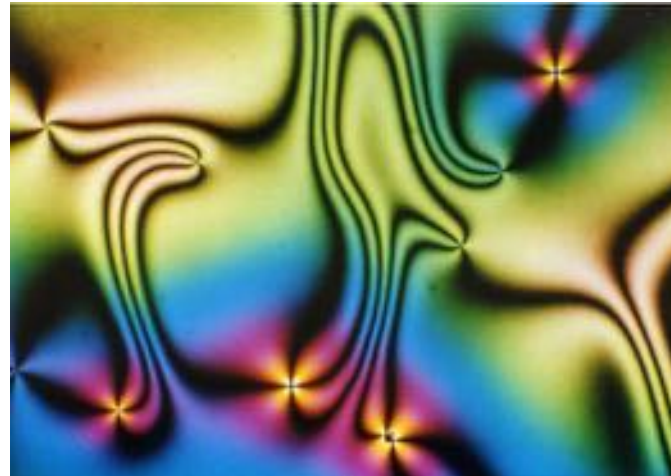
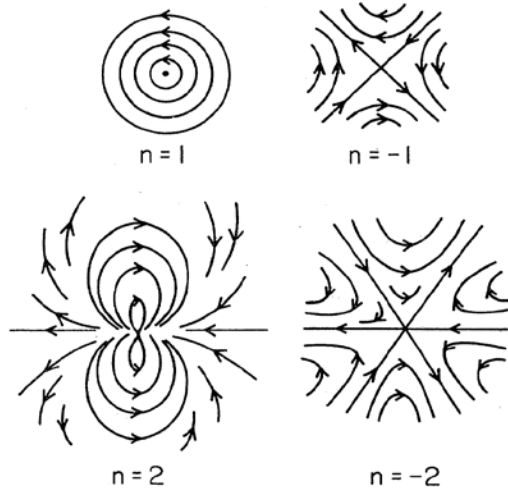


Non-equilibrium Thermodynamic Phase Transitions

Formation of defects



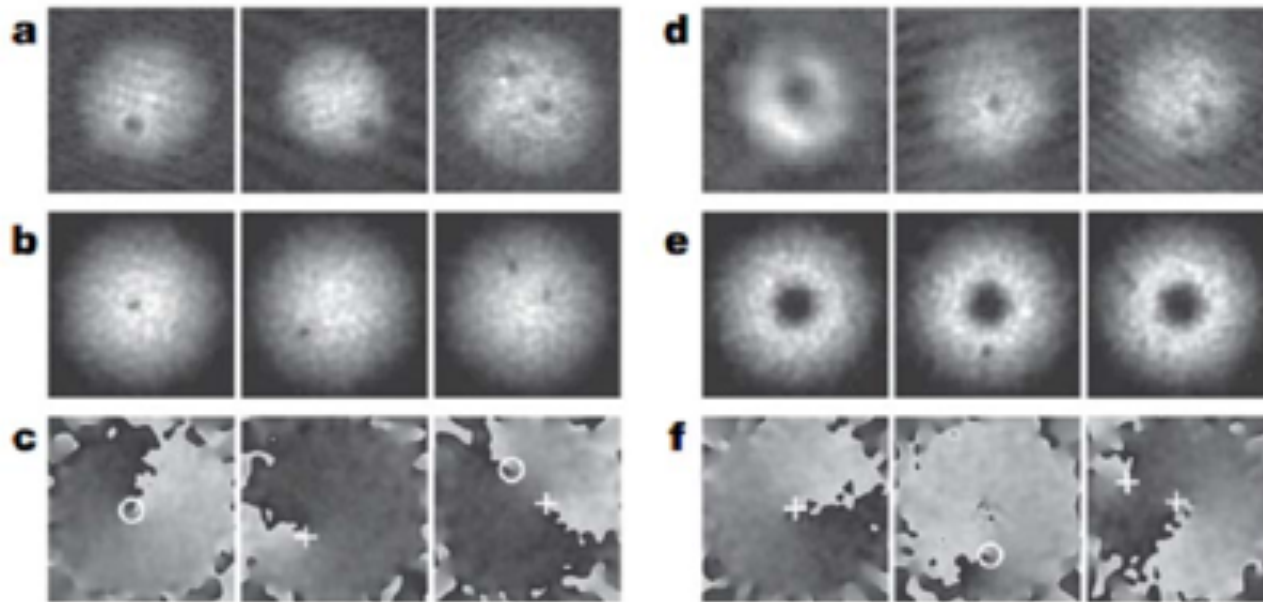
Defects in various systems



O.Lavrentovich/Kent State Univ.

Defects in various systems

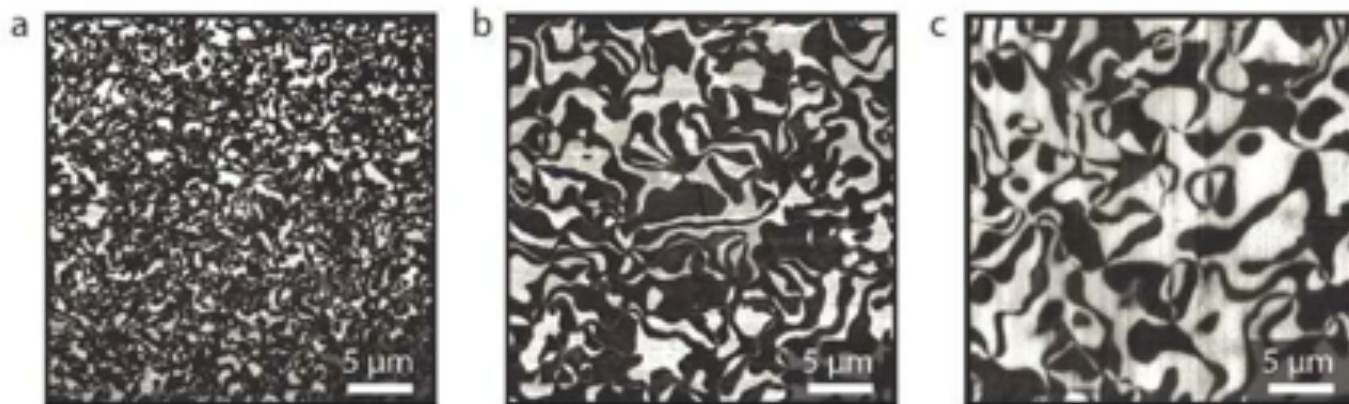
Bose-Einstein condensates



B. P. Anderson, Nature, 455, 948 (2008)

Defects in various systems

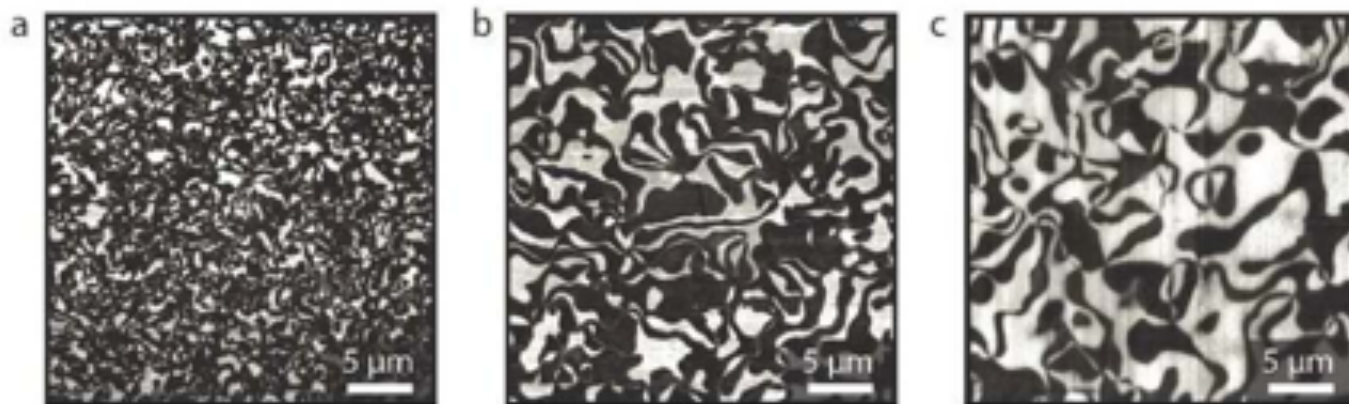
Ferroelectric domains of YMnO_3



N. A. Spaldin *et al*, Phys. Rev. X 2, 041022 (2012)

Defects in various systems

Ferroelectric domains of YMnO_3



Question: how does the probability of creating a defect depends on the rate of change of the control parameter?

Kibble-Zurek mechanism

How does the number of defects depends on the quench rate?

Cosmological experiments in superfluid helium?

W. H. Zurek

Theoretical Astrophysics, Los Alamos National Laboratory,
Los Alamos, New Mexico 87545, USA

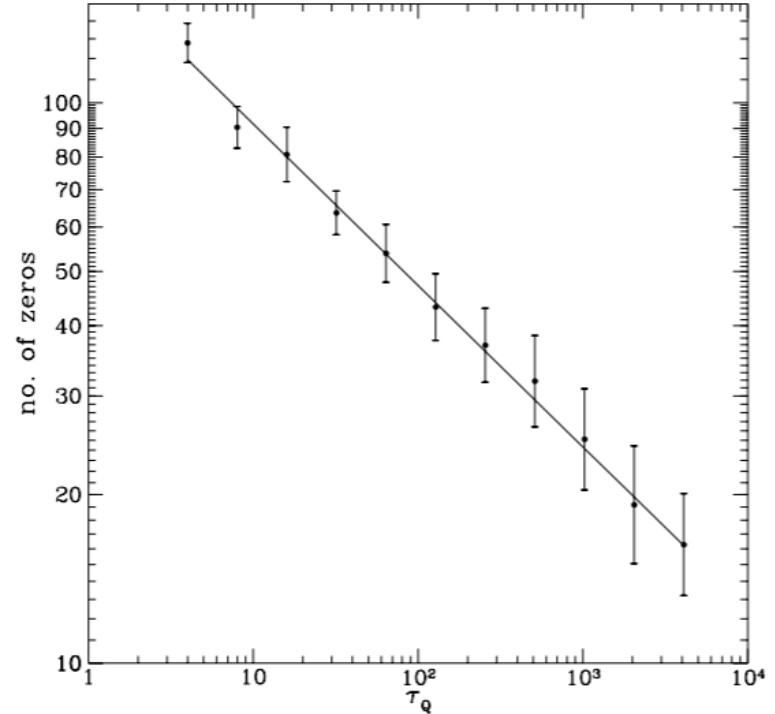
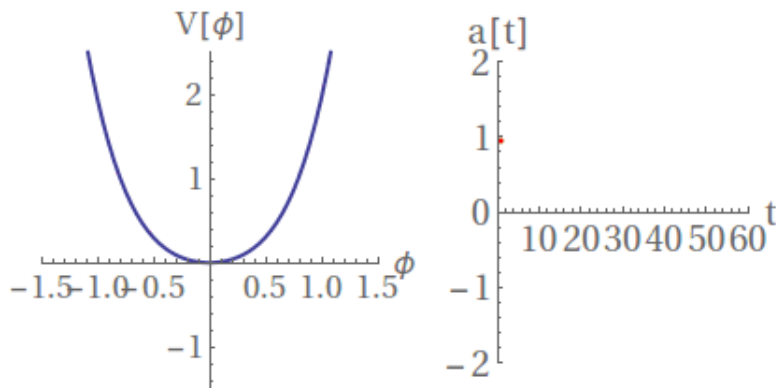
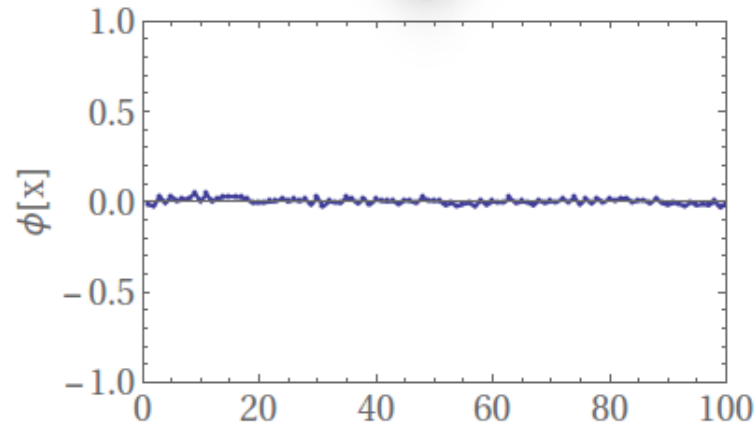
Symmetry breaking phase transitions occurring in the early Universe are expected to leave behind long-lived topologically stable structures such as monopoles, strings or domain walls^{1–6}. Here I discuss the analogy between cosmological strings and vortex lines in the superfluid, and suggest a cryogenic experiment which tests key elements of the cosmological scenario for string formation. In a superfluid obtained through a rapid pressure quench, the phase of the Bose condensate wavefunction—the ⁴He analogue of the broken symmetry of the field-theoretic vacuum—will be chosen randomly in domains of some characteristic size d . When the quench is performed in an annulus of circumference C the typical



Nature 317, 505–508
(1985)

Formation of domains during phase transitions

- Time Dependent Ginzburg Landau simulation



Phys. Rev. Lett. 78, 2519 (1996)

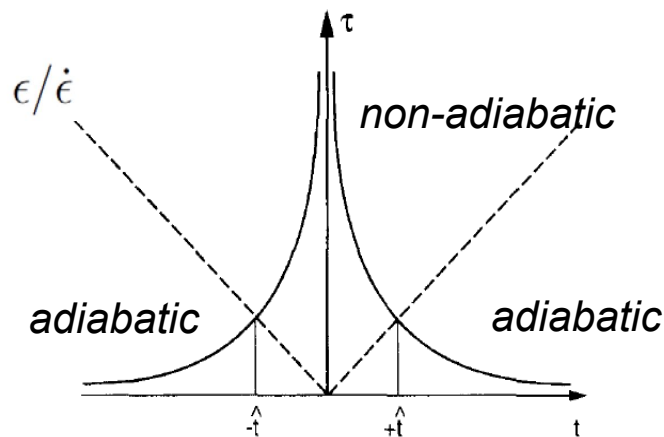
Kibble-Zurek mechanism

- Divergence of correlation length and relaxation time

$$\xi = \frac{\xi_0}{|\epsilon|^\nu} \quad \tau = \frac{\tau_0}{|\epsilon|^\mu} \quad \epsilon = \frac{T_C - T}{T_C}$$

- Linear quench $\epsilon(t) = -\frac{t}{\tau_Q}$

- Use the condition, $\tau(\hat{t}) = |\hat{t}|$, to signal the breakdown of adiabaticity



Kibble-Zurek mechanism

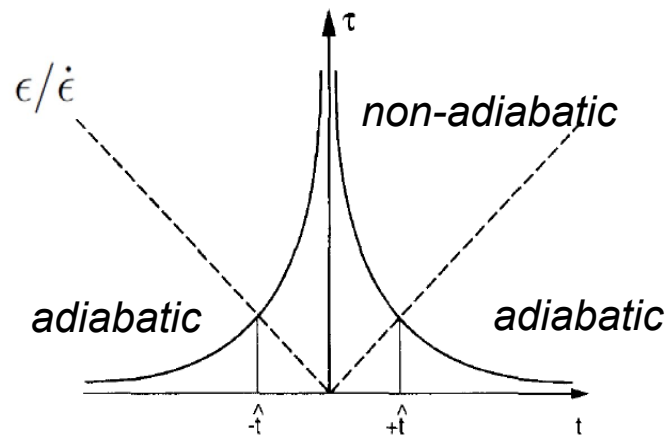
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- Linear quench $\epsilon(t) = -\frac{t}{\tau_Q}$

Kibble-Zurek mechanism

- Use the condition, $\tau(\hat{t}) = |\hat{t}|$ to signal the breakdown of adiabaticity



- Leads to maximum correlation length

$$\hat{\xi} \approx \xi_0 \left(\frac{\tau_Q}{\tau_0} \right)^{\nu/(1+\mu)}$$

Experimental tests of Kibble-Zurek scaling law

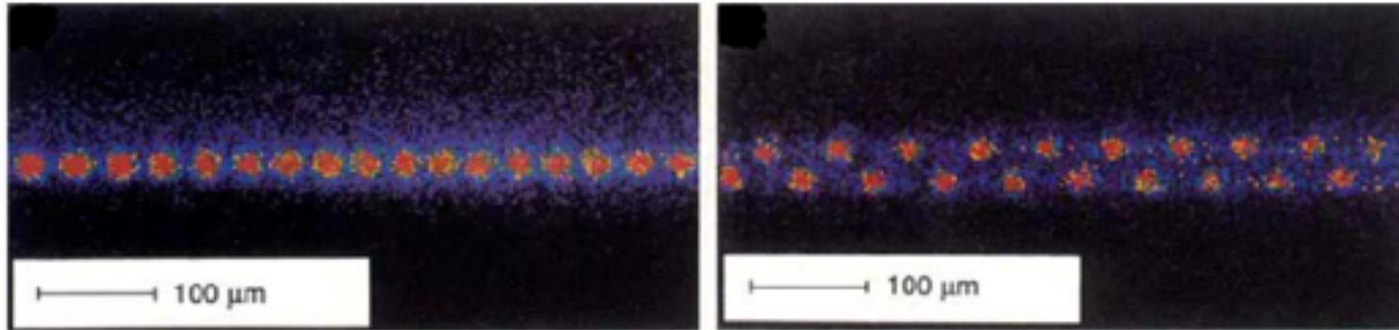
Challenges

- precise variation of the control parameter over several orders of magnitude
- Inhomogeneities and impurities in the system
- Finite size of the system
- Equilibrium critical exponents may be unknown

Examples of the systems where KZ mechanism has been observed

- Bose-Einstein condensates
- Ferroelectrics
- **Ion crystals**
- . . .

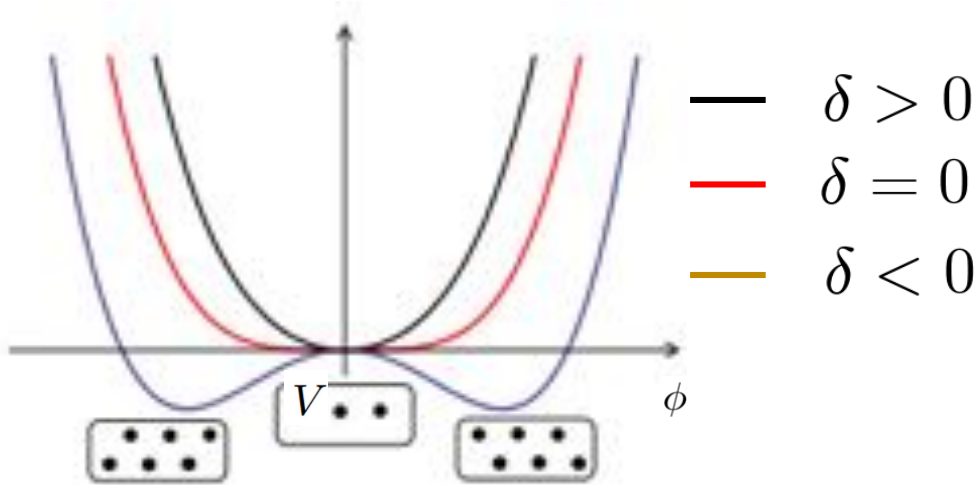
Linear to zigzag phase transition in Coulomb crystals



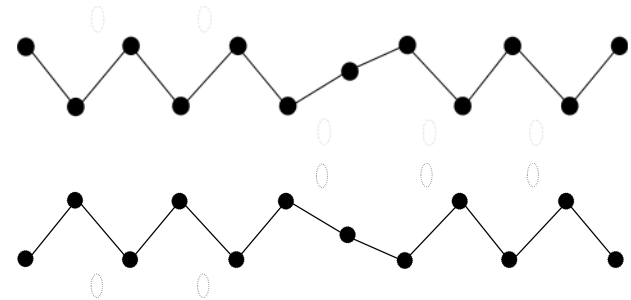
G.BirkI/MPQ

- Weakening of the confining potential induces PT
- Second order phase transition [Phys. Rev. B, 77, 064111 (2008)]
- Described by Ginzburg-Landau theory
- Both the static and dynamic critical exponents are known

Linear to zigzag transition

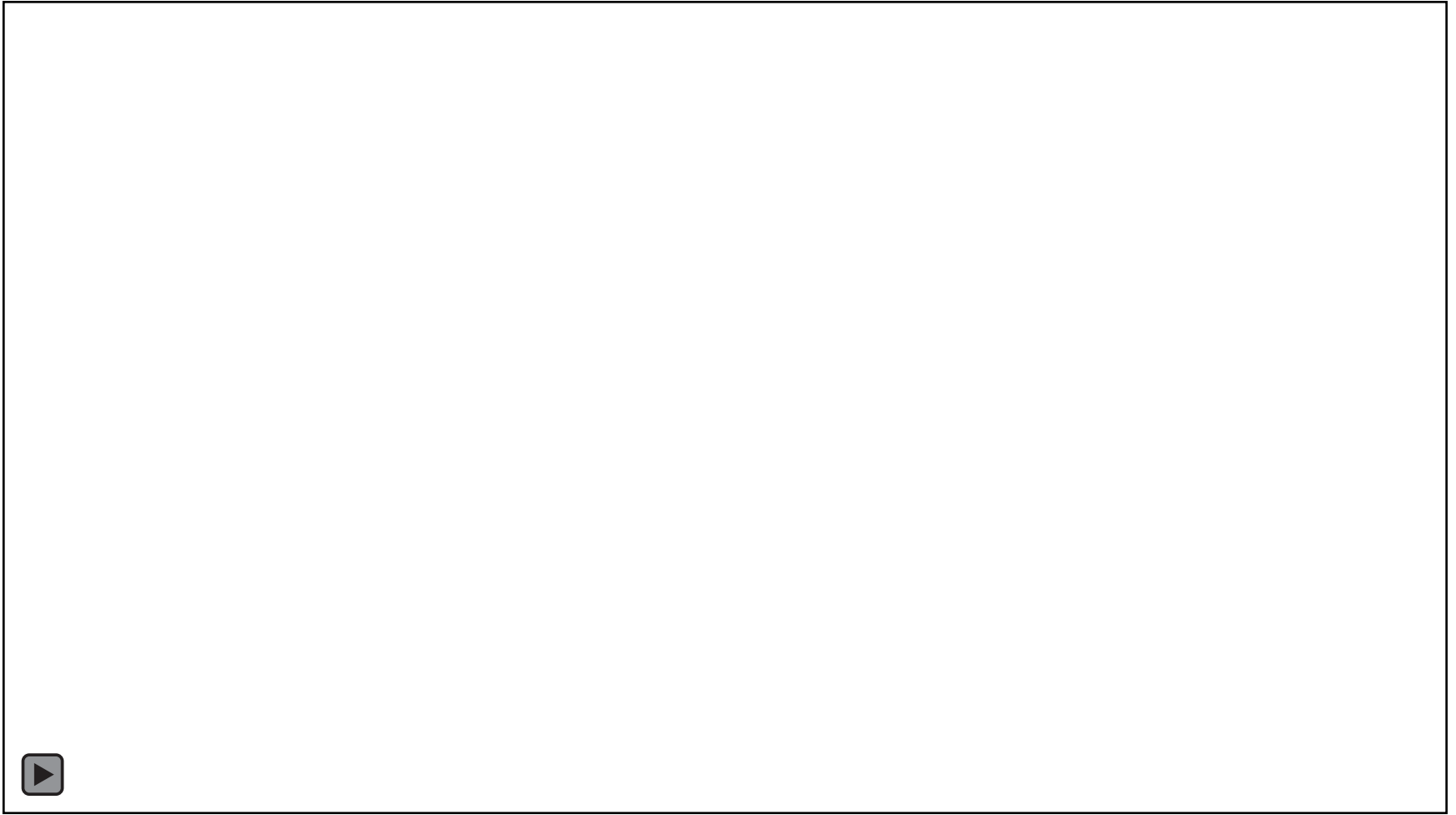


$$V = \delta\phi^2 + \phi^4$$



- Structure interpolates between two ground states
- Resistant to perturbations

Typical experimental runs



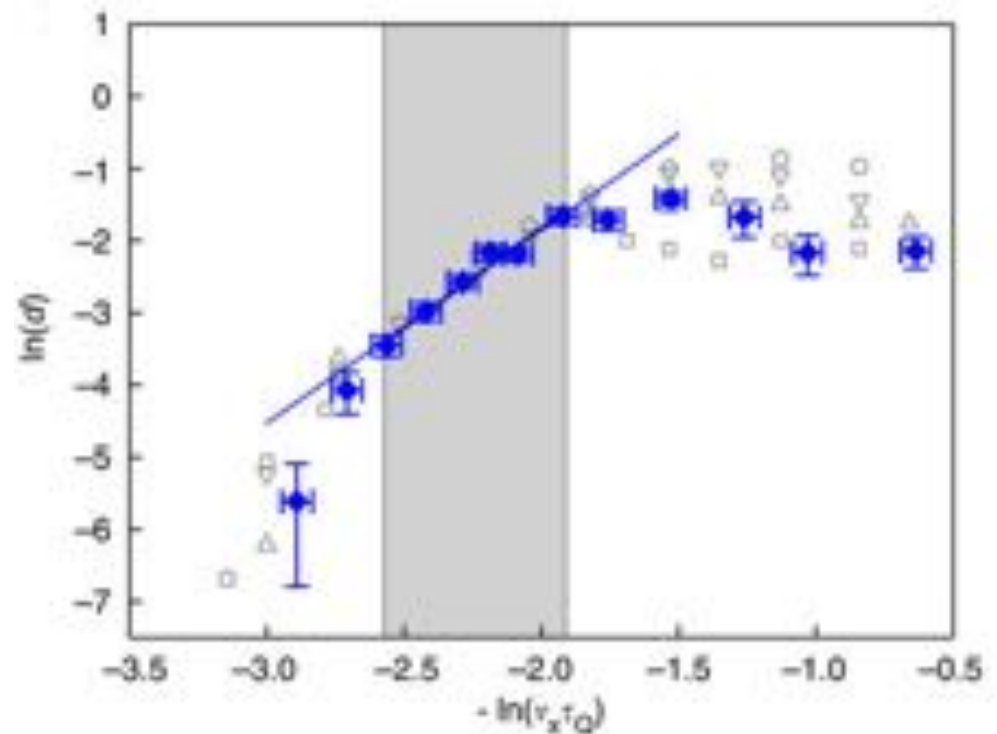
Nature Communications, 4, 2291, (2013)

Results

- KZ mechanism and scaling observed in ion crystals

However

- System is small – finite size effects
- System is inhomogeneous

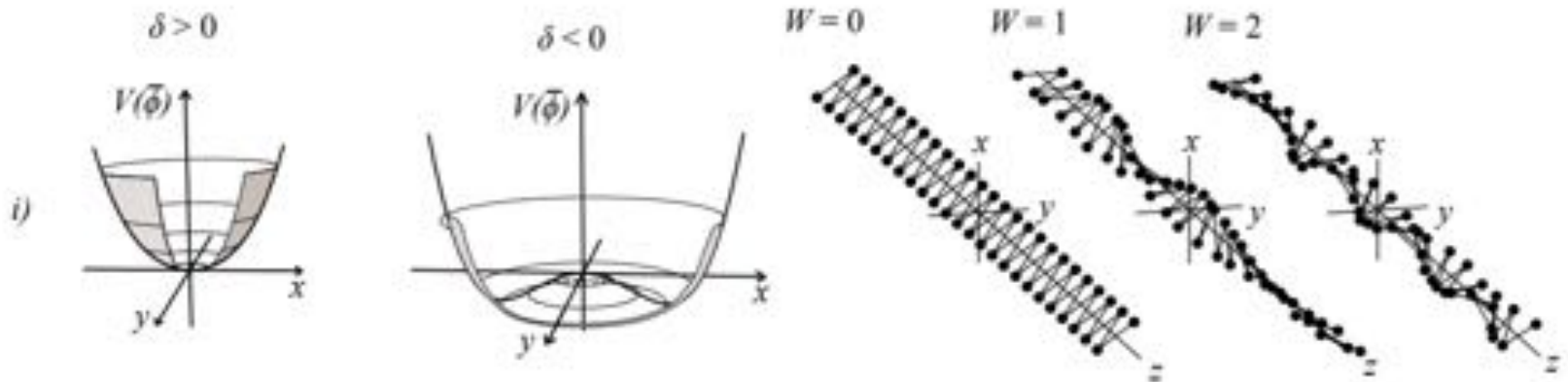


Further work

- Accounting for inhomogeneities and finite size effects
- Stochastic thermodynamics – entropy production
- Quantum regime
- First order phase transitions?
- Other geometries

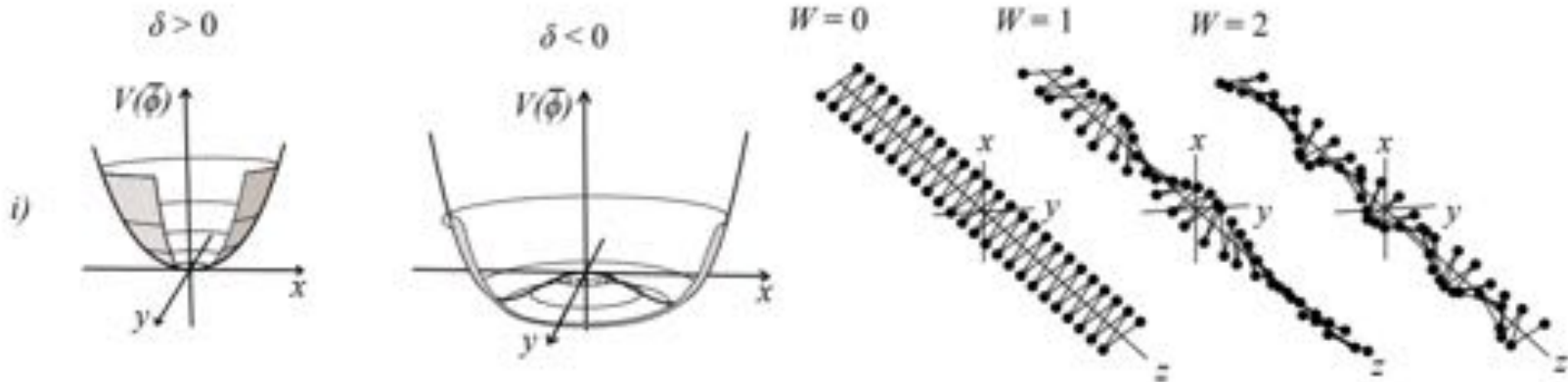
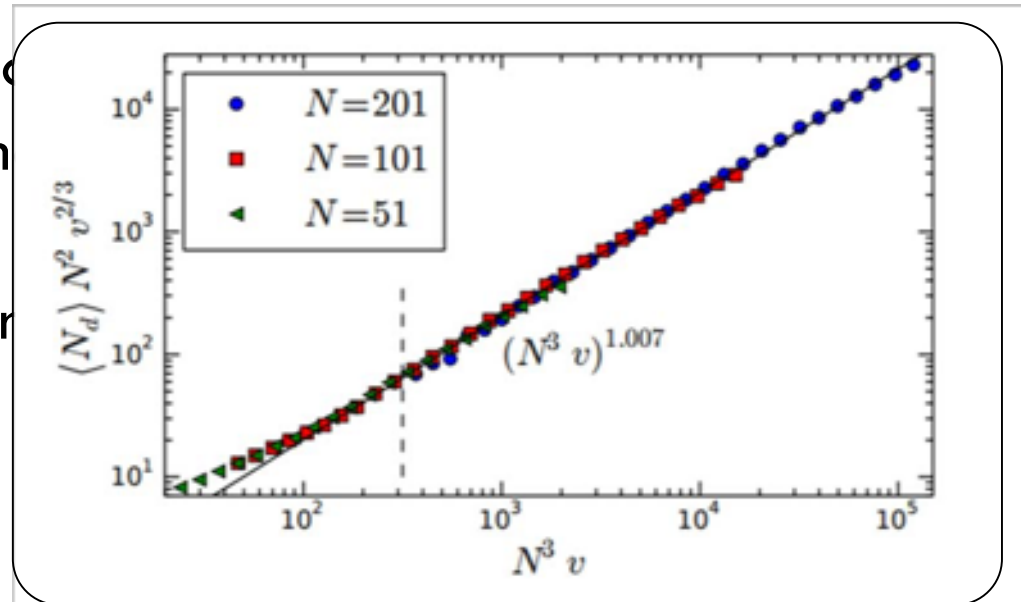
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Further work

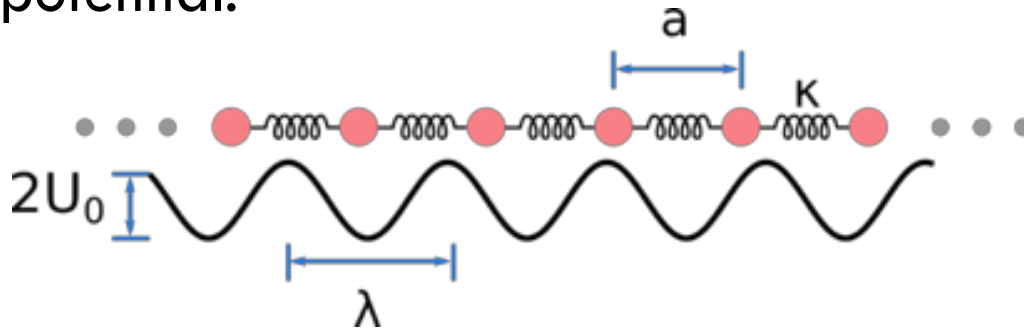
- Accounting for inhomogeneities
- Stochastic thermodynamics
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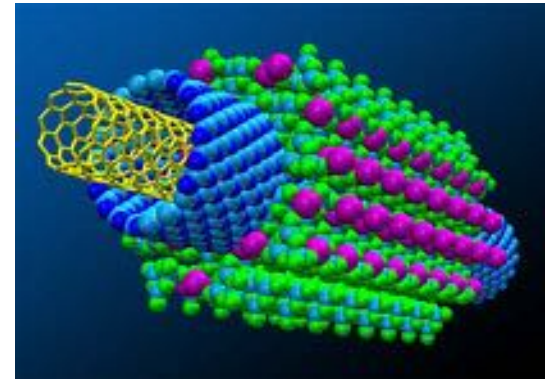
Collective phenomenon 2 – Aubry phase transition

Aubry phase transition

Consider a chain of coupled particles moving in a periodic potential.



This is a good model of nanofriction



For incommensurate ratio a/λ there exist a transition from pinned to freely sliding chain.

This is the **Aubry transition**.

Frenkel-Kontorova model

A simple mathematical model for this system is the Frenkel-Kontorova model

$$V = \sum_j \left(\frac{1}{2} (u_{j+1} - u_j)^2 + \frac{\lambda}{2} (1 - \cos(\pi u_j / a)) \right)$$

The equilibrium configurations are found by solving a system of equations

$$\frac{\partial V(\{u_j\})}{\partial u_j} = 0$$

i.e.
$$-u_{j+1} - u_{j-1} + 2u_j + (\lambda\pi/2a) \sin(\pi u_j / a) = 0$$

Frenkel-Kontorova model

The iterative map

$$-u_{j+1} - u_{j-1} + 2u_j + (\lambda\pi/2a) \sin(\pi u_j/a) = 0$$

Can be written as

$$p_{i+1} = p_i + (\lambda\pi/2a) \sin(\pi\theta_i/a)$$

$$\theta_{i+1} = p_i + \theta_i + (\lambda\pi/2a) \sin(\pi\theta_i/a) \bmod 2a$$

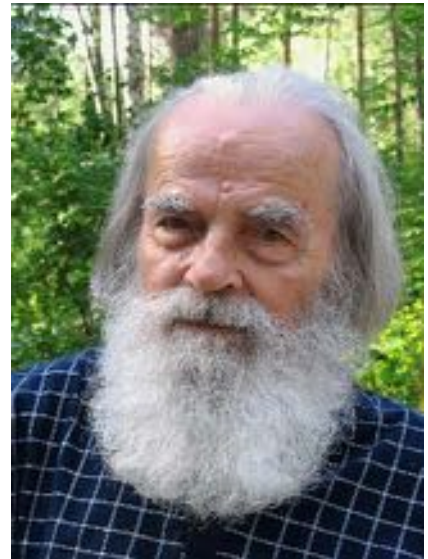
where $p_i \equiv u_i - u_{i-1}$ and $\theta_i \equiv u_i \bmod 2a$

Frenkel-Kontorova model

$$p_{i+1} = p_i + (\lambda\pi/2a) \sin(\pi\theta_i/a)$$

$$\theta_{i+1} = p_i + \theta_i + (\lambda\pi/2a) \sin(\pi\theta_i/a) \bmod 2a$$

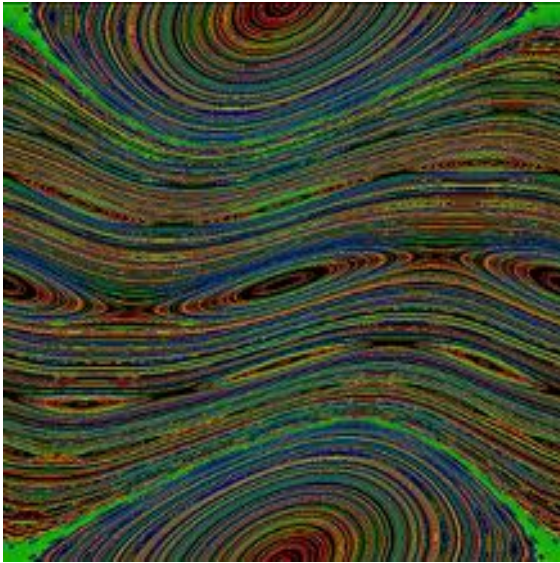
This is Chirikov's **standard map**!



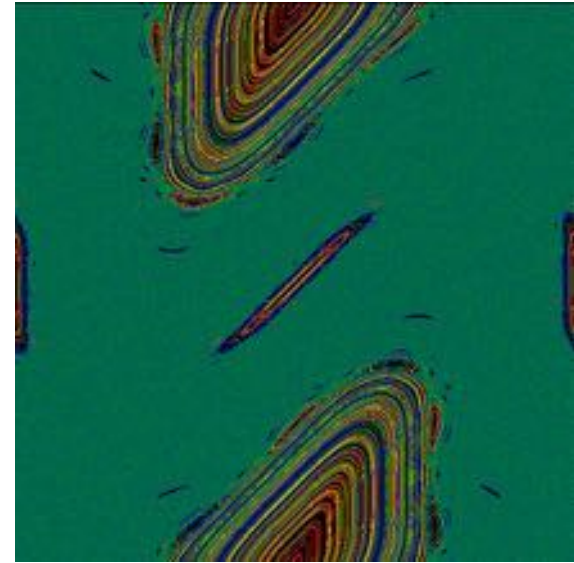
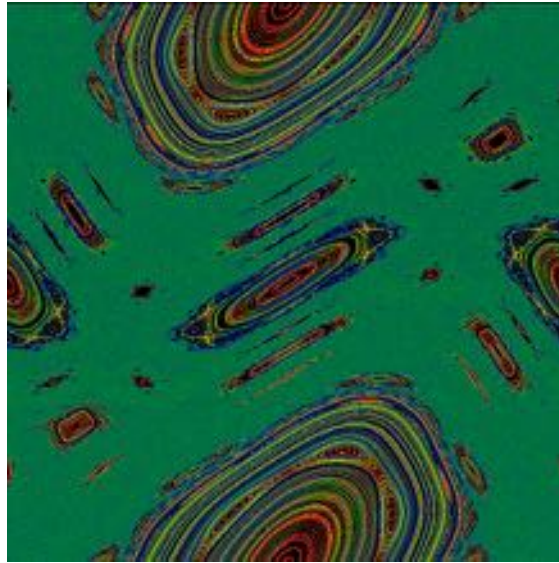
Standard Map

$$p_{i+1} = p_i + (\lambda\pi/2a) \sin(\pi\theta_i/a)$$

$$\theta_{i+1} = p_i + \theta_i + (\lambda\pi/2a) \sin(\pi\theta_i/a) \bmod 2a$$



order

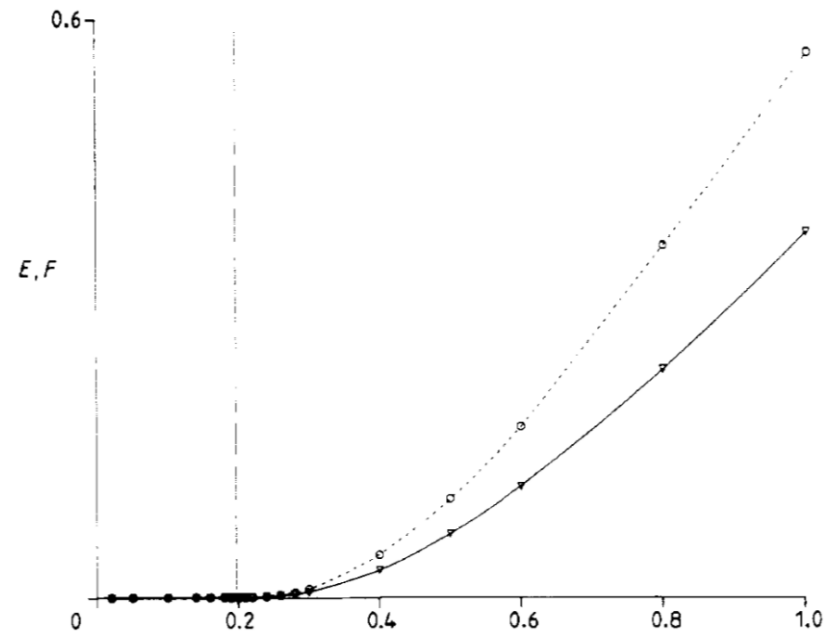
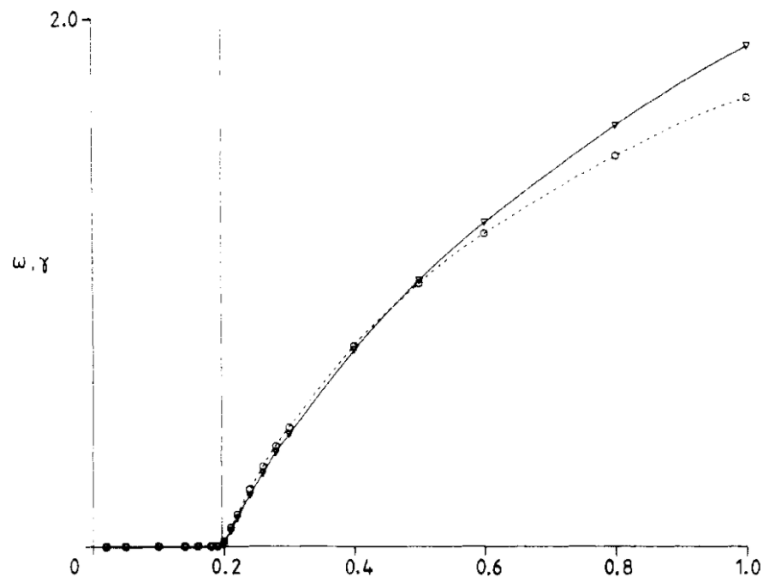


chaos

→
Increasing λ

Frenkel-Kontorova model

- Ordered phase is **frictionless**
- In the chaotic phase the particles are **pinned**. There are exponentially many degenerate states in the vicinity of the ground state – glassy phase.



J. Phys. C: Solid State Phys.
16, 1593 (1983)

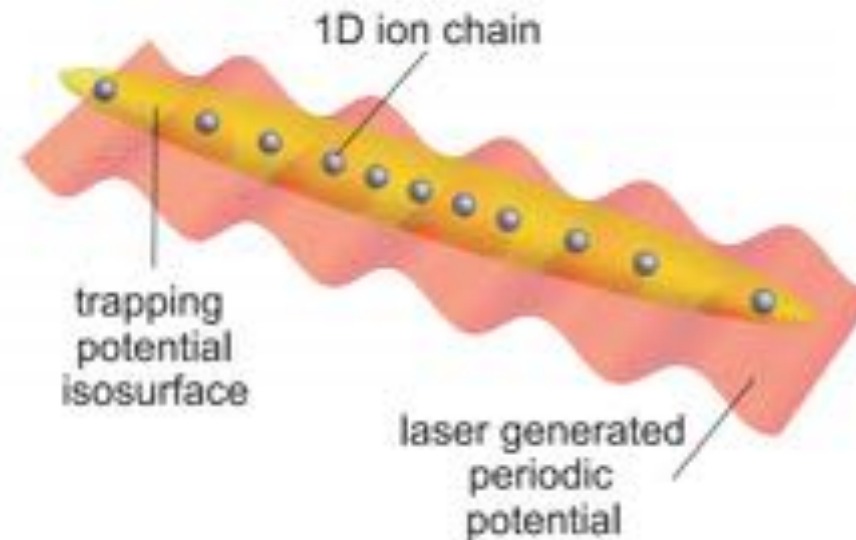
Aubry transition in ion traps with an additional optical lattice

Theoretical proposals:

- Garcia-Mata et al, Eur. Phys. J. D. 41, 325 (2007)
- Benassi et al, Nature Communications, 2 236 (2011)

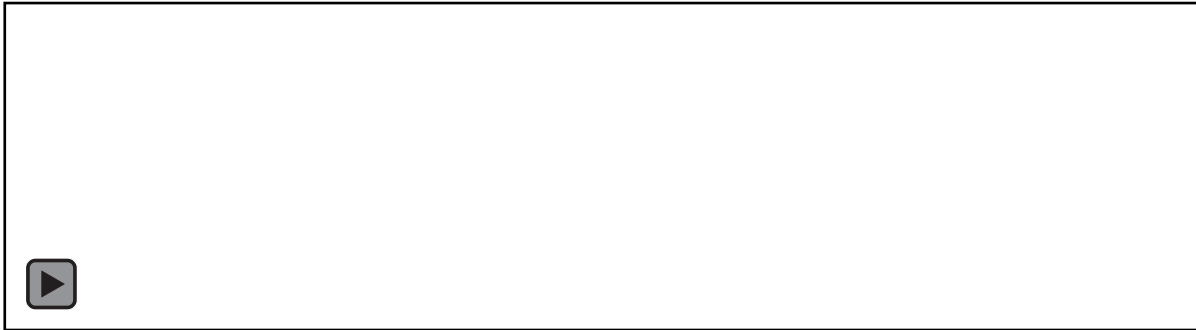
Experiments

- Science 348 (6239), 1115-1118 (2015)
- Nature Physics 11, 915-919 (2015)
- Nature Materials 15, 717-721 (2016)



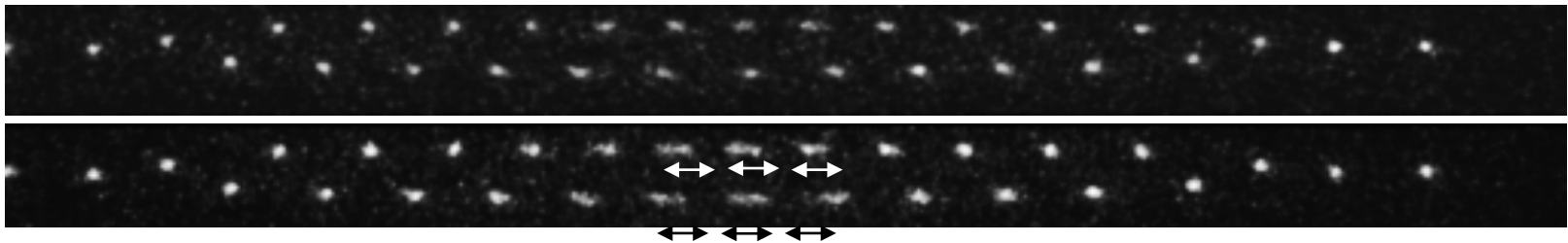
Our idea – use a zigzag crystal without an optical lattice

- Two row ion crystal can be used to study friction
- Shear force is introduced either by application of electric field or radiation pressure
- The distance between rows is controlled by varying the trapping potential

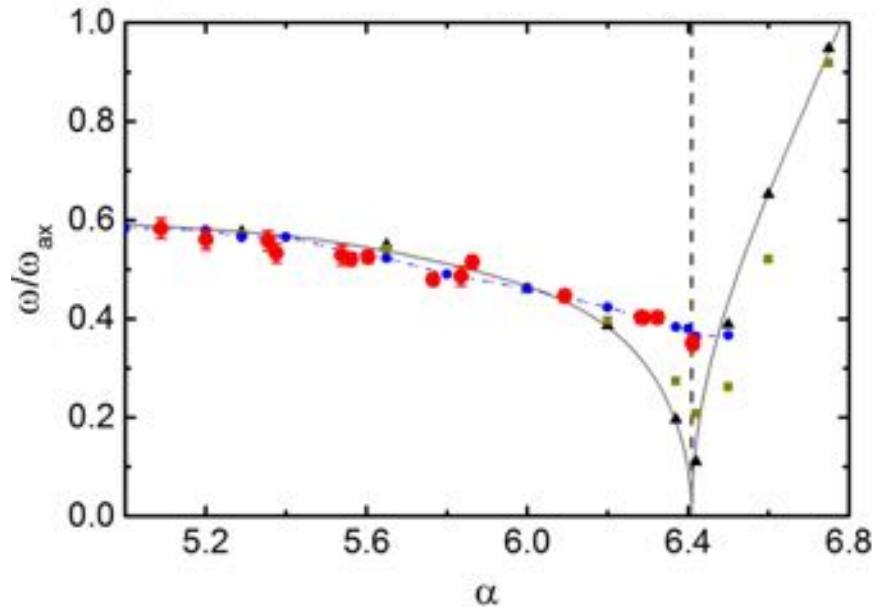


Results

The experiments were conducted in the National Metrology Laboratory in Braunschweig, Germany.



Shear mode, excited by intensity modulation of cooling beam



ratio of axial to radial confining frequency

- exp. Data (0.5 ± 0.4 mK)
- theory $T=0$ K
- ▲ sim. $T = 5 \mu\text{K}$
- sim. $T = 50 \mu\text{K}$
- sim. $T = 1$ mK

Kiethe et al., Nature Communications **8** 15364 (2017)

Conclusions and Future work

We have

- Introduced a novel model system for investigating friction in molecular fibres (e.g. proteins, DNA and other deformable nanocontacts.)
- Investigated the pinned to sliding phase transition in the self-organized ion Coulomb crystal

Future work

- Understand Aubry transition in the presence of backaction
- Understand the effect of inhomogeneities and of finite size
- Time dependent driving – kinetic friction
- More complex crystal geometries
- Quantum regime