# Non-Equilibrium Dynamics and Nanofriction in Ion Coulomb Crystals

Lars Timm<sup>1</sup>, Jan Kiethe<sup>2</sup>, Hendrik Weimer<sup>1</sup>, Luis Santos<sup>1</sup>, and <u>Tanja E. Mehlstäubler<sup>1,2</sup></u>

<sup>1</sup>Leibniz Universität Hannover, 30167 Hannover, Germany <sup>2</sup>PTB, 38116 Braunschweig, Germany



11. August 2022 – ECRYS Cargese





## PTB – National Metrology Institute

#### PTB / Braunschweig + Berlin

#### ca. 2200 employees



Founded 1887 by Werner von Siemens & Hermann von Helmholtz

## The Team "Quantum Clocks and Complex Systems"



#### Int. Collaborations:

NICT Toyko (J) University of Osaka (J) CMI (Prag, Cz) NPL (London, UK) W. Zurek (Los Alamos NL) R. Nigmatullin (Uni Sydney, Au) Haggai Landa (IBM, IL)



Visiting scientists: S. Ignatovich (ILP, Novosibirsk) N. Ohtsubo (NICT, Tokyo) M. Kitao (Osaka University) M. Doležal (CMI, Prag) L. Ye (JPL/CALTECH)





Bundesministerium für Bildung und Forschung

Industry Partners:

Grintech (Jena)

Naneo (Lindau)

D&G (Stuttgart)

Vacom (Jena)

Toptica (München)

mat





exchange with Osaka and Tokyo

**TRIAC** International Joint Laboratory for

International Joint Laboratory for Trapped-Ion Integrated Atomic-Photonic Circuits



## "Quantum Clocks and Complex Systems"



## Trapped Ions... (in our case <sup>172</sup>Yb<sup>+</sup>)



- $10^4$  K deep traps  $\rightarrow$  **long trapping times** for single ion (**up to months**)
- ions are trapped at  $E = 0 \rightarrow$  no systematic shifts to 1<sup>st</sup> order
- strong trap potential  $\rightarrow$  strong localization ( $\sigma \approx nm$ )
- high level control of internal (pseudo-spin) & external degrees of freedom (bosonic degree of motion)
- Laser-cooling to mK  $\rightarrow$  resolved sideband-cooling to quantum mechanical ground-state of motion!

Current world record in clock accuracy: Brewer et al., PRL 2019: accuracy  $\Delta v/v = 9.4 \times 10^{-19}$ 

## Micromotion in RF ion traps

**Quadrupol Potential** 

$$\Phi(r,z,t) = \frac{U_{AC}}{2r_0} \cos \Omega t \ (x^2 + y^2 - 2z^2)$$

Mathieu equation (writing  $\tau = \Omega t/2$ )

$$\frac{d^2}{d\tau^2} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \underbrace{(a_i + 2q_i \cos 2\tau)} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = 0$$



Ion motion in trap

$$x_{i}(t) \cong \underbrace{[x_{0i} + x_{1i}\cos(\omega_{i}t + \varphi_{i})]}_{\text{micromotion}} \underbrace{\left[1 + \frac{q_{i}}{2}\cos(\Omega t)\right]}_{\text{secular frequency}} + C\varphi_{AC}\sin(\Omega t)$$

## Micromotion in RF ion traps

**Quadrupol Potential** 

$$\Phi(r,z,t) = \frac{U_{AC}}{2r_0} \cos \Omega t \ (x^2 + y^2 - 2z^2)$$

Mathieu equation (writing  $\tau = \Omega t/2$ )

$$\frac{d^2}{d\tau^2} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \underbrace{(a_i + 2q_i \cos 2\tau)} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = 0$$

Ion motion in trap  $x_{i}(t) \cong [x_{0i} + x_{1i}\cos(\omega_{i}t + \varphi_{i})] \left[1 + \frac{q_{i}}{2}\cos(\Omega t)\right] + C\varphi_{AC}\sin(\Omega t)$ micromotion secular frequency (rf driven motion) (laser cool)

FIG. 9. (a) Photomicrograph of a Lissajous orbit in the r-z plane of a single charged particle of aluminum powder. The micromotion is visible. (b) Pattern of "condensed" Al particles (Wuerker and Langmuir, 1959).

Rev. Mod. Phys., Vol. 62, No. 3, July 1990





## New Quantum Clocks ?

<u>Now needed</u>: "experimental methods, that allow to manipulate and measure many-body quantum systems."



#### **Quantum Metrology** $\leftrightarrow$ **Quantum Simulation & Information**

Herschbach et al., Appl. Phys. B 107, 891 (2012)

## 2019: Measurement based multi-ion uncertainty budget



Keller et al., "Controlling systematic frequency uncertainties at the 10<sup>-19</sup> level in linear Coulomb crystals", PRA 99, 1 (2019)

## Summer 2021: First frequency ratio <sup>115</sup>In<sup>+</sup> - <sup>87</sup>Sr - <sup>171</sup>Yb<sup>+</sup>



10<sup>5</sup>

#### Frequency ratio measurement of <sup>115</sup>In<sup>+</sup> versus <sup>87</sup>Sr at NICT in Japan in 2020<sup>[1]</sup>





[1] Ohtsubo et al., *Opt. Lett.* **45**, 5950 (2020)
 [2] Dörscher et al., *Metrologia* **58** 015005 (2021)
 [3] Huntemann et al., *Phys. Rev. Lett.* **116**, 063001

 $\rightarrow$  2 orders of magnitude improvement

## Februar / March 2022 – International Campaign

#### Clock comparison **Braunschweig** versus **Paris and Torino** via **European Fiber Network**





74 % uptime, <sup>115</sup>In<sup>+</sup> vs. <sup>171</sup>Yb<sup>+</sup>



# Ion Coulomb Crystals



#### Hot Ion Plasma/Liquid

 $E_{kin} > E_{pot}$  !



#### Self-organized system! Nonlinear chaotic dynamics

# Ion Coulomb Crystals, $E_{pot} > E_{kin}$





#### Phases in Ion Coulomb Crystals



What happens when a system changes from one equilibrium condition to another?

- Examples for 2nd-order phase transitions:
  - ferro-magnetism  $\rightarrow$  para-magnetism
  - metal  $\rightarrow$  superconductor
  - early universe



#### Symmetry breaking phase transitions

What happens when a system changes from one equilibrium condition to another?

- Examples for 2nd-order phase transitions:
  - ferro-magnetism  $\rightarrow$  para-magnetism
  - metal  $\rightarrow$  superconductor
  - early universe

Spontaneous symmetry \_\_\_\_\_ breaking of Higgs field



Nature Physics 7, 2 (2011)

## Symmetry breaking in ion Coulomb crystals



#### The Kibble-Zurek Mechanism

- $\xi$ : correlation length
- $\tau$ : relaxation time
- defect density:  $d = \frac{\xi}{system \ size}$

• 
$$\tau \sim \left|\frac{\tau_0}{t}\right|^{\upsilon z}$$
  
•  $\xi \sim \left|\frac{\tau_0}{t}\right|^{\upsilon}$ 

- KZM: d from ξ at freezeout
- friction (laser cooling) negligible  $\implies v = \frac{1}{2}, z = 1$

test of KZM with defined  $\nu$ , z

del Campo et al., PRL 105, 075701 (2010) Fishman et al., PRB 77, 064111 (2008)

Quenching the control field



#### Harmonic Ion Traps – Inhomogeneous Case

 Ions in harmonic potential: phase transition spreads out from center!



• Phase front faster than speed of sound!

A. Del Campo et al., Phys. Rev. Lett. 105, 075701 (2010)

#### The Kibble-Zurek Mechanism

#### Prediction of KZM

Power law scaling of defect density:

$$d \sim \left|\frac{1}{\tau_Q}\right|^{\nu/(1+\nu z)}$$

test of KZM with defined v, z



#### Experiment: fast, non-adiabatic radial quenches



#### **Experimental details in:**

Pyka et al., Nat. Commun. 4, 2291 (2013)

 $v_{axial} = 24.6 \text{ kHz}$  $v_{rad} \approx 500 - 140 \text{ kHz}$ 

#### Monitor rf trapping voltage $\rightarrow$ quench rate



#### Scaling of Defect Creation

Defect Probability as Function of Ramp Velocity:



Nikoghosyan et al., Universality in the dynamics of second-order phase transitions, PRL 116, 080601 (2016)

Puebla et al., Fokker-Planck formalism approach to Kibble-Zurek scaling laws and nonequilibrium dynamics, PRB 95, 134104 (2017)

#### Topological defects in ion Coulomb crystals

#### Localized Defect $v_{rad}/v_z \approx 8$



Extended Defect  $v_{rad}/v_z \approx 5.5$ 

Pyka et al., Nat. Commun. 4, 2291 (2013)

#### Order Parameter $\Phi$

radial ion separation a:



#### **Topological Soliton:**

Langragian of Scalar Field:

$$L = \frac{1}{2} \left( \frac{\partial \Phi}{\partial t} \right)^2 - \frac{1}{2} \left( \frac{\partial \Phi}{\partial z} \right)^2 + \lambda \Phi^2 + A \Phi^4$$

- field configurations, such that their presence can be detected by looking at the values of the field far away from the defect
- cannot be removed by local deformations of the field



# Some features of topological defects

#### Stability of topological defects



#### Kinks for quantum information - Theory

Soliton physics with laser cooled ions:

defects behave like quasi-particles – addressable via gapped mode!



Long coherence times of localized internal modes:

#### Storage of Q-Info & Transport of Entanglement:

Landa et al., PRL **104**, 043004 (2010) Landa et al., PRL **113**, 053001 (2014)

#### E-field Creating Kink & Anti-Kink



E-field ramp

Partner et al., New J. Phys. **15**, 103013 (2013)

# The Aubry Phase Transition

# Friction at the Atomic Scale



**Complex, Self-Organized System with Back-Action** 

#### Theoretical models



Prandt-Tomlinson (1928)



Many-body effects: Frenkel-Kontorova (1938)

#### Many-body system: lattice forces can cancel



If **a** and  $\lambda$  are incommensurate?  $\rightarrow$  **superlubricity!** (1983)

#### Aubry phase transition (1983)

If **a** and  $\lambda$  are incommensurate:

- systems becomes **superlubric**
- analyticity breaking of hull function



## How can we experimentally realize nanofriction?

Vanossi et al., Modeling friction: From nanoscale to mesoscale, Rev. Mod. Phys. 85 (2013)

#### Proposal: use linear ion chain in optical corrugation potential

 Theory:
 Benassi et al., Nature Commun 2, 236 (2011)

 Puttivarasin et al., New J. Phys. 13, 075012 (2011)

 Fogarty et al., Phys. Rev. Lett. 115, 233602 (2015) ...



Standing optical wave in cavity

## Theory prediction for finite systems (qualitative) !

-mm .....

**Symmetry Breaking** from sliding to pinned phase<sup>[1]</sup>

#### Soft Mode !

2. Vanishing vibrational "soft mode" drives the transition from sticking to sliding regime<sup>[2]</sup>:

[1] Benassi et al., *Nature Commun* 2, 236 (2011)
[2] Puttivarasin et al., *New J. Phys.* 13, 075012 (2011)



#### **Experiments with ions in standing optical lattice:**

Bylinskii *et al., Science* 348, 1115 (2015) Gangloff *et al.,* Nature Physics 11, 915 (2015) Bylinskii *et al.,* Nature Materials 15, 717 (2016)



Gangloff et al., Nature Physics, 11 (2015)

## Our System: self-organized crystal with back-action



#### Self-organized crystal with back-action

Locally the kink disturbes the quasi-periodicity of the two atomic layers



 $D = m \omega_{ax}^2$  : ion trap  $\kappa \sim \frac{e^2}{\pi \epsilon_0} \frac{1}{ma^3}$  : ion interaction



Interaction between the ion layers gives corrugation potential!

#### Self-organized crystal with back-action

Locally the kink disturbes the quasi-periodicity of the two atomic layers



control parameter in experiment:

 $\alpha = \omega_{rad} / \omega_{axial}$ 





## **Experimental Observations**

Kiethe *et al.,* **Probing Nanofriction and Aubry-type Signatures in a Finite Self-Organized System,** Nat. Comm. 8, 15364 (2017) Kiethe *et al.,* **Nanofriction and Motion of Topological Defects in Coulomb Crystals,** New J. Phys. 20, 123017 (2018)

**Order parameter**  $\Phi$  := relative distance to closest ion in other layer



**Order parameter**  $\Phi$  := relative distance to closest ion in other layer





#### **Experimental observation:**

#### Peierls-Nabarro Barriers

= potential energy of kink soliton





Kiethe et al., NJP (2018)

0.3 0.0  $\alpha = 5.65$ -0.3 0.3 0.0  $\alpha = 6.38$ -0.3  $z_{\mathbf{j}}$  [a] 0.3 0.0  $\alpha = 6.43$ -0.3 0.3 0.0  $\alpha = 6.60$ -0.3 -0.2 0.0 0.1 0.2 -0.1 z<sub>j,0</sub> [a]

**Hull function** 

## Can we observe the Sliding Mode ?

#### Vibrational Shear Mode should drive the Phase Transition



First observation of the localized kink mode!

## **Observation of the Sliding Mode**



legend:
Hessian matrix T = 0K
simulations T = 5μK
▲ simulations T = 1mK
▼ exp. data

#### **PN-energy barriers of kink soliton:**

 $\rightarrow$  thermal energy allows for switching



Yes, but strong non-linearities due to finite temperature!

## **Friction Summary**

- Symmetry breaking & non-analytic hull function for the first time observed in self-organized Coulomb crystal
- Temperature induced non-linearities impact soft-mode
- $2^{nd}$  stage cooling to **T** =  $\mu$ K via ln<sup>+</sup> ions  $\rightarrow$  **go quantum**
- Defect reduces friction by more than an order of magnitude



#### Kink assisted DNA unfolding

Kühner et al., Biophysical Journal 92, 2491 (2007)

Follow-up work ...

## How does a soft mode couple to thermal phonon environment?

#### Finite temperature spectrum at the symmetry-breaking linear-zigzag transition

J. Kiethe,<sup>1</sup> L. Timm,<sup>2</sup> Haggai Landa,<sup>3,4</sup> D. Kalincev,<sup>1</sup> Giovanna Morigi,<sup>5</sup> and T. E. Mehlstäubler<sup>1,6</sup>,

<sup>1</sup> Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany
 <sup>2</sup> Institut für Theoretische Physik, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover, Germany
 <sup>3</sup> Institut de Physique Théorique, Université Paris-Saclay, CEA, CNRS, 91191 Gif-sur-Yvette, France
 <sup>4</sup> IBM Quantum, IBM Research Haifa, Haifa University Campus, Mount Carmel, Haifa 31905, Israel
 <sup>5</sup> Theoretische Physik, Saarland University, Campus E26, 66123 Saarbrücken, Germany
 <sup>6</sup> Institut für Quantenoptik, Leibniz Universität Hannover, Welfengarten 1, 30167 Hannover, Germany
 (Dated: December 22, 2020)



Fishman et al., PRB 77, 064111 (2008)

## Spectroscopy of phonons via resonant light forces



Photos of excitation of lowest energy phonons (1 node, 2 nodes, ...)

## Coupling of soft mode to thermal phonon environment

Equation of motion of phonon *i* under non-linear interaction:

$$V_4 = \frac{1}{2!} \sum_{i=1}^{3N} m\omega_i^2 \Theta_i^2 + \frac{1}{3!} \sum_{ijk=1}^{3N} L_{ijk} \Theta_i \Theta_j \Theta_k + \frac{1}{4!} \sum_{ijkl=1}^{3N} M_{ijkl} \Theta_i \Theta_j \Theta_k \Theta_l$$

$$\ddot{\Theta}_i = -\frac{1}{m} \frac{\partial V_4}{\partial \Theta_i} - \gamma_i \Theta_i + \Xi_i(t)$$

Time average over higher frequency phonons:

$$\ddot{\Theta}_{1} = -\tilde{\omega}_{1}^{2}\Theta_{1} - \frac{1}{2}\nu_{12}^{2}\Theta_{2} + \eta_{1} - \gamma_{1}\Theta_{1} + \Xi_{1}$$
$$\ddot{\Theta}_{2} = -\tilde{\omega}_{2}^{2}\Theta_{2} - \frac{1}{2}\nu_{12}^{2}\Theta_{1} + \eta_{2} - \gamma_{2}\Theta_{2} + \Xi_{2},$$

with 
$$\tilde{\omega}_i(T)^2 = \omega_i^2 + \nu_{\text{eff},i}^2 T$$
  $\nu_{\text{eff},i}^2 = \frac{1}{2m} \sum_{k \neq 1,2} M_{iikk} \frac{k_B}{m\omega_k^2}$ 

#### Theory for two lowest frequency modes:



dashed lines = new theory

## Coupling of soft mode to thermal phonon environment



#### Theory for two lowest frequency modes:

#### **Conclusion:**

also at Linear-to-Zigzag Transition...

- → soft mode is modified due to non-linear coupling to thermal phonon environment
- → soft-mode sees modified Coulomb environment due to oscillating phonon environment
- $\rightarrow$  Floquet physics



J. Kiethe, L. Timm, H. Landa, D. Kalincev, G. Morigi, T. E. Mehlstäubler <u>Finite-temperature spectrum at the symmetry-breaking linear to zigzag transition</u> Phys. Rev. B, **103**, 104106 (2021)

## For really low temperatures: Is there quantum nanofriction?

4 2 0 30 20 20 ~ 30 20 *z* (μm)

**PN-energy barriers of kink soliton:** 



L. Timm

L. Santos

In future:  $2^{nd}$  stage cooling to **T** =  $\mu$ **K** ٠ via polarization gradient cooling could be possible

Is tunneling over 10s of micrometer possible?

## Is there quantum nanofriction ?

#### Tunneling over 10s of micrometer? $\rightarrow$ collective excitation! $\rightarrow$ ions move by only a few nm while top. defect moves by 10s µm



Define effective mass of the quasi particle:

$$M_{\text{eff}}(X) = m \sum_{i} \left(\frac{d\vec{r}_{i,C}(X)}{dX}\right)^2$$

Solve Hamiltonian for quasi particle:

$$\hat{H}_s = \hat{P} \frac{1}{2M_{\text{eff}}(\hat{X})} \hat{P} + U(\hat{X})$$

L. Timm, L. A. Rüffert, H. Weimer, L. Santos, T. E. Mehlstäubler Quantum nanofriction in trapped ion chains with a topological defect, Phys. Rev. Research, 3, 043141 (2021)

## Quantum nanofriction





Sliding phase:

QUANTUM WORLD

Assumption: Kink = quantum particle in classical PN potential

- Harmonic eigenstates
- Equidistant spectrum

Tunneling regime:

- Barrier splits ground state wavefunction
- Sym. and antisym. pairs

Quasi-classical regime:

- Large barrier
   →tunneling negligible
- Localized states

**Consequences for observables in experiments?** 

## Quantum nanofriction

#### ENERGY SPECTRUM



- Quantum fluctuations: No "softmode"
- Tunneling regime: Eigenstate energy below barrier height but tunneling causes energy gap
- Quasi-classical regime: Degenerate sets of eigenstates, localized left/right

# → Spectroscopic measurement of the energy spectrum after ground-state cooling

#### **TUNNELING DYNAMICS**



for T =  $0.1 \,\mu\text{K}$ 

- Initialize a localized state in one potential minimum and monitor evolution
- Oscillation between left and right minimum due to tunneling
- Not observable in quasi-classical regime

#### $\rightarrow$ At low $\mu$ K temperatures tunneling dynamics is observed

#### Work by other groups

Kiethe *et al.,* **Probing Nanofriction and Aubry-type Signatures in a Finite Self-Organized System,** Nat. Communs. 8, 15364 (2017)

Brox et al., Spectroscopy and Directed Transport of Topological Solitons in Crystals of Trapped Ions, PRL 119, 153602 (2017)

Kiethe *et al., Nanofriction and Motion of Topological Defects in Coulomb Crystals,* New J. Phys. 20, 123017 (2018)

 $\rightarrow$  Symmetries in Ion Trap and Light Forces

#### Outlook: Energy Transport with Topological Defect



FIG. 2: Dynamics of the kinetic energy after a 1 µm displacement of ion 7 along z, calculated using Eq. (2), for (a)  $\alpha = 5.5$  (sliding phase) and (b)  $\alpha = 6.8$  (pinning phase).

Timm et al., Energy localization in interacting atomic chains with topological solitons, Phys. Rev. Res. (2020)

## The Team "Quantum Clocks and Complex Systems"

# Thank you for your attention!

Industry Partners:

Grintech (Jena)

Naneo (Lindau)

D&G (Stuttgart)

Vacom (Jena)

Toptica (München)

QUARTIQ (Berlin)

New:



FURA







Int. Collaborations: NICT Toyko (J) University of Osaka (J)

CMI (Prag, Cz) NPL (London, UK) W. Zurek (Los Alamos NL) R. Nigmatullin (Uni Sydney, Au) ILP and Uni Novosibirsk (R) Haggai Landa (IBM, IL)



Visiting scientists: S. Ignatovich (ILP, Novosibirsk) N. Ohtsubo (NICT, Tokyo) M. Kitao (Osaka University) M. Doležal (CMI, Prag) L. Ye (JPL/CALTECH)



Bundesministerium für Bildung und Forschung



Osaka and Tokyo

**International Joint Laboratory for Trapped-Ion Integrated Atomic-Photonic Circuits** 



TRIAC