



Ion Coulomb crystals: Thermodynamics, Quantum dynamics and Simulators

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One-component plasma (homogeneous system, 3D)

Coupling parameter:
$$\Gamma = e^2/akT$$

 $a = (3/4\pi n)^{1/3}$ Wigner-Seitz radius $\mathcal{E}_{\mathbf{F}_{1}}^{100}$
Strong correlations: $\Gamma \gg 1$

Crystallization (transition to spatial order): $\Gamma = 174$

D. Dubin and T. O'Neil, RMP 1999.

One-component plasmas in atomic physics

Bragg Diffraction from Crystallized Ion Plasmas

W. M. Itano,* J. J. Bollinger, J. N. Tan,† B. Jelenković,‡ X.-P. Huang, D. J. Wineland





Fig. 3. Histogram representing the numbers of peaks (not intensities) observed as a function of qa_{ws} , where $\mathbf{q} = \mathbf{k}_s - \mathbf{k}_l$ is the difference between the incident (\mathbf{k}_l) and scattered (\mathbf{k}_s) photon wave vectors. We analyzed 30 Bragg diffraction patterns from two approximately spherical plasmas having 270,000 and 470,000 ions. The dotted lines show the expected peak positions, normalized to the center of gravity of the peak at A ({110} Bragg reflections).



Fig. 4. Time-resolved Bragg diffraction pattern of the same plasma as in Fig. 2. Here and in Figs. 5 and 6 the small open circle marks the position of the undeflected laser beam. A bcc lattice, aligned along a (100) axis, would generate a spot at each intersection of the grid lines overlaid on the image. The grid spacing corresponds to an angular deviation of 2.54×10^{-2} rad. Here, $\omega_r = 2\pi \times 125.6$ kHz, $n_o = 3.83 \times 10^8$ cm⁻³, $N = 5 \times 10^5$, $\alpha = 0.98$, and $2r_o = 1.36$ mm.

Coulomb gas in atomic physics

 Gas of ionized atoms: usually singly-ionized alkali-earth metals (e.g. Berillium, Calcium, Magnesium).
 Radiation is absorbed and emitted in the visible.



Fig. 4. Time-resolved Bragg diffraction pattern of

Coulomb gas in atomic physics

1) Gas of ionized atoms: usually singly-ionized alkali-earth metals. Radiation is absorbed and emitted in the visible.

2) Confinement by external potentials: Paul (radiofrequency) or Penning traps.



Innsbruck Ion trap

Linear Paul trap:

 $\Phi_0 = U_{\rm dc} + V_{\rm ac} \cos(\Omega_{\rm rf} t)$

Effective harmonic force $\ \mathbf{F} \propto -\mathbf{r}$

Possibility to control the number of ions and the shape of the cloud

Coulomb gas in atomic physics

1) Gas of ionized atoms: usually singly-ionized alkali-earth metals. Radiation is absorbed and emitted in the visible.

2) Confinement by external potentials: Paul (radiofrequency) or Penning traps.

Crystallization:
 Low thermal energies are achieved by laser cooling.
 Cooling down to *few microKelvin*.

Crystals of ions in traps: Applications

High-precision measurements

Simulation of astrophysical systems

Ultracold chemistry

Quantum-based technologies

Quantum simulators, quantum metrology, Quantum computing.



Aarhus, Berkeley, Boulder, Freiburg, Erlangen, Innsbruck, London, Mainz, Marseille, Michigan, München, Oxford, Paris, PTB, Saarbrücken, Siegen, Sussex,

Cirac, Zoller, Retzker, Plenio, Altman, Porras, Solano, Duan, ...

Trapped ions and Nobel Foundation



The Nobel Prize in Physics 1989 was divided, one half awarded to Norman F. Ramsey *"for the invention of the separated oscillatory fields method and its use in the hydrogen maser and other atomic clocks"*, the other half jointly to Hans G. Dehmelt and Wolfgang Paul *"for the development of the ion trap technique"*.

The Nobel Prize in Physics 2012 was awarded jointly to Serge Haroche and David J. Wineland "for groundbreaking experimental methods that enable measuring and manipulation of individual quantum systems"

And also: Ramsey (1989), Chu, Cohen-Tannoudji, Phillips (1997), Haroche (2012)

Low dimensional structures

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PHYSICAL REVIEW LETTERS

30 MARCH 1992

Observation of Ordered Structures of Laser-Cooled Ions in a Quadrupole Storage Ring

I. Waki, (a) S. Kassner, G. Birkl, and H. Walther

Max-Planck-Institut für Quantenoptik, D-8046 Garching bei München, Federal Republic of Germany (Received 11 September 1991; revised manuscript received 16 December 1991)





[Birkl et al., Nature 357, 310 (1992)]

Phase diagram

Multiple-shell structures of laser-cooled ²⁴Mg⁺ ions in a quadrupole storage ring

G. Birkl, S. Kassner & H. Walther

Max-Planck-Institut für Quantenoptik, Garching bei München, Germany

Nature 357, 310 (1992)





Outline

1. Thermodynamics of ion chains

- the linear-zigzag instability, classical PT
- the linear-zigzag instability, quantum PT
- 2. Dynamics of ion chains across the instability
 - Classical quenches
 - Quantum quenches
- 3. Outlook. Topological Structural Transitions

Thermodynamics of ion chains

The ion chain

In textbooks (Ashcroft and Mermin):



Periodic distribution: Bloch theorem Long-range interaction (Coulomb): no sound velocity

The ion chain in a linear trap

(M. Drewsen and coworkers, Aarhus)

$$H = \sum_{j=1}^{N} \frac{\mathbf{p}_{j}^{2}}{2m} + \frac{1}{2} m \left(v^{2} x_{j}^{2} + v_{t}^{2} \left(y_{j}^{2} + z_{j}^{2} \right) \right) + \frac{1}{2} \sum_{j=1}^{N} \sum_{i \neq j} \frac{Q^{2}}{r_{i,j}}$$

$$\nu \ll \nu_{t} \quad \text{1D structure (ion chain)}$$

Inhomogeneous distribution: NO Bloch theorem

Long-range interaction:

pertubation theory with Bloch waves does not converge

Charge density at equilibrium

$$m\nu^2 x_i^{(0)} = -\sum_{j>i} \frac{Q^2}{(x_j^{(0)} - x_i^{(0)})^2} + \sum_{j$$

Continuum limit: mean field description for 1D



Linear density: $n_L(x) = \frac{3}{4} \frac{N}{L} \left(1 - \frac{x^2}{L^2} \right)$

Length of the chain: $L(N)^{3} = 3\left(\frac{Q^{2}}{m\nu^{2}}\right) N \log N$

at leading order in 1/log N

D. Dubin, PRE 1997.

Spectra of excitations





Spectra of excitations



Spectra of excitations



Statistical Mechanics

Quantization of the vibrations

$$\hat{H}_{n} = \sum_{n=1}^{N} \hbar \omega_{n}^{\parallel} \hat{N}_{n}^{\parallel} + \sum_{n=1}^{N} \hbar \omega_{n}^{\perp} (\hat{N}_{n,y}^{\perp} + \hat{N}_{n,z}^{\perp})$$

M

Canonical ensemble

$$\rho = \frac{1}{Z} \exp(-\beta H)$$
$$F = -k_B T \log Z$$

ΔŢ

One-dimensional behaviour: $k_B T \ll \hbar \omega_{\min}^{\perp}$

Thermodynamic limit: $\nu \sim \sqrt{\log N}/N$ as $N \to \infty$ Density in the center $n(0) = \frac{3}{4} \frac{N}{L}$ fixed

Specific Heat



Non extensive behaviour at low temperatures in the thermodynamic limit: $c_a \propto 1/\sqrt{\ln N}$

•Due to long-range Coulomb interaction

•It is a quantum effect (at high-T Dulong-Petit holds)

Ion chains are thermal reservoirs?

• In the *harmonic* chain the dynamics is integrable

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VOLUME 6, NUMBER 4 APRIL 1965

Statistical Mechanics of Assemblies of Coupled Oscillators*

G. W. FORD[†]

Department of Physics, University of Michigan, Ann Arbor, Michigan

M. KAC

The Rockefeller Institute, New York, New York

AND

P. MAZUR

Lorentz Institute for Theoretical Physics, Leiden, The Netherlands (Received 25 September 1964)

It is shown that a system of coupled harmonic oscillators can be made a model of a heat bath. Thus a particle coupled harmonically to the bath and by an arbitrary force to a fixed center will (in an appropriate limit) exhibit Brownian motion. Both classical and quantum mechanical treatments are given.

 The rest of the chain acts as a bath for a single ion (when thermalization rate is faster than recurrence)

Ion chain as quantum reservoir

Langevin equation:

$$\frac{d^2 X_{\pm}}{dt^2} + \int_0^t \Gamma_{\pm}(t - t') \frac{dX_{\pm}}{dt'} dt' + (1 - \Gamma_{\pm}(0)) X_{\pm}(t) = F_{\pm}(t) - \Gamma_{\pm}(t) X_{\pm}(0)$$

damping kernel

Spectral density (Fourier transform of the damping kernel)

$$J_{\pm}(\omega) = \omega \int_{0}^{\infty} \Gamma_{\pm}(t) \cos(\omega t) dt$$

B. Taketani, T. Fogarty, E. Kajari, A. Wolf, T. Busch, G.M. PRA (2014)



distance d=5a, chain of 50 ions in a thermal state (ions: Calcium, impurity defects: Indium).

T. Fogarty, E. Kajari, B. Taketani, A. Wolf, T. Busch, G.M. PRA (2013)

Scaling with the distance



linear decay with the distance

T. Fogarty, E. Kajari, B. Taketani, A. Wolf, T. Busch, G.M. PRA (2013)

Linear-zigzag instability





[Birkl et al., Nature 357, 310 (1992)]

Preamble: Ring

No axial confinement: periodic distribution Modes are phononic waves with quasimomentum *k* in BZ



Transition chain-zigzag

decrease transverse confinement ν_t

Linear chain





Transition chain-zigzag

decrease transverse confinement



Transition chain-zigzag

decrease transverse confinement



Sh. Fishman, G. De Chiara, T. Calarco, GM, PRB 2008

Chain to Zig-Zag: second-order phase transition?



Symmetry breaking: line to plane



Order parameter: Distance from the axis Control field: Transverse frequency



Soft mode: Zigzag mode

J. Eschner and coworkers, Barcelona & Saarbrücken

Potential at the instability

Ansatz: the zigzag mode is the soft mode.

Expand the potential at 4th order in plane waves Study new minima as a function of transverse freq.



Potential of the zigzag mode

Derivation of the effective potential for the zigzag mode:

$$V^{\text{soft}} = \mathcal{V}[(\Psi_0^y)^2 + (\Psi_0^z)^2] + A[(\Psi_0^y)^2 + (\Psi_0^z)^2]^2$$



$$\mathcal{V} = \frac{m}{2}\beta_0 = \frac{1}{2}m(\nu_t^2 - \nu_t^{(c)2})$$
$$A = \frac{3}{2}\frac{31}{32}\zeta(5)\frac{Q^2}{a^5}$$

The other modes are stably trapped by a harmonic potential (microscopic derivation of Landau model)

Sh. Fishman, G. De Chiara, T. Calarco, G.M., PRB 2008

Summary: classical phase transition

- Microscopic derivation of the Landau model.
- Second-order phase transition.
- Critical exponents of Landau model.
- Soft mode: zigzag mode.

Sh. Fishman, G. De Chiara, T. Calarco, G.M., PRB 2008

Classical phase transition





Quantum phase transition

$$\nu_t^{(c) \ 2} = 2\left(\frac{2Q^2}{ma^3}\right) \sum_{j=1}^N \frac{1}{j^3} \sin^2 \frac{j \ \pi}{2}$$

linear Tunneling: disorder zigzag






Quantum fluctuations at the mechanical instability (2D)

Soft mode: $y_j^{\text{soft}} = (-1)^j y_0$

Modes close to the instability:

 $y_j = (-1)^j a \phi_j$

Effective potential: $V[\{\phi_j\}] \approx \sum_{j=1}^{N} V_0(\phi_j) + \frac{1}{2}K \sum_{j=1}^{N} (\phi_j - \phi_{j+1})^2$ $V_0(\phi) = -\frac{1}{2}m(\nu_c^2 - \nu_t^2)a^2\phi^2 + \frac{1}{4}ga^4\phi^4$

E. Shimshoni, G.M., S. Fishman PRL 2011

Mapping to an Ising model in the transverse field

 $\phi_j = \phi_0 \sigma_j^z \! + \! \delta \phi_j$

 $Z \approx Z_0 \int \mathcal{D}\sigma \exp\left(-S_I[\sigma]/\hbar\right)$ action of an Ising model

Effective Hamiltonian $H_{I} = -\sum_{j=1}^{N} (J\sigma_{j}^{z}\sigma_{j+1}^{z} + h\sigma_{j}^{x})$ $h \approx C_{h} (U_{P}U_{K}^{2})^{1/3} \text{ transverse field (tunneling)}$ $J = K\phi_{0}^{2} = C_{J}U_{P}\varepsilon \text{ exchange coupling (Coulomb interaction)}$

E. Shimshoni, G.M., S. Fishman PRL 2011

DMRG results

$$egin{aligned} ilde{H} &= rac{1}{2} \sum_{i=1}^L \left[ilde{p}_i^2 + \left(ilde{\omega}^2 - \mathcal{M}_1
ight) ilde{y}_i^2 \ &+ \mathcal{M}_2 \left(ilde{y}_i + ilde{y}_{i+1}
ight)^2 + \mathcal{M}_3 \ ilde{y}_i^4
ight] \end{aligned}$$

| | Quantity | Computed | Theory [11] |
|----------------------|----------------------|-------------------|-------------|
| η | Anomalous dimension | 0.258 ± 0.012 | 0.25 |
| $\boldsymbol{\beta}$ | Spont. magnetization | 0.126 ± 0.011 | 0.125 |
| ν | Correlation length | 1.03 ± 0.05 | 1 |
| \boldsymbol{c} | Central charge | 0.487 ± 0.015 | 0.5 |

Theory: critical exponents of Ising model with transverse field

P. Silvi, G. De Chiara, T. Calarco, G.M., S. Montangero, Ann. Phys. (2013)

Quantum effects



DMRG and RG flow analysis are in excellent agreement

D. Podolsky, E. Shimshoni, P. Silvi, S. Montangero, T. Calarco, GM, S. Fishman, PRB 2014

Quantum effects



ions: quantum effects are negligible

D. Podolsky et al, PRB 2014

Dynamics:

classical and quantum quenches

Classical quenches

at the linear-zigzag instability

Preamble: scaling at the classical phase transition



Preamble: scaling at the classical phase transition



Preamble: scaling at the classical phase transition



Dynamical properties at criticality



Dynamics of the order parameter:

Landau Ginzburg equation in presence of damping (laser cooling)

$$\partial_t^2 \psi - h(x)^2 \partial_x^2 \psi + \eta \partial_t \psi + \delta(x, t) \psi + 2\mathcal{A}(x) \psi^3 = \varepsilon(t)$$

A. Del Campo, G. De Chiara, G.M., M. Plenio, A. Retzker, PRL 2010

Kibble-Zurek mechanism



Kibble-Zurek hypothesis: $\tau \sim (\nu_t - \nu_t^{(c)})^{-1}$

System follows the quench adiabatically till the relaxation time becomes slower than the quench.

Freeze-out time: $\tau(\hat{t}) = \hat{t}$ Density of defects: $d_o \sim \frac{1}{\hat{\xi}_o}$

A. Del Campo, G. De Chiara, G.M., M. Plenio, A. Retzker, PRL 2010

Density of defects after the quench

Scaling of the density of defects as a function of the quench rate:



[Laguna and Zurek, PRL 1999]

A. Del Campo, G. De Chiara, G.M., M. Plenio, A. Retzker, PRL 2010

Experimental quenches



T. Mehlstäubler and coworkers (PTB)

See also: Schätz (Freiburg) and Schmidt-Kaler (Mainz)

Experimental quenches



T. Mehlstäubler and coworkers (PTB)

What's next: spectroscopy and control of the kinks

See also: Schätz (Freiburg) and Schmidt-Kaler (Mainz)

Sudden quenches

in a linear chain

I $e^{ik_L y_1} |e\rangle\langle e|$

Initial state: $|\Psi(0)
angle = |g,0
angle$

II Ô Ô Q Q Ô Ô Q Q Ô Ô Q Q

 $\begin{array}{c|c} \mathrm{I} & & & & |e\rangle \\ & & & |g\rangle \\ \end{array} & & & |g\rangle \\ \mathrm{II} & & & |e\rangle\langle e| \\ \mathrm{II} & & & |\psi(t_{\mathrm{pulse}})\rangle = \frac{1}{\sqrt{2}} \left(|g,0\rangle + |e,\alpha\rangle\right) \\ & & & \hat{\mathbb{O}} \otimes \mathbb{O} \\ \end{array}$

 $\begin{array}{c} \text{III} \\ \bigcirc & \mathbb{Q} \stackrel{Q}{\circ} \stackrel{\circ}{\circ} \stackrel{\circ}{\circ} \stackrel{Q}{\circ} \stackrel{Q}{\circ} \stackrel{\circ}{\circ} \stackrel{\circ}{$

I Initial state: $|\Psi(0)\rangle = |g,0\rangle$ $\begin{aligned} & \widehat{\mathbf{T}}_{e^{ik_L y_1} | e \rangle \langle e |} \\ & |\Psi(t_{\text{pulse}}) \rangle = \frac{1}{\sqrt{2}} \left(|g, 0 \rangle + | e, \alpha \rangle \right) \\ & \widehat{\mathbf{O}} \bigotimes \widehat{\mathbf{O}} \bigotimes \widehat{\mathbf{O}} \widehat{\mathbf{O}} \bigotimes \widehat$ Π $\Psi(t+t_{\text{pulse}}) \rangle = \frac{1}{\sqrt{2}} \left(|g,0\rangle + \mathrm{e}^{\mathrm{i}\phi}|e,\alpha \mathrm{e}^{-\mathrm{i}\nu t} \rangle \right)$ III

Initial state: $|\Psi(0)\rangle = |g,0\rangle$ Ι Π $|\Psi(t+t_{\text{pulse}})\rangle = \frac{1}{\sqrt{2}} \left(|g,0\rangle + \mathrm{e}^{\mathrm{i}\phi}|e,\alpha\mathrm{e}^{-\mathrm{i}\nu t}\rangle\right)$ III Probability to be in the ground state: $\mathcal{P}_g(t) = \frac{1}{2} \left[1 + \operatorname{Re} \left\{ e^{\mathrm{i}\phi} \mathcal{S}(t) \right\} \right]$

Cat-states in spin-dependent potentials

Quantum superposition of two internal states in a spin-dependent potential

$$V_{\text{pot}} = \sum_{j=1}^{N} |g\rangle_{j} \langle g| \ V_{g}(\mathbf{r}_{j}) + |e\rangle_{j} \langle e| \ V_{e}(\mathbf{r}_{j})$$

Cat-state of ion structures

$$\left|\Psi(t)\right\rangle = \frac{1}{\sqrt{2}} \left(\left|ggg\right\rangle \left|0\right\rangle_{zz} + \left|geg\right\rangle \left|\phi(t)\right\rangle\right)$$

J. Baltrusch, C. Cormick, G. De Chiara, T. Calarco, GM, PRA (2011)

Cat-states in spin-dependent potentials



Ramsey contrast

Ramsey contrast gives the overlap between the two motional states across the transition



J. Baltrusch, C. Cormick, G. De Chiara, T. Calarco, G.M, PRA (2011)



Visibility gives the overlap of the states across the quench

 $\mathcal{O}_0(t) = {}_g \langle \underline{0} | U_e(t) | \underline{0} \rangle_g$



J. Baltrusch, C. Cormick, and GM, PRA (2012)



Visibility gives the overlap of the states across the quench

 $\mathcal{O}_0(t) = {}_g \langle \underline{0} | U_e(t) | \underline{0} \rangle_g$



J. Baltrusch, C. Cormick, and GM, PRA (2012)

Fourier transform of the Visibility signal

10 tin μs



J. Baltrusch, C. Cormick, GM, PRA (2012)

Single-mode sq

0.2

0.1 0

-0.1 -0.2

Multi-mode sq.

Quantum Quenches



Picture: Chris Monroe's group

Based on engineering the coupling between phonons and spins (Wunderlich, Porras, Cirac)

Experiments: Blatt, Bollinger, Monroe, Schätz,

Topological Phase Transitions in Ion Crystals

Planar instability



D.H.E. Dubin, PRL 1993

Continuous transition from a single to three planes

Order parameter



order parameter $z_i = \operatorname{Re}\left[\psi e^{i\mathbf{K}\cdot\mathbf{r}_i}\right]$

Symmetries and Model



Symmetries and Model



Ginzburg-Landau free energy

 $\frac{f_{\rm GL}}{\mathcal{K}} = \frac{\gamma}{2} |\nabla \psi|^2 + r|\psi|^2 + u|\psi|^4 + v|\psi|^6 + \frac{w}{2} \left[\psi^6 + (\psi^*)^6\right]$

6-state clock model

D. Podolsky, E. Shimshoni, GM, S. Fishman, 2015

Phase diagram



Phase diagram



Conclusions

Structural transitions in ion crystals: "natural" quantum simulators of solid-state models

Ion crystals: laboratory for studying far-off equilibrium statistical mechanics

Interfacing phonons and photons: novel quantum phases of matter
Exotic phases of photons and ions



Typical length of crystallization is incommensurate with cavity wave length (figure from Cetina et al, NJP 2013)

Exotic phases of photons and ions



Exotic model of friction



T. Fogarty, C. Cormick, H. Landa, V. M. Stojanovic, E. A. Demler, GM, arXiv:1504.00265

Collaborations

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Fogar



Baltrusch



