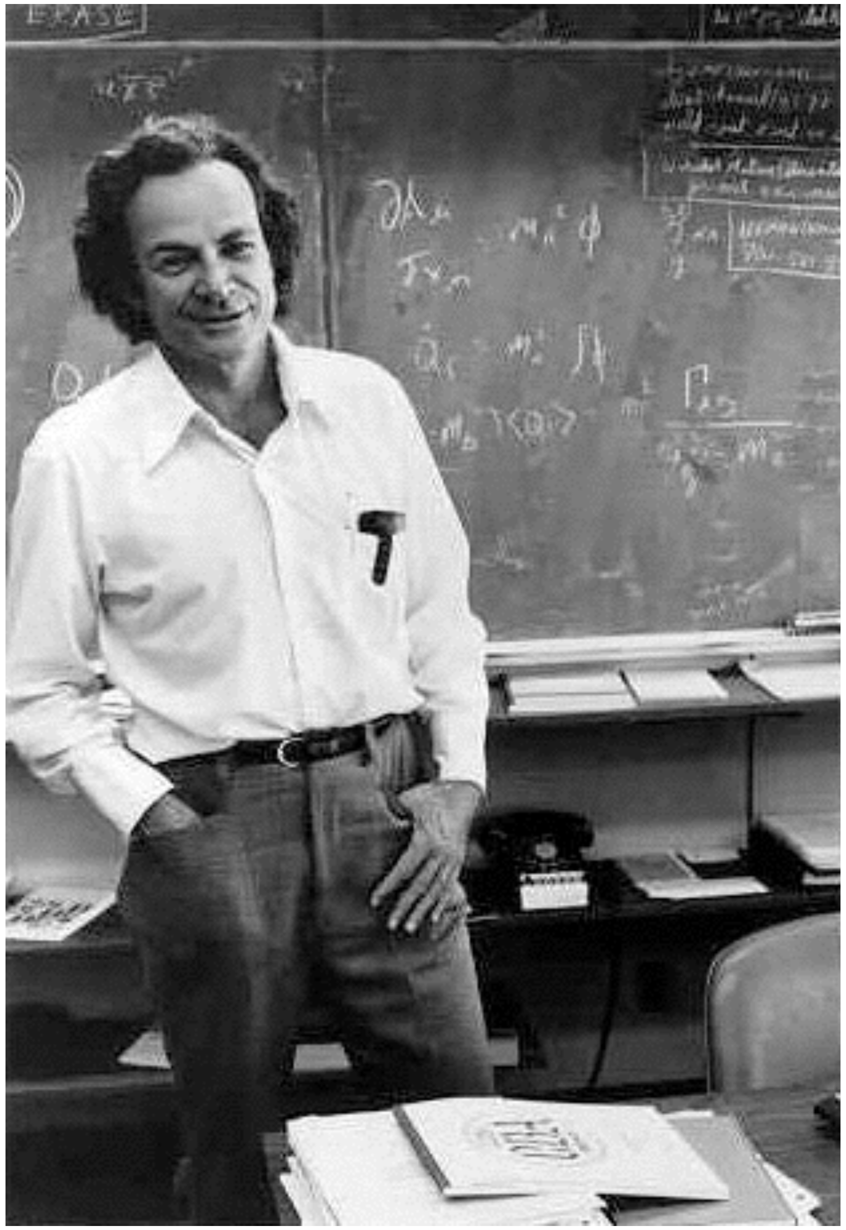
Quantum mechanical systems out of equilibrium

Viewpoints on Emergence in Nonequilibrium Systems meeting, Edinburgh, 23 June 2014

Jean-Sébastien Caux
Universiteit van Amsterdam

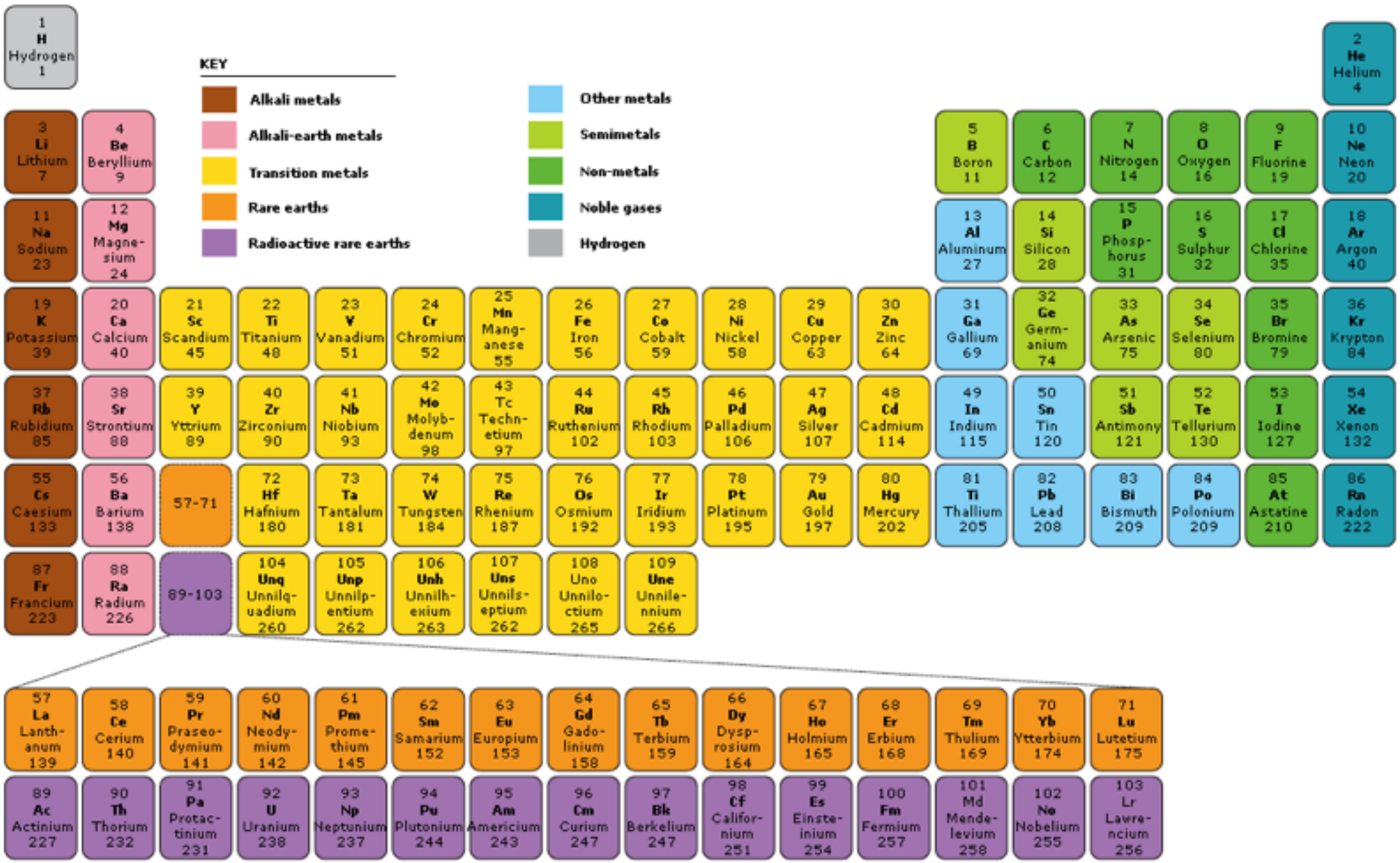
Main challenges and goals



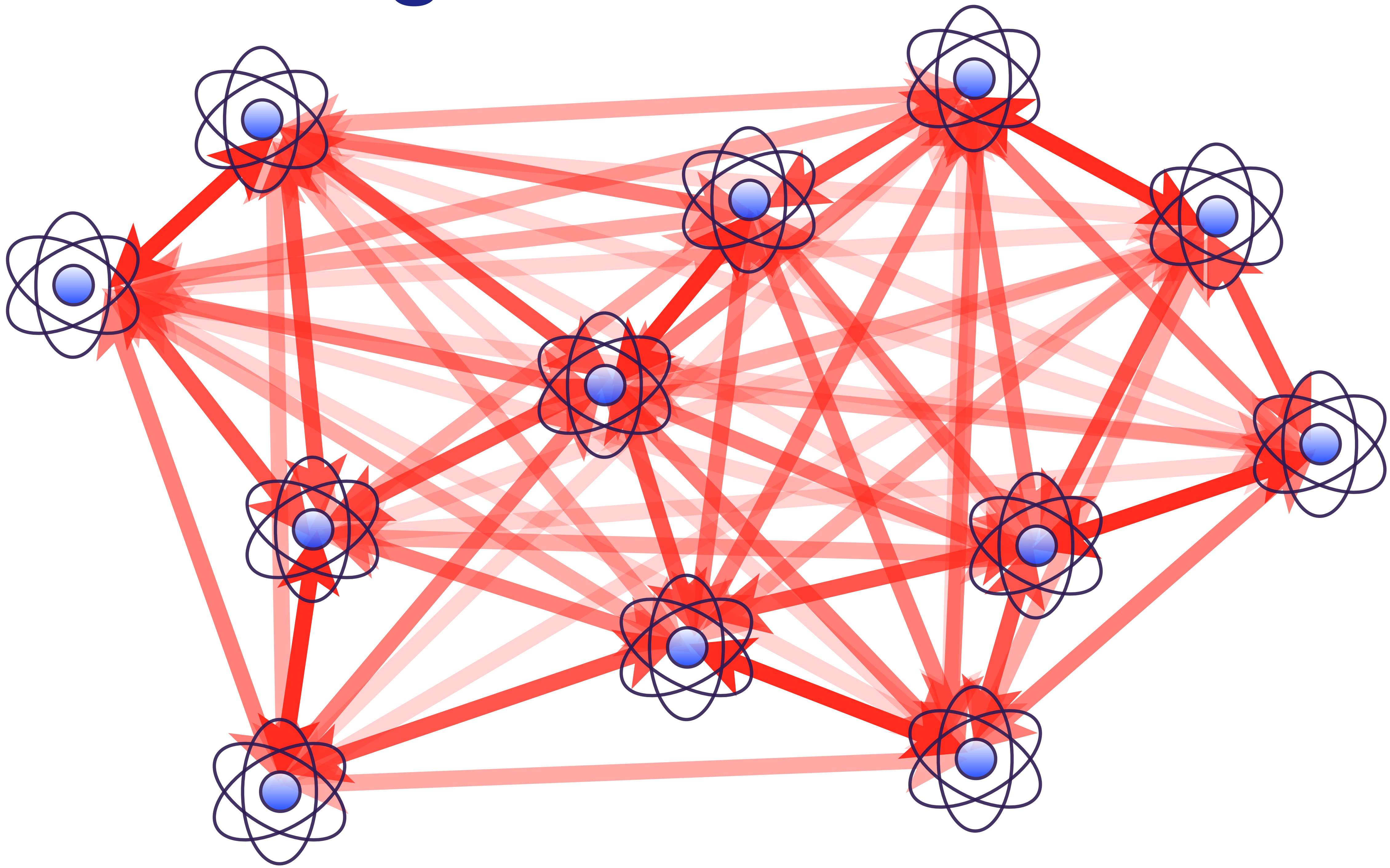
Now, the name of this talk is ``There is Plenty of Room at the Bottom"---not just ``There is Room at the Bottom." What I have demonstrated is that there is room---that you can decrease the size of things in a practical way. I now want to show that there is plenty of room.

Richard Feynman, APS talk 1959

It’s not just that there is plenty of room, it’s also that there are *many ways to fill it*…

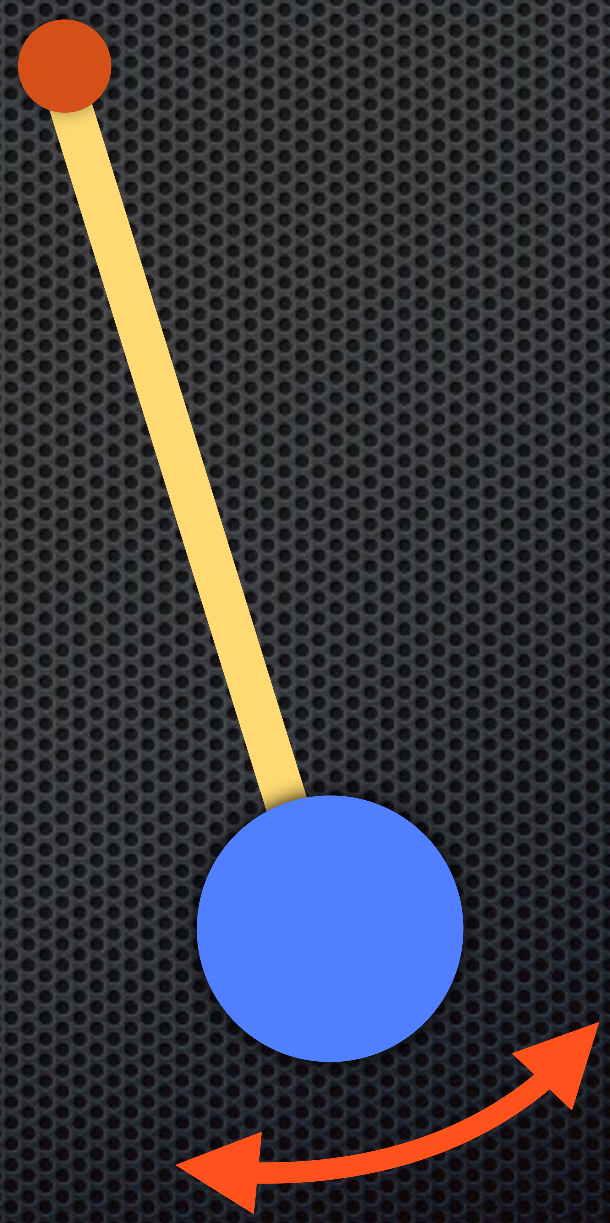


The strong correlations ‘minefield’



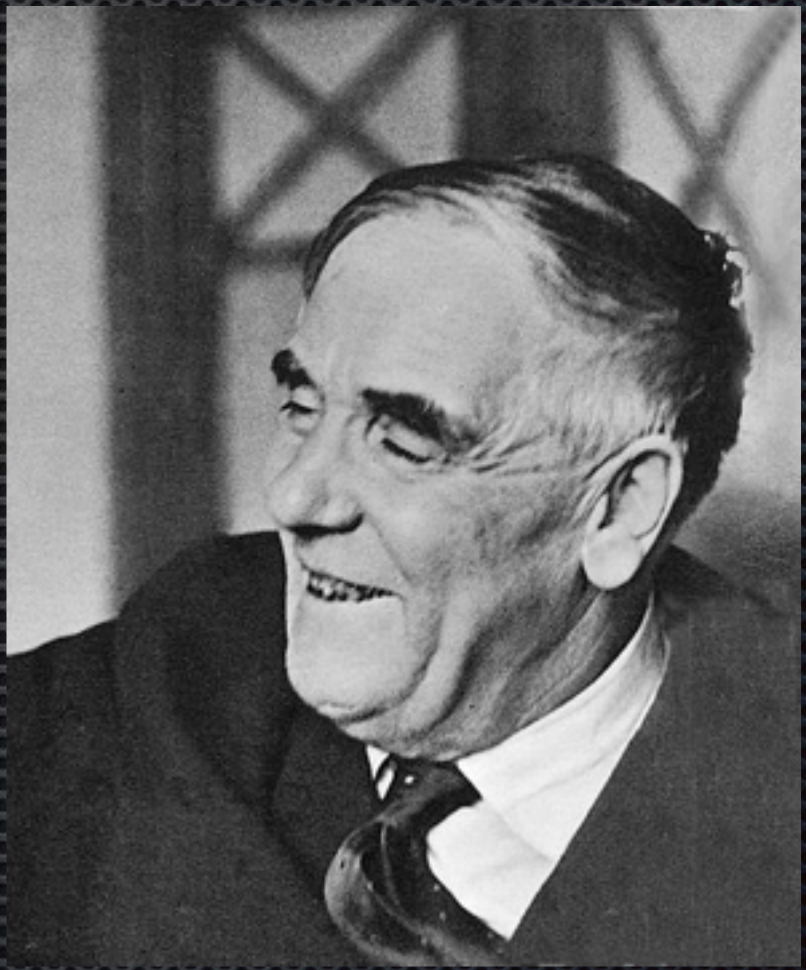
Many particles + interactions =
emergent state, difficult to describe

One of the only things we really understand



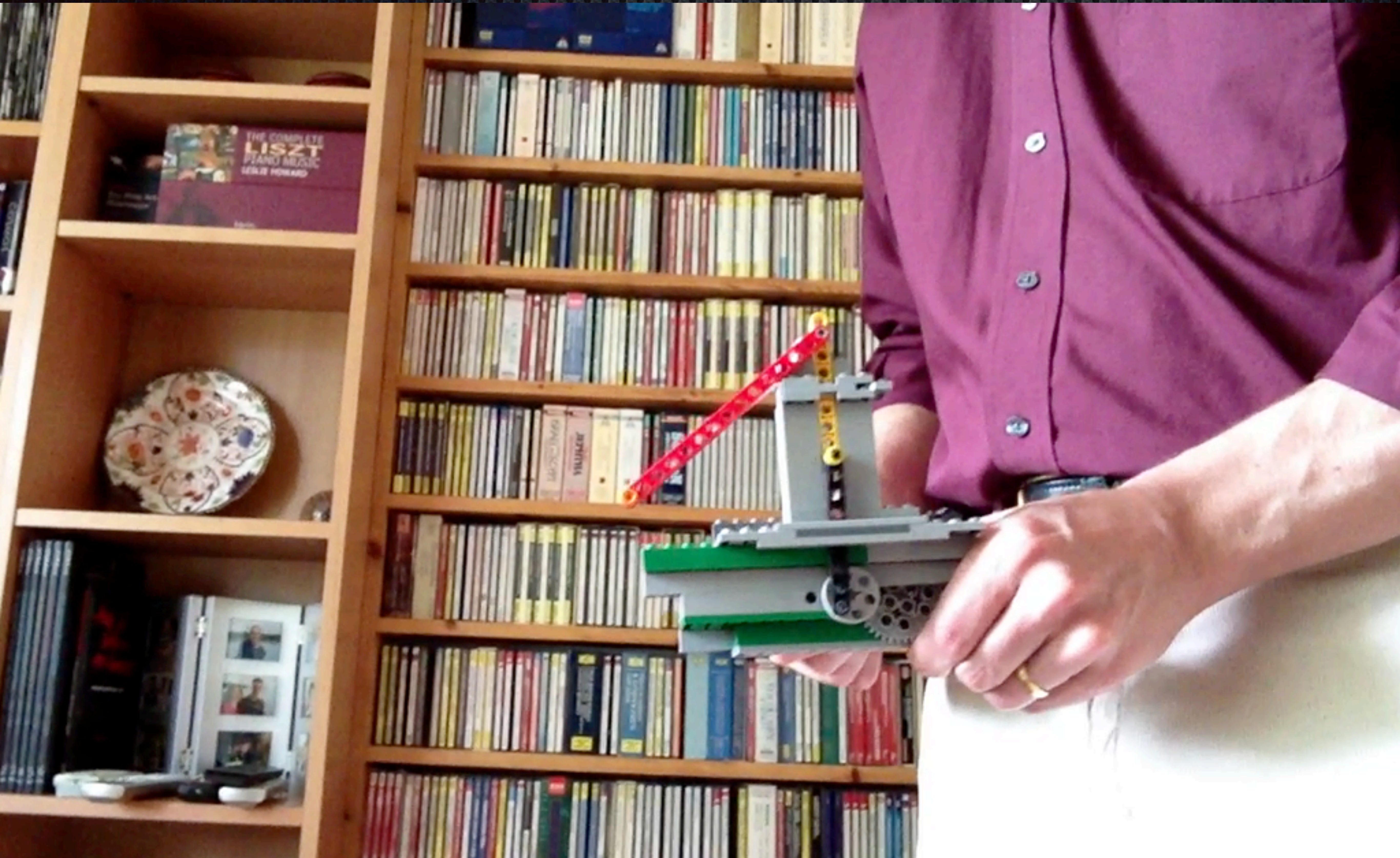
The simple pendulum on its head

Kapitsa pendulum, 1951



Pyotr L. Kapitsa
(8/7/1894-8/4/1984)

The Kapitza pendulum



Main goals of this research area

- **Understand how ‘many’, ‘quantum’, ‘driven’ relate to and impact one another**
- **Identify and create new quantum states with interesting properties**
- **Classify the possible states, phases and (quasi)particles in out-of-equilibrium systems**
- **Translate these new properties into new functionalities**
- **At more fundamental level: enrich our understanding of quantum many-body physics**

arXiv cond-mat year 1994

arxiv.org/year/cond-mat/94

Cornell University Library

We gratefully acknowledge support from the Simons Foundation and member institutions

arXiv.org > cond-mat > 1994

Search or Article-id (Help | Advanced search)

All papers Go!

Condensed Matter

Article statistics for 1994

Available montly lists with counts of **cond-mat articles** + *cross-listings to cond-mat* in 1994 (each '|' represents 20 articles):

- 9401 |||| **77** + *10* (Jan 1994)
- 9402 |||||| **114** + *8* (Feb 1994)
- 9403 |||||! **95** + *24* (Mar 1994)
- 9404 |||||! **102** + *16* (Apr 1994)
- 9405 |||||! **90** + *27* (May 1994)
- 9406 ||||||! **123** + *12* (Jun 1994)
- 9407 ||||||! **124** + *15* (Jul 1994)
- 9408 |||||! **102** + *10* (Aug 1994)
- 9409 ||||||| **124** + *18* (Sep 1994)
- 9410 ||||||! **118** + *15* (Oct 1994)
- 9411 ||||||||! **131** + *40* (Nov 1994)
- 9412 ||||||| **123** + *23* (Dec 1994)

1994 totals: **1323 articles** + *218 cross-lists*

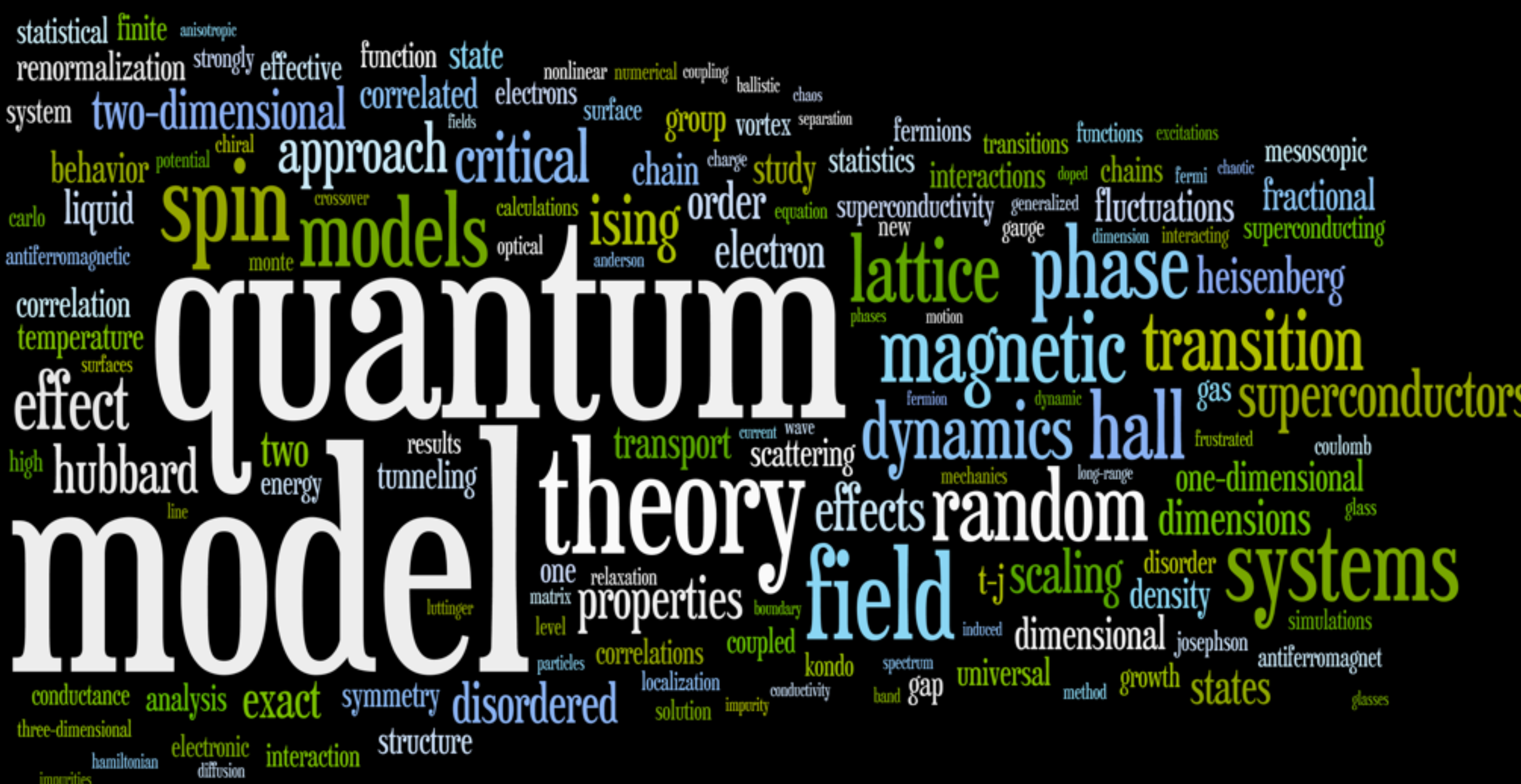
Other years: 2014 2013 2012 2011 2010 2009 2008 2007 2006 2005 2004 2003 2002 2001 2000 1999 1998 1997 1996 1995 1994 1993 1992

Link back to: arXiv, form interface, contact.

1994 abstracts (all 1541)

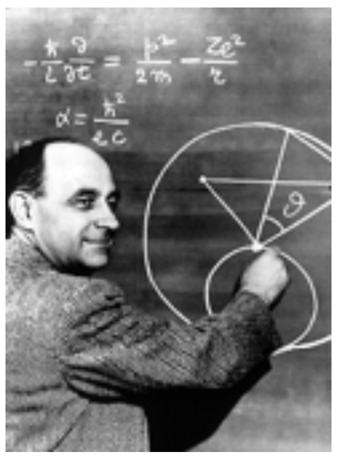
http://arxiv.org/list/cond-mat/94?show=1541

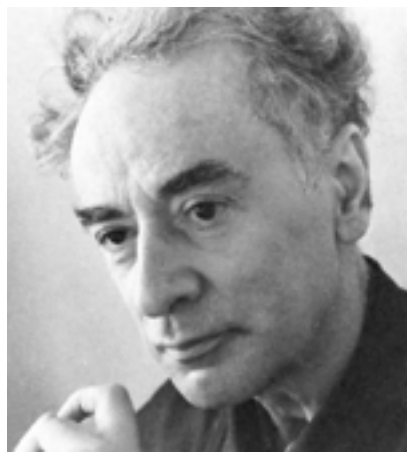
arxiv 1994 (cond-mat) word cloud (1529 article titles)



Existing theory frameworks

- Fermi liquid theory



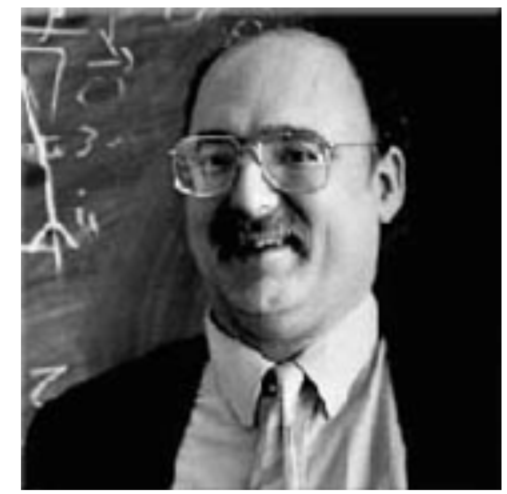


- Fermi sea

- Fermion-like quasiparticles

The rule rather than the exception in high-dimensional systems

- Luttinger liquid theory



- Quantum liquid

- Spin-charge separation

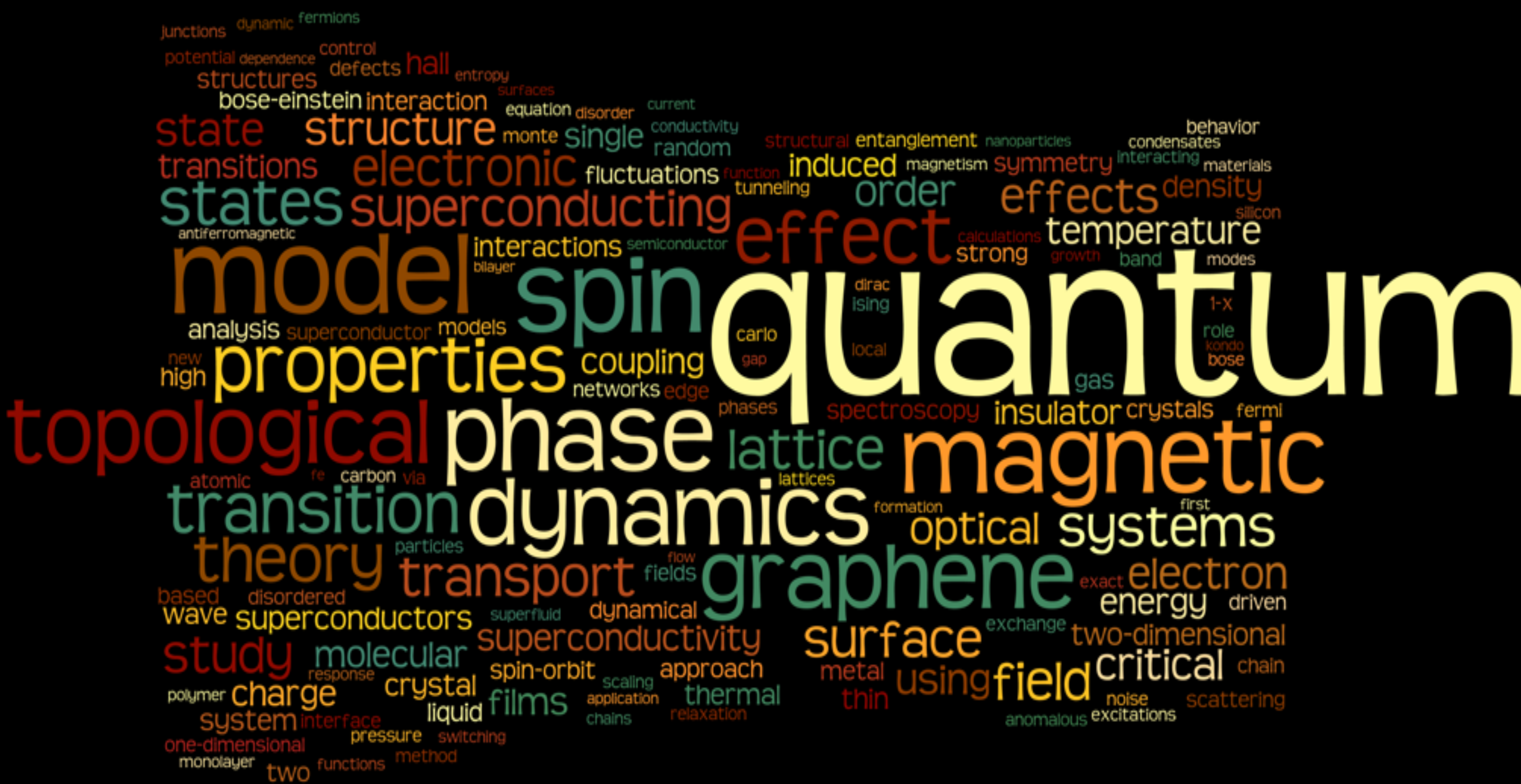
The rule rather than the exception in low-dimensional systems

Focus: low-energy, 'universal' features
Description breaks down away from E ~ 0
or out of equilibrium

Notable developments

- **The cold atoms revolution**
  - unprecedented tunability
  - a theoretician’s wet dream: idealized is realized!
- **Nanodevices**
  - quantum dots
  - nanowires
  - NV centers
- **Great strides in (experimental) magnetism**
  - neutrons getting better and better
  - new techniques like RIXS
- **Numerical methods**
  - emergence of amazingly efficient algorithms (DMRG,… ‘rise of the machines’)

arxiv 2014 (cond-mat) word cloud (first 2000 of 7129 article titles)

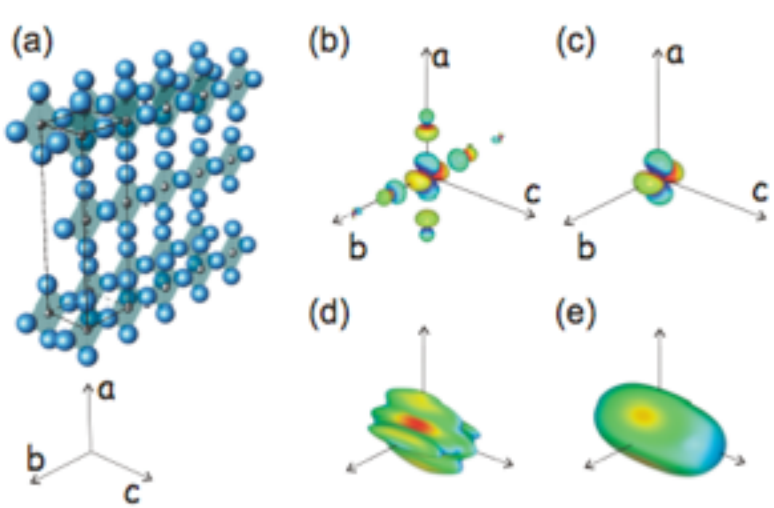


Critical assessment:

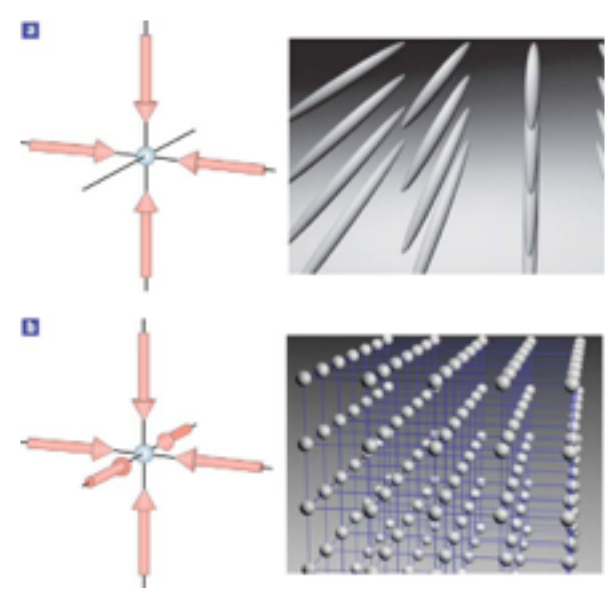
experimental work is far ahead, theory a bit stuck

Missing: reliable theory framework with quantitative predictive power, beyond low-energy/equilibrium limit

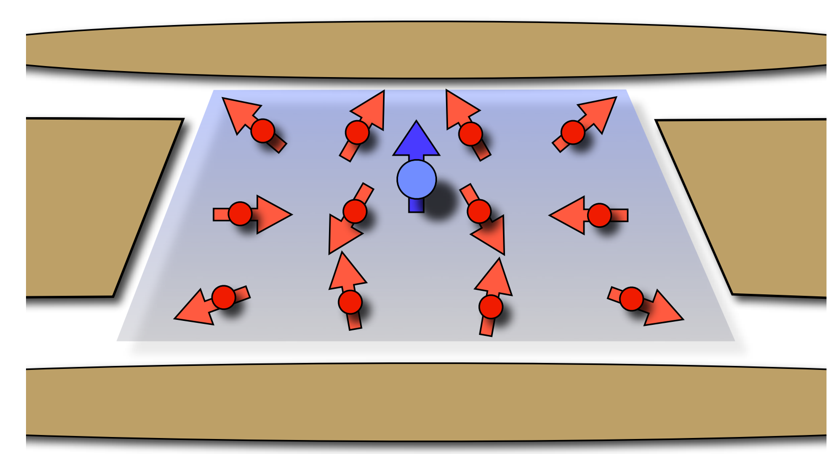
Urgently needed to describe ongoing experiments



Quantum magnetism

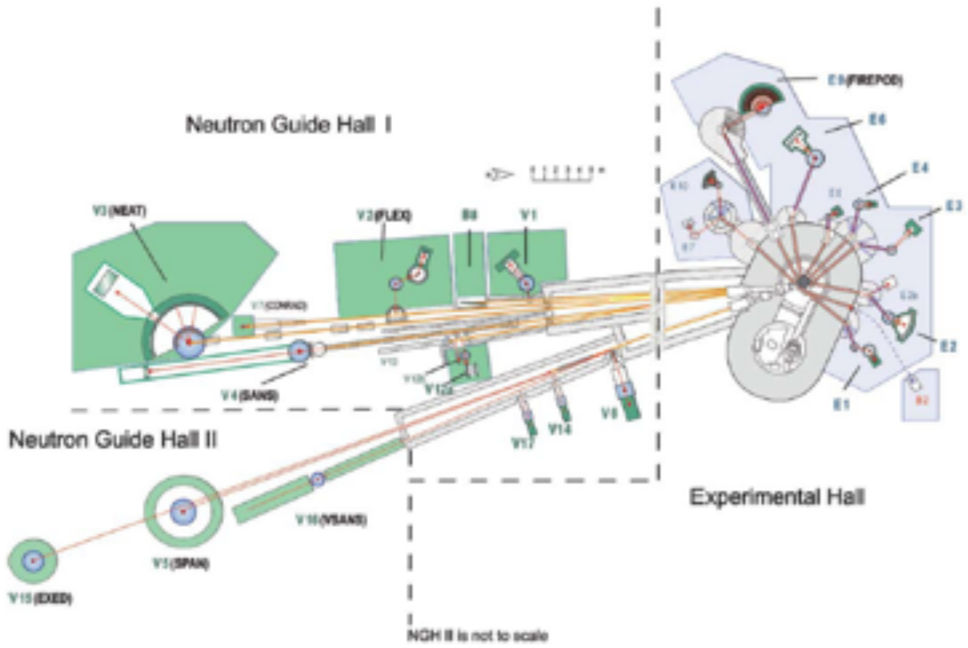


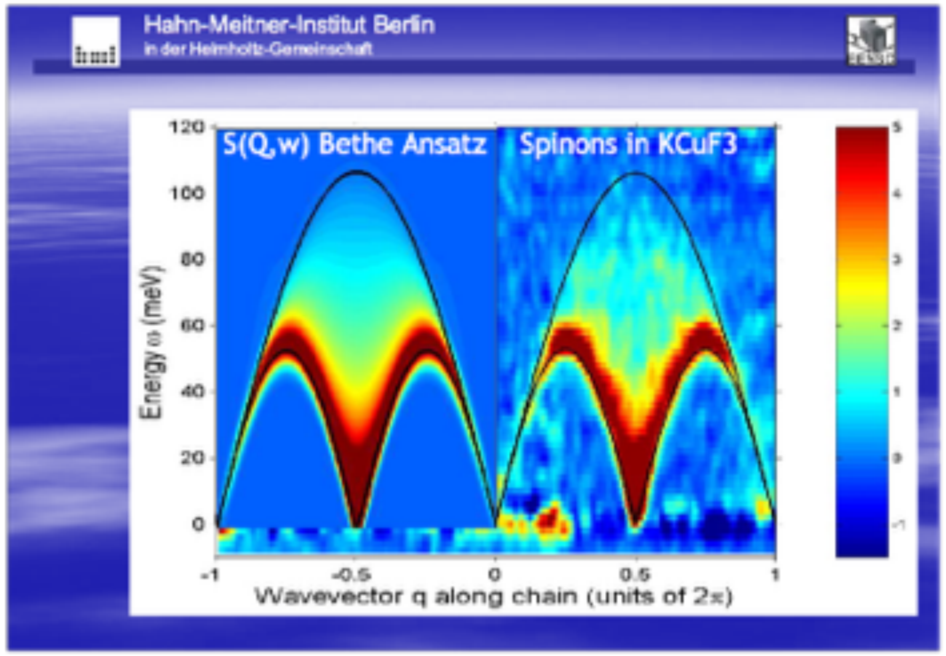
Cold atoms



Quantum dots, nanodevices

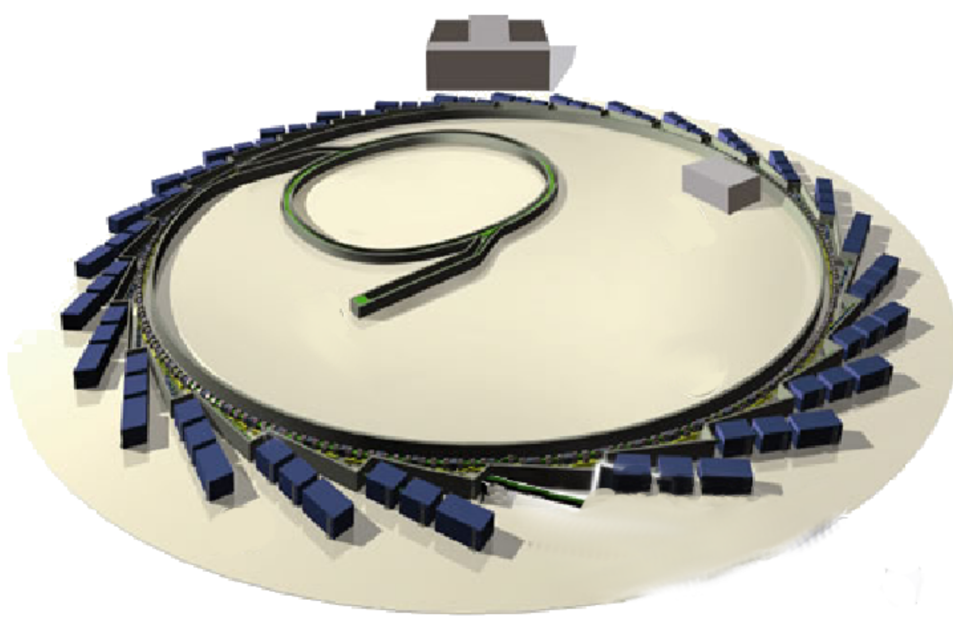
Experiments (I): Quantum magnetism/neutrons



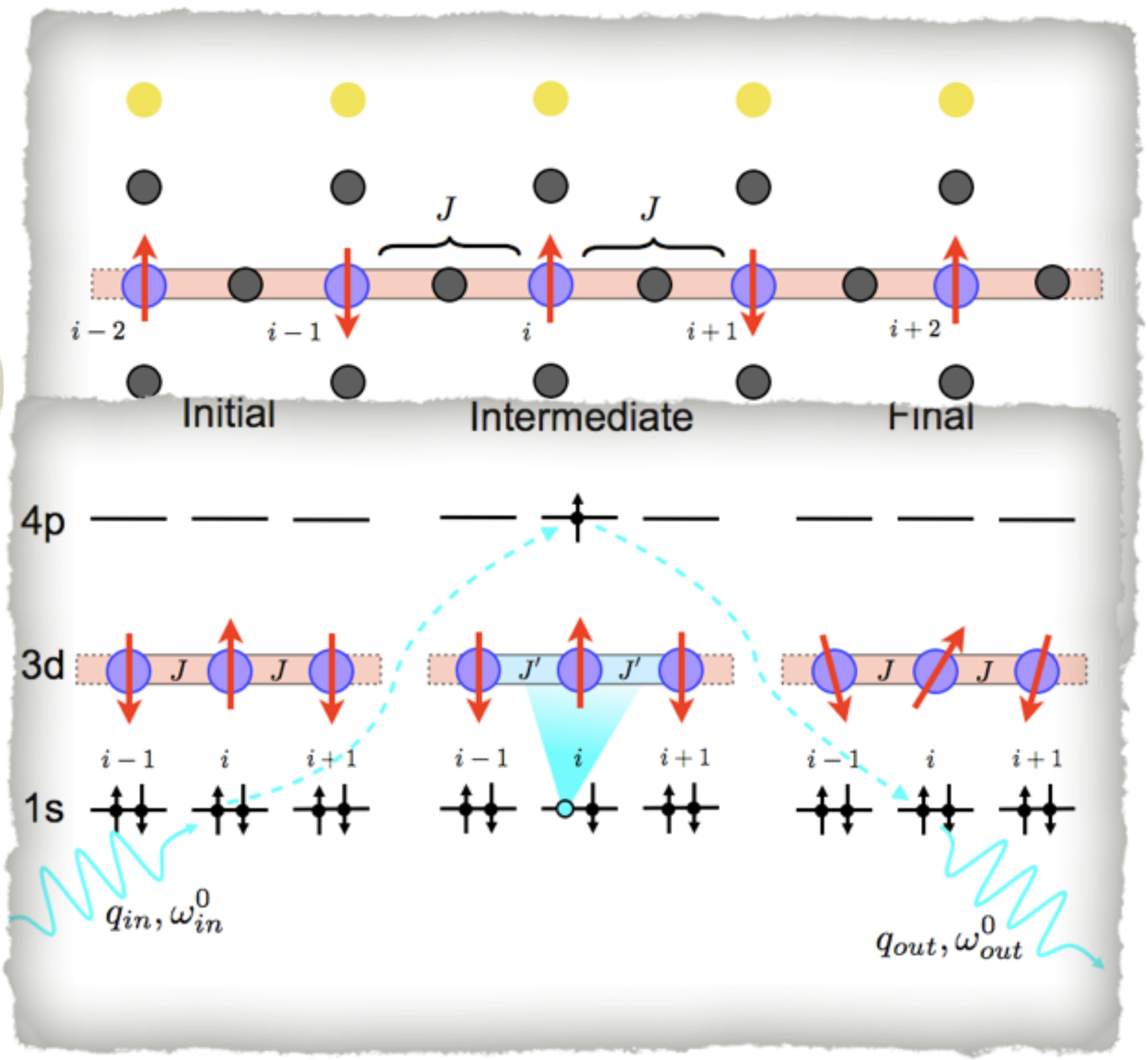


RIXS
(resonant inelastic X-ray scattering)

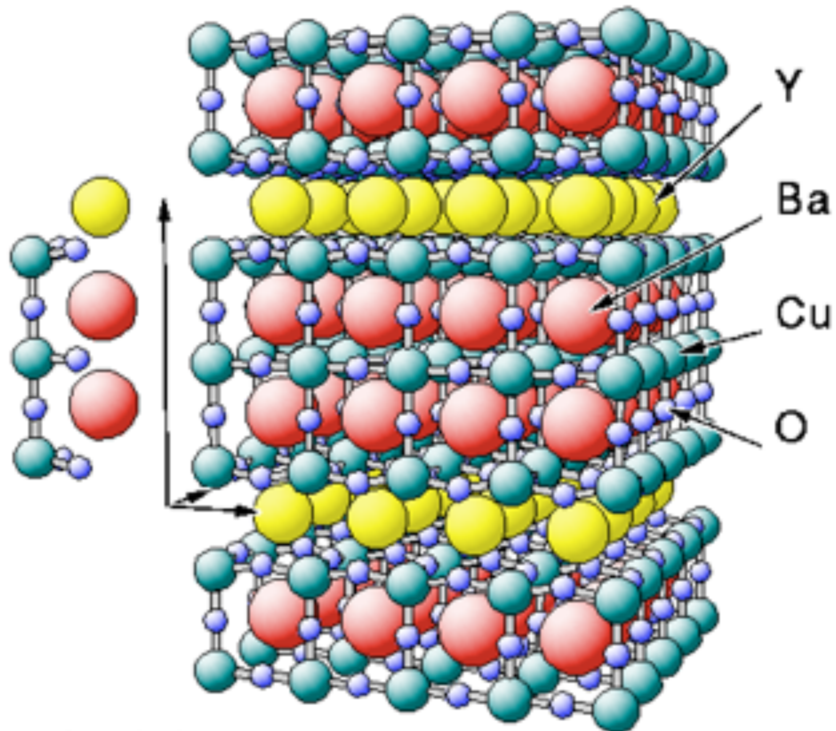
Synchrotron



X-ray induces a 1s-4p transition on copper, modifying exchange term



Example question: does a room-temperature superconductor exist?

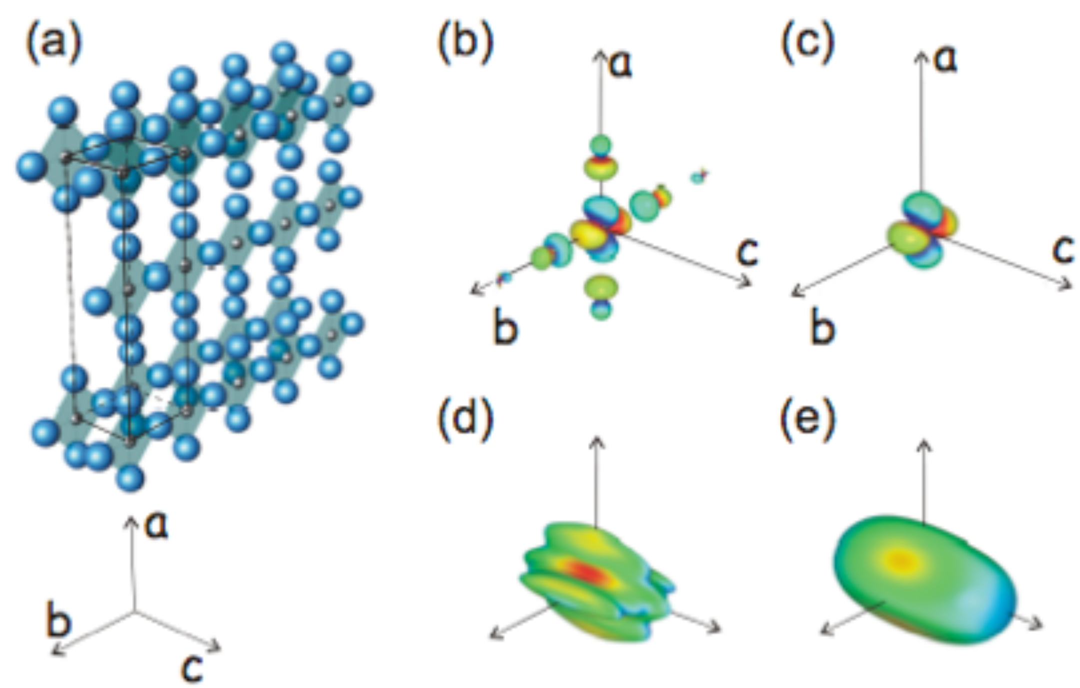


$YBa_2Cu_3O_7$ (.3) lattice

YBCO: high-Tc (93K)superconductor

No theory up to now
How to proceed?

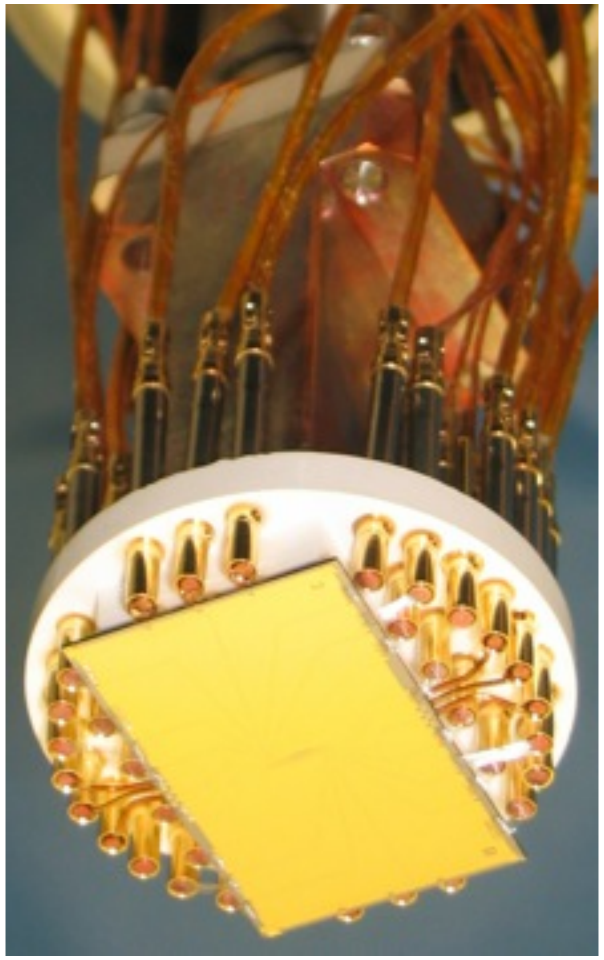
Strategy: start by understanding simpler (1d) materials displaying related properties.
Magnetism-driven pairing?

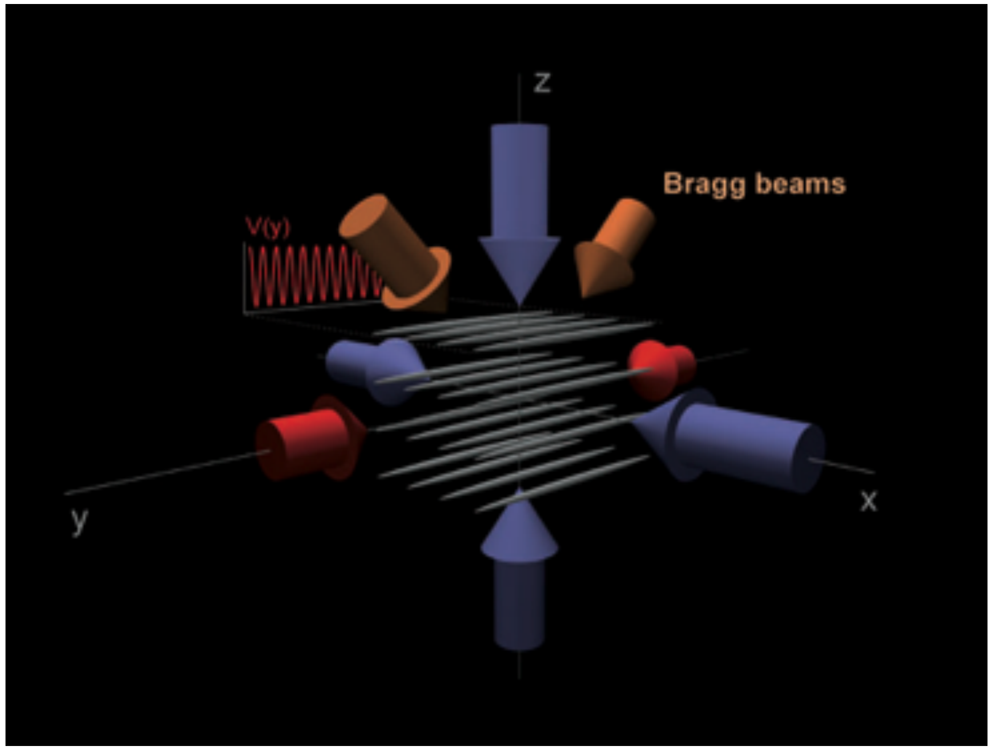


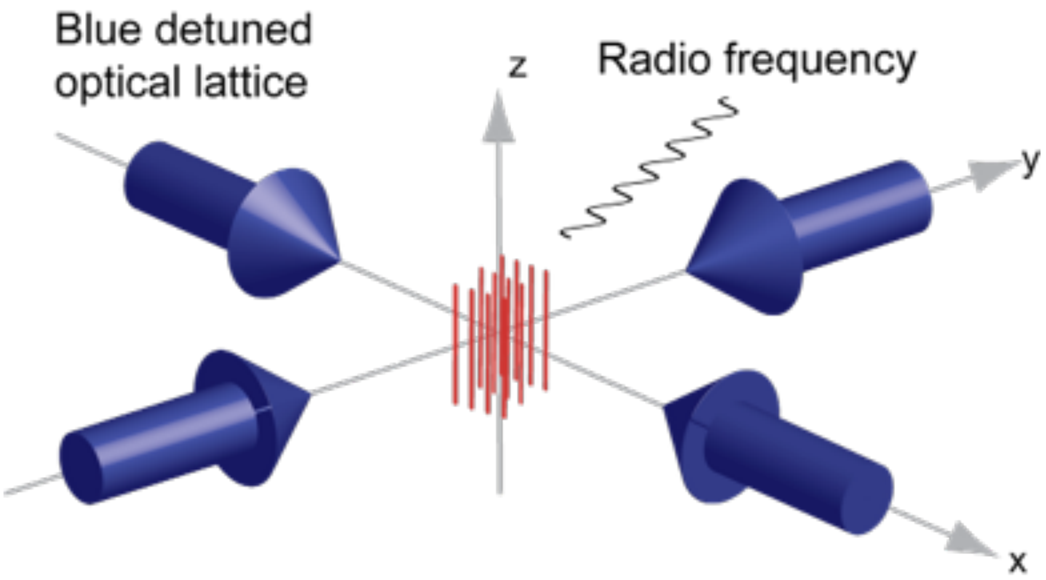
Sr_2CuO_3

Walters, Perring, Caux, Savici, Gu, Lee, Ku, Zaliznyak, NATURE PHYSICS 2009

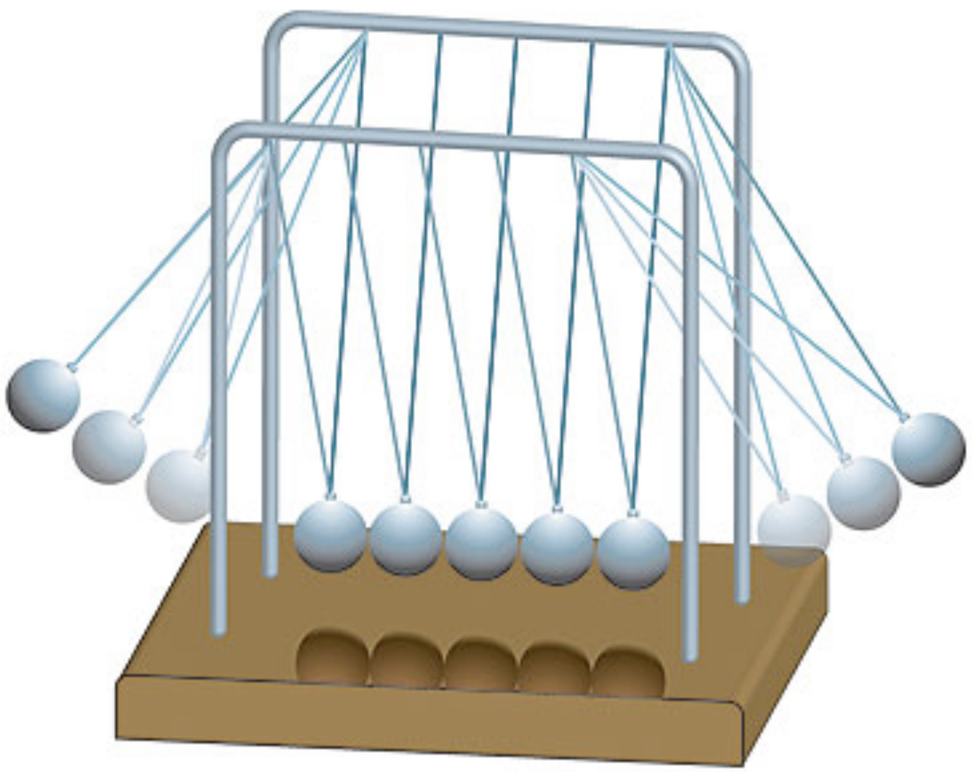
Experiments (II): Cold atoms



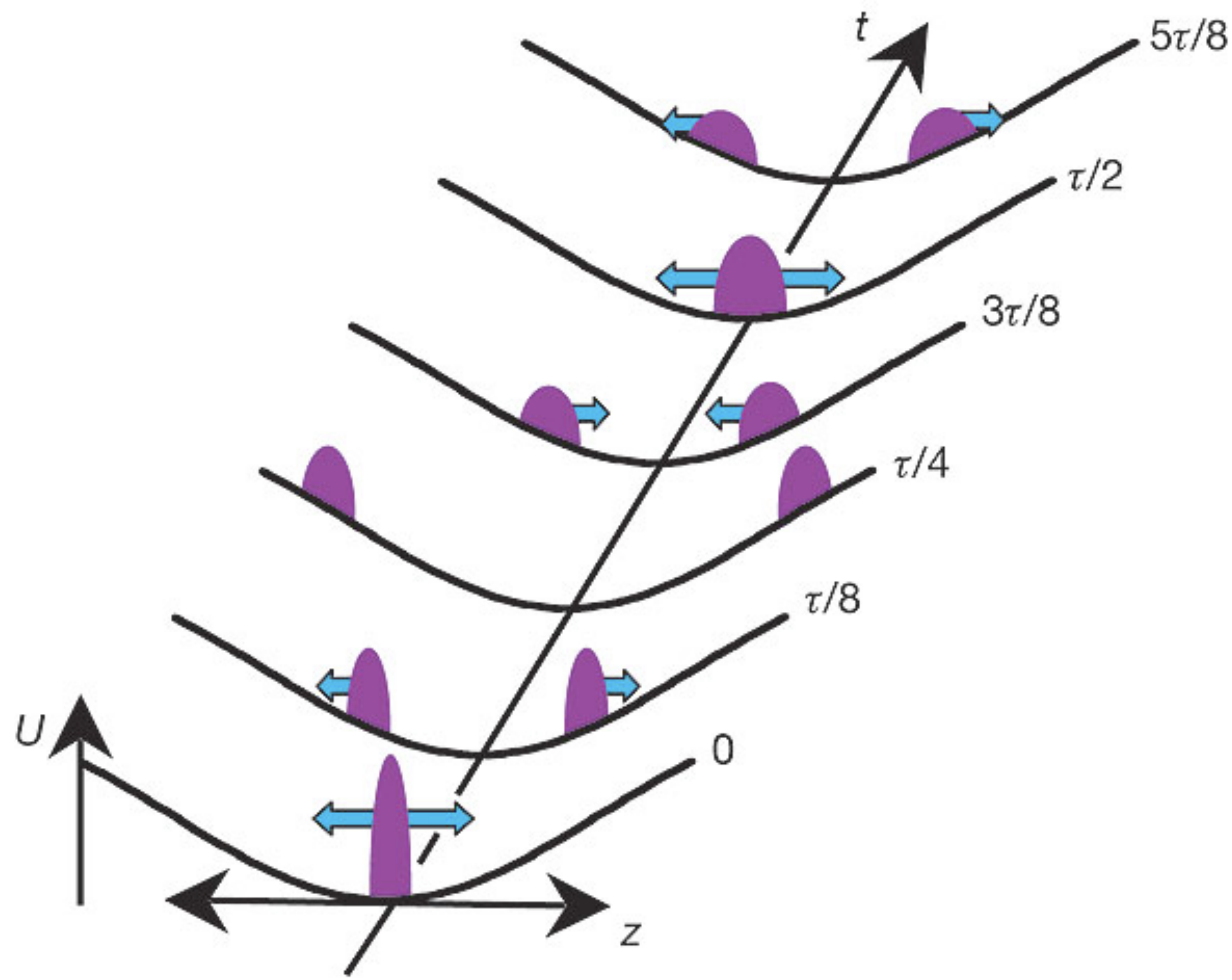




David Weiss's quantum Newton's cradle experiment



Ergodicity in interacting quantum systems close to an integrable model

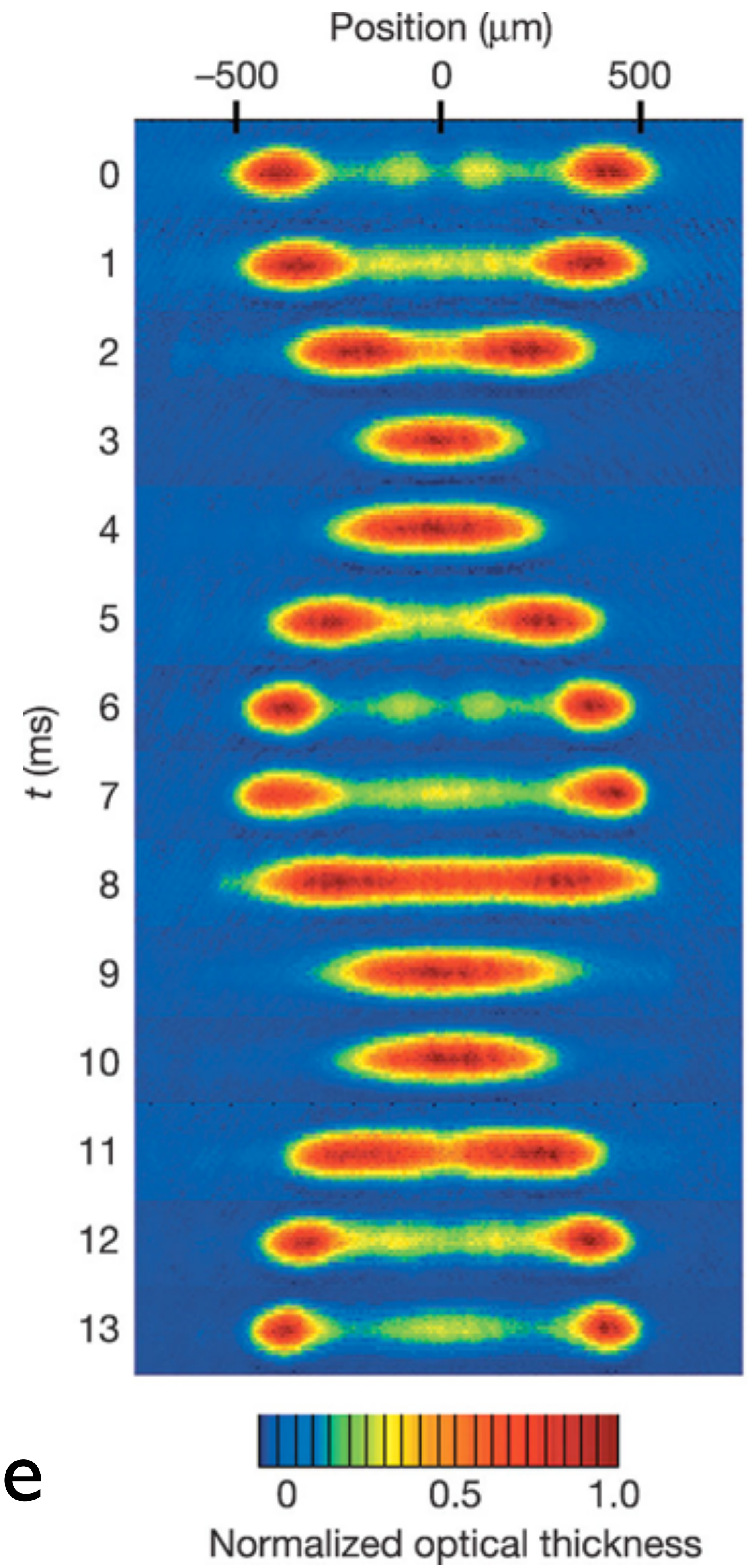


Atoms do not thermalize during the experimental time scale (about 50 cycles)

Experimentally possible to 'break' integrability in different ways, to test relaxation and ergodicity

Does there exist a quantum KAM theorem ?

Nonequilibrium & quench physics experimentally accessible



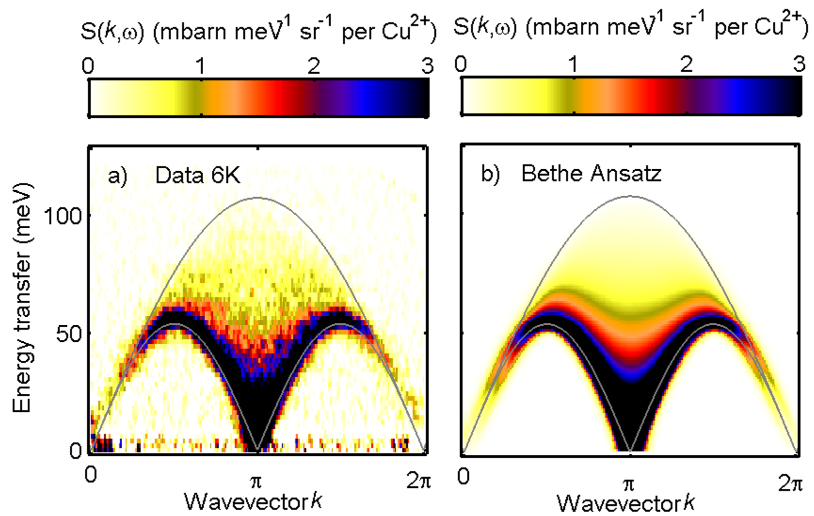
Useful theoretical paradigms

Mea culpa: focused on 1d

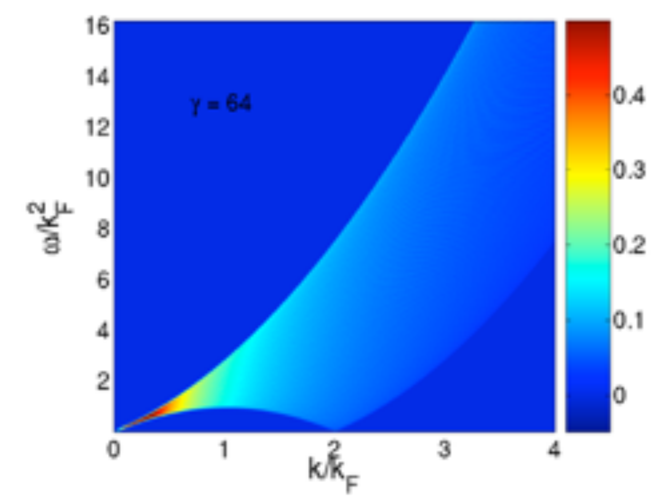
~~*Mea culpa:*~~ *can really do something here!*

- **Nonperturbative solutions (integrability)**
- **Extensions of Luttinger theory to higher energies (by including nonlinearities)**
- **Numerical methods**

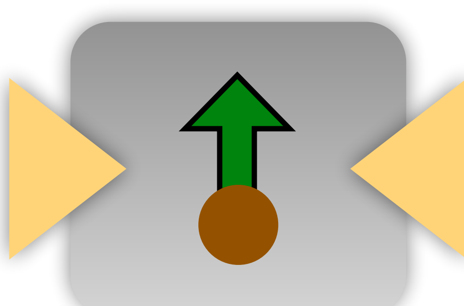
Applications of integrability in many-body physics



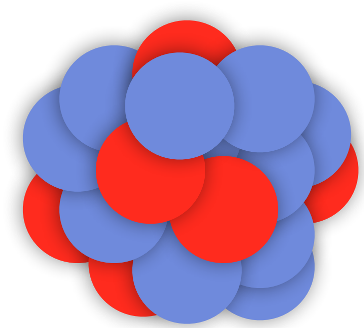
Quantum magnetism



Ultracold atoms



Quantum dots, NV centers

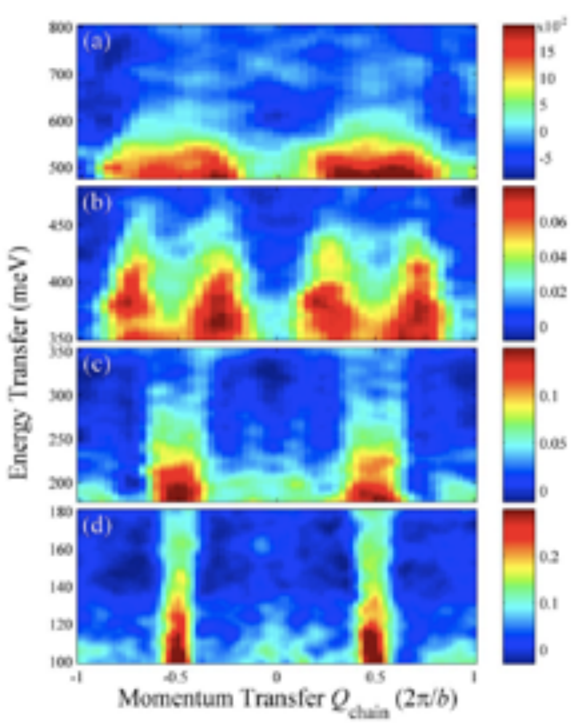


Atomic nuclei

Quantum spin chains

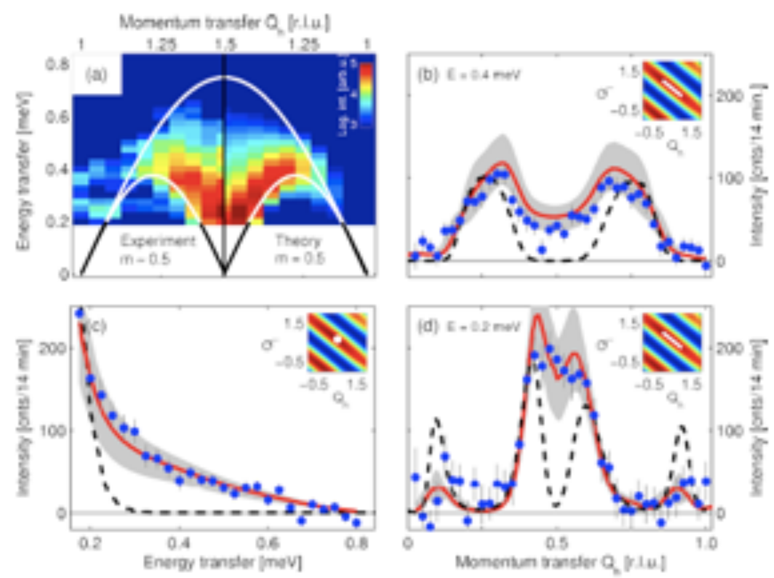
Correlations, experiments (INS, RIXS), prefactors, ...

Sr_2CuO_3



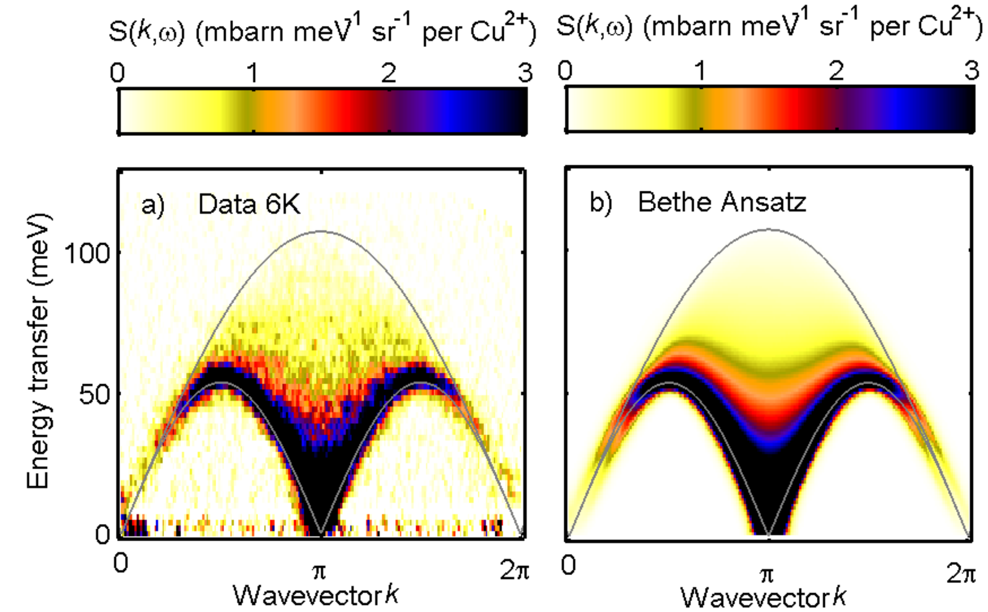
Walters, Perring, Caux, Savici, Gu, Lee, Ku, Zaliznyak, NATURE PHYSICS 2009

$(C_5D_{12}N)_2CuBr_4$

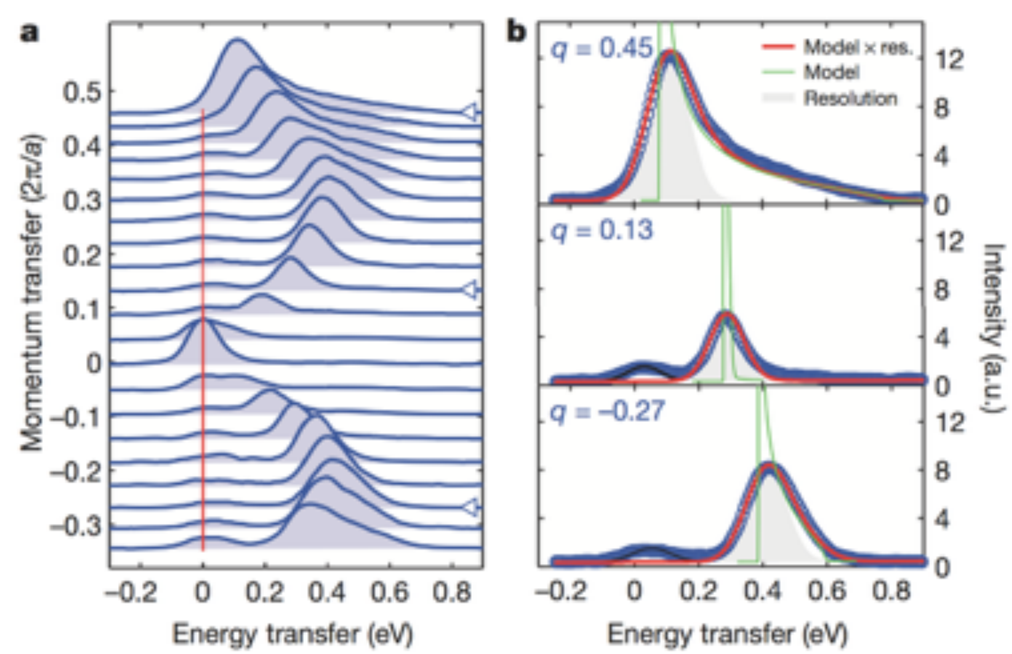


Thielemann, Rüegg, Rønnow, Läuchli, Caux, Normand, Biner, Krämer, Güdel, Stahn, Habicht, Kiefer, Boehm, McMorrow, Mesot, PRL 2009

$KCuF_3$



Lake, Tennant, Caux, Barthel, Schollwöck, Nagler, Frost 2013



Sr_2CuO_3 (RIXS)

Schlappa, Wohlfeld, Zho, Mourigal, Haverkort, Strocov, Hozoi, Monney, Nishimoto, Singh, Revcolevschi, Caux, Patthey Rønnow, van den Brink, Schmitt, NATURE 2012

Counting fractional spinon excitations in the quantum Heisenberg antiferromagnetic chain

Martin Mourigal,[1,2,3,*] Mechthild Enderle,[1] Axel Klöpperpieper,[4]
Jean-Sébastien Caux,[5] Anne Stunault,[1] and Henrik M. Rønnow[2]

(Nature Physics 2013)

$CuSO_4 \cdot 5D_2O$

Roger Hiorns, *Seizure*

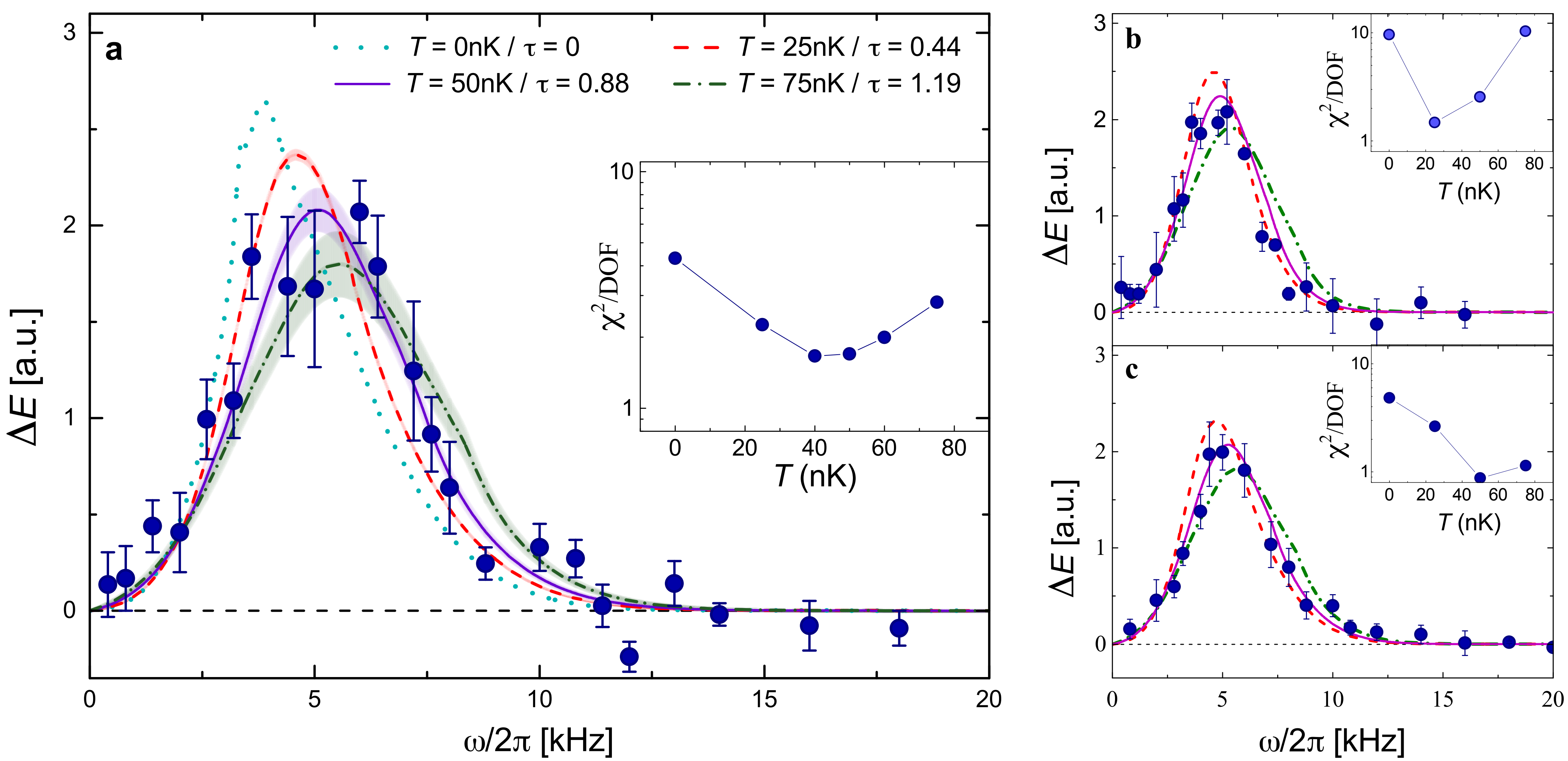
Cold atoms

Observing elementary excitations of correlated one-dimensional Bose gases

N. Fabbri, M. Panfil, D. Clément, L. Fallani, M. Inguscio, C. Fort and J.-S. Caux

arxiv:1406.2176

Density correlations using Bragg spectroscopy



Cold atoms

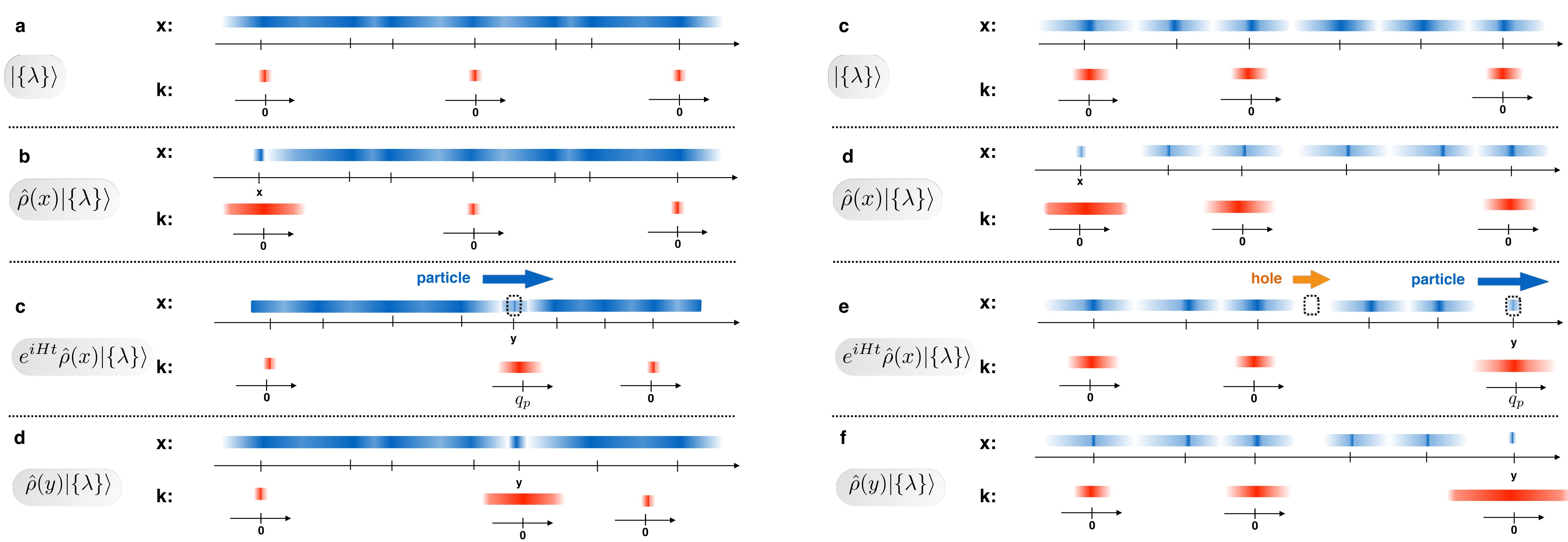
Observing elementary excitations of correlated one-dimensional Bose gases

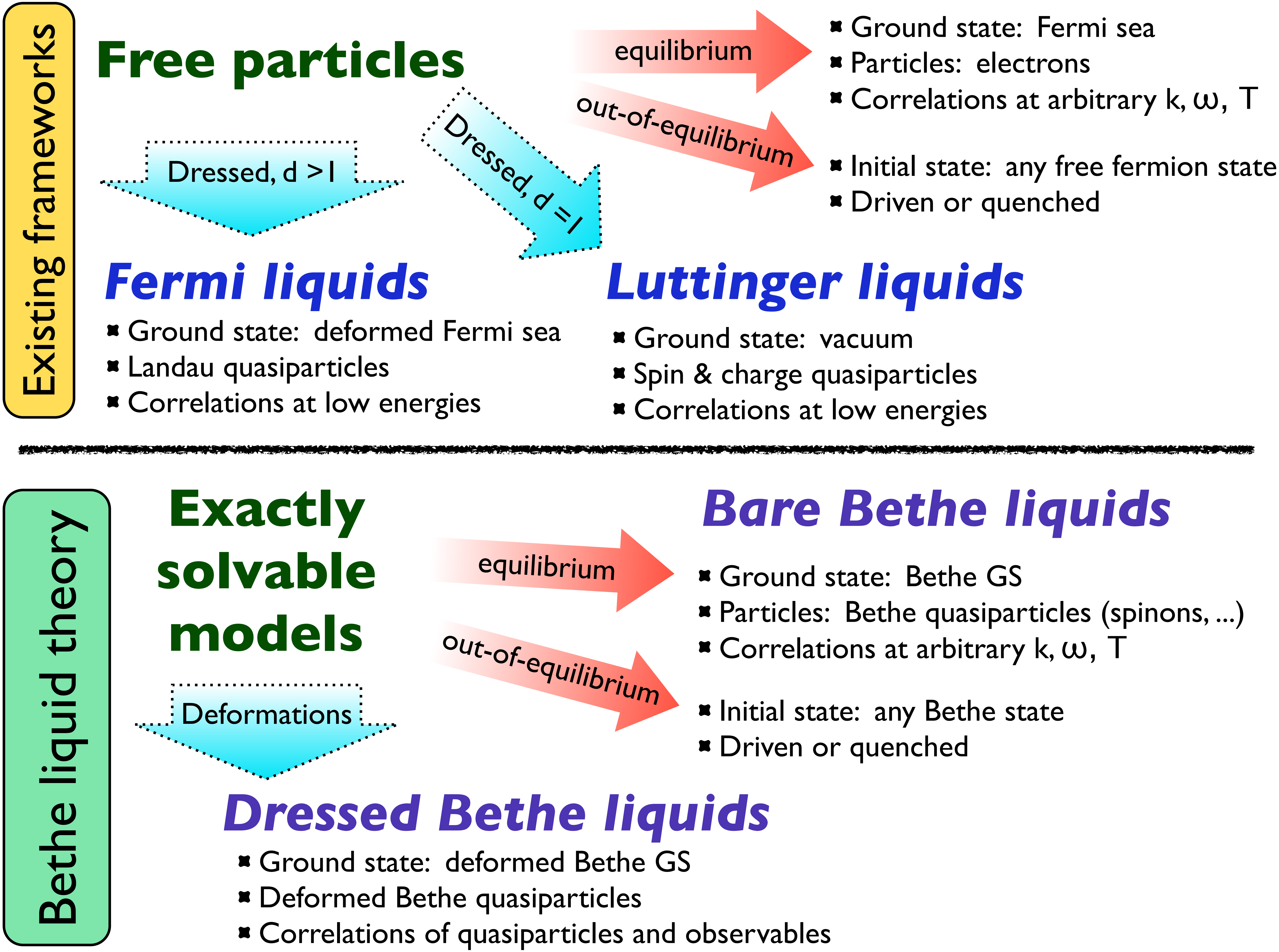
N. Fabbri, M. Panfil, D. Clément, L. Fallani, M. Inguscio, C. Fort and J.-S. Caux

arxiv:1406.2176

Intuitive picture of correlations: from ‘quasiparticles’

weak interactions | strong interactions



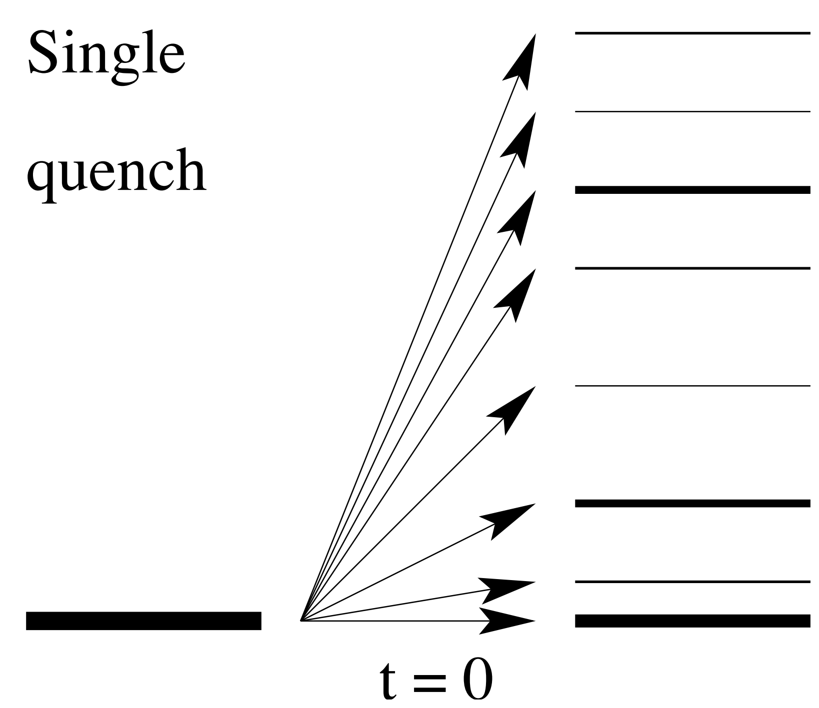

Existing frameworks
Free particles
equilibrium
Ground state: Fermi sea
Particles: electrons
Correlations at arbitrary k, ω, T
out-of-equilibrium
Initial state: any free fermion state
Driven or quenched
Dressed, d > 1
Dressed, d = 1
Fermi liquids
Ground state: deformed Fermi sea
Landau quasiparticles
Correlations at low energies
Luttinger liquids
Ground state: vacuum
Spin & charge quasiparticles
Correlations at low energies
Bethe liquid theory
Exactly solvable models
equilibrium
Bare Bethe liquids
Ground state: Bethe GS
Particles: Bethe quasiparticles (spinons, ...)
Correlations at arbitrary k, ω, T
out-of-equilibrium
Initial state: any Bethe state
Driven or quenched
Deformations
Dressed Bethe liquids
Ground state: deformed Bethe GS
Deformed Bethe quasiparticles
Correlations of quasiparticles and observables

Example of a (very) current challenge: post-quench steady states: GGE or not?

Quenches

Sudden change of interaction/global parameter

$$H_g \longrightarrow H_{g'}$$



- explore quantum systems in fundamentally different ways than traditional local probes
- open up many interesting questions about quantum relaxation, equilibration/thermalization
  (Eigenstate thermalization hypothesis, Mazur inequality, Generalized Gibbs ensemble, ...)
- provide whole new set of challenges for theory (old toolbox not enough)

First question: what is the steady state long after the quench?

Fundamental issue: does the system relax? thermalize?

Can we obtain an effective/simplified understanding?

Crucial point: *time evolution in the presence of myriads of constraints (due to integrability) is special*

Conjecture: *after a quantum quench, a generalized Gibbs ensemble (GGE) describes state at asymptotically large time*

$$\lim_{t\to\infty} \bar{\mathcal{O}}(t) = \langle \mathcal{O} \rangle_{GGE} = \frac{\mathrm{Tr}\{\mathcal{O} e^{-\sum_n \beta_n Q_n}\}}{\mathrm{Tr}\{e^{-\sum_n \beta_n Q_n}\}}$$

Rigol, Dunjko, Yurovsky, Olshanii, PRL 2007

see also Jaynes, Phys. Rev. 1957

GGE implementation

Generalized inverse temperatures to be set using the initial conditions on conserved charges

$$\langle \hat{Q}_m \rangle = \mathrm{Tr}\left\{ \hat{Q}_m e^{-\sum_n \beta_n \hat{Q}_n} \right\} / \mathcal{Z}_{GGE} \quad m = 0, 1, 2, \ldots$$

where $\mathcal{Z}_{GGE} = \mathrm{Tr} e^{-\sum_n \beta_n \hat{Q}_n}$

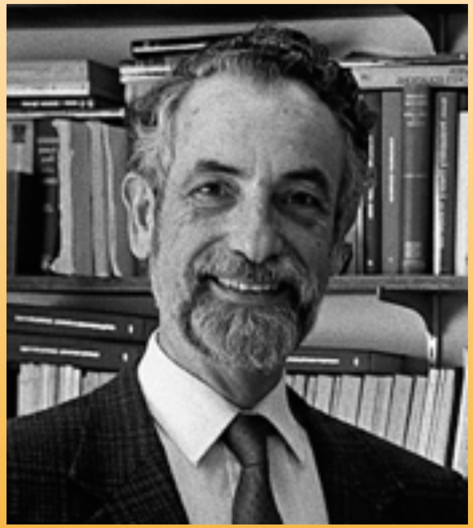
In reality, two major difficulties:

- Conserved charges are generically nontrivial
- Self-consistency problem difficult to solve

In practice: implementable for free theories only (charges: momentum occupation modes)

For interacting cases: not understood in general.

BEC to repulsive Lieb-Liniger quench



Interacting Bose gas (Lieb-Liniger)

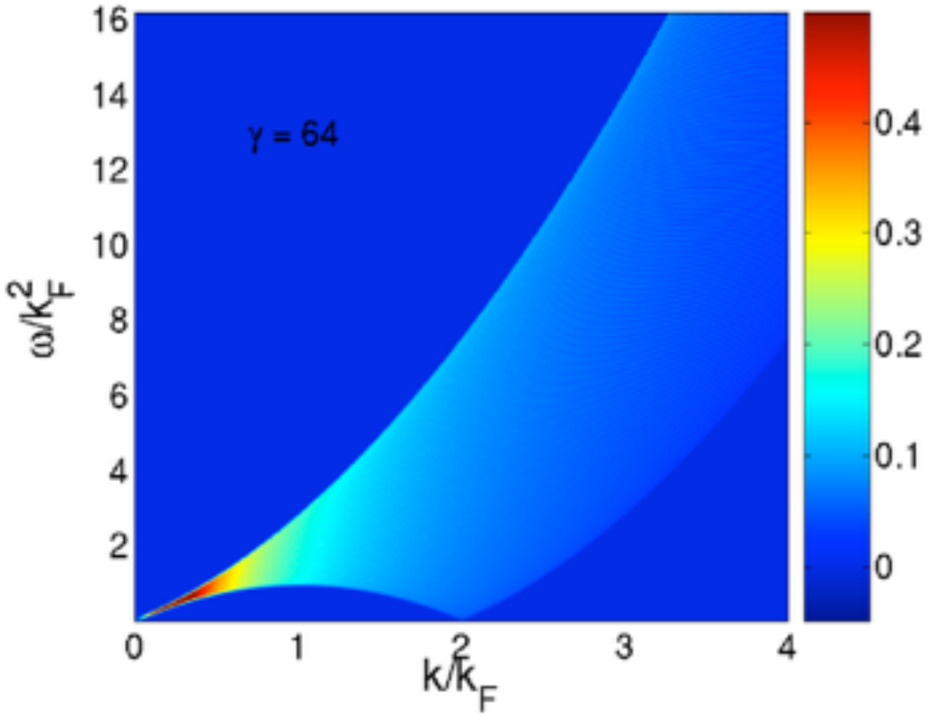
$$\mathcal{H}_N = -\sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + 2c \sum_{1\leq j<l\leq N} \delta(x_j - x_l)$$

Exact eigenstates from Bethe Ansatz:

$$\Psi(\mathbf{x}|\boldsymbol{\lambda}) = F_\lambda \sum_{P\in S_N} A_P(\mathbf{x}|\boldsymbol{\lambda}) \prod_{j=1}^{N} e^{i\lambda_{P_j} x_j}$$

$$F_\lambda = \frac{\prod_{j>k=1}^{N}(\lambda_j - \lambda_k)}{\sqrt{N! \prod_{j>k=1}^{N}\left((\lambda_j-\lambda_k)^2 + c^2\right)}}$$

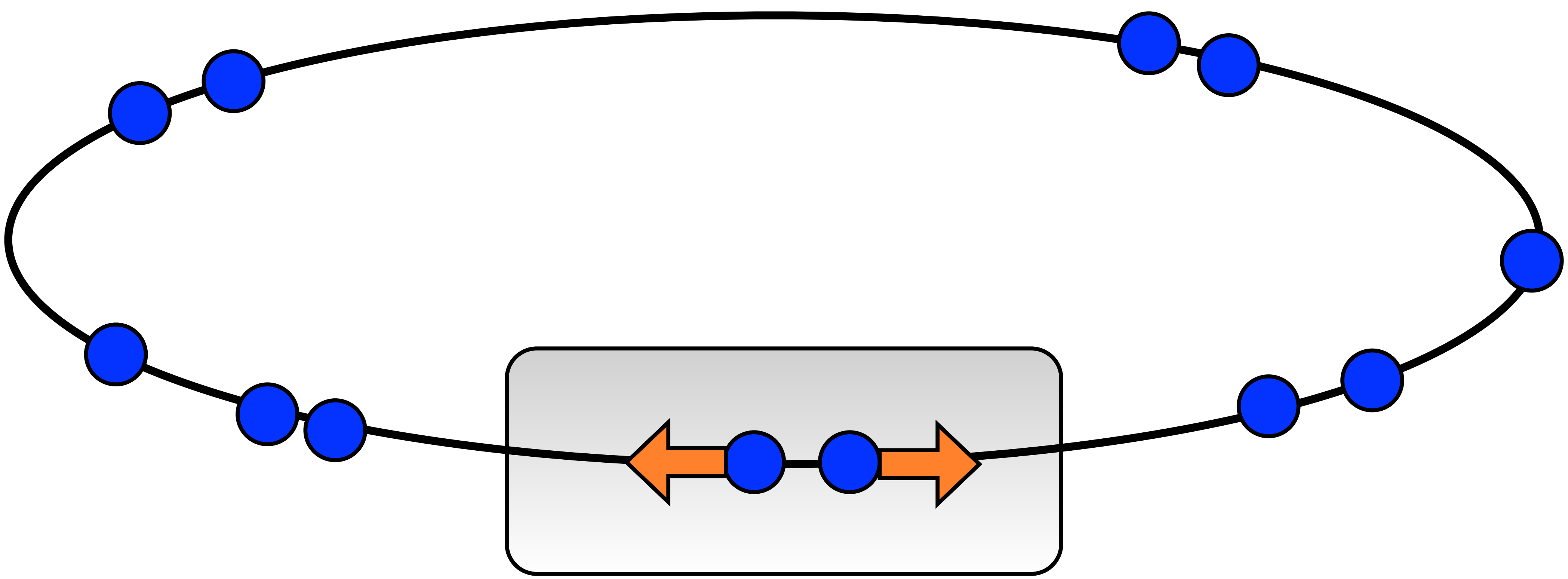
$$A_P(\mathbf{x}|\boldsymbol{\lambda}) = \prod_{j<k=1}^{N}\left(1 - \frac{ic\ \mathrm{sgn}(x_j - x_k)}{\lambda_{P_j} - \lambda_{P_k}}\right)$$



Quench from BEC to repulsive gas

Start from GS of noninteracting theory, $$|0_N\rangle \equiv \frac{1}{\sqrt{L^N N!}} \left(\psi^\dagger_{k=0}\right)^N |0\rangle$$

Turn repulsive interactions on from t=0 onwards:



particles 'repel away' from each other,
system heats up, momentum distribution broadens, ...

This is a difficult problem to treat...

1) Generalized Gibbs ensemble logic

Kormos, Shashi, Chou and Imambekov, arxiv:1204.3889

Conserved charges:

$$\hat{Q}_n : \qquad \hat{Q}_n|\{\lambda\}_N\rangle = Q_n|\{\lambda\}_N\rangle$$

$$Q_n(\{\lambda\}_N) = \sum_{j=1}^{N} \lambda_j^n$$

Davies 1990; Davies and Korepin

GGE inapplicable, charges take infinite values!

J-S C + J. Mossel, unpublished

2) GGE on lattice, q-deformed model

Works, partial results only (using a few charges)

Kormos, Shashi, Chou, JSC, Imambekov, arxiv:1305.7202

The ‘quench action’ approach

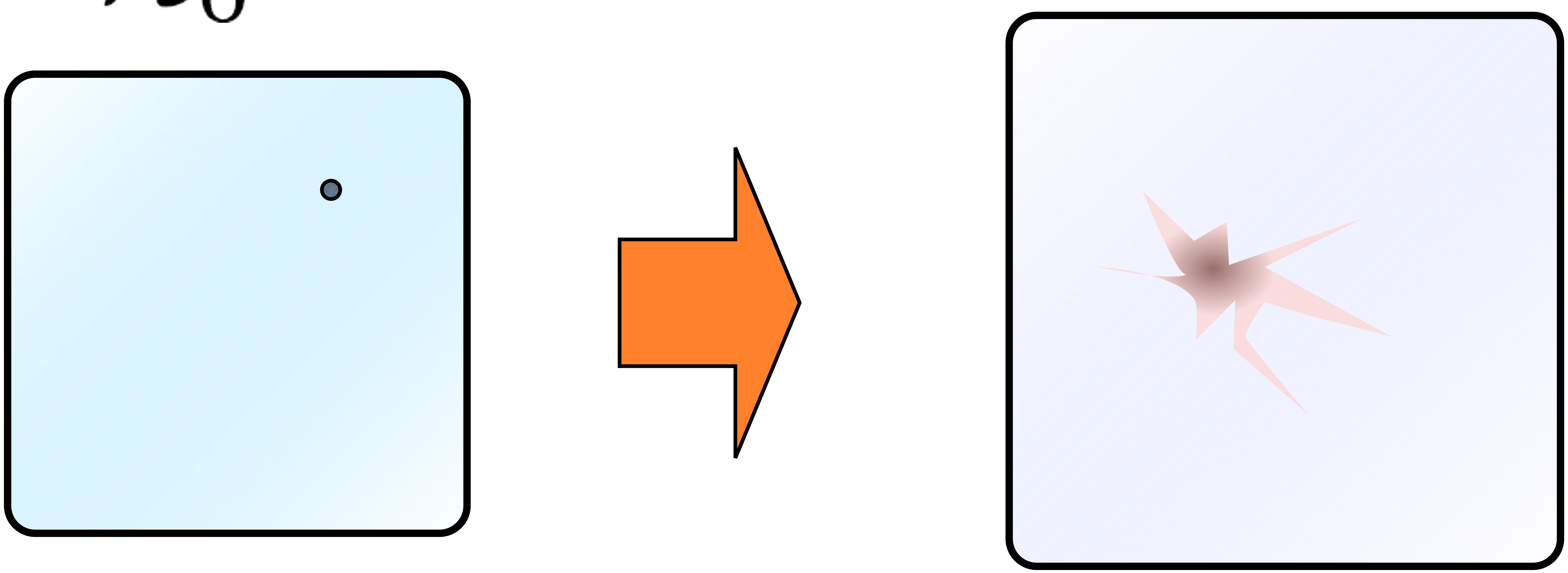
J-SC & F.H.L. Essler, PRL 2013

in pictures...

$\mathcal{H}_0$

Initial state:

$\mathcal{H}$



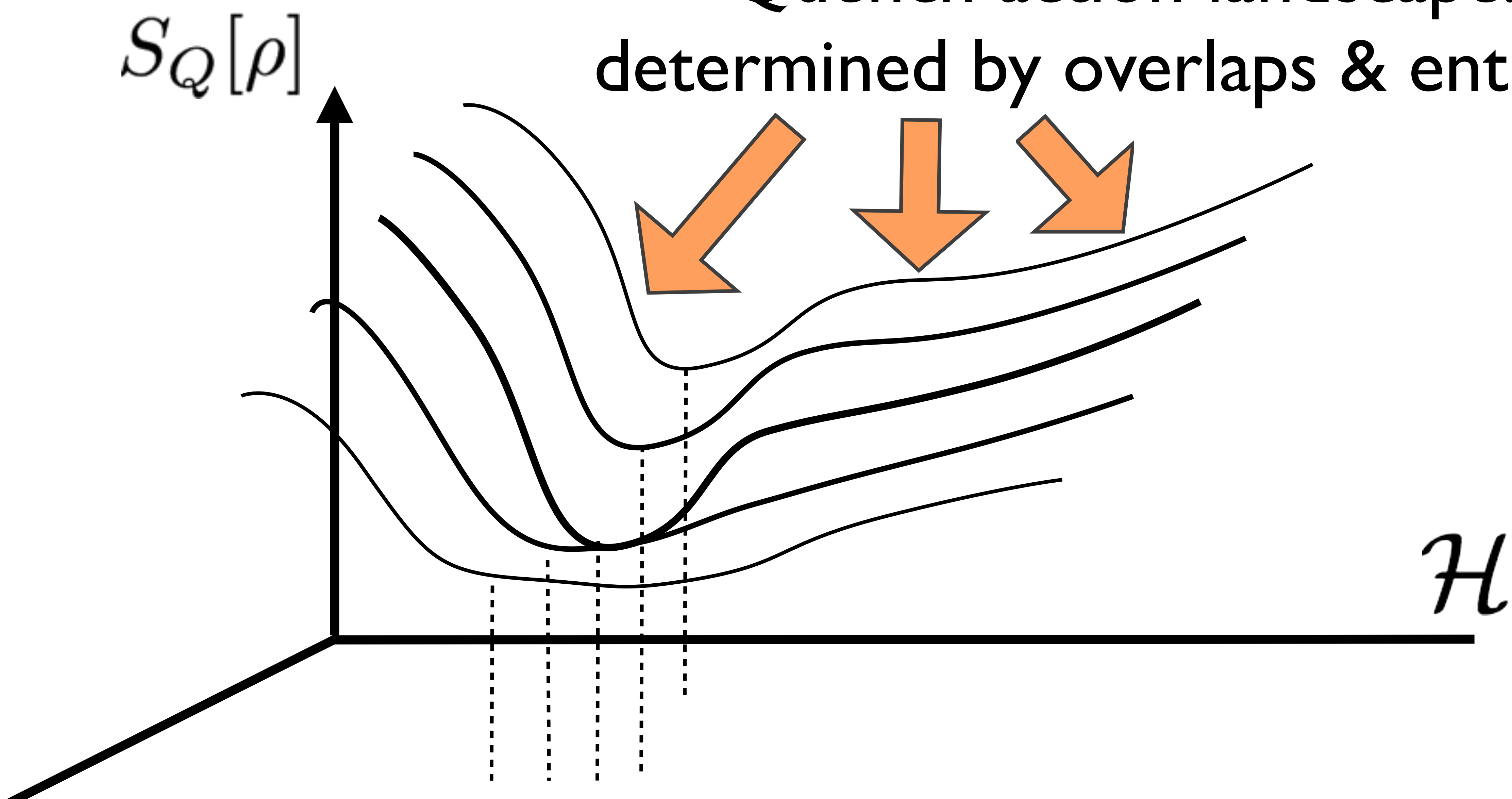
in pre-quench
Hilbert space basis

in post-quench
Hilbert space basis

The ‘quench action’ approach

J-SC & F.H.L. Essler, PRL 2013

Quench action landscape:
determined by overlaps & entropy

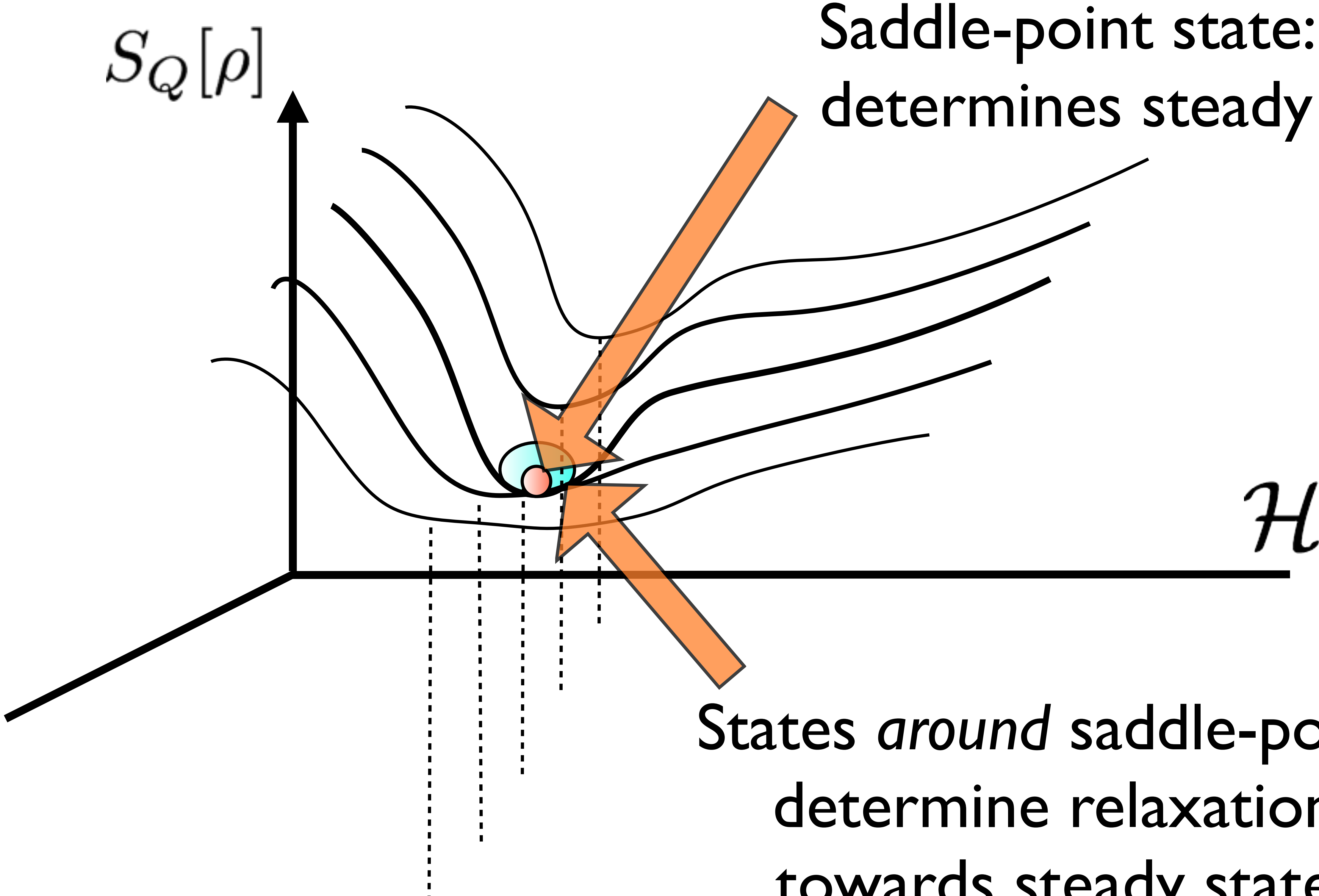


Variational approach, implemented by a
‘Generalized thermodynamic Bethe Ansatz’

J. Mossel and J-SC, JPA 2012; J-SC & R. Konik, PRL 2012,
see also Fioretto & Mussardo NJP 2010, Pozsgay JSTAT 2011

The ‘quench action’ approach

J-SC & F.H.L. Essler, PRL 2013



Saddle-point state: ρ_{sp}
determines steady state

States *around* saddle-point:
determine relaxation
towards steady state

The quench action approach: gives full post-quench dynamics

$$\lim_{Th} \bar{\mathcal{O}}(t) = \lim_{Th} \frac{1}{2} \sum_{\{\mathbf{e}\}} \Big[e^{-\delta S_{\{\mathbf{e}\}}[\rho_{sp}] - i\omega_{\{\mathbf{e}\}}[\rho_{sp}]t} \langle \rho_{sp} | \mathcal{O} | \rho_{sp}; \{\mathbf{e}\} \rangle + e^{-\delta S^*_{\{\mathbf{e}\}}[\rho_{sp}] + i\omega_{\{\mathbf{e}\}}[\rho_{sp}]t} \langle \rho_{sp}; \{\mathbf{e}\} | \mathcal{O} | \rho_{sp} \rangle \Big]$$

Main message: the *full* time dependence is recoverable using a minimal amount of data

- saddle-point distribution (from GTBA)
- excitations in vicinity of sp state (easy)
- differential overlaps
- selected matrix elements

Back to BEC-LL quench

Explicit result:

J. De Nardis, B. Wouters, M. Brockmann & J-SC, PRA 89, 2014

M. Brockmann JPA 2014

$$\langle \{\lambda_j\}_{j=1}^{N/2}, \{-\lambda_j\}_{j=1}^{N/2} | 0 \rangle = \sqrt{\frac{(cL)^{-N} N!}{\det_{j,k=1}^{N} G_{jk}}} \frac{\det_{j,k=1}^{N/2} G_{jk}^{Q}}{\prod_{j=1}^{N/2} \frac{\lambda_j}{c} \sqrt{\frac{\lambda_j^2}{c^2} + \frac{1}{4}}}$$

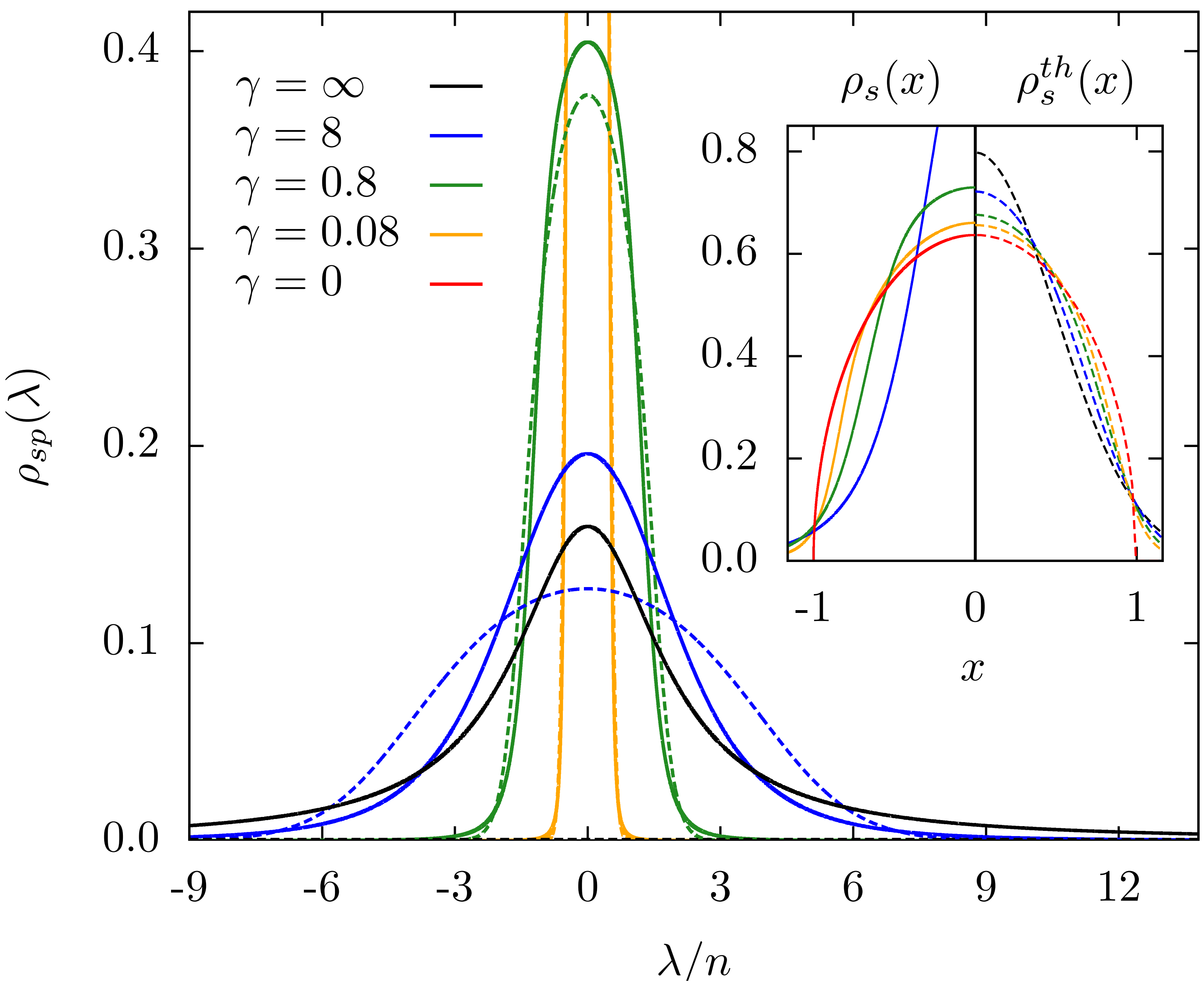
(reminiscent of Gaudin formula)

with matrix $$G_{jk}^{Q} = \delta_{jk} \left(L + \sum_{l=1}^{N/2} K^{Q}(l_j, l_l) \right) - K^{Q}(l_j, l_k)$$

$$K^{Q}(\lambda, \mu) = K(\lambda - \mu) + K(\lambda + \mu) \qquad K(\lambda) = \frac{2c}{\lambda^2 + c^2}$$

Quench action solution to BEC-LL quench

J. De Nardis, B. Wouters, M. Brockmann & J-SC, PRA 89, 2014



Subplot: scaled fn

$$\rho_s(x) = \sqrt{\gamma}\rho(c\sqrt{\gamma}x/2)/2$$

Large c:

$$\rho(\lambda) = \frac{1}{2\pi}\frac{4n^2}{\lambda^2 + 4n^2}$$

Small c: semicircle

$$\rho(\lambda) \sim \frac{1}{\pi\sqrt{\gamma}}\sqrt{1 - \frac{\lambda^2}{4\gamma n^2}}$$

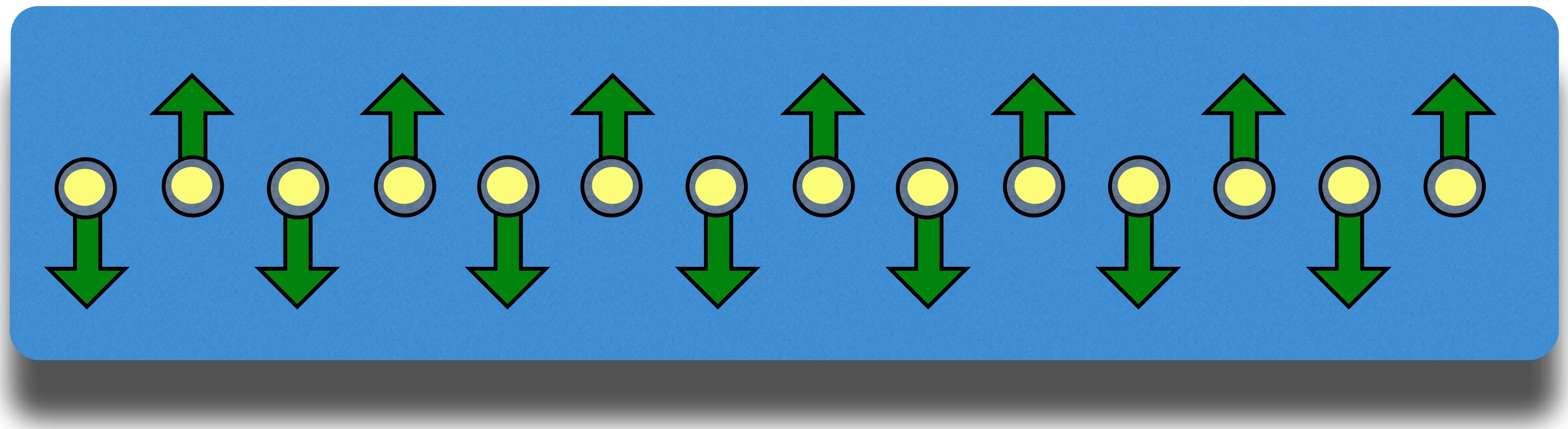
Asymptotics as from q-bosons: $2\pi\rho(\lambda) \sim \frac{n^4\gamma^2}{\lambda^4} + \frac{n^6\gamma^3(24-\gamma)}{4\lambda^6} + \dots$

Exact solution despite inapplicability of GGE!!

Néel to XXZ quench

Quench from Néel to XXZ

Start from Néel state:



From t=0 onwards, evolve with XXZ Hamiltonian

$$H = \sum_{j=1}^{N} \left[J(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z) - H_z S_j^z \right]$$

Can one treat this problem exactly?

Quench action approach to Néel-XXZ quench

First step: exact overlaps of Néel state with XXZ eigenstates

Tsuchiya JMP1998; Kozlowski & Pozsgay JSTAT 2012; Pozsgay arxiv 2013

(Gaudin-like form again!) M. Brockmann, J. De Nardis, B. Wouters & J-SC JPA 2014

$$\frac{\langle \Psi_0 | \{\pm\lambda_j\}_{j=1}^{M/2} \rangle}{\| \{\pm\lambda_j\}_{j=1}^{M/2} \|} = \sqrt{2} \left[\prod_{j=1}^{M/2} \frac{\sqrt{\tan(\lambda_j + i\eta/2)\tan(\lambda_j - i\eta/2)}}{2\sin(2\lambda_j)} \right] \sqrt{\frac{\det_{M/2}(G_{jk}^{+})}{\det_{M/2}(G_{jk}^{-})}}$$

$$G_{jk}^{\pm} = \delta_{jk} \left(N K_{\eta/2}(\lambda_j) - \sum_{l=1}^{M/2} K_{\eta}^{+}(\lambda_j, \lambda_l) \right) + K_{\eta}^{\pm}(\lambda_j, \lambda_k)$$

$$K_{\eta}^{\pm}(\lambda, \mu) = K_{\eta}(\lambda - \mu) \pm K_{\eta}(\lambda + \mu) \qquad K_{\eta}(\lambda) = \frac{\sinh(2\eta)}{\sin(\lambda + i\eta)\sin(\lambda - i\eta)}$$

The steady state: Néel to XXZ

B. Wouters, M. Brockmann, J. De Nardis, D. Fioretto & J-SC, 1405.0172

see also B. Pozsgay et al, arxiv 1405.2843

Solid lines:
quench action

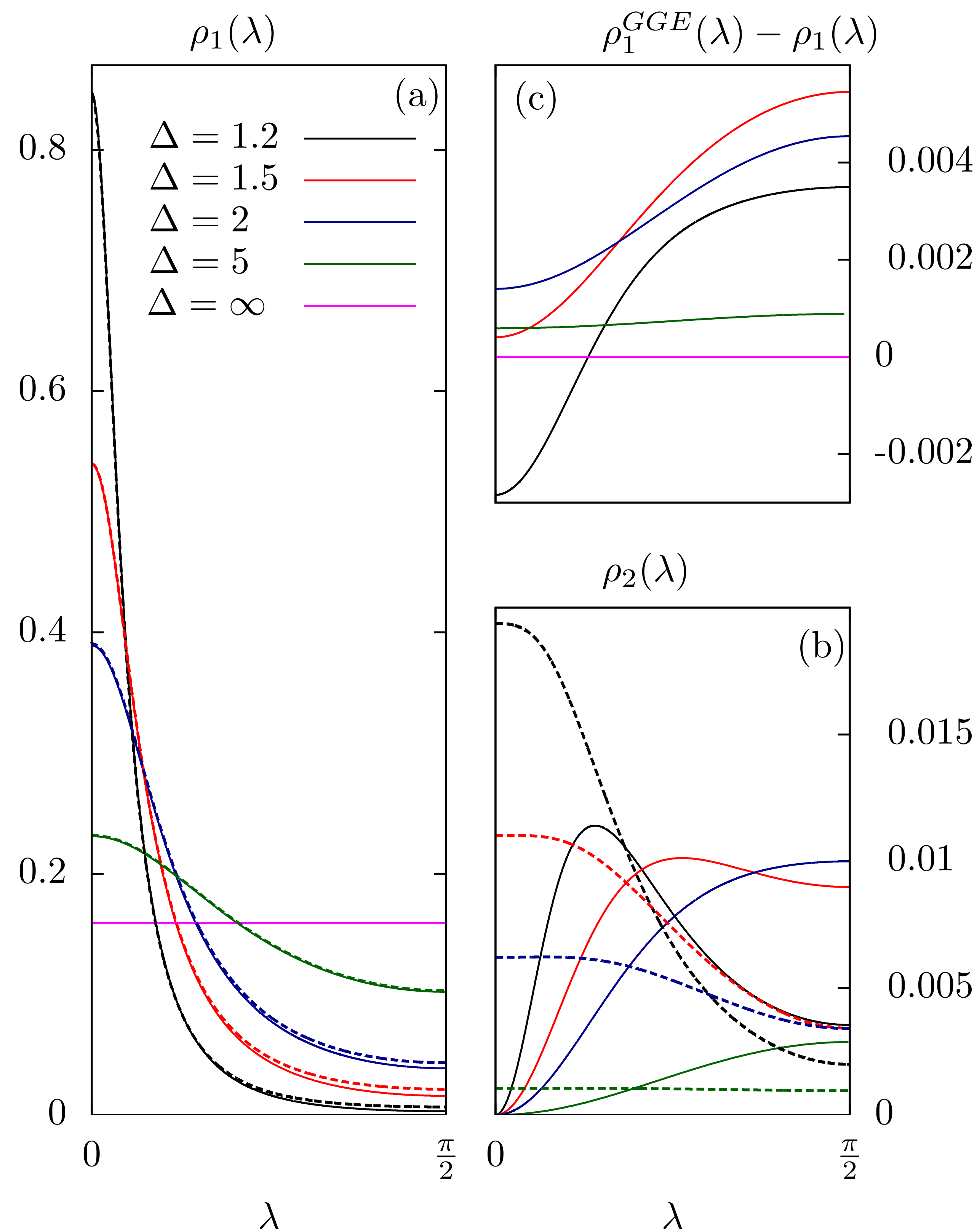
Dashed lines:
GGE (local charges)

QA and GGE have different saddle-point densities

Large Delta expansion:

$$\rho_1^{GGE} - \rho_1^{sp} = \frac{1}{4\pi\Delta^2} + O(\Delta^{-3}),$$

$$\rho_2^{GGE} - \rho_2^{sp} = \frac{1 - 3\sin^2(\lambda)}{3\pi\Delta^2} + O(\Delta^{-3}).$$



What's going on?

Néel to XXZ: current situation

- *quench action solution gives correct expectation value for all conserved charges, directly from microscopics*
- *quench action and (local) GGE steady state distributions do not coincide*
- *these different distributions lead to different observable expectation values*

Possible explanation of this mismatch:

- *GGE converges to QA once all (nonlocal*) charges are added*

Are our intuitions on (non)locality misleading?

* *of which there are exponentially many more than local ones!*

Looking ahead, 20 years from now

Wish list for experiments

- **Magnetism: ability to create controlled out-of-equilibrium conditions, and to observe time-dependent behaviour (pump-probe neutrons?)**
  cold-atom-like capabilities for tailoring states

- **Magnetism: push ‘new’ methods like RIXS**

- **Cold atoms: ability to create ‘cleaner’ settings (w/o trap effects, lower T for fermions, …)**
  the interesting physics is not in the trapping!

- **Cold atoms: enlarge toolbox of observables**
  magnetism-like capabilities for probing states

Wish list for theory/numerics

- **Expand the reach of nonperturbative methods**
  - quantitative results on many more systems/observables
  - steady-state universality classes (using quench action?)
  - examples of truly driven systems fully under control
  - quantum integrability: better understanding
  - quantum KAM theorem
  - ability to perturb around exactly solved points
  - dream on: exact solutions in higher d
- **Field theory-based methods**
  - adapt nonlinear Luttinger theory to off-equilibrium
  - nonperturbative results in higher d
- **Numerical methods**
  - DMRG equivalents in higher dimensions
  - better time-dependent simulations

THANK YOU FOR YOUR ATTENTION