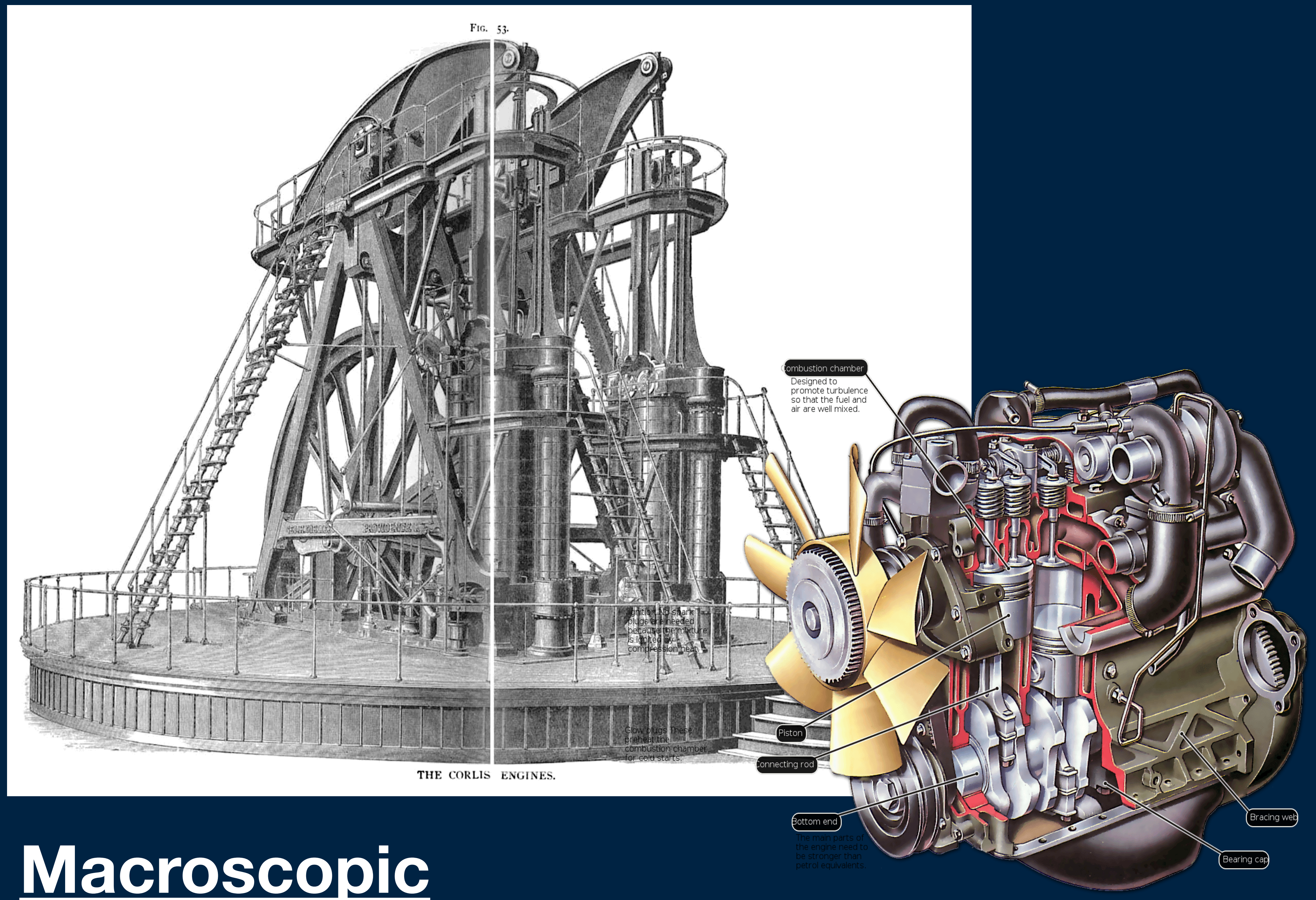
Thermodynamics in a quantum world

Nelly Ng, Nanyang Assistant Professor, SPMS NTU

Outline

Quantum thermodynamics at a glance → Taking the information-theoretic approach → Taking the physics-oriented approach → Building the measurement toolbox for quantum fields

Thermodynamics — then and now

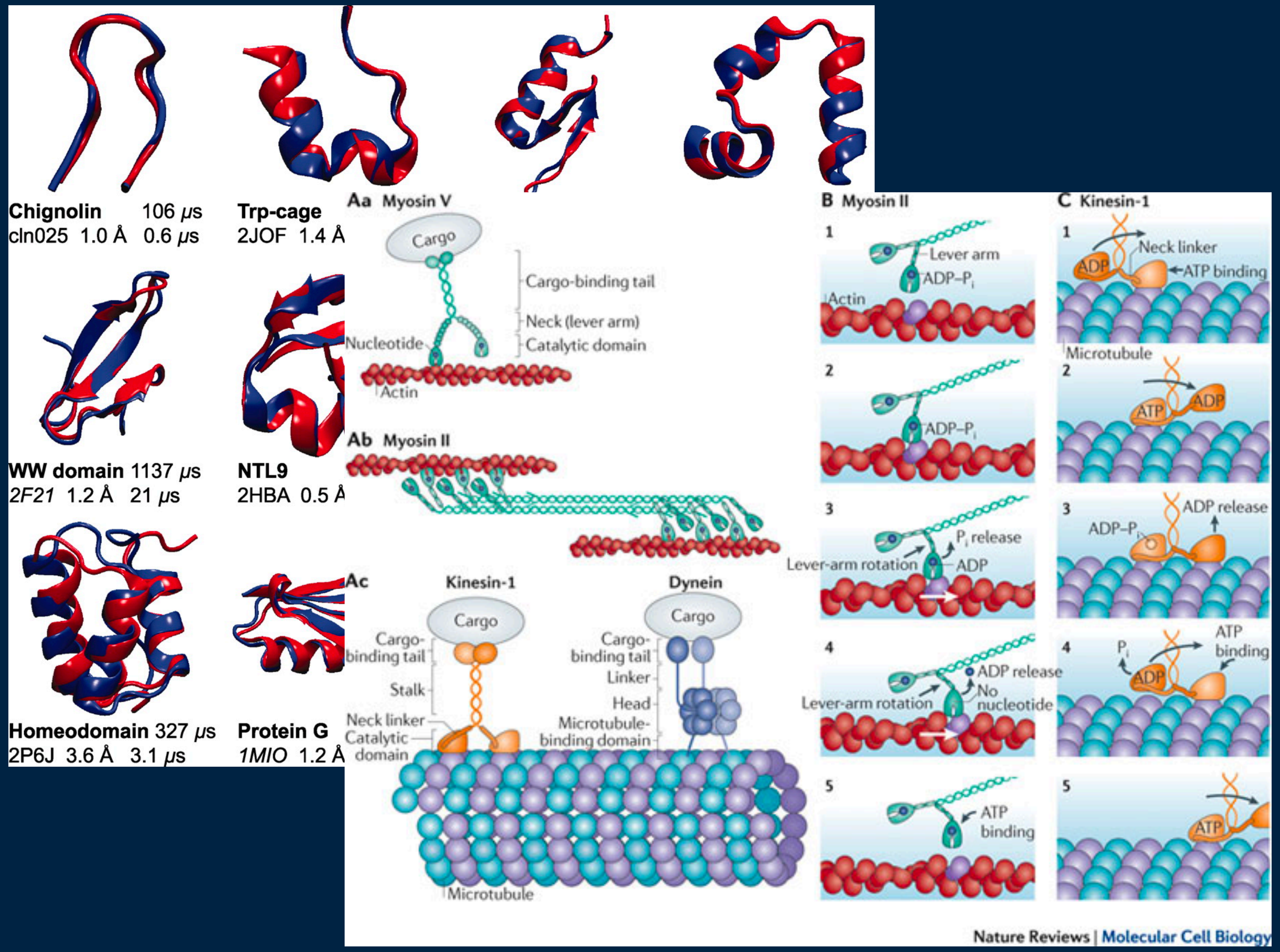


Macroscopic

❖Thermodynamic limit

❖Variables (energy, entropy, pressure etc)

❖Steady state limit/ensemble average behaviour



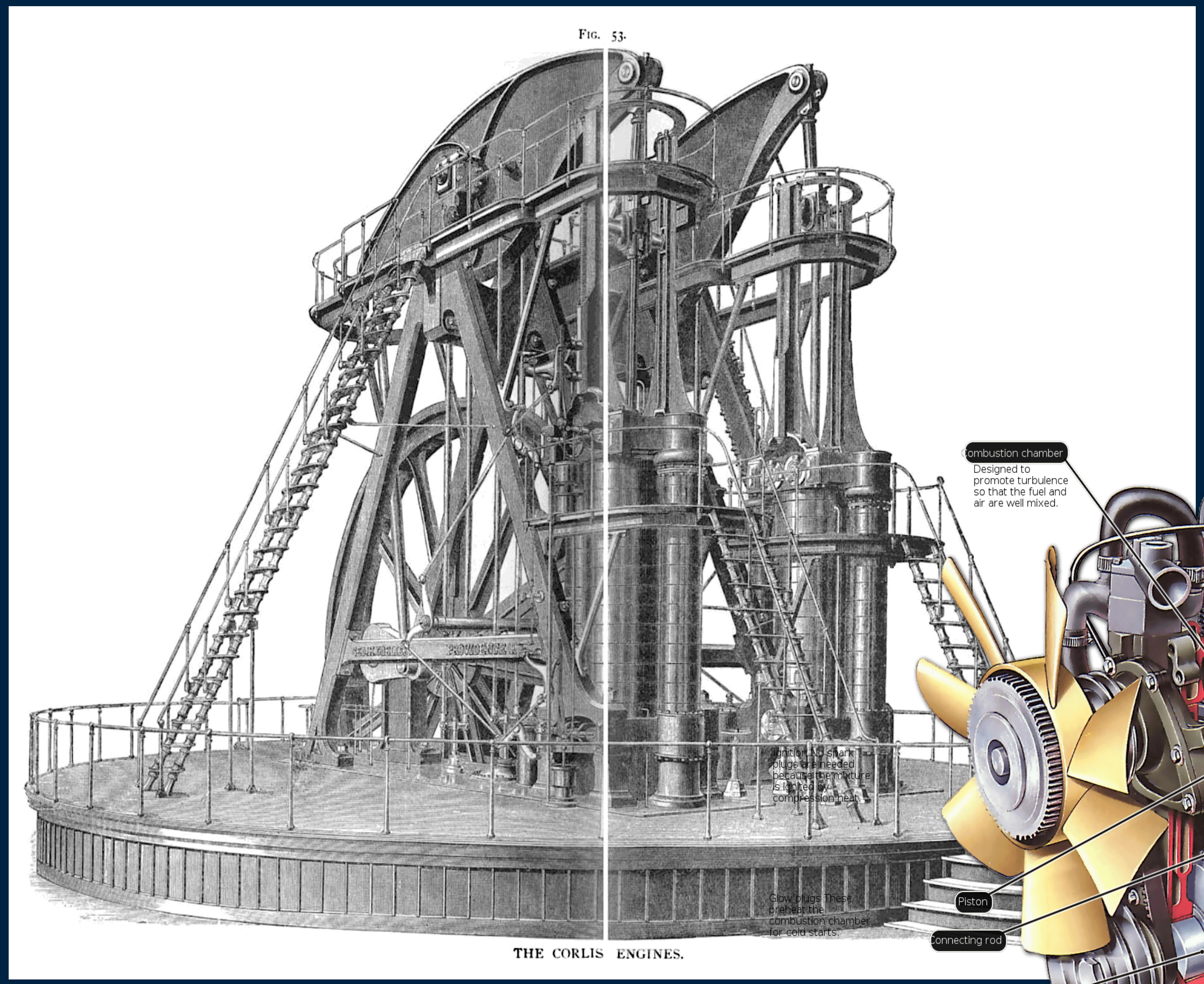
Mesoscopic/Stochastic

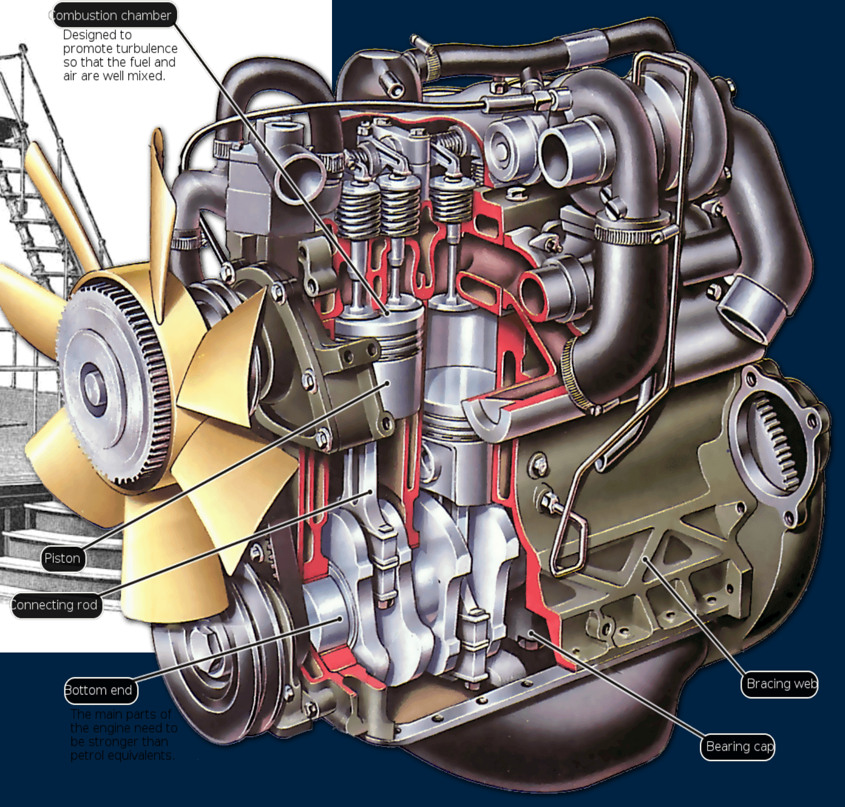
❖ Out-of-equilibrium behavior

❖ Models for system-bath interaction

❖ Refined second law for individual phase space trajectories (fluctuation theorems)

Thermodynamics — then and now





Macroscopic

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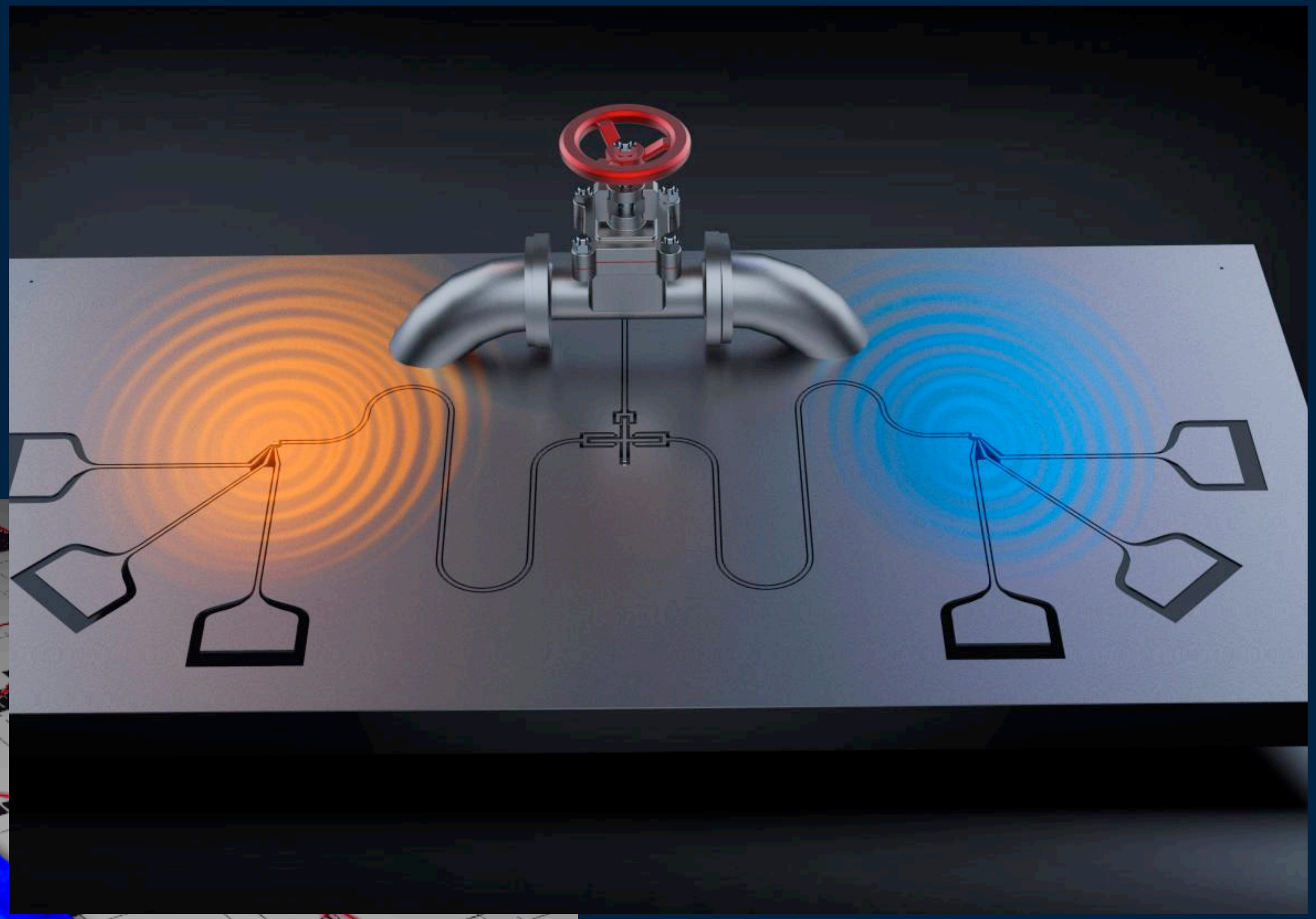
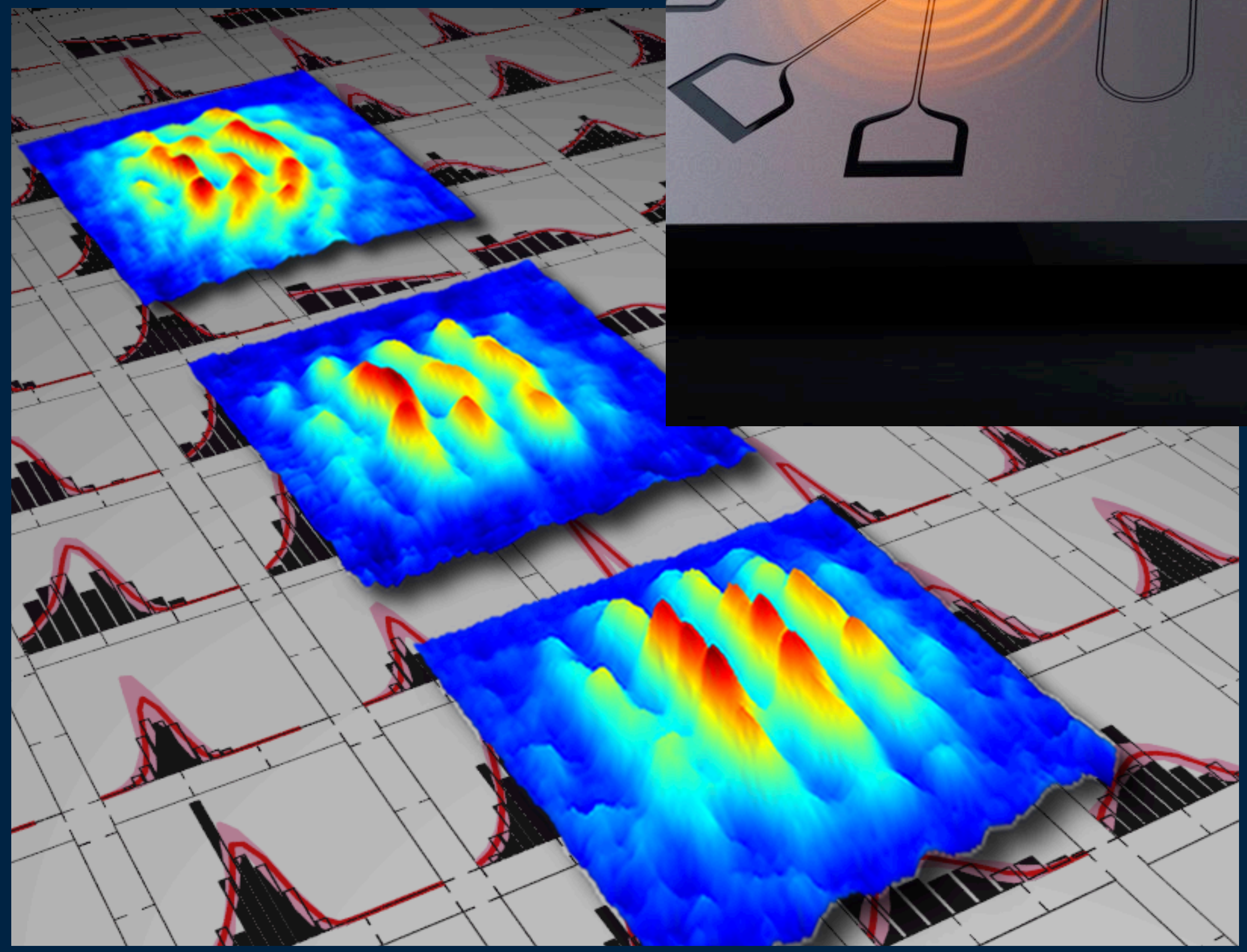


Heat valve connecting superconducting qubits, Source: EurekaAlert, Credit: Jorden Senior / Aalto University



Rubidium atoms on a chip, Source: Schmiedmayer group, Vienna.

Quantum

- ❖ Highly non-negligible energy fluctuations
- ❖ Finite-sized environments/baths
- ❖ Entanglement, coherence, and their effects on thermal machines

Goals of quantum thermodynamics

Understanding the mechanism of thermalisation

"Why do we observe thermalization-like behavior" when quantum mechanics give rise to unitary dynamics?

(almost) well understood at the level of local observables

There are strongly interacting systems which do not thermalise!

Ex: Emergence of canonical ensembles
PRE 79, 061103 (2009)

- Central to statistical mechanics
- Assumption on subjective knowledge
- Can be justified by *entanglement between systems,*
  - For most states $|\psi\rangle \in \mathscr{H}_R \otimes \mathscr{H}_S$,

$$\mathrm{tr}_R(|\psi\rangle\langle\psi|_{RS}) \approx \mathrm{tr}_R \frac{\mathbb{I}_{RS}}{d_R d_S}$$

  - Similar result for physically motivated states: MPS, k-designs

Goals of quantum thermodynamics

Understanding the mechanism of thermalisation

"Why do we observe thermalization-like behavior" when quantum mechanics give rise to unitary dynamics?

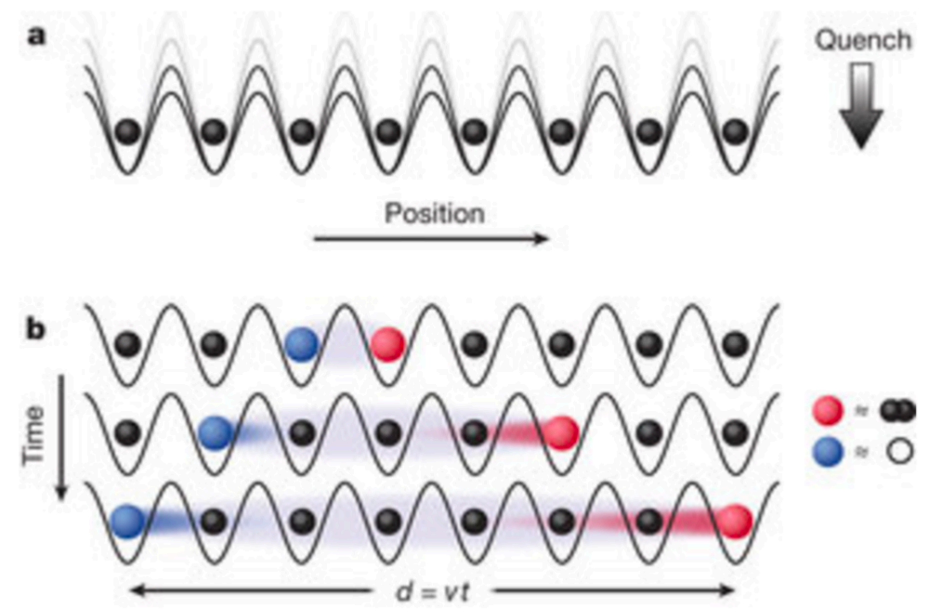
(almost) well understood at the level of local observables

There are strongly interacting systems which do not thermalise!

Ex: equilibration time scales

❖ Lieb-Robinson bounds
  Commun. Math. Phys. (1972) 28: 251
  Nature 481, 484–487 (2012)

Figure 1: **Spreading of correlations in a quenched atomic Mott insulator.**



❖ Decoupling theorems
  PRL 108, 070501 (2012)

Detailed review:
Rep. Prog. Phys. 79, 056001 (2016)

Goals of quantum thermodynamics

Ex: Landauer's principle

➢ Erasure of information requires work input

➢ Szilard engine

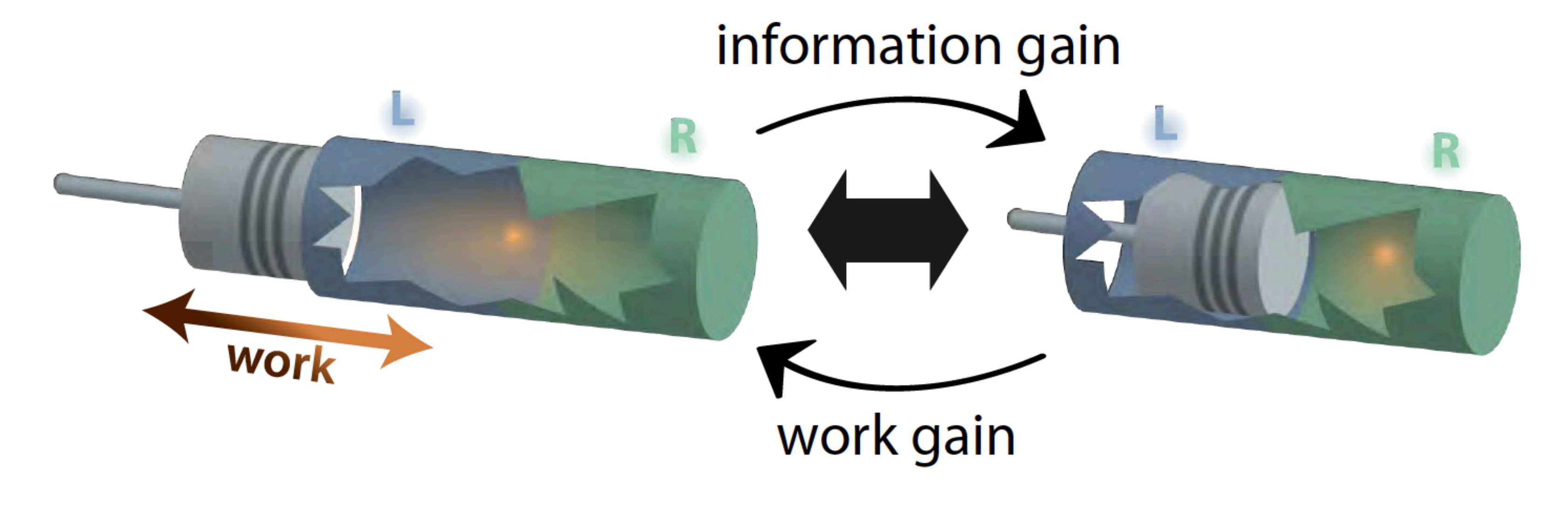
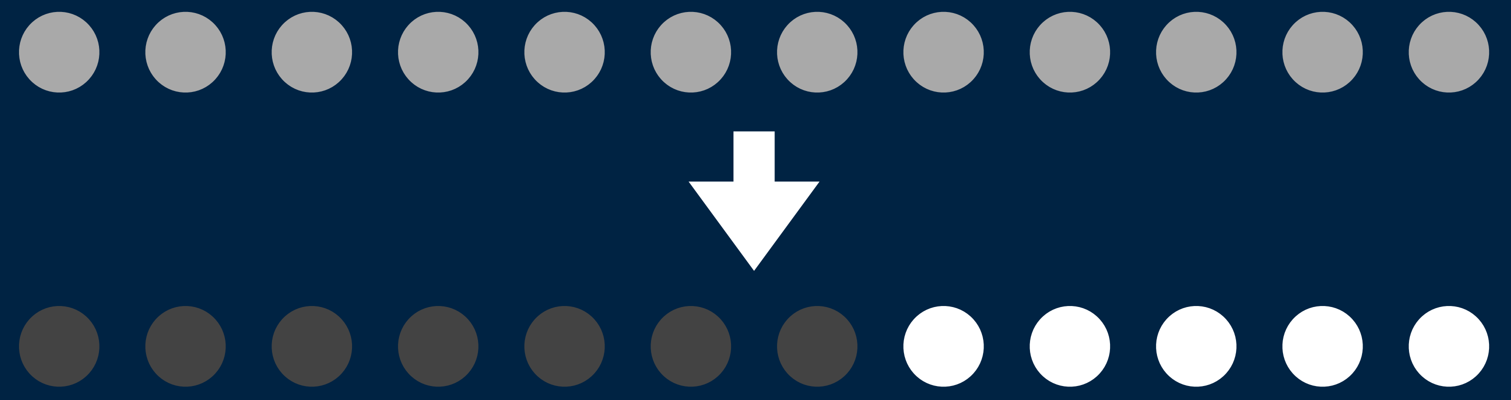


Fig: P.Faist, PhD Thesis

➢ Data compression
NJP 13, 053015 (2013)



Identically noisy states

Unitary compression

Distilled states which are very close to being pure, with some high entropy states

➢ Storing work in terms of information
Nature 474, 61--63 (2011)

➢ Operational meaning for conditional entropy being negative

Landauer's principle vs Szilard engine: trading between work and information

Deriving fundamental energetic principles that are independent of system-specifics

Fundamental limitations to tasks such as work extraction or cooling

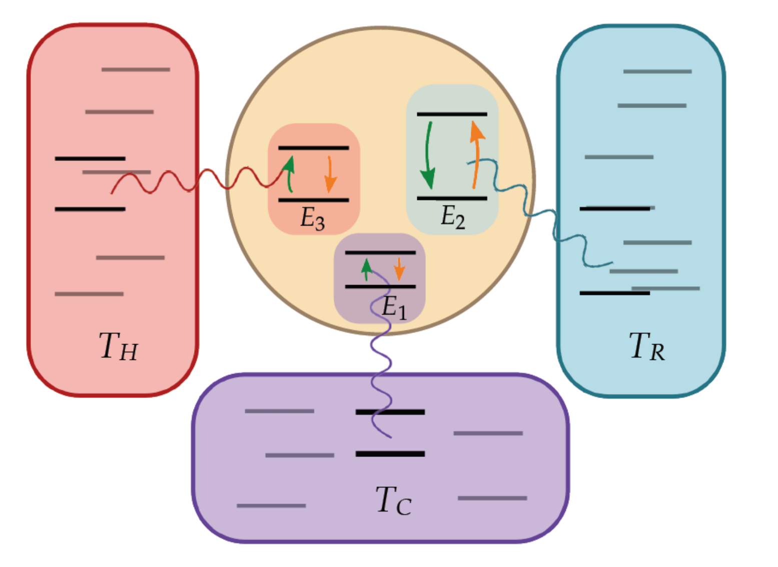
Goals of quantum thermodynamics

Building interesting quantum thermal machines

Understanding the role of entanglement and coherence in machine performance

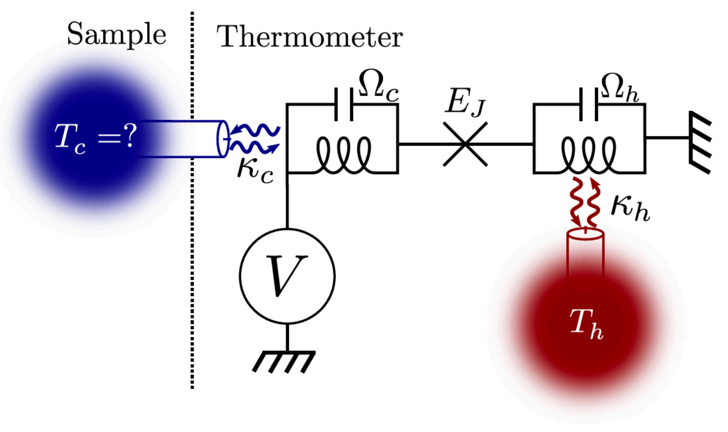
Various platforms – see AVS Quantum Sci. 4, 027101 (2022) for a comprehensive review!

Refrigerator
Smallest possible quantum fridge
PRL 105, 130401 (2010)
Entanglement enhances cooling
PRE 89, 032115 (2014)



Coherence assisted, single-shot cooling
New J. Phys. 17 (2015) 115013

Thermometry
Phase estimation
PRA 82, 011611 (2010)
PRA 96, 062103 (2017)
Quantum fridge, cQED implementation
PRL119(9), 090603 (2017)



Coherence helps!
Scientific reports, 5(1), 14413
NJP 17 115013 (2015)

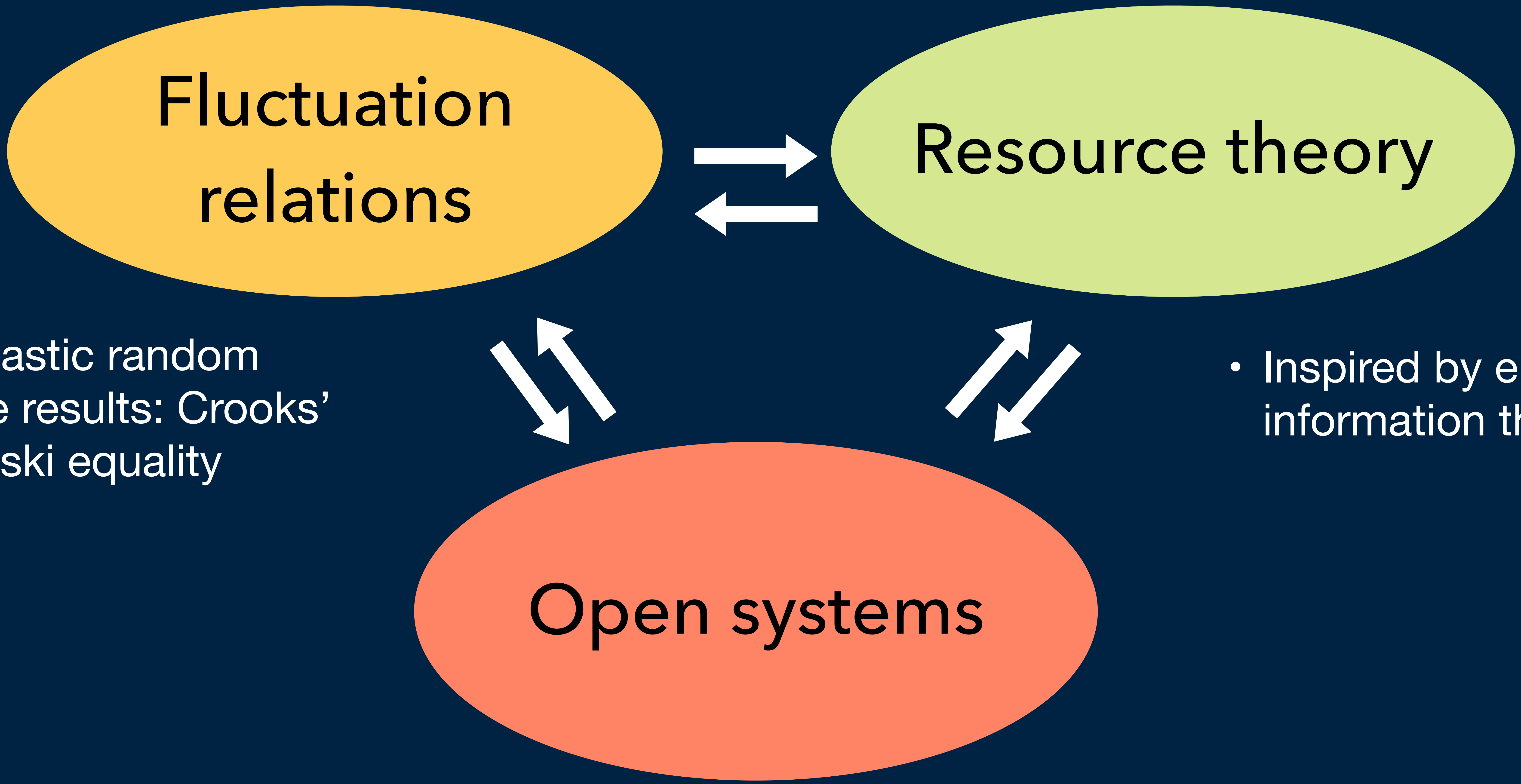
Entanglement is useful!
PRE 89, 032115 (2014)

Hard to analyze

PRX 5 (2), 021001
NJP 18 (2), 023045
PRL 113, 150402 (2014)

Backaction reduces efficiency
PRE 95, 062131 (2017)
PRX 7, 031022 (2017)

Various approaches to theoretical quantum thermo



- Work as a stochastic random variable, notable results: Crooks' theorem, Jarzynski equality
- Inspired by entanglement/ information theory
- Differential equations modelling specifics of system-bath interaction

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My journey started in information theory…

Free operations

+

Free states

State transition conditions:

When is $\rho \to \rho'$ possible?

- Usually in terms of monotones

Necessary (N) conditions

$$\rho \to \rho' \implies M(\rho) \leq M(\rho')$$

Sufficient (S) conditions

$$\rho \to \rho' \impliedby M(\rho) \leq M(\rho')$$

Necessary and sufficient (N&S) conditions

$$\rho \to \rho' \iff M(\rho) \leq M(\rho')$$

- Applied to entanglement theory, manipulation of coherence, non-Gaussianity, complexity and various quantum resources!

Resources ;)

REVIEWS OF MODERN PHYSICS, VOLUME 91, APRIL–JUNE 2019

Quantum resource theories

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(published 4 April 2019)

Quantum Physics

[Submitted on 8 Feb 2024]

Resources of the Quantum World

Gilad Gour

This book delves into the burgeoning field of quantum resource theories, a novel and vibrant area of research within quantum information science that seeks to unify diverse quantum phenomena under a single framework. By recognizing various attributes of physical systems as "resources," this approach offers a fresh perspective on quantum phenomena, transforming our understanding and application of concepts such as quantum entanglement, coherence, and more. With a focus on the pedagogical, the book aims to equip readers with the advanced mathematical tools and physical principles needed to navigate and contribute to this rapidly evolving field. It covers a wide range of topics, from the foundational aspects of quantum mechanics and quantum information to detailed explorations of specific resource theories, including entanglement, asymmetry, and thermodynamics. Through rigorous mathematical exposition and a unique axiomatic approach, the book provides deep insights into the operational and conceptual frameworks that underpin quantum resource theories, making it an invaluable resource for graduate students, early-career researchers, and anyone interested in the cutting-edge developments in quantum information science.

Comments: 956 Pages (including appendices), Preliminary Version, Feedback and comments are most welcome especially typos, errors, and missing references

Subjects: **Quantum Physics (quant-ph)**; Information Theory (cs.IT); Mathematical Physics (math-ph)

Cite as: arXiv:2402.05474 **[quant-ph]**

(or arXiv:2402.05474v1 **[quant-ph]** for this version)

https://doi.org/10.48550/arXiv.2402.05474

Resource theoretic quantum thermodynamics

$$[U_{\mathrm{AR}}, \hat{H}_{\mathrm{A}} + \hat{H}_{\mathrm{R}}] = 0$$

Energy preserving unitaries

❖1st law: energy preservation

+

Gibbs states of fixed temperature

Why should we use energy preserving unitaries only?

- Accounting for all sources of work we may input during the thermodynamic process explicitly, e.g. number of non-E-preserving channels, or appending athermal states
- seems incompatible with some strong coupling scenarios, in particular when system-bath interaction remains strong all the time
  - In this case, our notion of the thermodynamic system S should **include** the strongly interacting part of the environment

Resource theoretic quantum thermodynamics

$$[U_{\mathrm{AR}}, \hat{H}_{\mathrm{A}} + \hat{H}_{\mathrm{R}}] = 0$$

Energy preserving unitaries

❖ 1^{st} law: energy preservation

+

Gibbs states of fixed temperature

Why should we use Gibbs states only as free states?

$$\tau_R = \frac{1}{\mathrm{tr}\left(e^{-\beta \hat{H}_R}\right)} e^{-\beta \hat{H}_R}$$

- Gibbs states τ_β are passive, i.e. for any unitary U,

$$\mathrm{tr}(\hat{H} U \tau_\beta U^\dagger) \geq \mathrm{tr}(\hat{H} \tau_\beta)$$

- Importance of passivity: if a state is not passive, we can easily extract work from it
- Furthermore, Gibbs states are completely passive, i.e. $\tau_\beta^{\otimes n}$ is also passive for any n
- Lastly, Gibbs states are also the only states which are completely passive….

Resource theoretic quantum thermodynamics

$$[U_{\mathrm{AR}}, \hat{H}_{\mathrm{A}} + \hat{H}_{\mathrm{R}}] = 0$$

Energy preserving unitaries

❖ 1st law: energy preservation

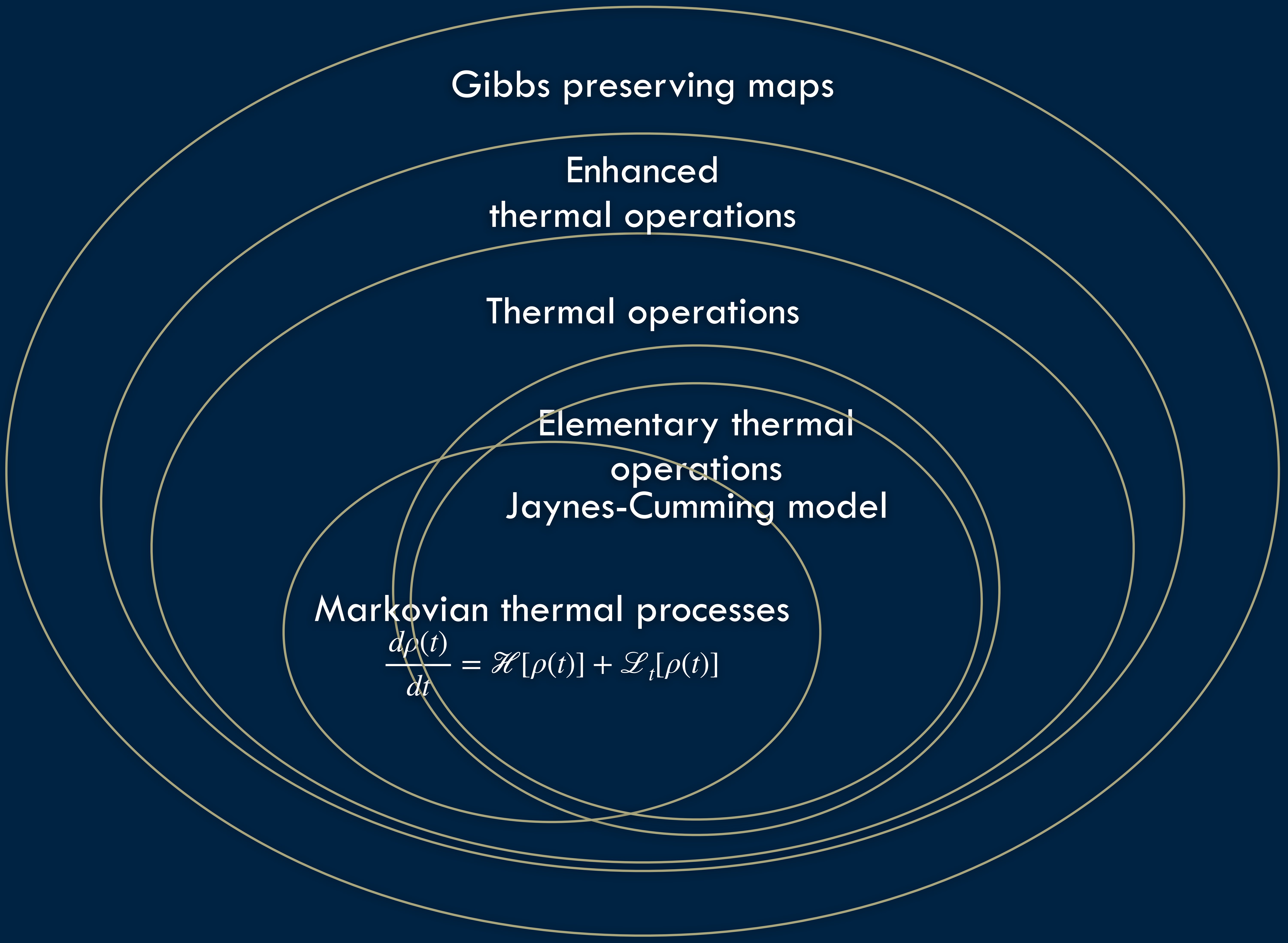
+

Gibbs states of fixed temperature

State transition conditions

- ❖ Classical 2nd law still holds i.e. free energy is a monotone.
- ❖ … but more constraints exist!
  - ❖ Thermo-majorization, Rényi relative entropies, etc
  - ❖ 3rd law: consequence of generalized 2nd law!

A hierarchy of thermal processes



We want single-shot reversibility!

Motivated by generalisation, easy characterization and reversibility

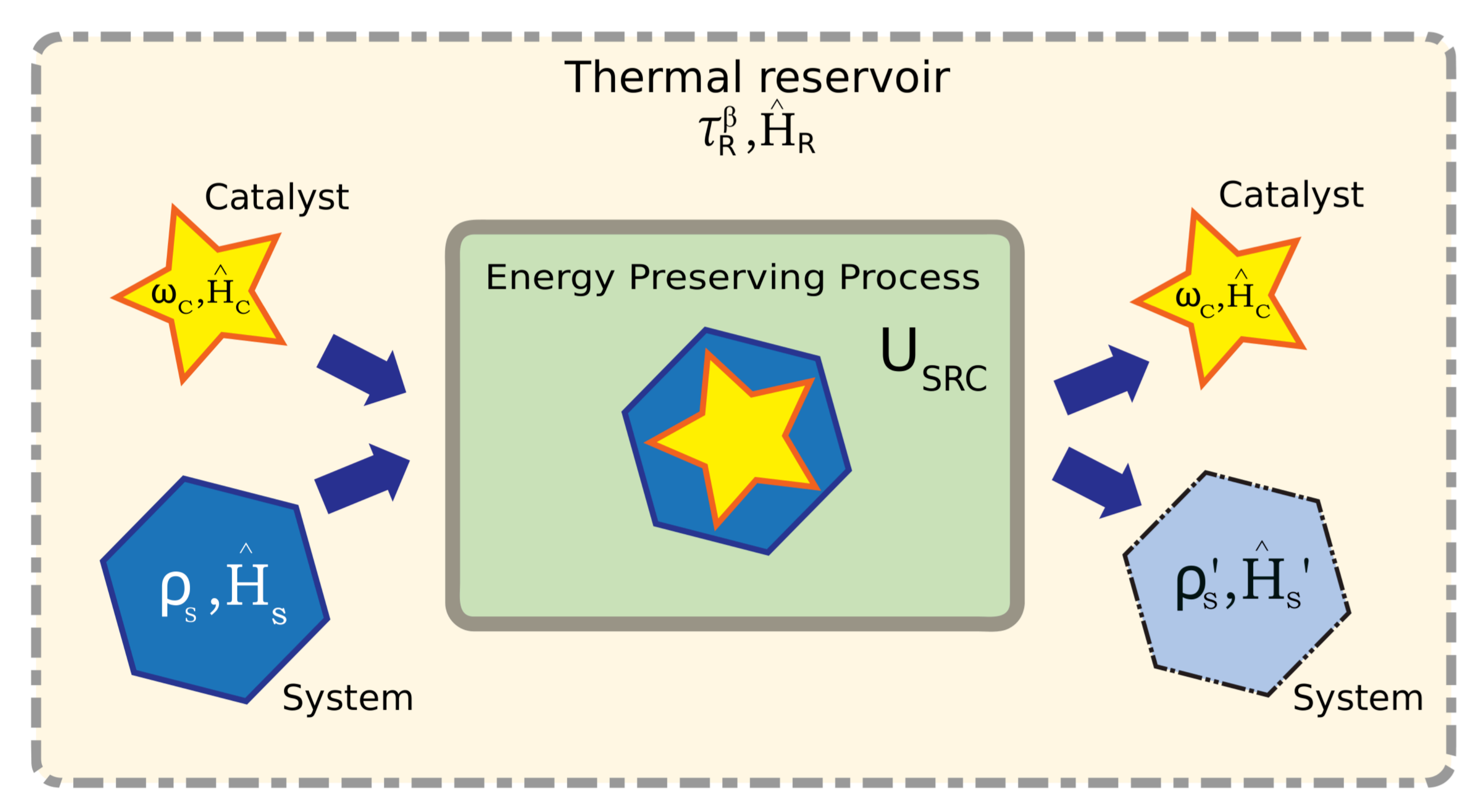
Physical meaning?

More complex characterization for state transitions

Motivated by feasibility and experimental-friendliness

We want realistic implementations!

Emergence of catalysis in quantum thermodynamics



- a source of **non-Markovianity** (e.g. a daemon)
- The **working body** of a heat engine that undergoes a cyclic process
- The **clock** that controls the implementation of a unitary by turning on and off some interaction Hamiltonian
- A catalyst can sometimes be seen as a coarse-grained version of a **battery** too!

Usage of correlations in bypassing Jarzynski equality

Limits to cooling, formulation of the third law for quantum thermo

Changes in system Hamiltonian

Efficiency of small heat engines

Detailed review: RMP 96, 025005 (2024)

The limitations of resource theoretic QT

- Obvious limitations, despite making very fundamental and all-encompassing statements…
- Too abstract; is it useful at all in helping us designing “real quantum thermal machines”?
  - (i) real quantumness: quantum mechanics is required to derive an appropriate effective physical model describing its dynamics,
    - with genuine quantum correlations potentially playing a major role,
  - (ii) real thermodynamics: it is infeasible to control its every single degree of freedom.

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Quantum thermodynamics at a glance → Taking the information-theoretic approach → **Taking the physics-oriented approach** → Building the measurement toolbox for quantum fields

- Talk to experimentalists, focus on a particular many-body platform,
- study its thermodynamical behaviour + how to analyze its performance as a thermal machine

Studying a blueprint for quantum thermal machines

System Specs

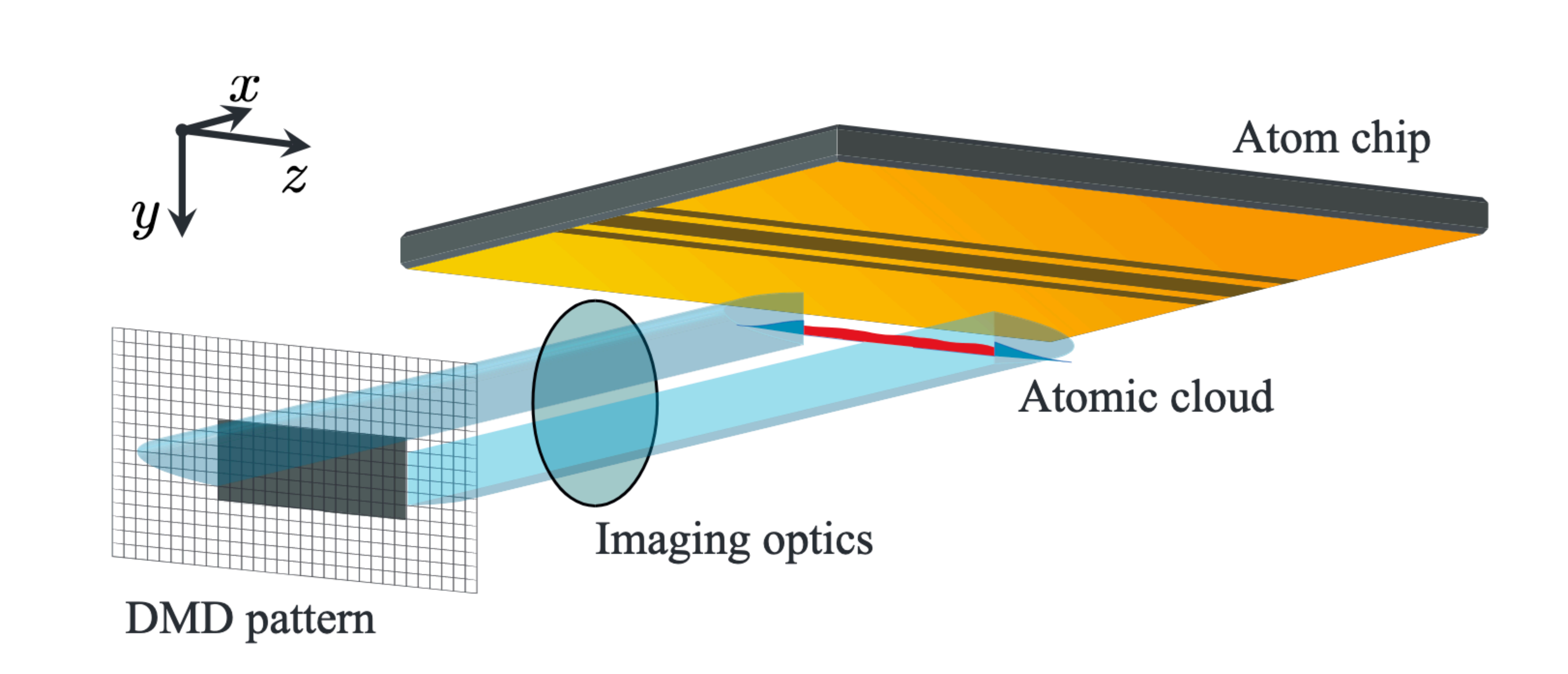
Quantities of interest vs Data readout

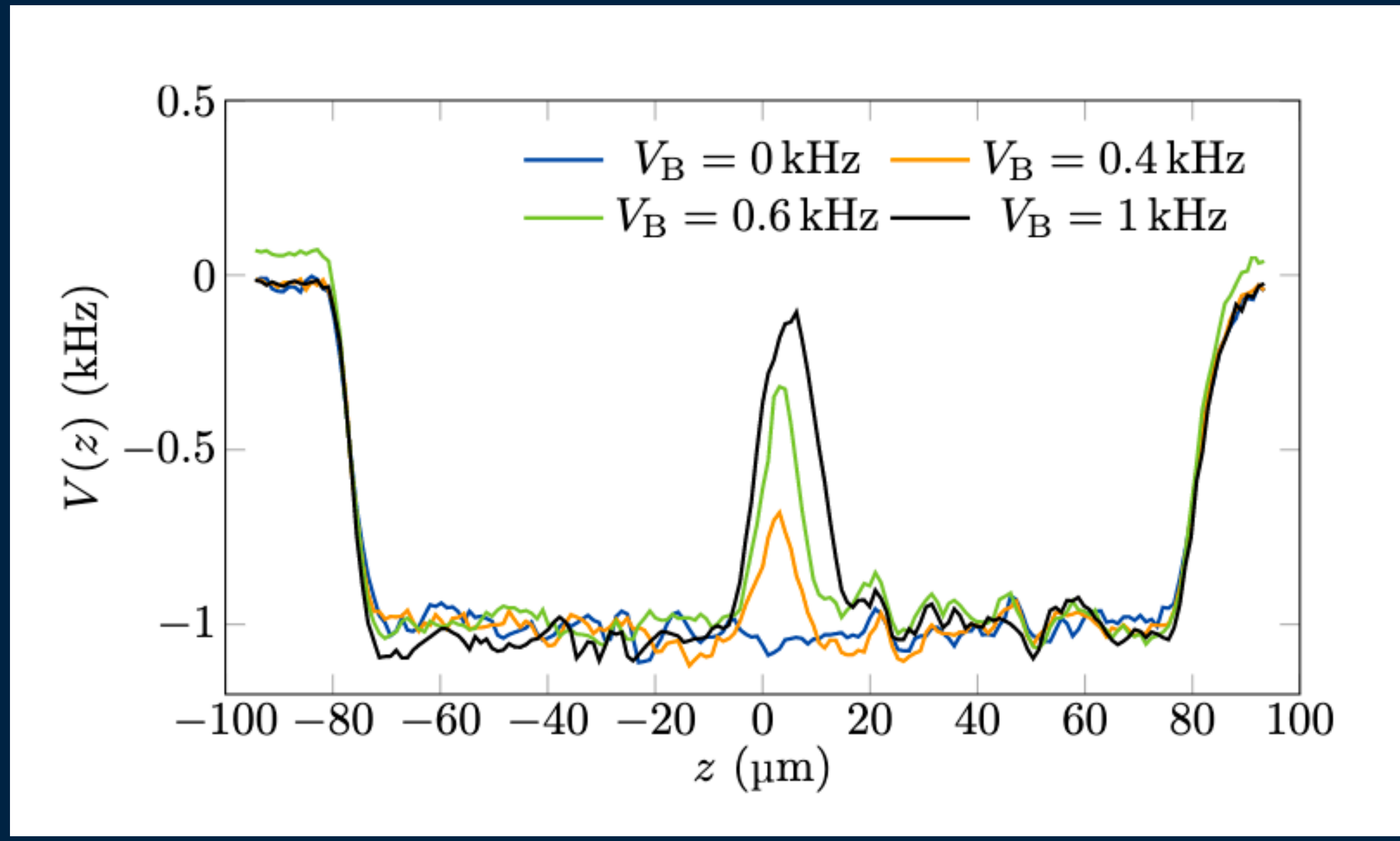
Protocols/
Operations

Future Questions
/Outlook

Ultra-cold atoms on an atom chip @ ATI, Vienna

- Rb atoms transversally trapped, 1-D system
  - Collective excitations
  - Well-approximated by non-interacting theory for quasi-particles
  - Digital mirror device for programmable potentials





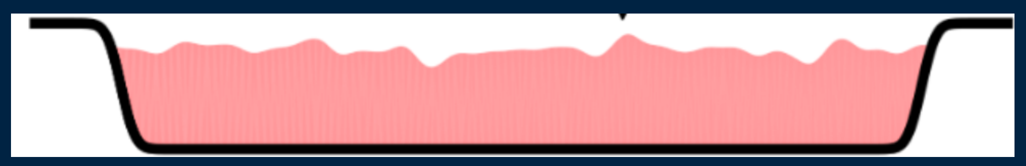
[figures from: Tajik et al, Optics Express 27, 33474 - 33487 (2019)]

Ultra-cold atoms on an atom chip @ ATI, Vienna

- Why are they interesting?
  - Potential **quantum simulator** for Sine-Gordon theory
    - [Schweigler et al, Nature 545, 323–326 (2017)]
  - Observe many-body **non-thermal equilibration** (GGE)
    - [Langen et al, Science 348 (2015) 207-211]
  - **Recurrences** of many-body observables
    - [Rauer et al, Science, 360, 307-310 (2018)]

Model: Luttinger Hamiltonian

System Specs



$$\hat{\Psi}(z) = e^{i\hat{\phi}(z)}\sqrt{\hat{\rho}(z)},$$

$$\hat{\rho}(z) = \rho_0(z) + \delta\hat{\rho}(z)$$

- Lieb-Liniger model + Bogoliubov theory

$$\hat{H}_{\mathrm{LL}} = \int \mathrm{d}z \hat{\Psi}^\dagger(z) \left[\frac{-\hbar^2}{2m}\partial_z^2 + V(z,t) - \mu + \frac{g(z)}{2}\hat{\Psi}^\dagger(z)\hat{\Psi}(z) \right] \hat{\Psi}(z)$$

- Low energy approximation

$$\hat{H}[n_{\mathrm{GP}}] = \int \mathrm{d}z \left[\frac{\hbar^2 n_{\mathrm{GP}}(z)}{4m} \left(\partial_z \hat{\phi}(z) \right)^2 + g(z)\ \delta\hat{\rho}(z)^2 \right]$$

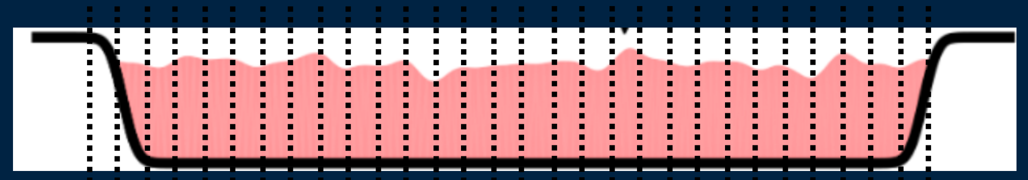
$$= \sum_{k>0} \hbar\omega_k \left(\hat{\phi}_k^2 + \delta\hat{\rho}_k^2 \right) + g\delta\hat{\rho}_0^2$$

Eigenmode rep.

Ex:
homogeneous gas,
linear dispersion relation

Gaussian dynamics and states

Quantities of interest vs Data readout



- Discretised derivation of Luttinger Hamiltonian

  [Mora, Castin, Phys. Rev. A 67, 053615 (2003)]

$$\hat{H}[n_{\mathrm{GP}}] = \Delta z \sum_{i=1}^{N-1} \frac{\hbar^2 \eta_i}{4m} \left[\frac{\hat{\phi}_i - \hat{\phi}_{i+1}}{\Delta z} \right]^2 + \Delta z \sum_{i=1}^{N} g(z_i) \delta\hat{\rho}_i^{\,2} \qquad \eta_i = \sqrt{\rho_i \rho_{i+1}}$$

  - Choice of Δz is like a frequency cut-off

- Approximately linear DR (for fraction of eigenmodes)

Simulation vs experimental observables

Quantities of interest vs Data readout

- Covariance matrix (Γ) formalism

$$\Gamma = \begin{pmatrix} \Gamma_{\rho\rho} & \Gamma_{\rho\phi} \\ \Gamma_{\phi\rho} & \Gamma_{\phi\phi} \end{pmatrix}$$

Total energy, $E_{\text{total}} = \mathrm{tr}(\hat{H}\Gamma)$

Energy per pixel, $E_{\text{pp}}(z_i) = \Delta z \cdot (\hat{H}\Gamma)_{i,i}$

Entropy $S(\rho) := -\,\mathrm{tr}(\rho \log \rho)$

Relative entropy w.r.t. thermal state (free energy when σ is thermal state) $D(\rho \| \sigma) := \mathrm{tr}(\rho \log \rho - \rho \log \sigma)$

Function of symplectic eigenvalues of $\Gamma_\rho, \Gamma_\sigma$, and $\mathrm{tr}(\hat{H}\Gamma_\rho)$

Simulation vs experimental observables

Quantities of interest vs Data readout

$$\Gamma = \begin{pmatrix} \Gamma_{\rho\rho} & \Gamma_{\rho\phi} \\ \Gamma_{\phi\rho} & \Gamma_{\phi\phi} \end{pmatrix}$$

- Density absorption imaging gives access to $\Gamma_{\rho\rho}$

$$\hat{H}[n_{\mathrm{GP}}] = \sum_{k>0} \hbar\omega_k \left(\hat{\phi}_k^2 + \delta\hat{\rho}_k^2 \right) + g\delta\hat{\rho}_0^2$$

$$\delta\hat{\rho}_k(t) = \cos(\omega_k t)\delta\hat{\rho}_k(0) - \sin(\omega_k t)\hat{\phi}_k(0)$$

Harmonical rotation of eigenmodes

$\longrightarrow$ Tomography on phonons

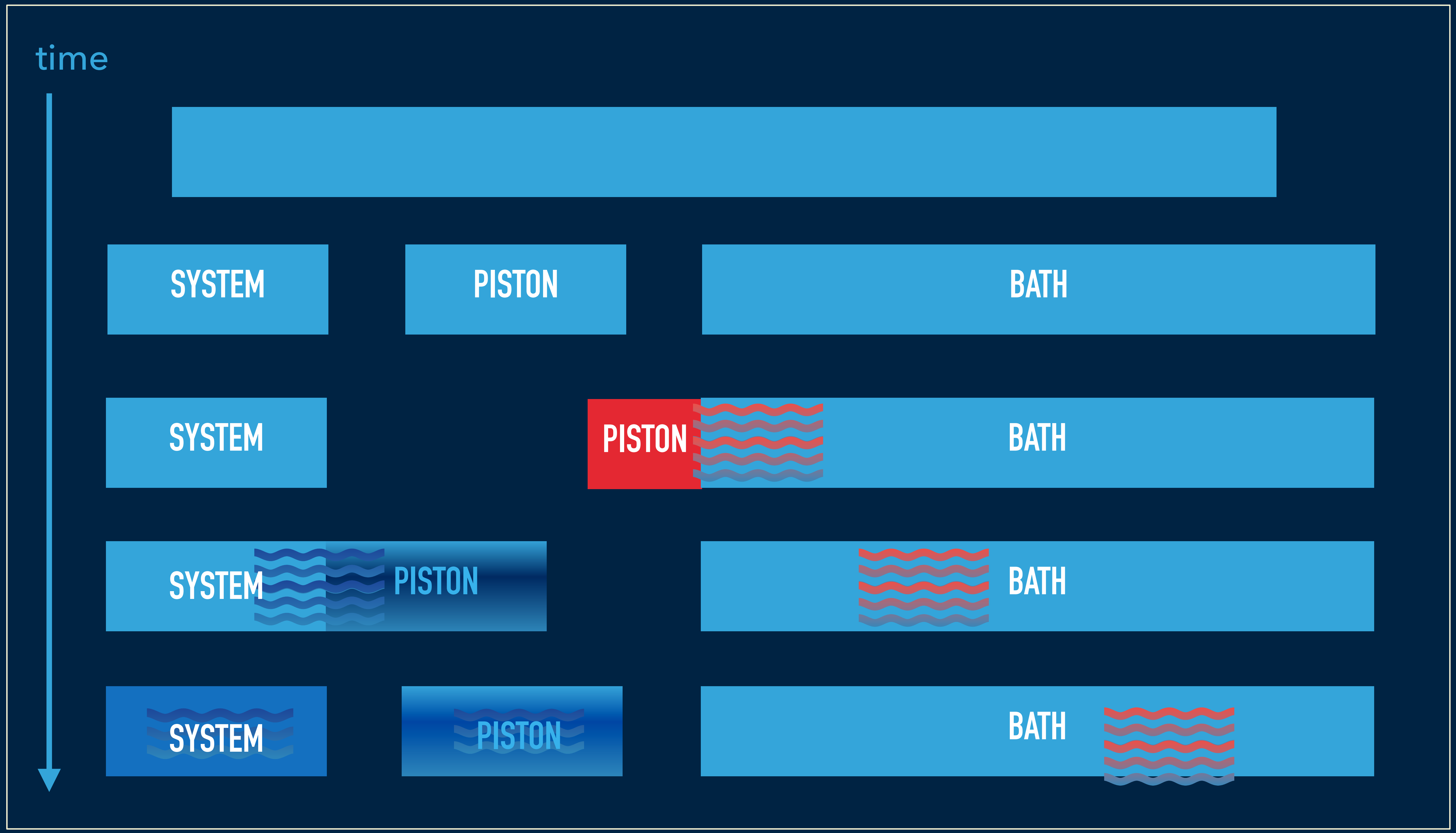
[M. Gluza et al, Comm. Phys, 3, 12 (2020)]

Operations & Protocols

Goal: a refrigeration cycle

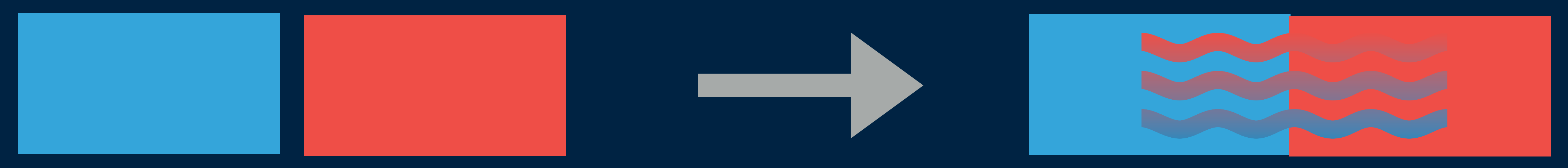
- Target: achieve extremely low temperatures for quantum many-body system (ex: Bose gas)
  - ground state preparation, low noise simulations etc
- How?
  - Evaporative cooling
  - Dissipative dynamics
  - But there are still fundamental limits…

Can we run a reverse Otto cycle on superfluids?



Splitting, merging, compressing

- Simple models (e.g. linear ramp transforming from one Hamiltonian to another)

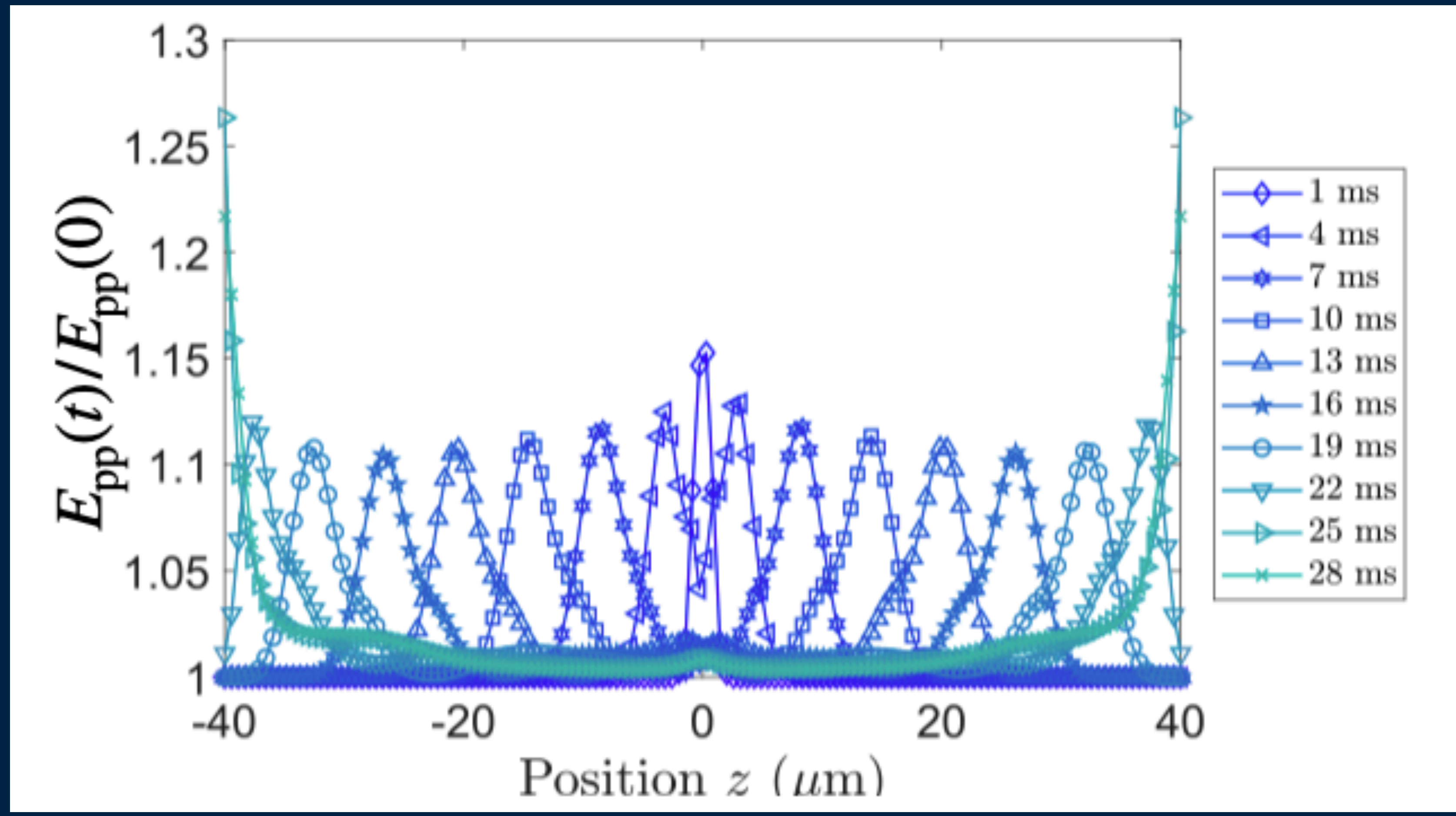


$H_{\text{decoupled}} = \hat{H}[n_{\text{GP(A)}}] + \hat{H}[n_{\text{GP(B)}}]$ $\qquad$ $H_{\text{joint}} = \hat{H}[n_{\text{GP(A)}} + n_{\text{GP(B)}}]$

$$H(t) = \left(1 - \frac{t}{t_{\text{m}}}\right)\hat{H}_{\text{decoupled}} + \frac{t}{t_{\text{m}}}\hat{H}_{\text{joint}}, \quad t_{\text{m}} = \text{merging time}$$

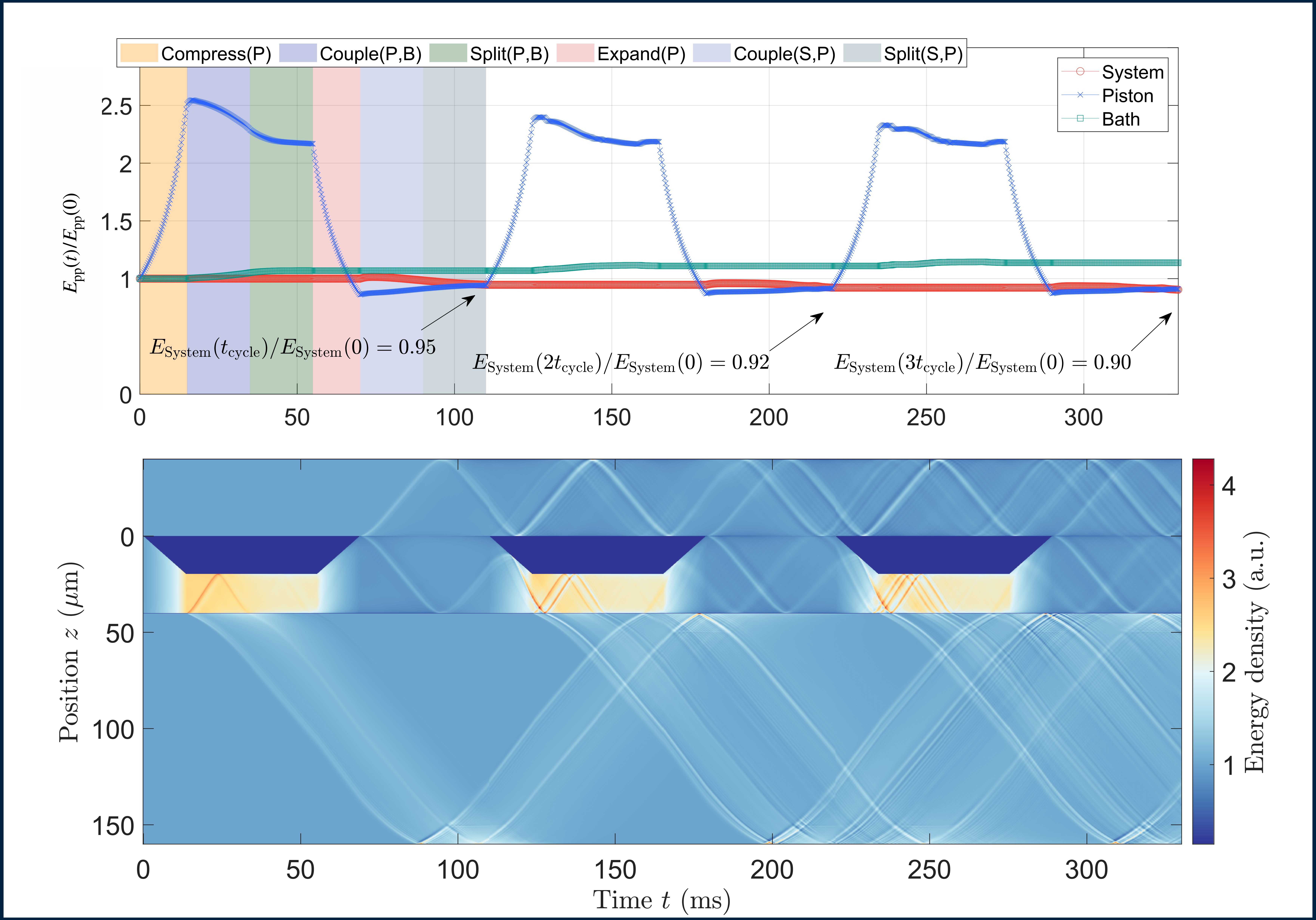
Recall:

$$\hat{H}[n_{\text{GP}}] = \Delta z \sum_{i=1}^{N-1} \frac{\hbar^2 \eta_i}{4m}\left[\frac{\hat{\phi}_i - \hat{\phi}_{i+1}}{\Delta z}\right]^2 + \Delta z \sum_{i=1}^{N} g(z_i)\delta\hat{\rho}_i^{\,2}$$



- Even with the most simplistic model, nontrivial amounts of energy are injected to joint system, waves packets travel ballistically out from interface
- The need to model explicit buffer region
  - Realistic profile for experiments
  - Lower amount of injected energy
  - Smaller contribution from high momentum modes, less dispersion

An idealized simulation of a quantum field refrigerator



Experimental execution of Landauer erasure

July 2024

Experimentally probing Landauer's principle in the quantum many-body regime

Stefan Aimet,[1,*] Mohammadamin Tajik,[2,*] Gabrielle Tournaire,[1,3] Philipp Schüttelkopf,[2] João Sabino,[2] Spyros Sotiriadis,[4,1] Giacomo Guarnieri,[5,1] Jörg Schmiedmayer,[2] and Jens Eisert[1]

[1]*Dahlem Centre for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany*
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[3]*Department of Physics and Astronomy, and Stewart Blusson Quantum Matter Institute, University of British Columbia, V6T1Z1 Vancouver, Canada*
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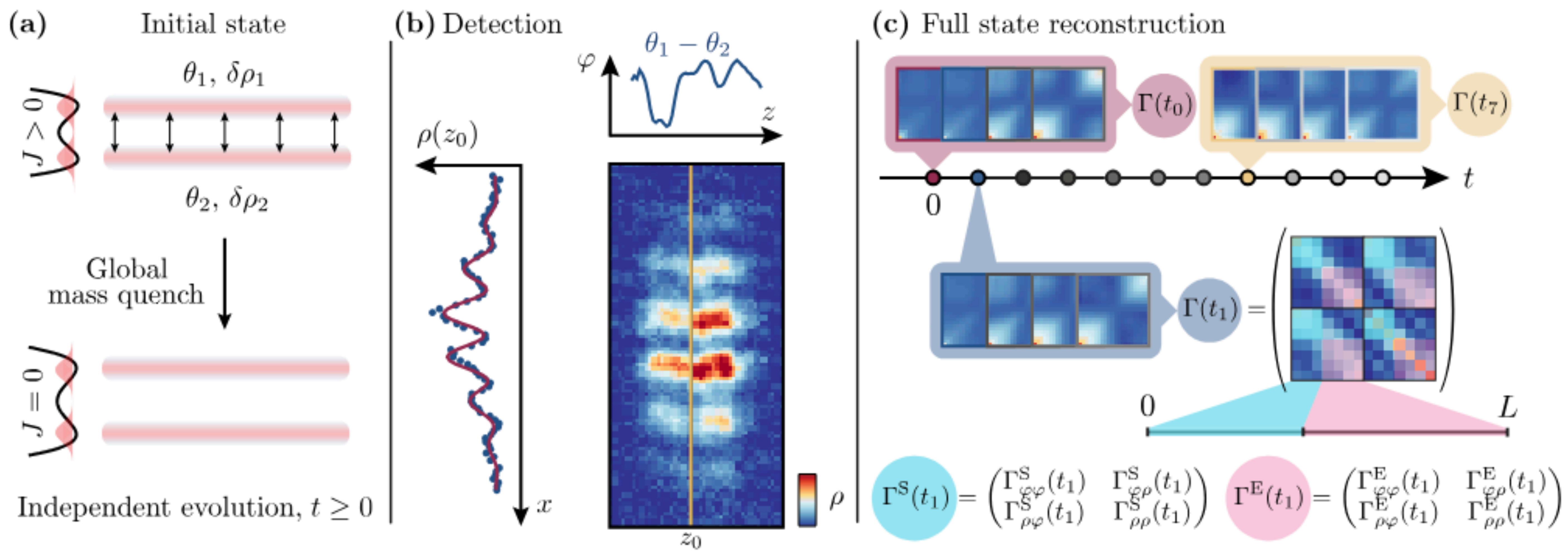

FIG. 1. **Schematic of the experimental protocol.** **a,** The experimental system consists of two tunnelling-coupled ultracold ^{87}Rb gases, with a single-particle tunnelling rate J, initially prepared in an initial state described by a global thermal state of the massive Klein-Gordon Hamiltonian. By ramping up a barrier between the condensates, a global mass quench is performed, and the condensates evolve independently under the post-quench Tomonaga-Luttinger liquid Hamiltonian for $t \geq 0$. **b,** The atomic clouds are released, and they interfere as they expand. We obtain integrated 2D atomic density via absorption imaging, from which the relative phase profiles are obtained. As an **c,** Using the measured phase-phase correlations, we dynamically reconstruct the full state. By successively shifting the observation window, we fit the covariance matrix $\Gamma(t)$ for different times t. The covariance matrices of system S and environment E are defined accordingly.

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The gaping problem when engaging experiments

Huge limitations on the measurement toolbox

- Measurements are almost always destructive (e.g. time-of-flight),
- We lose the gas after, hence no sequential measurements available
- Reconstruction limited and non-optimal
  - Various assumptions made to simplify reconstruction
  - Raises questions about reliability

The challenge statement when engaging experiments

In demand

A. Can we **rigorously test** the reliability state-of-the-art measurements, under the approximations previously made?

B. Can we **enhance state-of-the-art measurements**? For example by increasing the accuracy or extracting more information from the system.

C. If we can indeed improve the measurement toolbox, **what new physical phenomena can we probe**?

Hacking away

A. Can we **rigorously test** the reliability state-of-the-art measurements, under the approximations previously made?

Condensed Matter > Quantum Gases

[Submitted on 8 Mar 2024 (v1), last revised 9 May 2024 (this version, v2)]

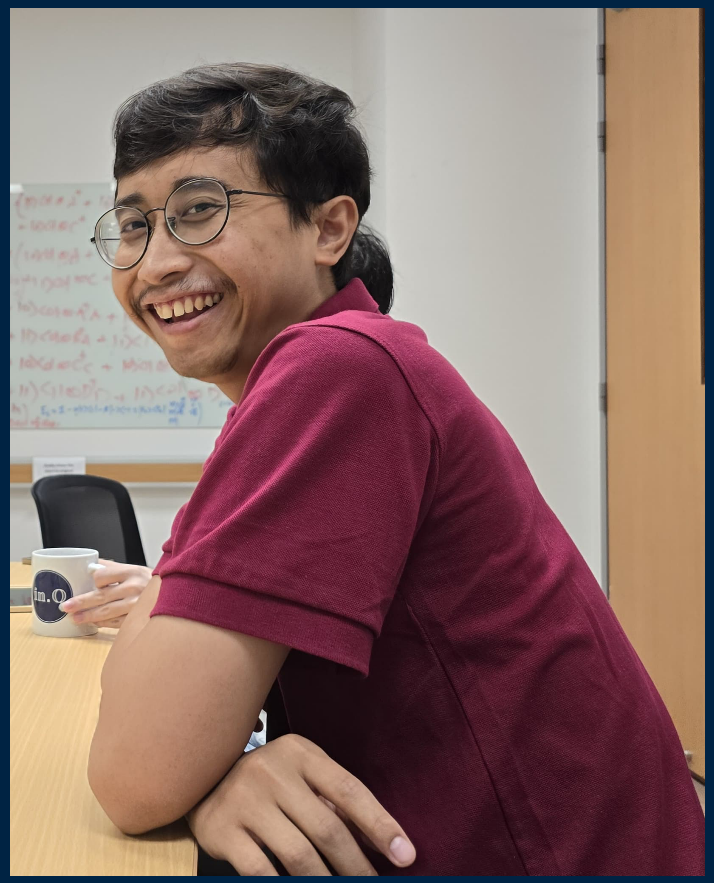
Systematic analysis of relative phase extraction in one-dimensional Bose gases interferometry

Taufiq Murtadho, Marek Gluza, Khatee Zathul Arifa, Sebastian Erne, Jörg Schmiedmayer, Nelly H.Y. Ng

Spatially resolved relative phase measurement of two adjacent 1D Bose gases is enabled by matter-wave interference upon free expansion. However, longitudinal dynamics is typically ignored in the analysis of experimental data. We provide an analytical formula showing a correction to the readout of the relative phase due to longitudinal expansion and mixing with the common phase. We numerically assess the error propagation to the estimation of the gases' physical quantities such as correlation functions and temperature. Our work characterizes the reliability and robustness of interferometric measurements, directing us to the improvement of existing phase extraction methods necessary to observe new physical phenomena in cold-atomic quantum simulators.

Comments: Significant updates from v1, contains new results section on the effect of image processing, 21+12 pages, 22 figures
Subjects: **Quantum Gases (cond-mat.quant-gas)**; Quantum Physics (quant-ph)
Cite as: arXiv:2403.05528 **[cond-mat.quant-gas]**
(or arXiv:2403.05528v2 **[cond-mat.quant-gas]** for this version)
https://doi.org/10.48550/arXiv.2403.05528

Let's do A for my first year during PhD…



Hacking away

B. Can we **enhance state-of-the-art measurements**? For example by increasing the accuracy or extracting more information from the system.

Condensed Matter > Quantum Gases

[Submitted on 7 Aug 2024 (v1), last revised 15 Oct 2024 (this version, v2)]

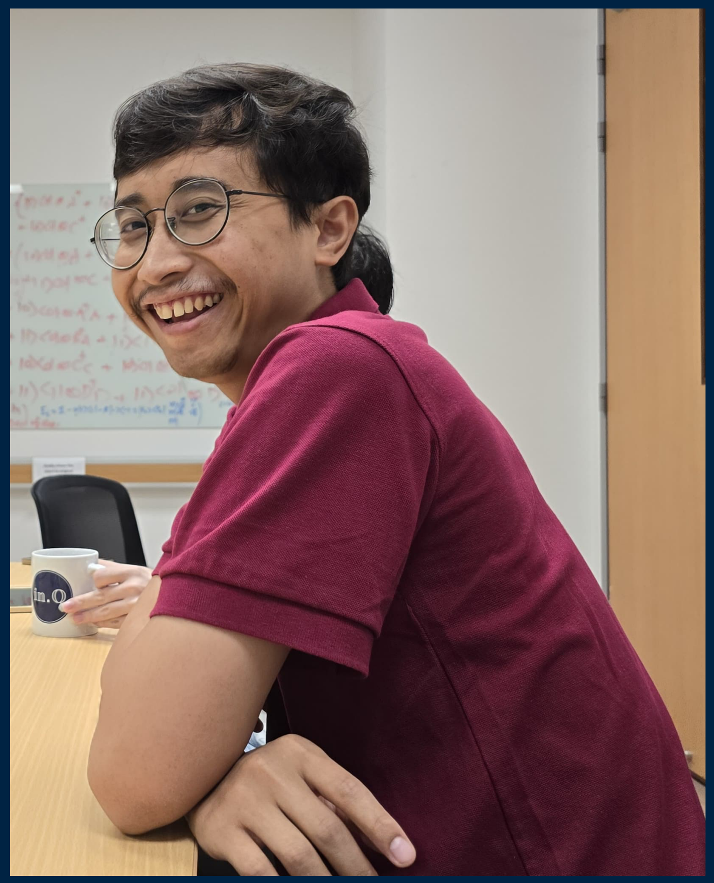
Measurement of total phase fluctuation in cold-atomic quantum simulators

Taufiq Murtadho, Federica Cataldini, Sebastian Erne, Marek Gluza, Mohammadamin Tajik, Jörg Schmiedmayer, Nelly H.Y. Ng

Studying the dynamics of quantum many-body systems is often constrained by the limitations in probing relevant observables, especially in continuous systems. A powerful method to gain information about such systems is the reconstruction of local currents from the continuity equation. Here we extend this approach to extract the total phase fluctuation of adjacent Bose gases. We validate our technique numerically and demonstrate its effectiveness by analyzing data from selected experiments simulating 1D quantum field theories through the phase difference of two 1D Bose gases probed by interference. Our analysis reveals the previously hidden sector of the sum mode of the phase, which is important for studying long-time thermalization and out-of-equilibrium dynamics of the system, thereby expanding the scope and capabilities of cold-atomic quantum simulators.

Comments: 5+9 pages, 12 figures
Subjects: **Quantum Gases (cond-mat.quant-gas)**; Quantum Physics (quant-ph)
Cite as: arXiv:2408.03736 **[cond-mat.quant-gas]**
(or arXiv:2408.03736v2 **[cond-mat.quant-gas]** for this version)
https://doi.org/10.48550/arXiv.2408.03736

And then tackle B for my second year …

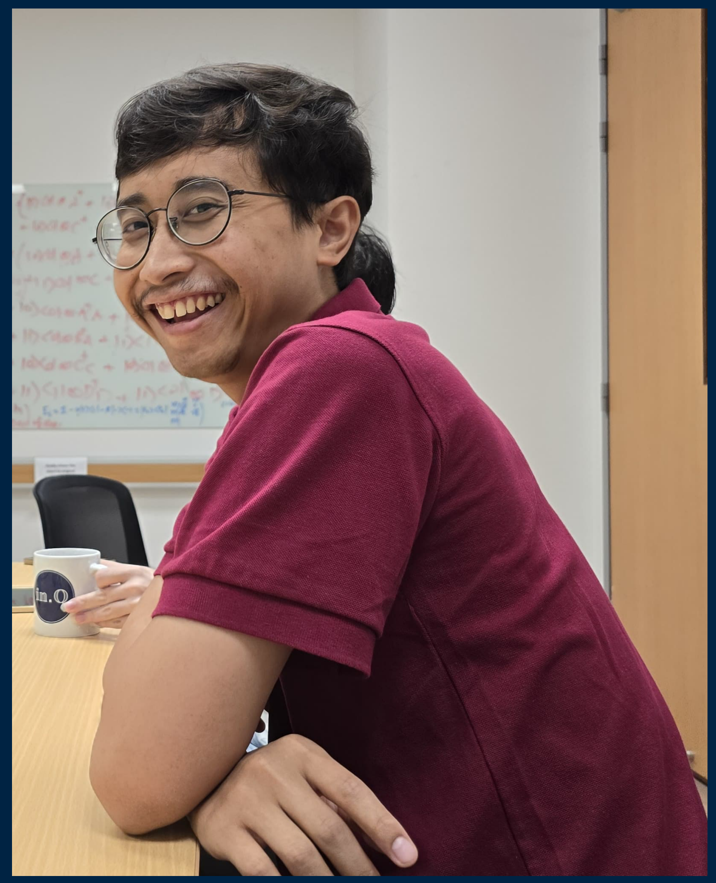


Hacking away

C. If we can indeed improve the measurement toolbox, **what new physical phenomena can we probe**?

What's next?

And now explore C with others who may be interested!



Thanks for listening!
Happy to take some questions