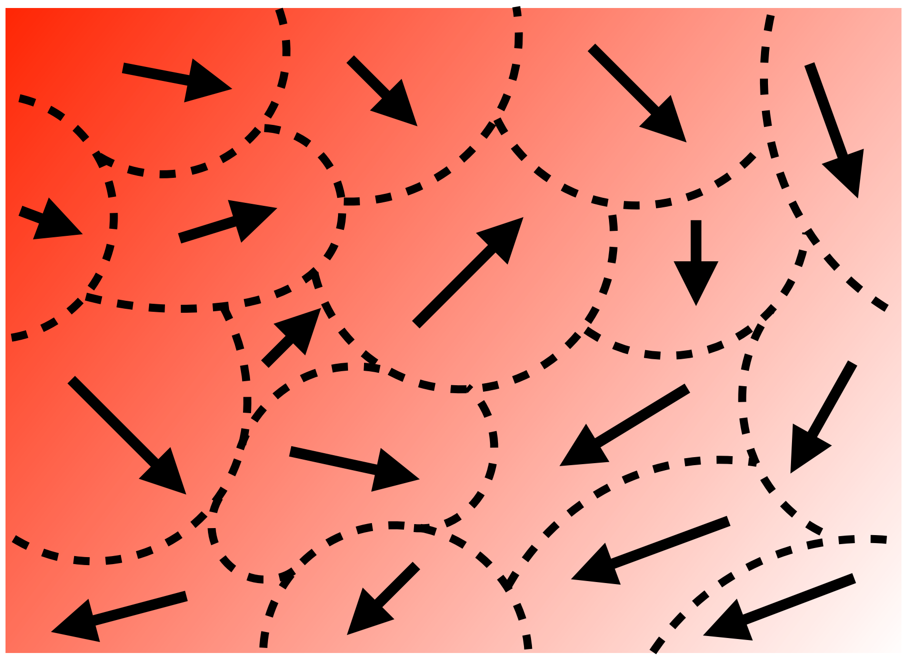
Hydrodynamics from local thermal pure quantum states



$$|\lambda_t; t\rangle$$

Masaru Hongo (Univ. of Illinois at Chicago)

Quantum Information Entropy in Physics @YITP, 2022/03/24

Based on S. Tsutsui, M. Hongo, S. Sato, T. Sagawa, arXiv:2106.12777 [cond-mat.stat-mech]

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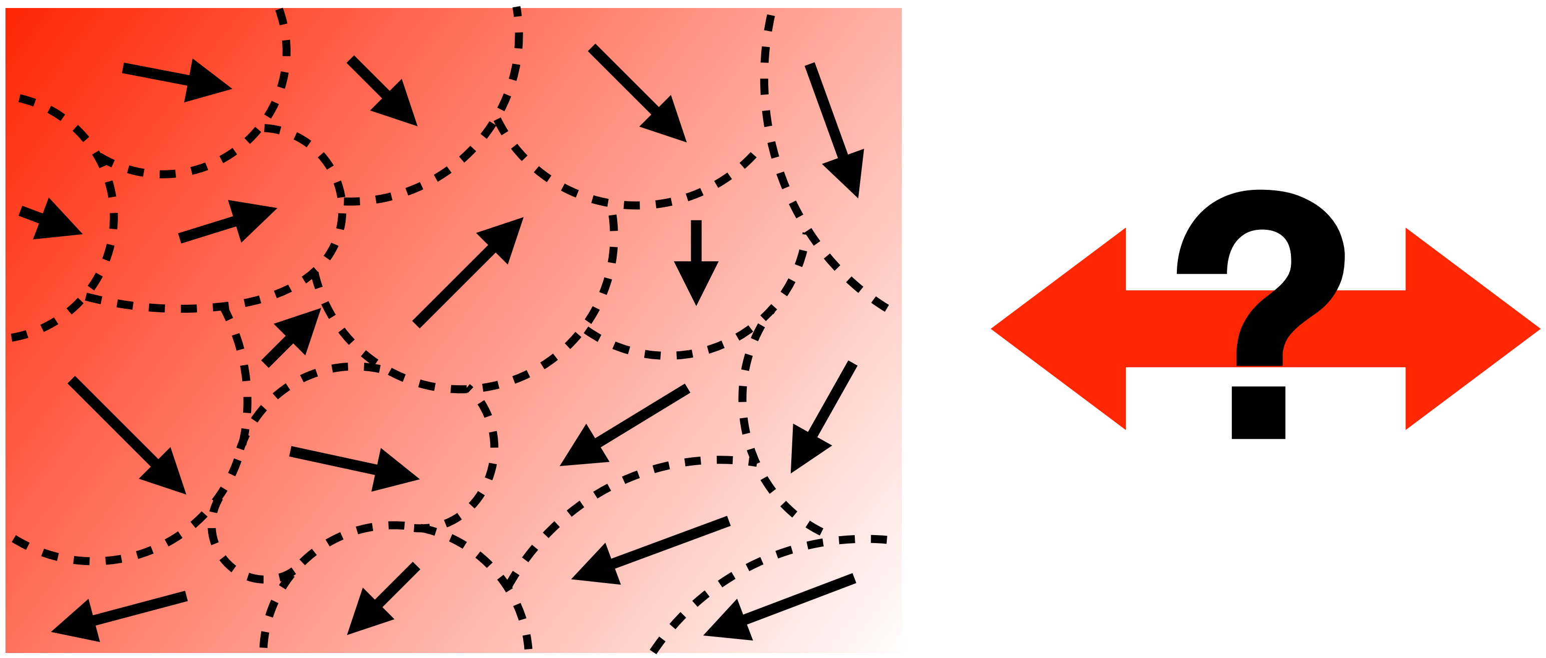

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Masaru Hongo (Univ. of Illinois at Chicago)

→ Niigata Univ. (from April)

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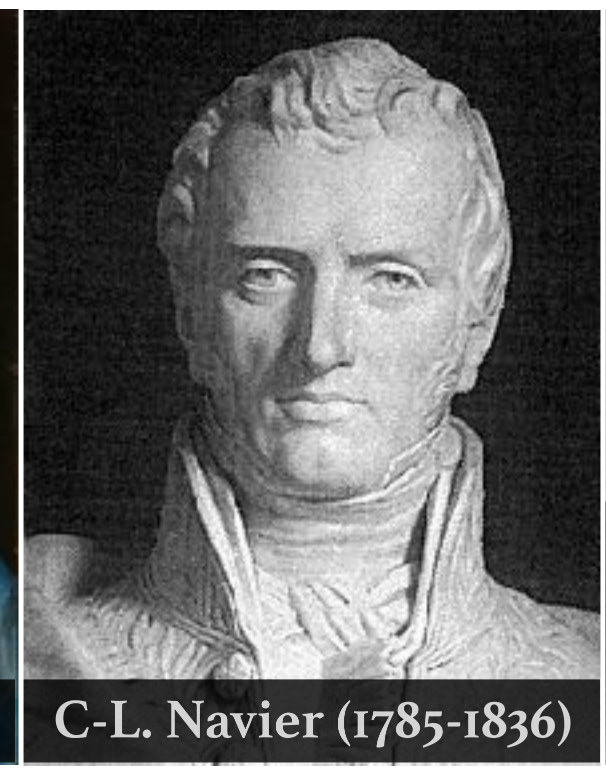
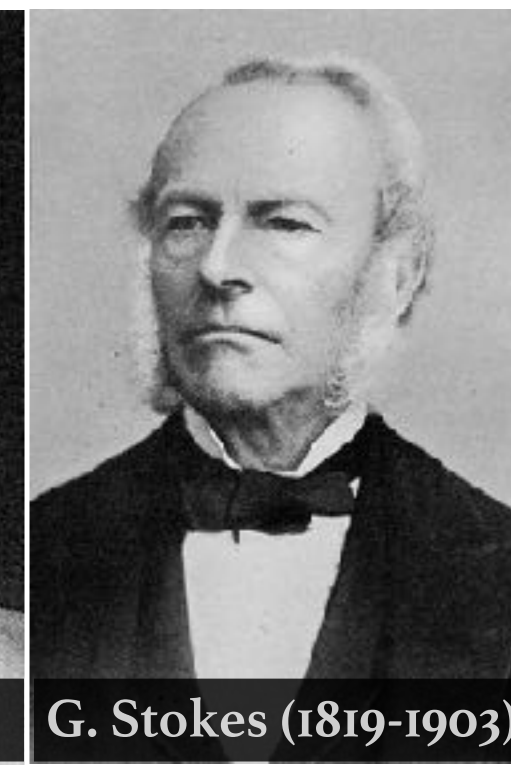
What is hydrodynamics?

The oldest but state-of-the-art phenomenological field theory





Pascal's law

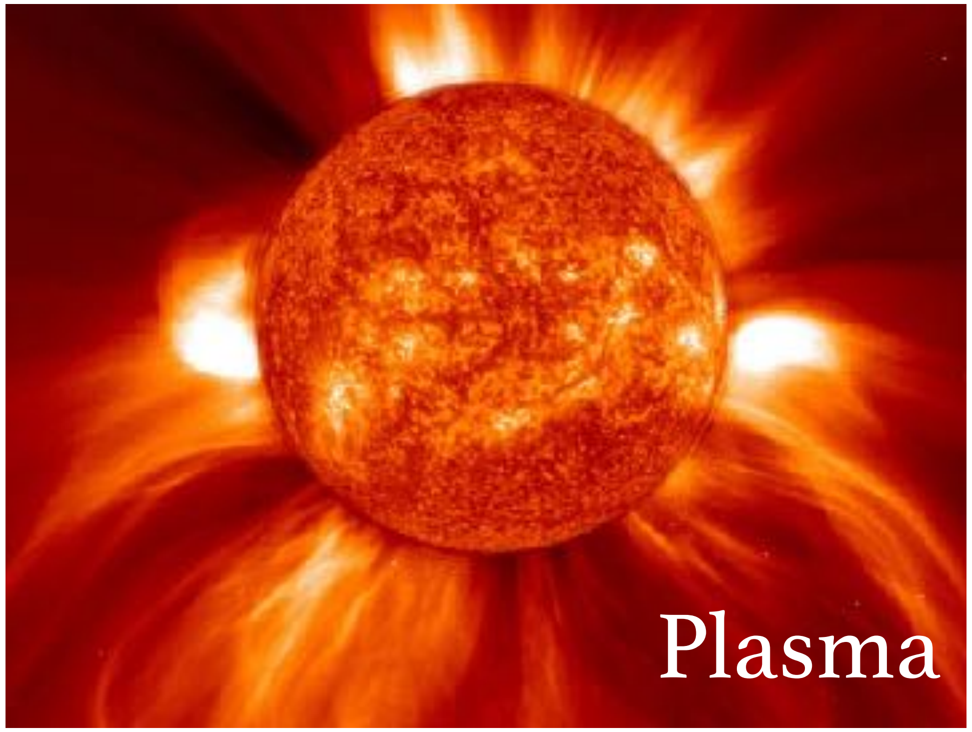
Hydro*dynamics*

Euler equations
(Perfect fluid)

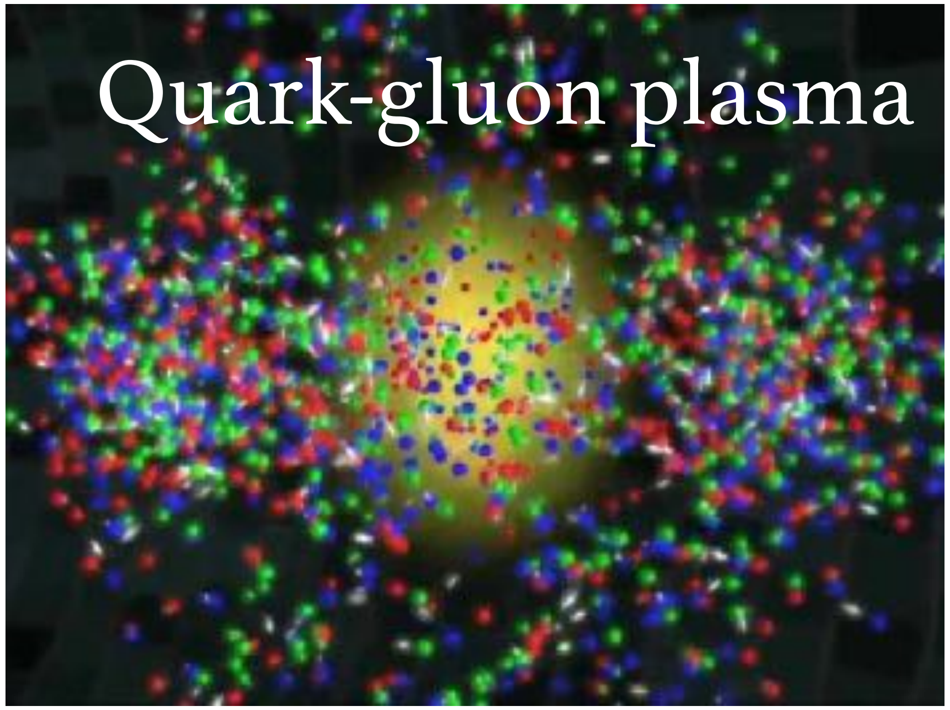
Navier-Stokes equations
(Viscous fluid)

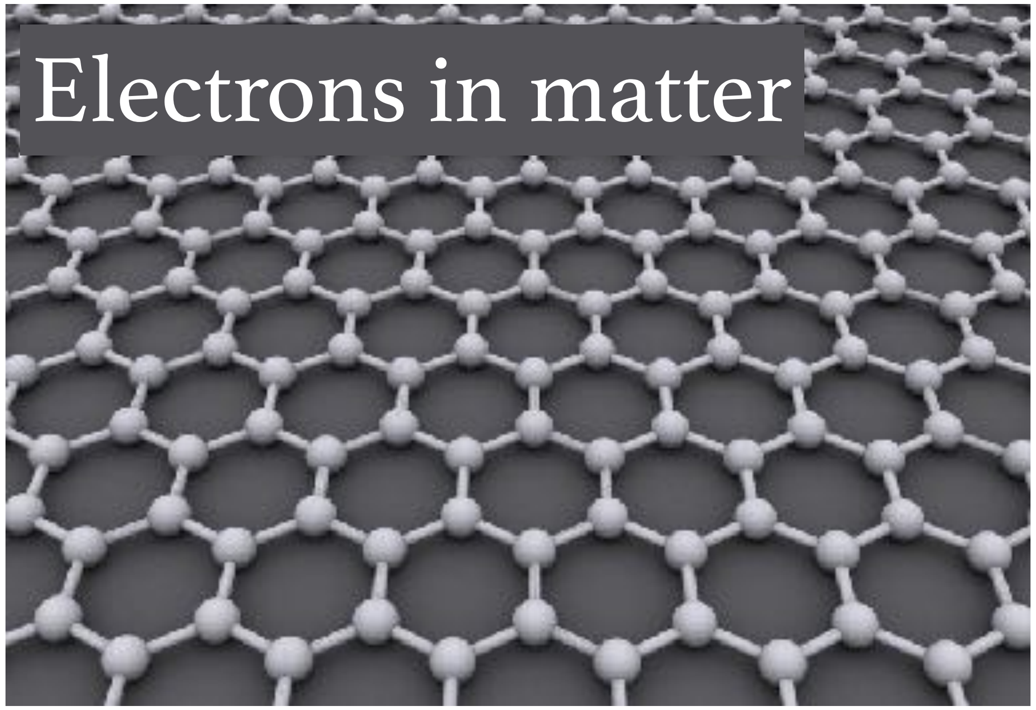
1600 — 1700 — 1800 — 1900

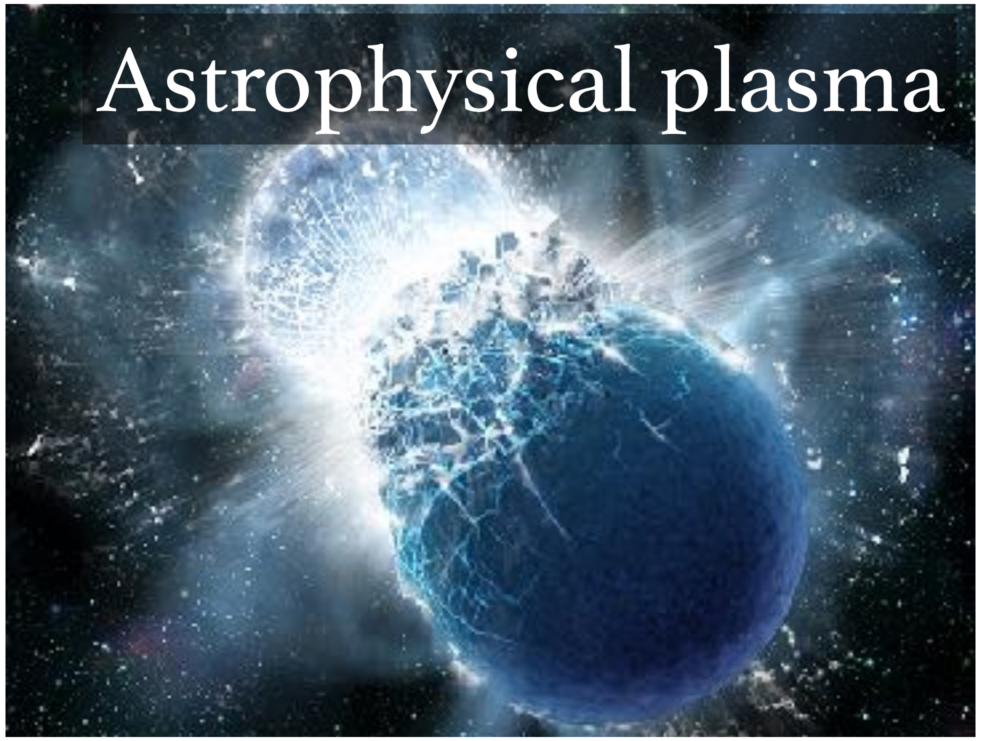
Classical hydrodynamic objects

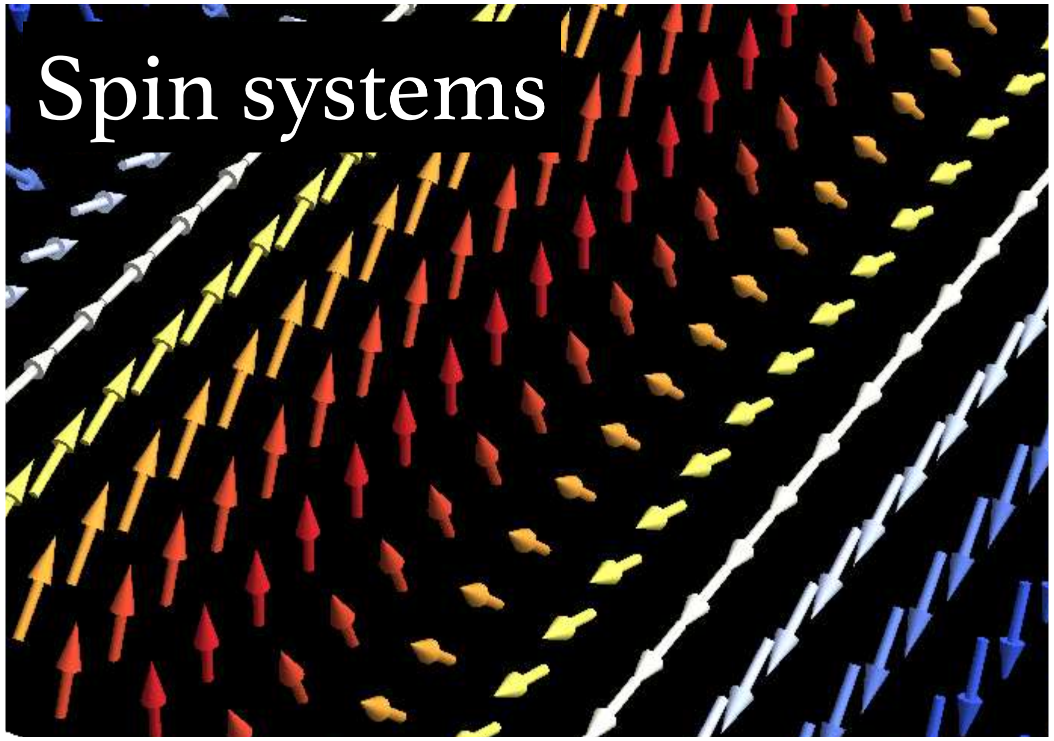


Modern hydrodynamic object

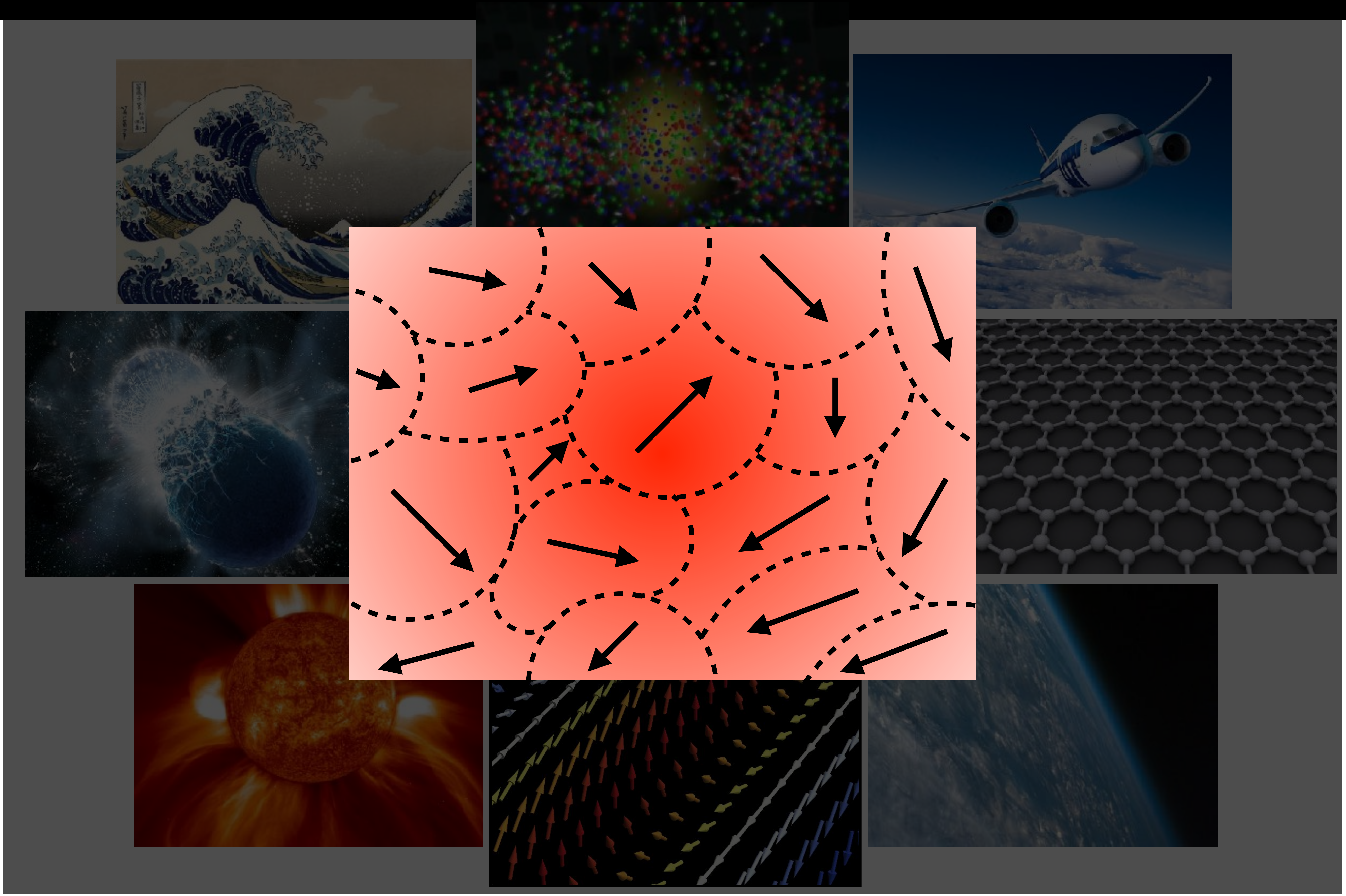








What hydrodynamics does is



Motivation

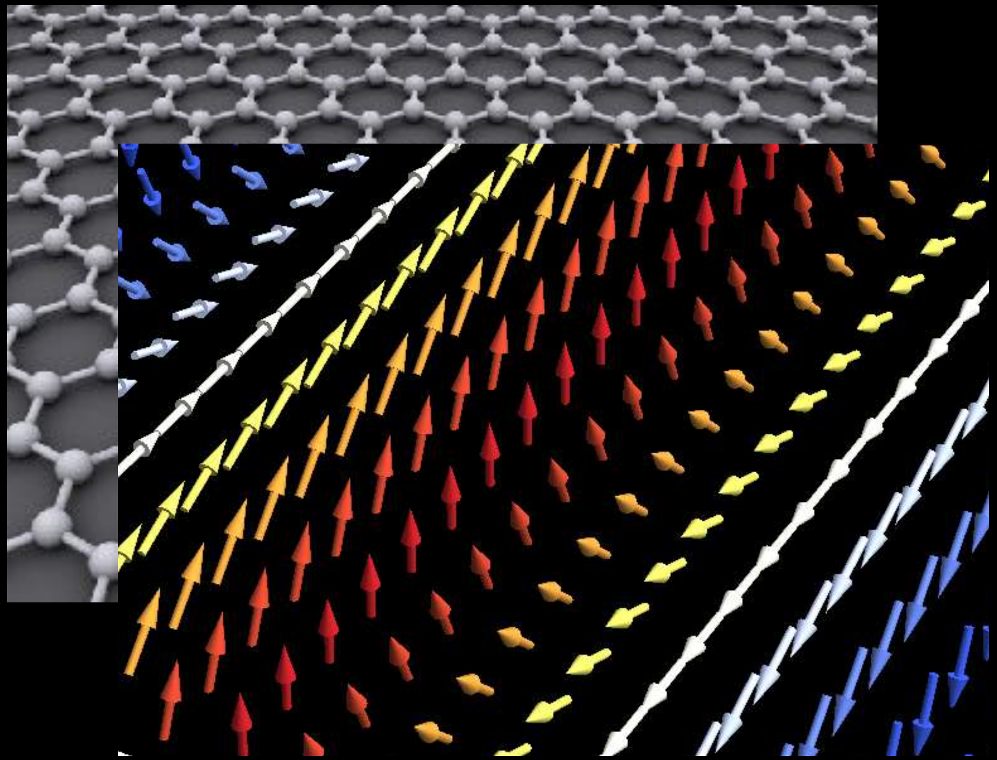
Microscopic

$$\hat{H}_{\mathrm{micro}}$$

Quantum theory

d.o.f.

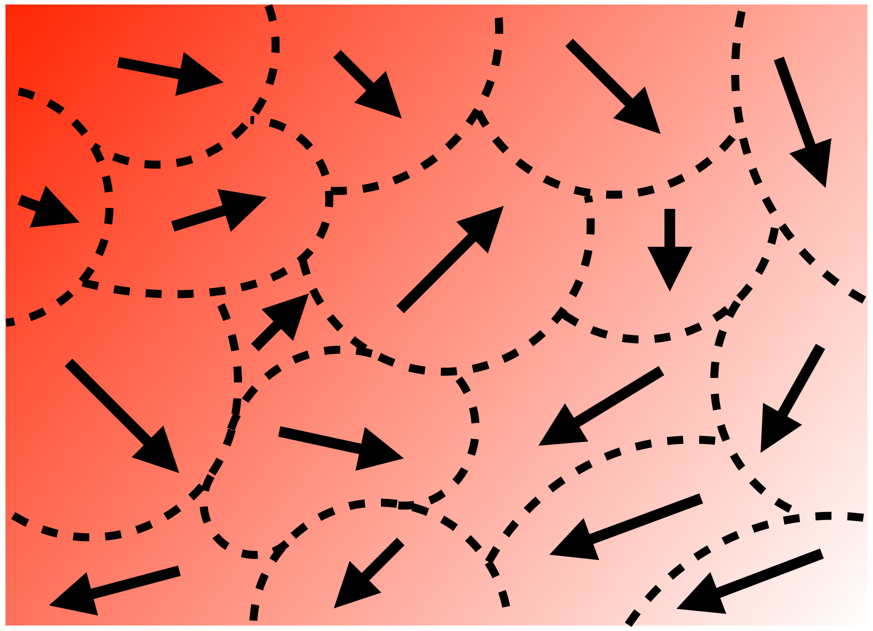
Electron, spin, ...



Question.

How to bridge the gap between micro and macro?

Macroscopic

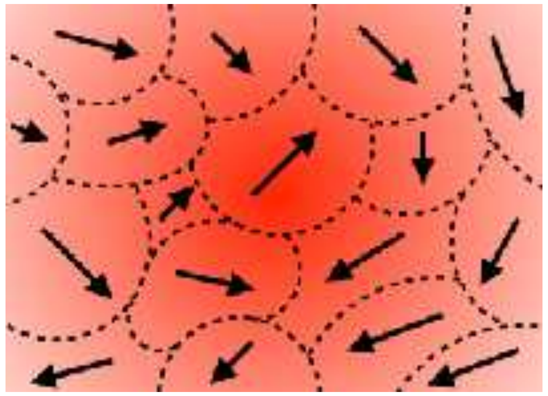


Hydrodynamics

d.o.f.

$T(x),\ \vec{v}(x),\ \mu(x)$

Hydro from pure state?

	Ensemble formulation	Pure state formulation
Global equilibrium $T = \text{const.}$	**Gibbs ensemble** $$\hat{\rho}_{\mathrm{G}} = \frac{1}{Z} \mathrm{e}^{-\beta \hat{H}}$$	**Eigenstate thermalization hypo.** Rigol-Dunjko-Olshanii (2008), … **Thermal pure quantum state** $$\lvert \beta \rangle \equiv \exp\left(-\frac{N\beta \hat{h}}{2} \right) \sum_{\alpha} z_{\alpha} \lvert \alpha \rangle$$ Bocchieri-Loinger (1959), Hams-De Raedt (2000), Popescu-Short-Winter (2006), Sugiura-Shimizu (2012-)
Lobal equilibrium 	**Local Gibbs ensemble** $$\hat{\rho}_{\mathrm{LG}} = \frac{1}{Z} \mathrm{e}^{-\int \mathrm{d}x \beta(x) \hat{h}(x)}$$ Nakajima (1957), Mori (1958), McLennan (1960) Zubarev et al. (1979), Becattini et al. (2015) Hayata-Hidaka-MH-Noumi (2015), MH(2017)	**?** **Local thermal pure quantum state** Tsutsui-MH-Sato-Sagawa, arXiv:2106.12777 [cond-mat.stat-mech]

Short Summary

◆ Formulation

[Tsutsui-MH-Sato-Sagawa, arXiv:2106.12777 [cond-mat.stat-mech]]

Local thermal pure quantum (ℓTPQ) state

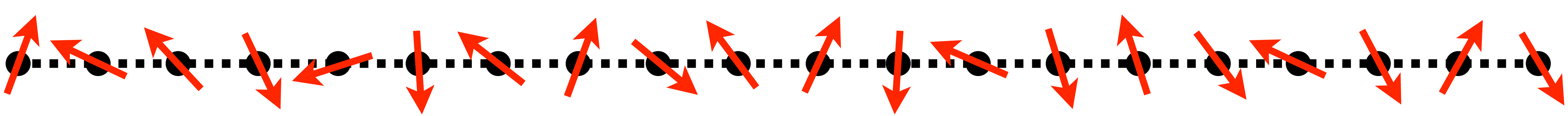
for nonintegrable systems (a finite number of local conserved quantities)

⇒ Hydrodynamics, 2nd law, and quantum fluctuation theorem

◆ Application

ℓTPQ state formulation covers various quantum systems including ones described by relativistic QFTs

⇒ Application to the simple nonintegralbe spin chain



Setup

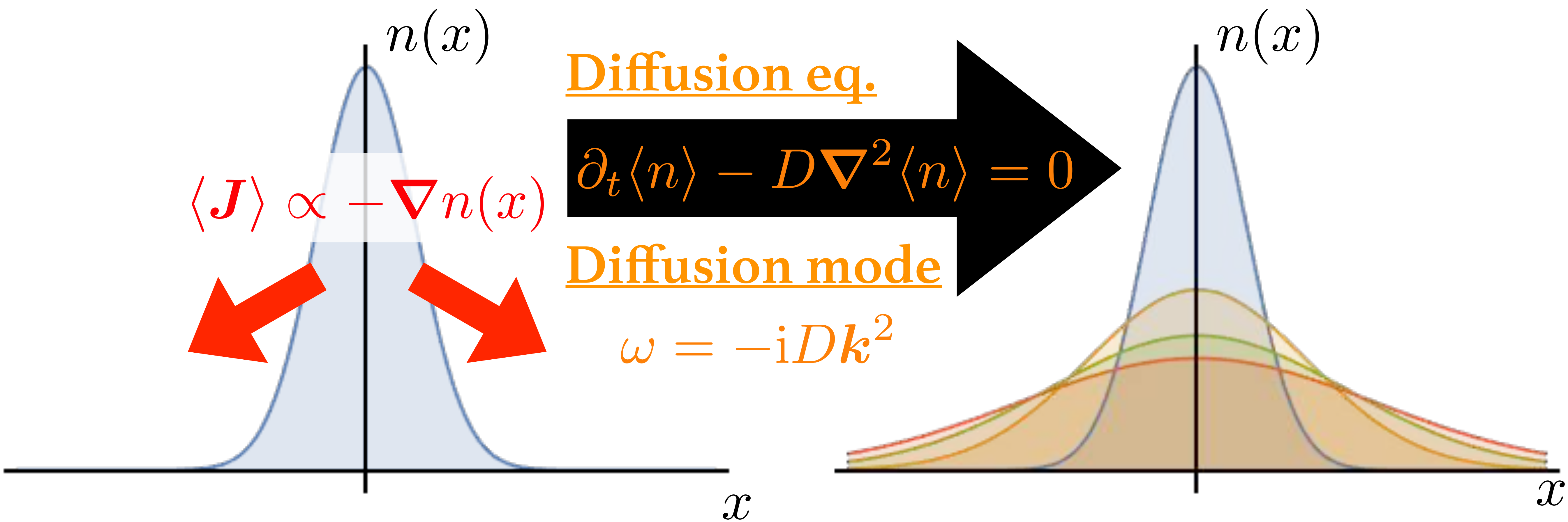
Primer to hydrodynamics

◆ Building blocks of hydrodynamic equation

(1) Conservation law: $\partial_t \langle n \rangle + \boldsymbol{\nabla} \cdot \langle \boldsymbol{J} \rangle = 0$

(2) Constitutive relation: $\langle \boldsymbol{J} \rangle = -D \boldsymbol{\nabla} n$

(3) Physical properties: Value of diffusion constant D



From microscopic view

◆ **Conservation laws**

$$\partial_0 \hat{c}_a + \partial_i \hat{\mathcal{J}}^i{}_a = 0$$

$$\begin{cases} \hat{c}_a & : \text{charge density} \\ \hat{\mathcal{J}}^i{}_a & : \text{charge current} \end{cases}$$

Need to clarify what $\langle \cdots \rangle$ does mean!

⇒ Local Gibbs ensemble, ℓTPQ state, etc.

◆ **Constitutive relation + Physical properties**

$$\langle \hat{\mathcal{J}}^i{}_a \rangle = \mathcal{J}^i{}_a[\langle \hat{c}_a \rangle] = \mathcal{J}^i{}_a[\lambda^a]$$

- Equation of state
- Values of transport coefficient

Local Gibbs (LG) ensemble

◆ **local Gibbs ensemble**

- **Average value:** $\langle \hat{\mathcal{O}} \rangle^{\mathrm{LG}}_{\lambda_t} \equiv \mathrm{Tr}\left(\hat{\rho}_{\mathrm{LG}}[\lambda_t; t]\hat{\mathcal{O}}\right)$
- **Density operator:** $\hat{\rho}_{\mathrm{LG}}[\lambda_t; t] \equiv \mathrm{e}^{-\hat{S}_{\mathrm{LG}}[\lambda_t; t]}$
- **Entropy operator:** $\hat{S}_{\mathrm{LG}}[\lambda_t; t] \equiv \hat{K}[\lambda_t; t] + \log Z_{\mathrm{LG}}[\lambda_t]$
- **Partition functional:** $Z_{\mathrm{LG}}[\lambda_{t_0}] \equiv \mathrm{Tr}\, \mathrm{e}^{-\hat{K}[\lambda_{t_0}; t_0]}$
- **Khat operator:** $\hat{K}[\lambda_t; t] \equiv \lambda^a(t)\hat{c}_a(t) \to \int \mathrm{d}^d x \beta(t, \boldsymbol{x})\hat{h}(t, \boldsymbol{x})$

⇒ **Assuming the initial LG distribution, we can derive hydro!**

[See, e.g., Hayata-Hidaka-MH-Noumi (2015), MH(2017) for the derivation of relativistic hydrodynamics]

ℓTPQ state

◆ ℓTPQ state formulation

- **Average value:** $\langle \hat{\mathcal{O}} \rangle^{\ell\mathrm{TPQ}}_{\lambda_t} \equiv \dfrac{1}{Z_{\ell\mathrm{TPQ}}[\lambda_t]} \langle \lambda_t; t | \hat{\mathcal{O}} | \lambda_t; t \rangle$

- **ℓTPQ state:** $|\lambda_t; t\rangle \equiv \sum_\alpha z_\alpha \mathrm{e}^{-\frac{1}{2}\hat{K}[\lambda_t;t]} |\alpha_t\rangle$ $\begin{cases} z_\alpha \equiv (z'_\alpha + \mathrm{i} z''_\alpha)/\sqrt{2} \\ |\alpha_t\rangle : \text{any orthonormal state} \end{cases}$

- **Entropy operator:** $\hat{S}[\lambda_t; t] = \hat{K}[\lambda_t; t] + \log Z_{\ell\mathrm{TPQ}}[\lambda_t]$

- **Partition functional:** $Z_{\ell\mathrm{TPQ}}[\lambda_t] \equiv \langle \lambda_t; t | \lambda_t; t \rangle$

- **Khat operator:** $\hat{K}[\lambda_t; t] \equiv \lambda^a(t) \hat{c}_a(t) \to \int \mathrm{d}^d x \beta(t, \boldsymbol{x}) \hat{h}(t, \boldsymbol{x})$

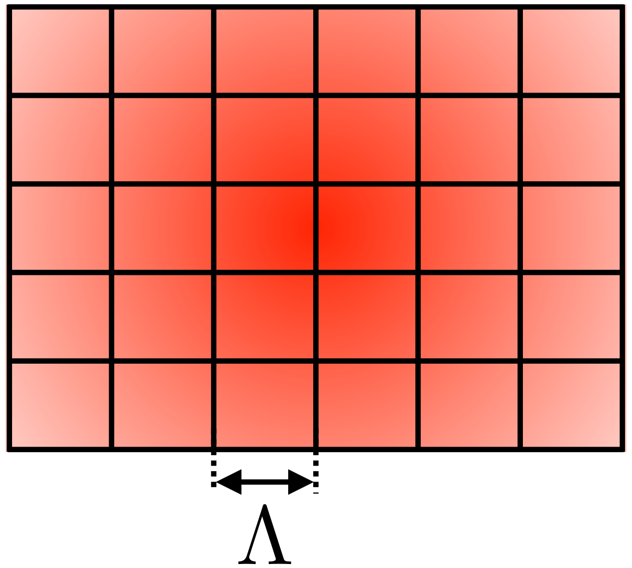
Q. Does ℓTPQ formulation correctly describes hydrodynamics?

Result 1: LG-ℓTPQ equivalence

◆ <u>Large fluid-cell limit</u>

All fluid cells should be large enough,
so that local thermodynamics is applicable

$$\Lambda \to \infty$$



◆ **Equivalence between LG and ℓTPQ formulations**

$$Z_{\ell\mathrm{TPQ}}[\lambda_t] \xrightarrow{P} Z_{\mathrm{LG}}[\lambda_t]$$

$$\langle \hat{\mathcal{O}} \rangle^{\ell\mathrm{TPQ}}_{\lambda_t} \xrightarrow{P} \langle \hat{\mathcal{O}} \rangle^{\mathrm{LG}}_{\lambda_t}$$

⇒ **Behaviors of thermodynamic properties and average of local operators are equivalent between the LG and ℓTPQ formulations!**

Result 2: Fluctuation theorem

◆ The 2nd law of thermodynamics

$$\langle \hat{S}[\lambda_t; t] - \hat{S}[\lambda_{t_0}; t_0] \rangle \geq O(\mathrm{e}^{-A_1 V_{\mathrm{cell}}})$$

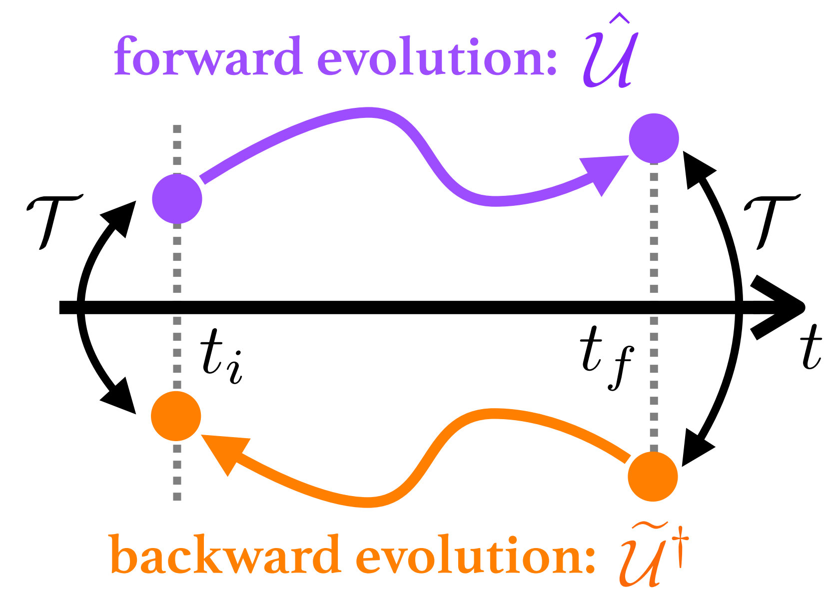
◆ Quantum fluctuation theorem

$$\left| G_F^{\ell\mathrm{TPQ}}(z) - G_B^{\ell\mathrm{TPQ}}(-z + \mathrm{i}) \right| = O(\mathrm{e}^{-A_2 V_{\mathrm{cell}}})$$

<u>Generating functions for the entropy production</u>

$$G_F^{\ell\mathrm{TPQ}}(z) = \langle \hat{\mathcal{U}}^\dagger(t) \mathrm{e}^{\mathrm{i}z\hat{S}[\lambda_t; t_0]} \hat{\mathcal{U}}(t) \mathrm{e}^{-\mathrm{i}z\hat{S}[\lambda_{t_0}; t_0]} \rangle_{\lambda_{t_0}}^{\ell\mathrm{TPQ}}$$

$$G_B^{\ell\mathrm{TPQ}}(z) = \langle \widetilde{\mathcal{U}}(t) \mathrm{e}^{\mathrm{i}z\hat{S}[\tilde{\lambda}_{t_0}; t]} \widetilde{\mathcal{U}}^\dagger(t) \mathrm{e}^{-\mathrm{i}z\hat{S}[\tilde{\lambda}_t; t]} \rangle_{\tilde{\lambda}_t}^{\ell\mathrm{TPQ}}$$



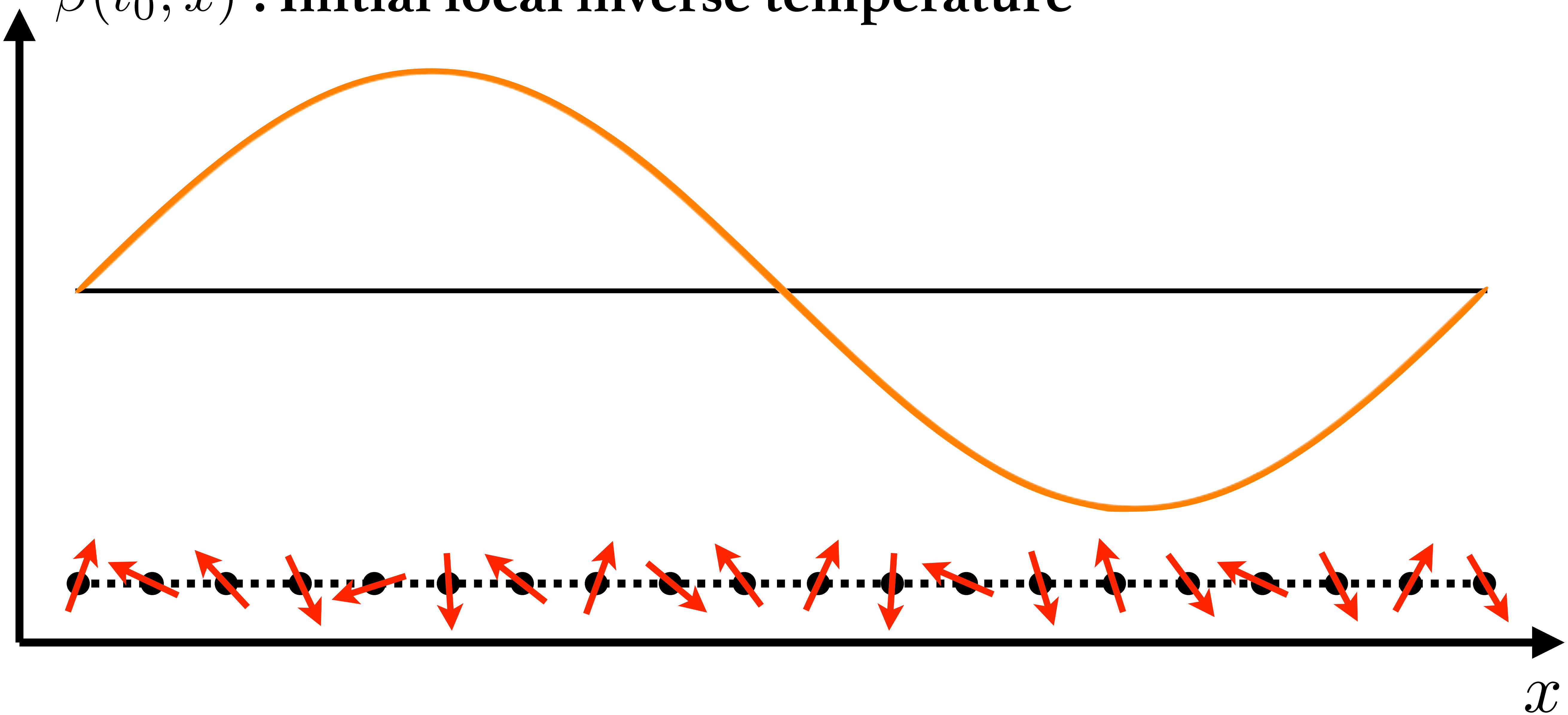
[In the LG ensemble formalism, both are exact, see MH J.Statist.Phys (2019)]

Application to spin chain

Model: spin chain

$$\hat{H} = \sum_{n=1}^{N} \left[J_z \sigma_n^z \sigma_{n+1}^z + D(\sigma_n^z \sigma_{n+1}^x - \sigma_n^x \sigma_{n+1}^z) + \Gamma \sigma_n^x + B \sigma_n^z \right]$$

$\beta(t_0, x)$ **: Initial local inverse temperature**



“Coarse-graining”

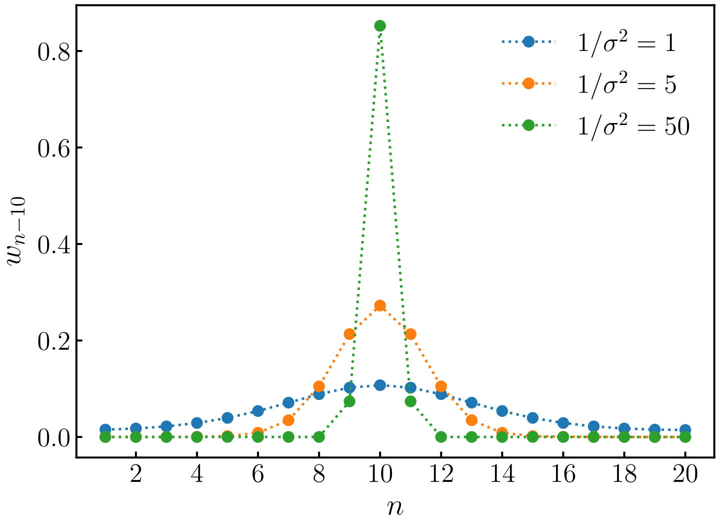
◆ **Microscopic conservation law**

$$\partial_t \hat{h}(t,n) + \nabla_x \hat{J}_E(t,n) = 0$$

$$\begin{cases} \hat{h}(n) = J_z \sigma^z_n \sigma^z_{n+1} + D(\sigma^z_n \sigma^x_{n+1} - \sigma^x_n \sigma^z_{n+1}) + \Gamma \sigma^x_n + B\sigma^z_n \\ \hat{J}_E(n-1/2) = -2D^2(\sigma^x_{n-1}\sigma^y_n\sigma^z_{n+1} - \sigma^z_{n-1}\sigma^y_n\sigma^x_{n+1}) + \cdots \end{cases}$$

“Coarse-graining”

$$\bar{\mathcal{O}}(t,n) \equiv \frac{1}{\tau}\int_t^{t+\tau} \mathrm{d}t' \sum_{n=1}^{N} w_{n-m} \hat{\mathcal{O}}(t',m)$$



◆ **Coarse-grained conservation law**

$$\partial_\tau \langle \bar{h}(t,n)\rangle + \nabla_x \langle \bar{J}_E(t,n)\rangle = 0 \quad \begin{cases} \partial_\tau \langle \bar{h}(t,n)\rangle = \dfrac{\langle \bar{h}(t+\tau,n)\rangle - \langle \bar{h}(t,n)\rangle}{\tau} \\ \nabla_x \langle \bar{J}_E(t,n)\rangle \equiv \langle \bar{J}_E(t,n+1/2)\rangle - \langle \bar{J}_E(t,n-1/2)\rangle \end{cases}$$

should be described by the hydrodynamic equation!

Time evolution from ℓTPQ state

◆ **Initial ℓTPQ state**

$$|\{\beta(n)\}\rangle \equiv \exp\left(-\frac{\sum_{n=1}^{N}\beta(n)\hat{h}(n)}{2}\right)\sum_{\alpha} z_\alpha |\alpha\rangle$$

$$\beta(t_0, n) = \bar{\beta} + \Delta\beta \sin\frac{2\pi(n-1)}{N} \quad (n = 1, \ldots, N)$$

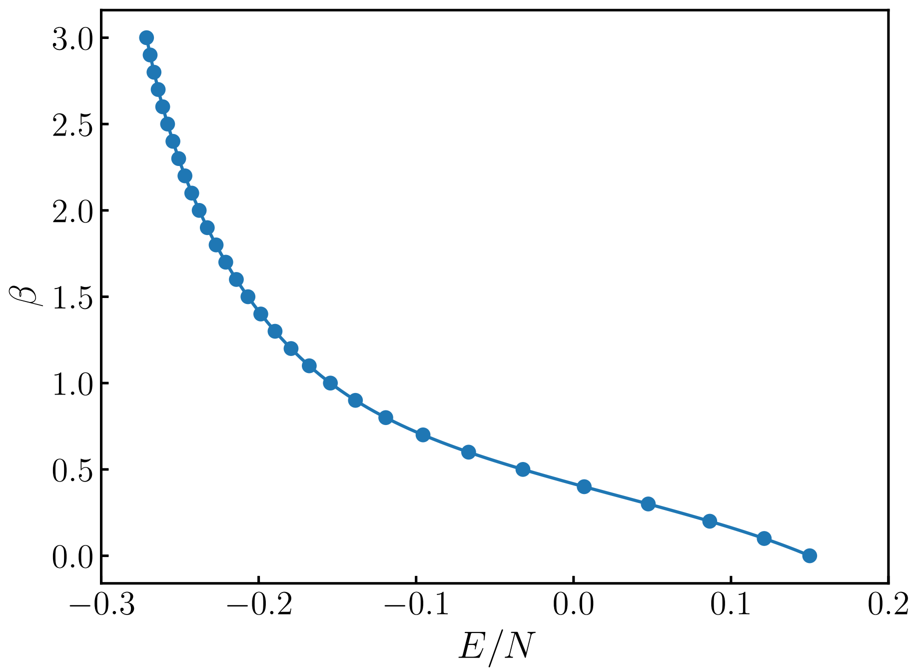
Solve the Schrödinger equation by the fourth order Runge-Kutta method

We can evaluate

$$\langle \bar{h}(t, n)\rangle \leftrightarrow T(t, n - 1/2)$$

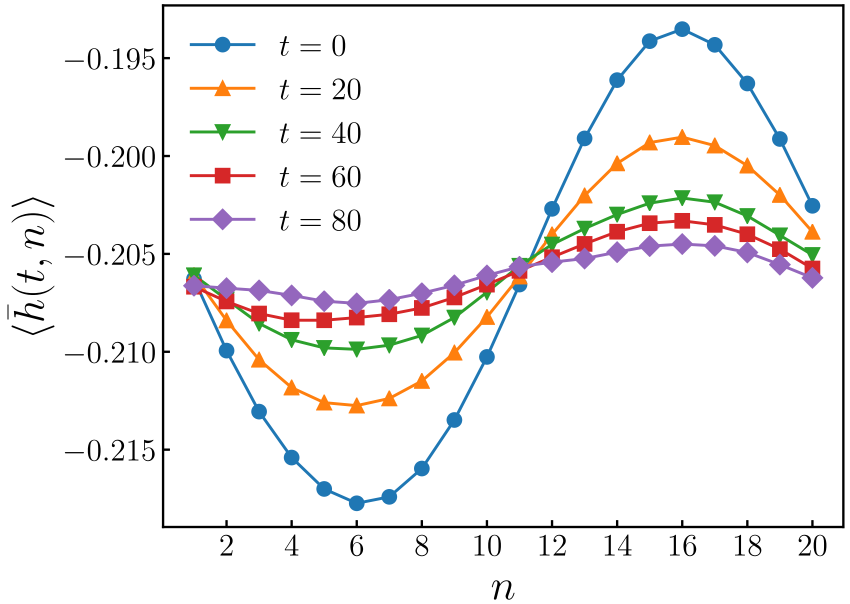
$$\langle \bar{J}_E(t, n - 1/2)\rangle \overset{?}{\simeq} -\kappa\nabla_x T(t, n - 1/2)$$

to investigate the validity of hydro

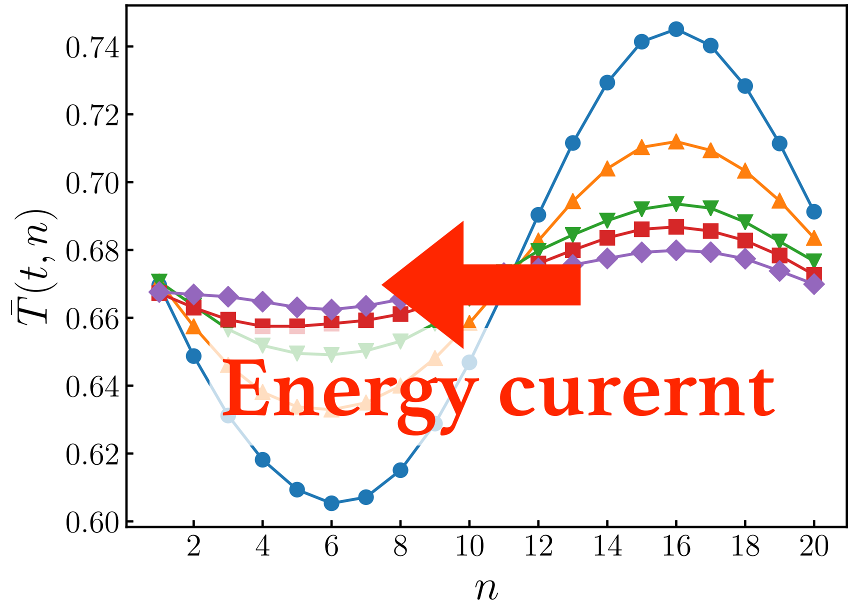


Time evolution

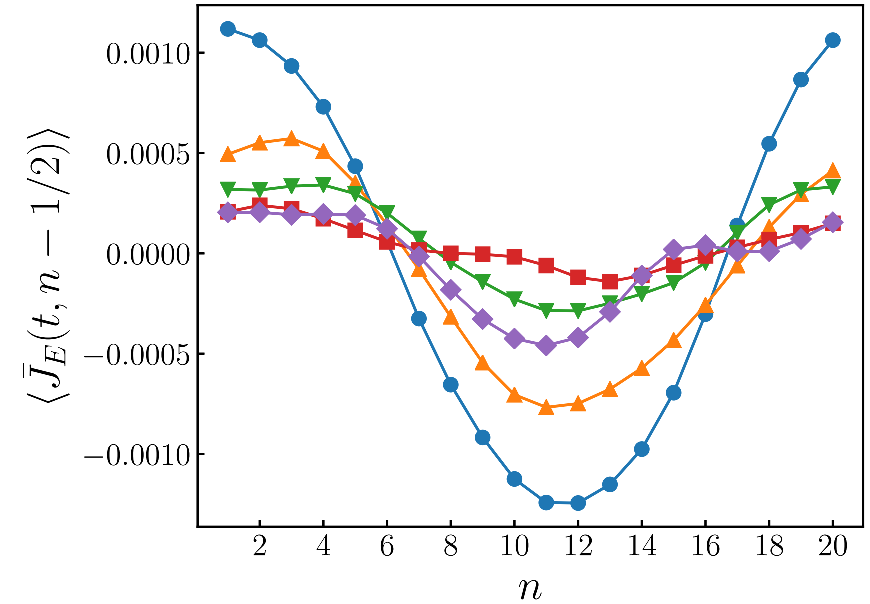
Energy density



Local temperature



Energy current

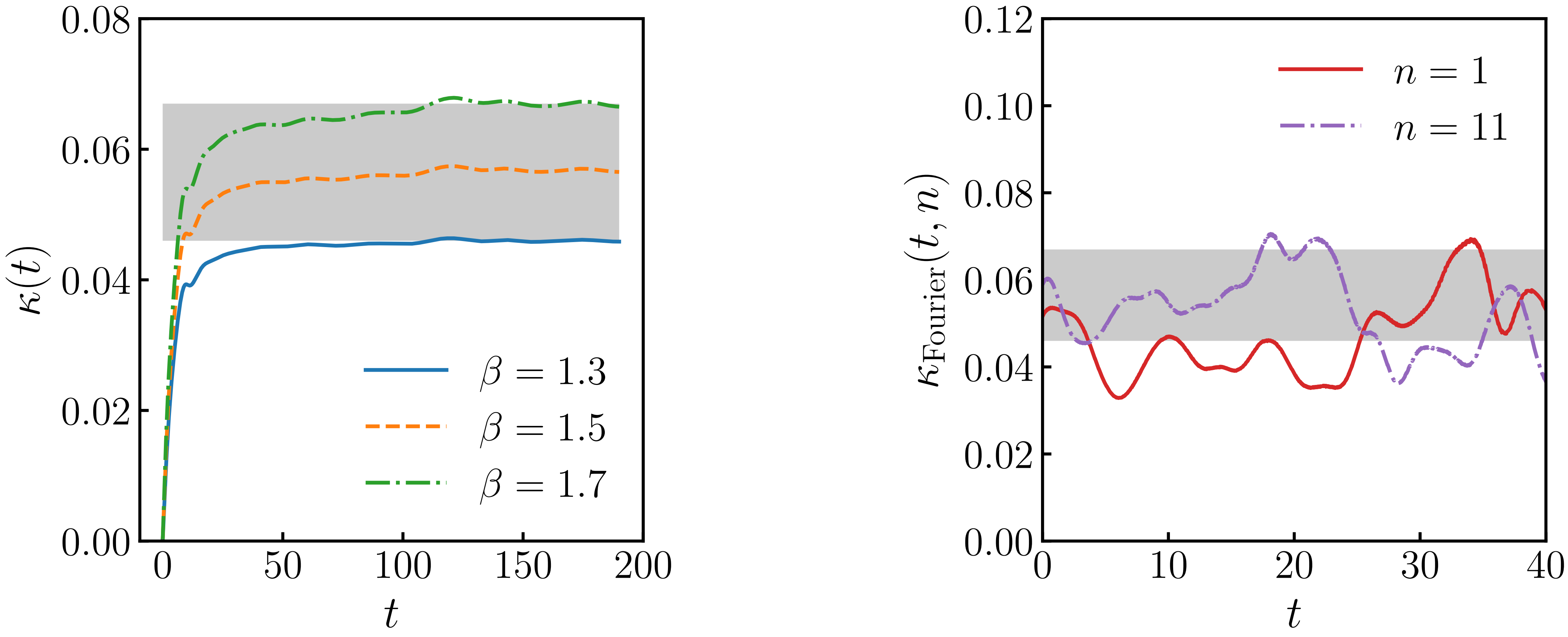


- **Relaxation of the inhomogeneous energy distribution occur**
- **Energy current is induced by the temperature gradient**

$$\langle \bar{J}_E(t, n-1/2) \rangle \simeq -\kappa \nabla_x T(t, n-1/2)$$

⇒ We can extract the value of a thermal conductivity κ !

Thermal conductivity



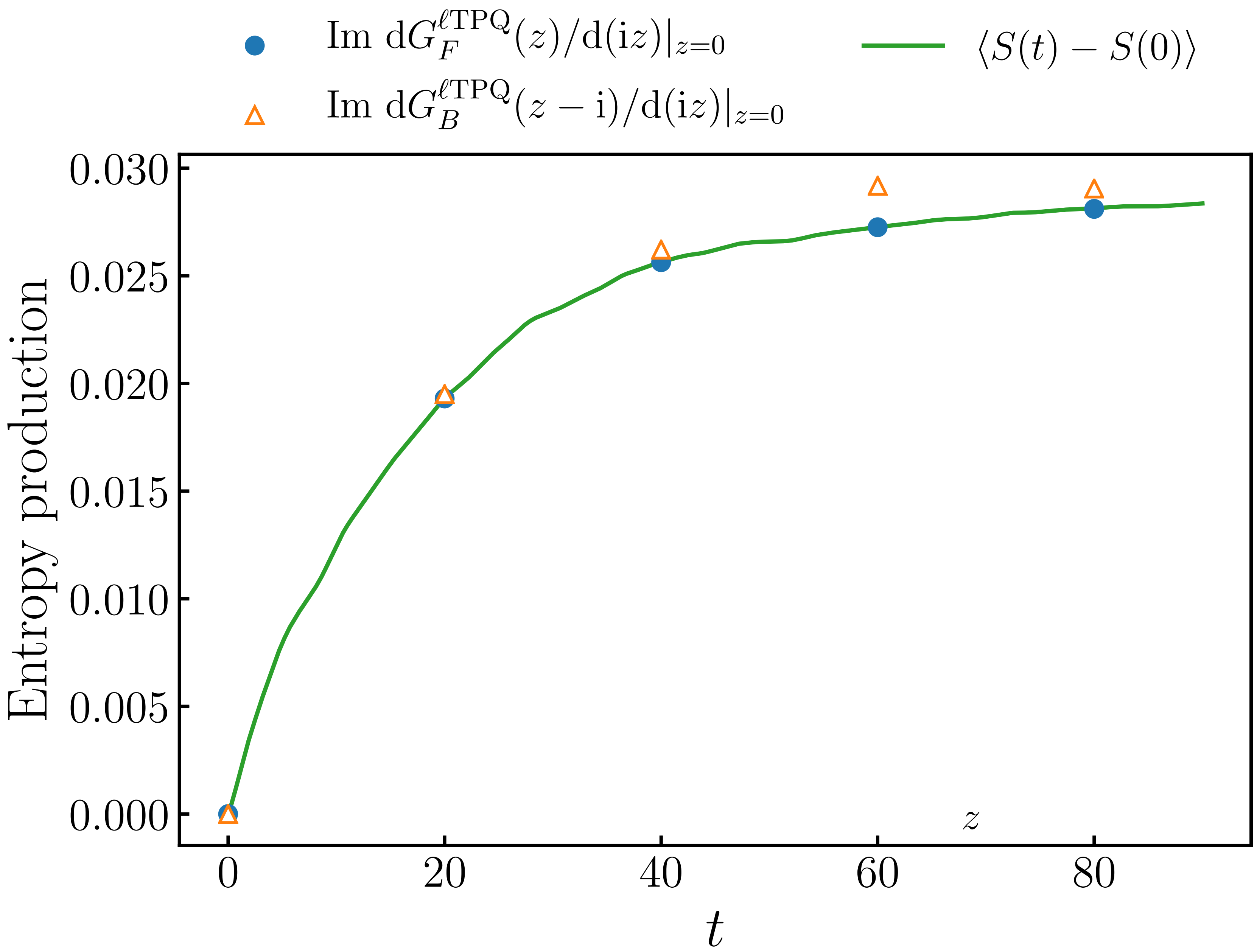
◆ **Two ways to estimate the thermal conductivity κ**

(i) $\langle \bar{J}_E(t, n - 1/2) \rangle \simeq -\kappa \nabla_x T(t, n - 1/2)$

(ii) Green-Kubo formula: $\kappa(t, n) = \frac{\beta(t,n)^2}{4N} \lim_{\tau \to \infty} \int_{-\tau}^{\tau} \mathrm{d}t \langle \{ \delta \hat{\mathrm{J}}_E(t), \delta \hat{\mathrm{J}}_E(t_0) \} \rangle^{\mathrm{TPQ}}_{\beta(t,n)}$

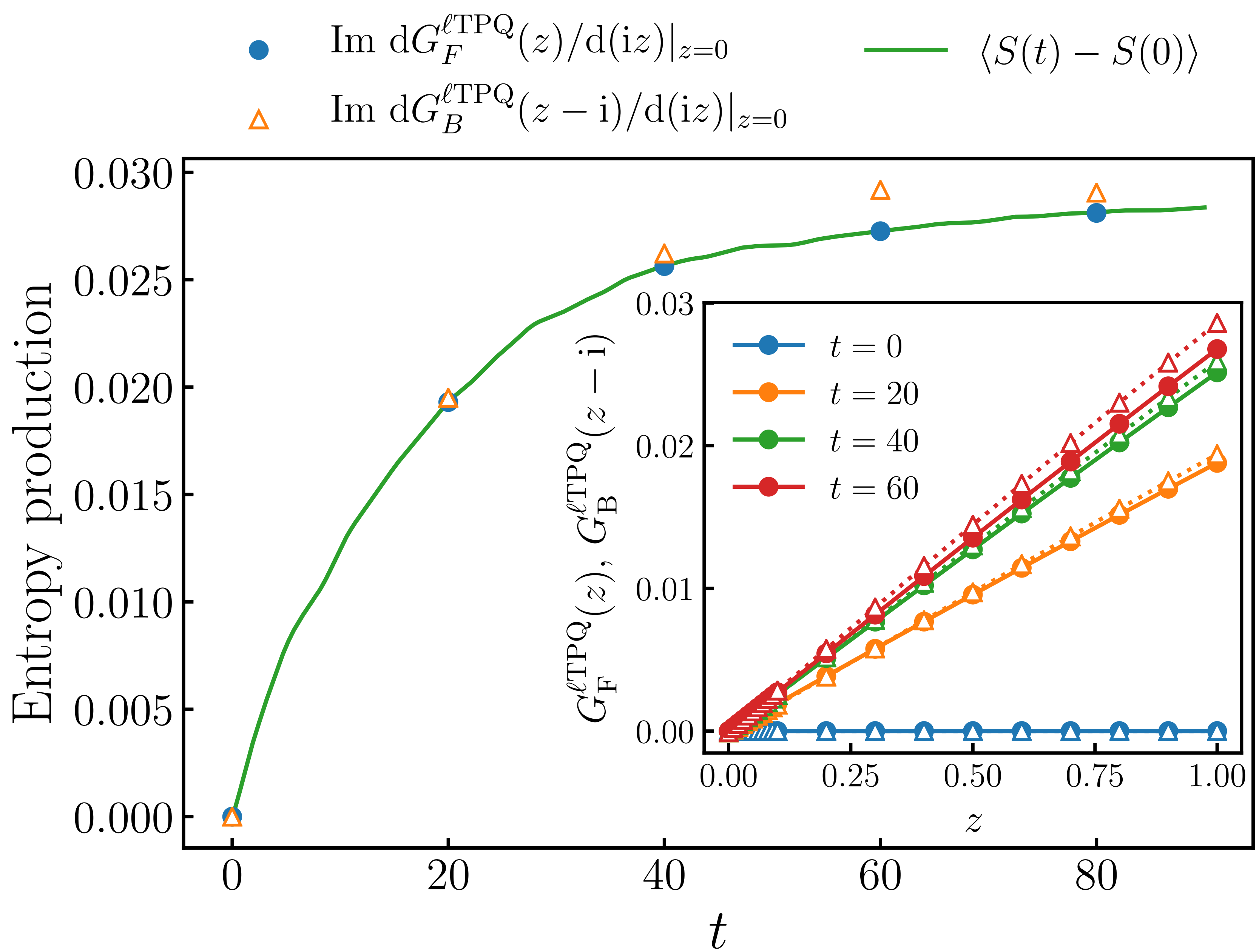
⇒Two results shows a good agreement! Hydro works!!

2nd law & Fluctuation Thm.



- **Entropy production: Direct evaluation vs generating function**

2nd law & Fluctuation Thm.



- **Entropy production: Direct evaluation vs generating function**
- **Fluctuation theorem:** $\left|G_F^{\ell\mathrm{TPQ}}(z) - G_B^{\ell\mathrm{TPQ}}(-z+\mathrm{i})\right| = O(\mathrm{e}^{-A_2 V_{\mathrm{cell}}})$

Summary & Outlook

Summary

◆ Main result

[Tsutsui-MH-Sato-Sagawa, arXiv:2106.12777 [cond-mat.stat-mech]]

(1) We construct a special pure (ℓTPQ) state reproducing hydrodynamics

(1-1) Equivalence between the LG and ℓTPQ state formulations

(1-2) The 2nd law of thermodynamics & Quantum fluctuation theorem

(2) We perform the ℓTPQ simulation for the nonintegrable spin chain

(2-1) Observe the hydrodynamic relaxation of the energy density

(2-2) Numerical confirmation of the 2nd law and fluctuation theorem

Outlook

Simulation in more general setups

Fermion systems, Systems with multiple conserved charge, …

Limitation of hydrodynamics

Coarse-graining size dependence, long-range interactions, integrable systems & generalized hydrodynamics, …

Eigenstate thermalization hypothesis (ETH)

Can we generalize the ETH to the local equilibrium to give a solid basis of hydrodynamics?