Nonintegrability and the Fourier heat conduction law

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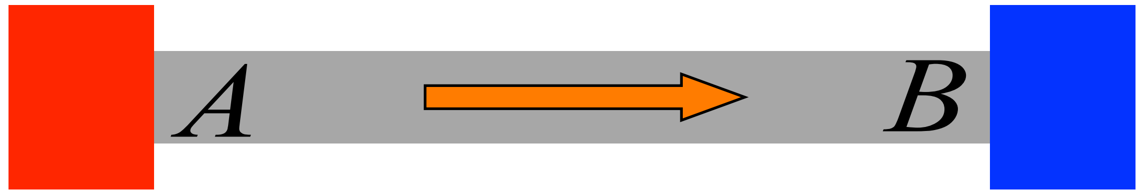
OUTLINE

Fourier-like behavior in 1D momentum-conserving systems (gases or lattices) close to an integrable limit

Application: fast growth (linear with the system size) of the thermoelectric figure of merit ZT (Fourier-like regime more favorable than the hydrodynamic regime)

Fourier Heat Conduction Law (1808)

"Théorie de la Propagation de la Chaleur dans les Solides"



T_H T_L

$$\boxed{\boldsymbol{J} = -\kappa \nabla T}$$

$\boldsymbol{J}$: heat flux

∇T: temperature gradient

κ : thermal conductivity

An old problem, and a long history

1808 - J.J. Fourier: study of the earth thermal gradient

19 century: Clausius, Maxwell, Boltzmann,
kinetic theory of gas, Boltzmann transport equation

1914 - P. Debye: $\kappa \sim Cvl$, conjectured the role of nonlinearity to ensure finite transport coefficients

1936 - R. Peierls: reconsidered Debye's conjecture

1953 - E. Fermi, J. Pasta and S.Ulam: **(FPU) numerical experiment** to verify Debye's conjecture

"It seems there is no problem in modern physics for which there are on record as many false starts, and as many theories which overlook some essential feature, as in the problem of the thermal conductivity of (electrically) nonconducting crystals."

R. E. Peierls (1961),
Theoretical Physics in the Twentieth Century.

QUESTION:

Can one derive the Fourier law of heat conduction from dynamical equations of motion without any statistical assumption?

REMARK:

(Normal) heat flow obeys a simple diffusion equation which can be regarded as a continuous limit of a discrete random walk

Randomness should be an essential ingredient of thermal conductivity

deterministically random systems are tacitly required by the transport theory

Ding-a-ling model

chaos for $\omega^2/E \gg 1$

Free electron gases at the reservoirs with Maxwellian distribution of velocities

$$f(v) = \frac{m\,|v|}{T}\exp\left(-\frac{mv^2}{2T}\right)$$

Heat flux $\quad J = \lim_{t\to\infty}\frac{1}{t}\sum_i \Delta E_i$

Internal temperature $\;T_i = \langle v_i^2 \rangle \qquad (m = k_B = 1)$

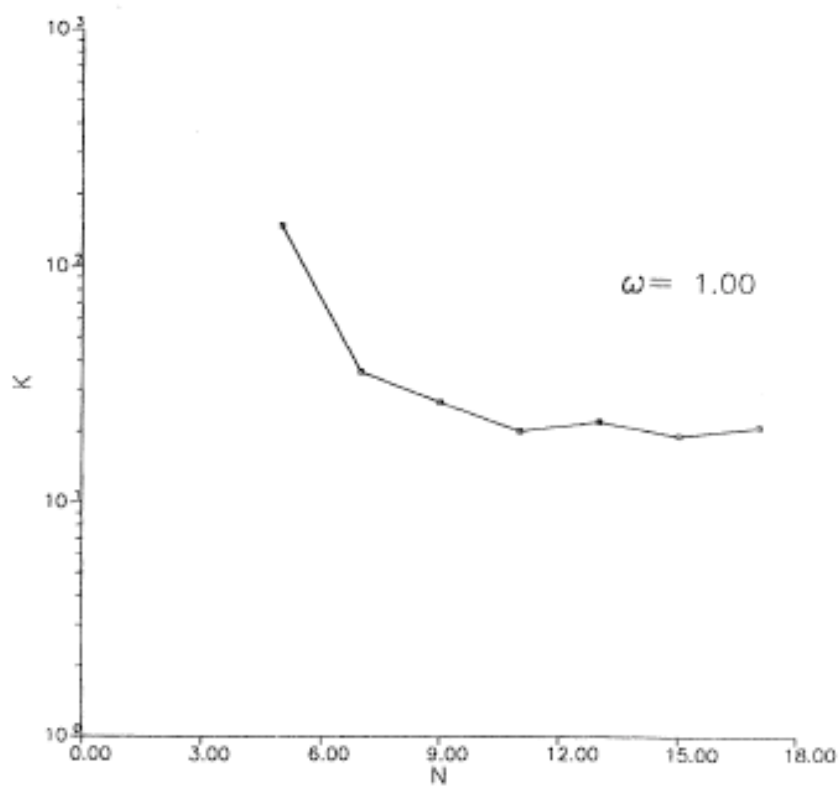


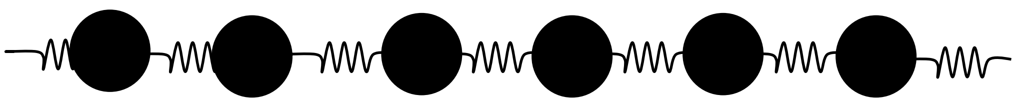
FIG. 3. Behavior of the coefficient of thermal conductivity as a function of the particle number N.

(G. Casati, J. Ford, F. Vivaldi, W.M. Visscher, PRL **52**, 1861 (1984))

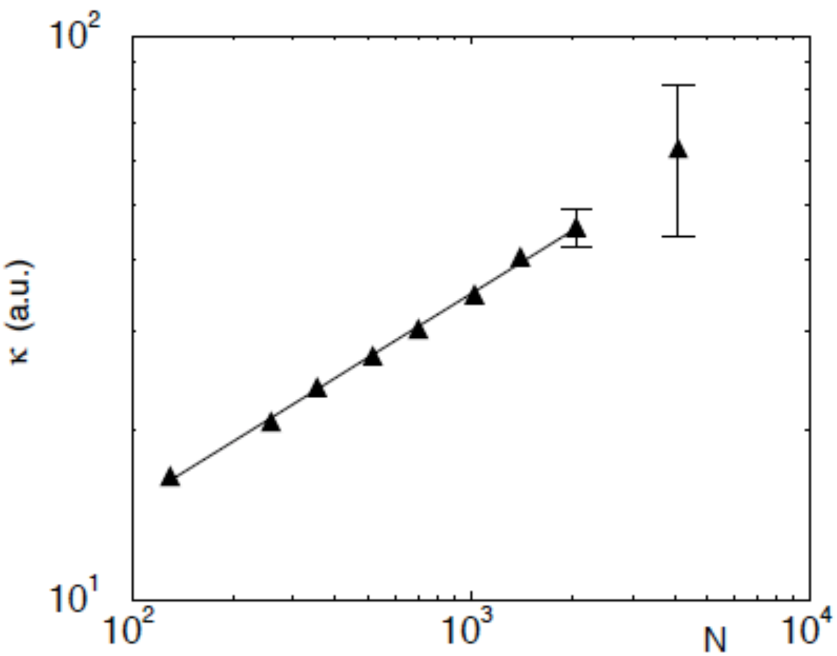
Momentum-conserving systems

Slow decay of correlation functions, diverging transport coefficients
(Alder and Wainwright, PRA **1**, 18 (1970))

FPU revisited: chaos is not sufficient to obtain Fourier law
(Lepri, Livi, Politi, EPL **43**, 271 (1998))



$$V(y) = \frac{1}{2}m\omega_0^2 y^2 + \frac{1}{4}gy^4$$



For momentum-conserving systems

3D $\kappa \sim L^0$ (**normal** heat conduction)

2D $\kappa \sim \ln(L)$ (**anomalous** heat conduction)

1D $\kappa \sim L^\alpha$ (**anomalous** heat conduction)

For **1D** momentum conserving systems

$$\kappa \sim L^{\alpha} \qquad \alpha > 0$$ (**anomalous** heat conduction)

Debate on the Universality of the exponent

Renormalization group analysis $\alpha = \frac{1}{3}$

PRL 89, 200601 (2002)

Kinetic theory $\alpha = \frac{2}{5}$

PRE 68, 056124 (2003), Commun. Pure Appl.Math. 61,1753 (2008)

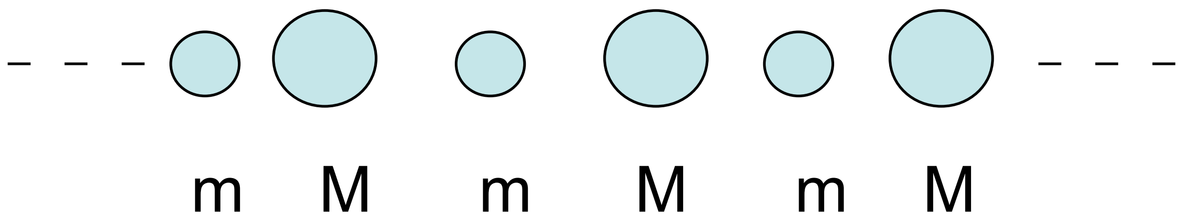
Mode coupling theory

$\alpha = \frac{1}{3}$ (for asymmetric potential)

$\alpha = \frac{1}{2}$ (for symmetric potential)

Recent numerical results: normal heat conduction observed in 1D momentum conserving lattice models with asymmetric interparticle interactions (Zhong et al., PRE **85**, 060102(R) (2012))

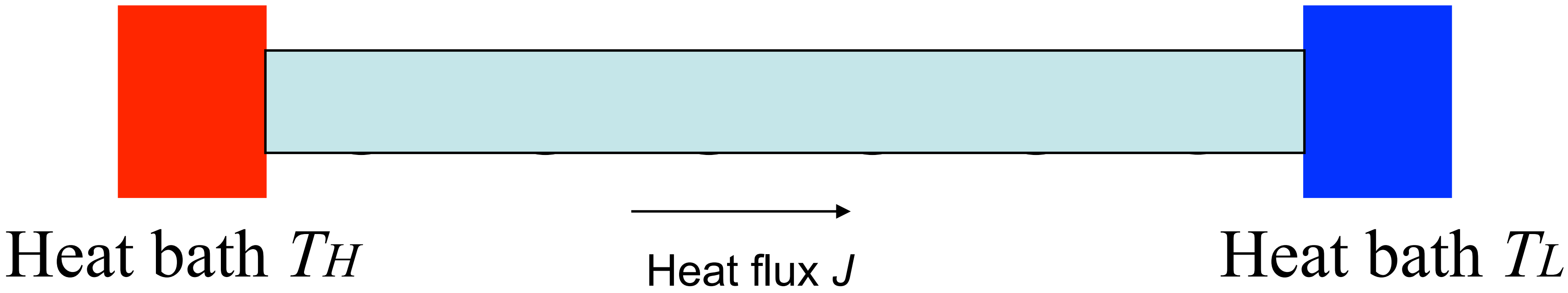
1D diatomic hard-point gas model

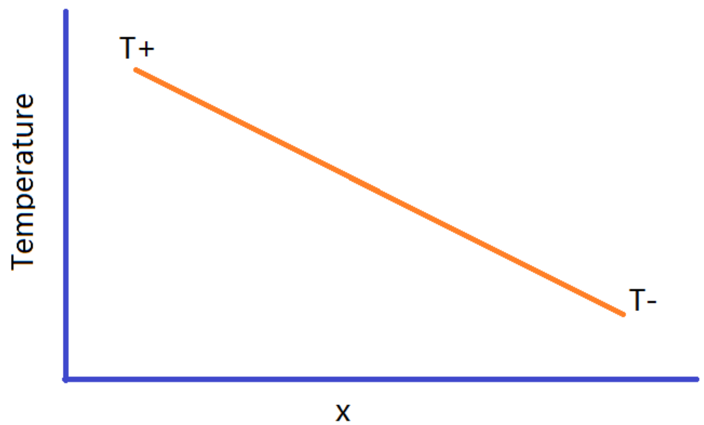


If M=m, the system is integrable

If M≠m, the system is non-integrable

Methods: nonequilibrium simulations





(Maxwellian heat baths)

$$J = -\kappa \nabla T \rightarrow \kappa \approx -\frac{JL}{\Delta T}$$

S. Lepri, et al, Phys. Rep. 377, 1 (2003); A. Dhar, Adv. Phys. 57, 457 (2008)

Methods: equilibrium simulations

Green-Kubo formula:

$$\kappa_{GK} = \lim_{\tau\to\infty}\lim_{N\to\infty}\frac{1}{T^2 N}\int_0^{\tau} < J(t)J(0) > dt \ ,$$

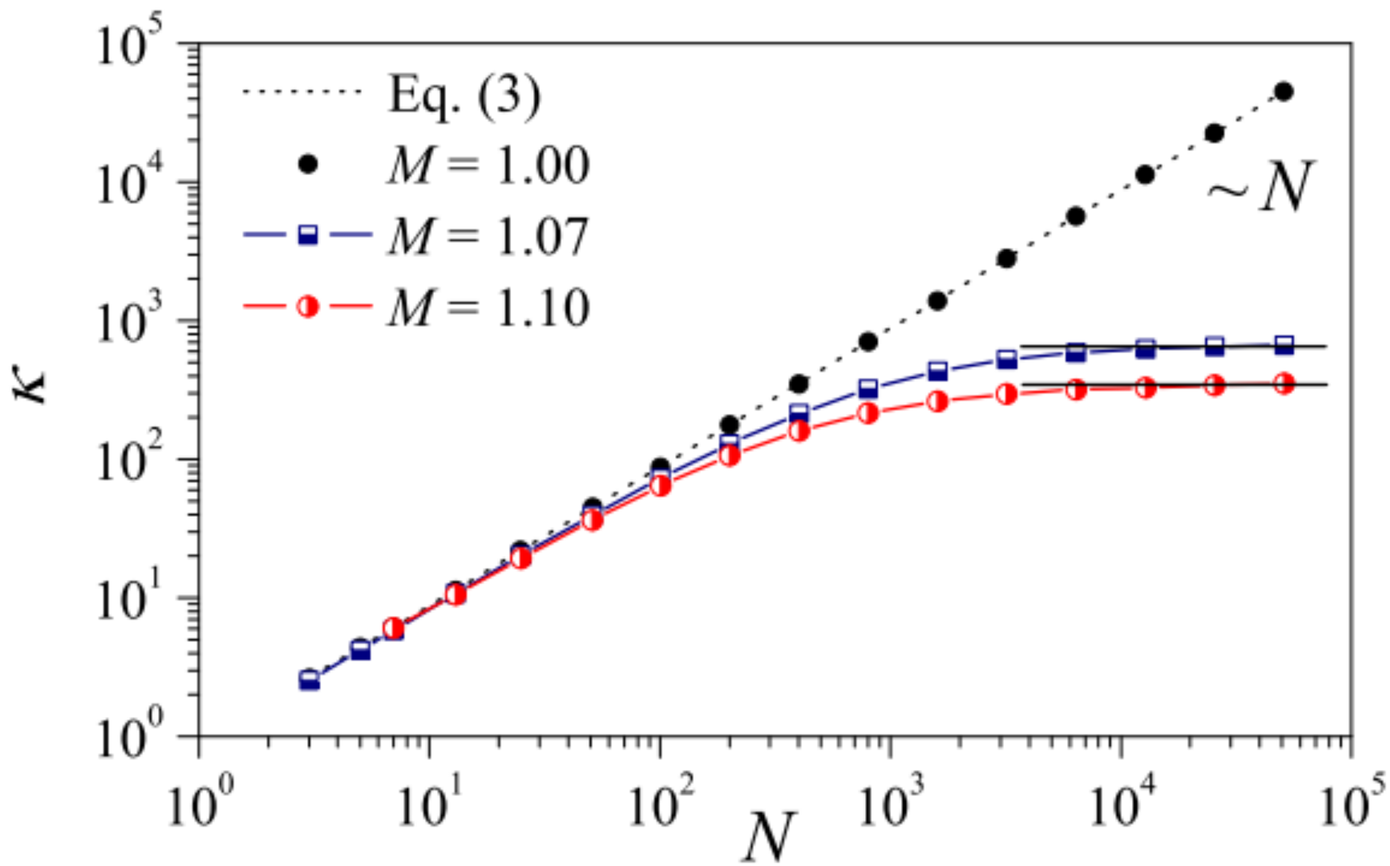
$$J(t) = \sum_{i=1}^{N} J_i(t)$$

$$< J(t)J(0) > /N \sim t^{-\gamma} \quad \begin{cases} 0 \le \gamma \le 1 & \text{anomalous heat conduction} \\ \gamma > 1 & \text{normal heat conduction} \end{cases}$$

S. Lepri, et al, Phys. Rep. 377, 1 (2003); A. Dhar, Adv. Phys. 57, 457 (2008)

Fourier law close to the integrable limit?

Results of nonequilibrium simulations for the hard-point gas model:



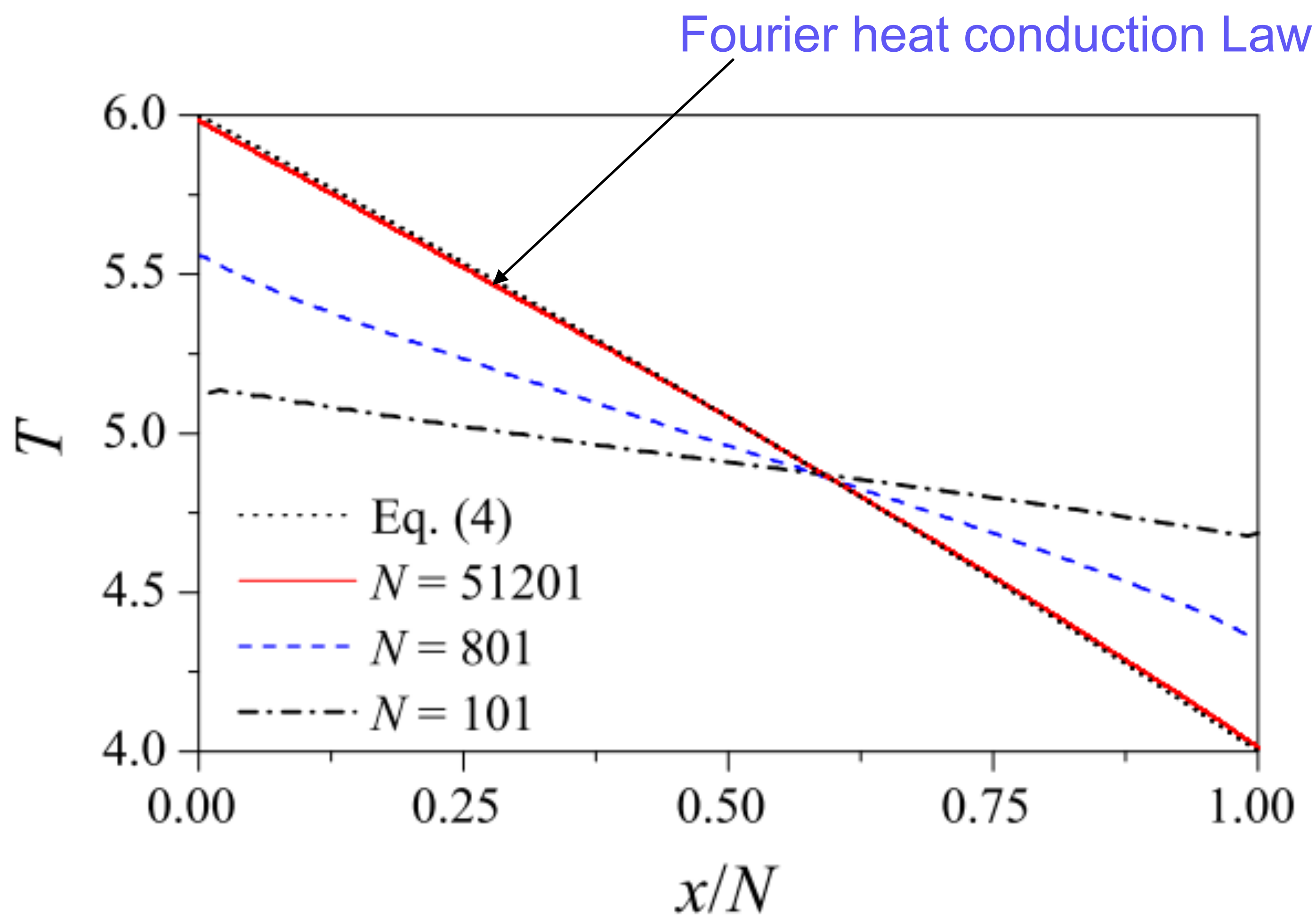
(m=1)

(Average particle density such that L=N)

$$\kappa_{\text{int}} = N\sqrt{\frac{2k_B^3}{m\pi}} \Bigg/ \left(\frac{1}{\sqrt{T_L}} + \frac{1}{\sqrt{T_R}}\right). \qquad (3)$$

(S. Chen, J. Wang , G. Casati, G.B., PRE **90**, 032134 (2014))

Temperature profiles

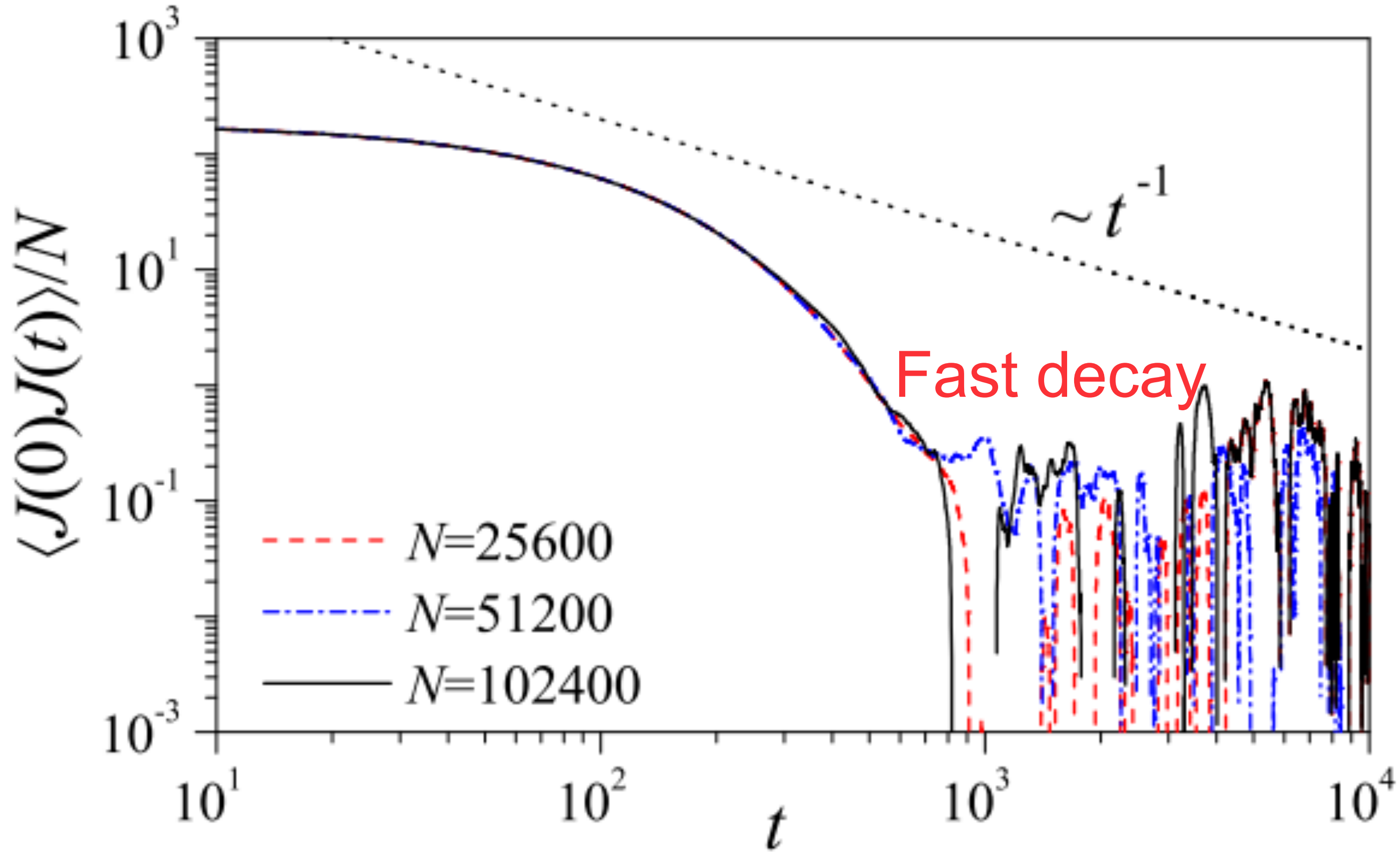


$$T(x) = \left[T_L^{3/2} \left(1 - \frac{x}{N} \right) + T_R^{3/2} \frac{x}{N} \right]^{2/3}. \qquad (4)$$

(S. Chen, J. Wang , G. Casati, G.B., PRE **90**, 032134 (2014))

Heat current correlation function

Results of equilibrium simulations for the diatomic hard-point gas model:



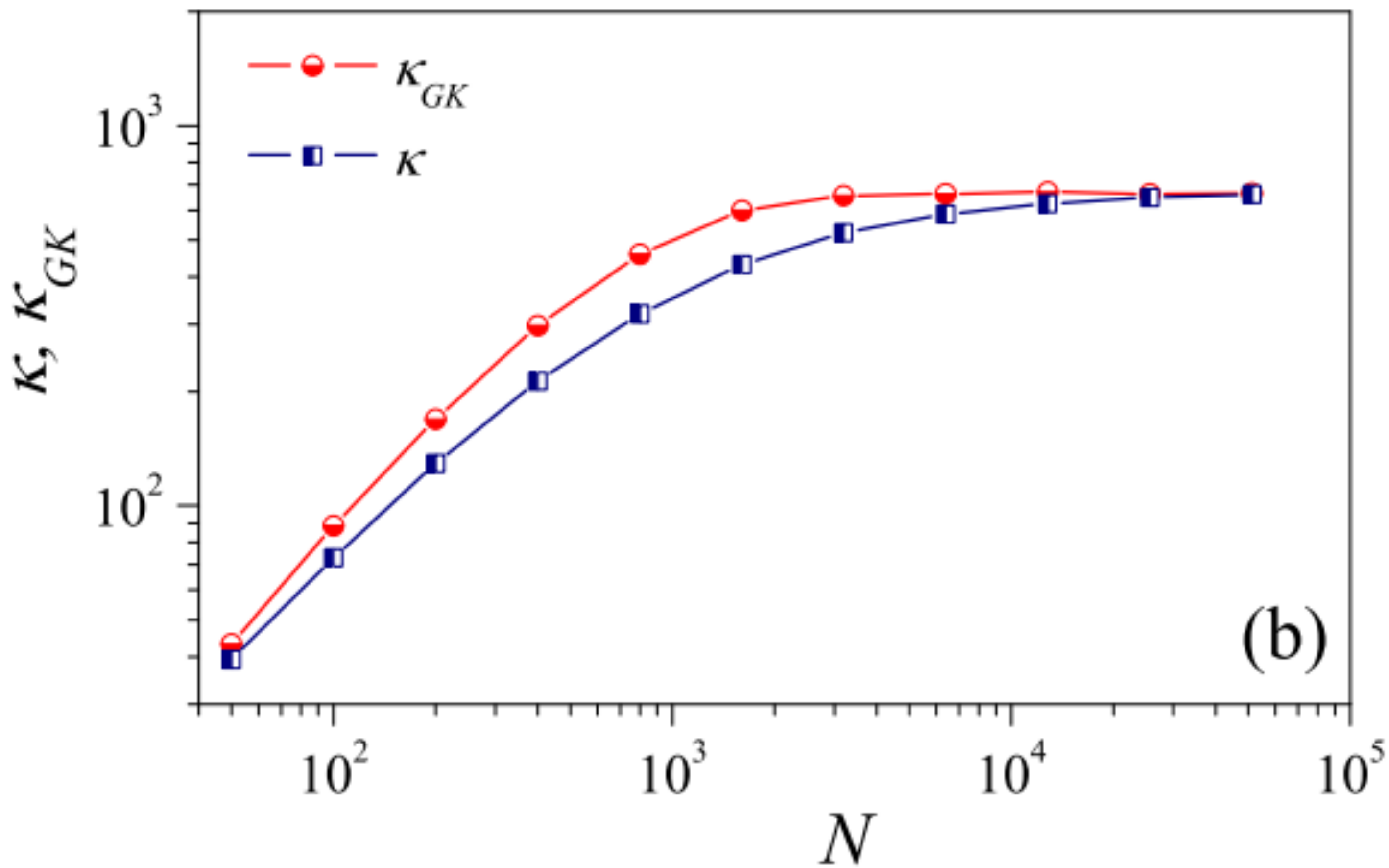
M=1.07

(m=1)

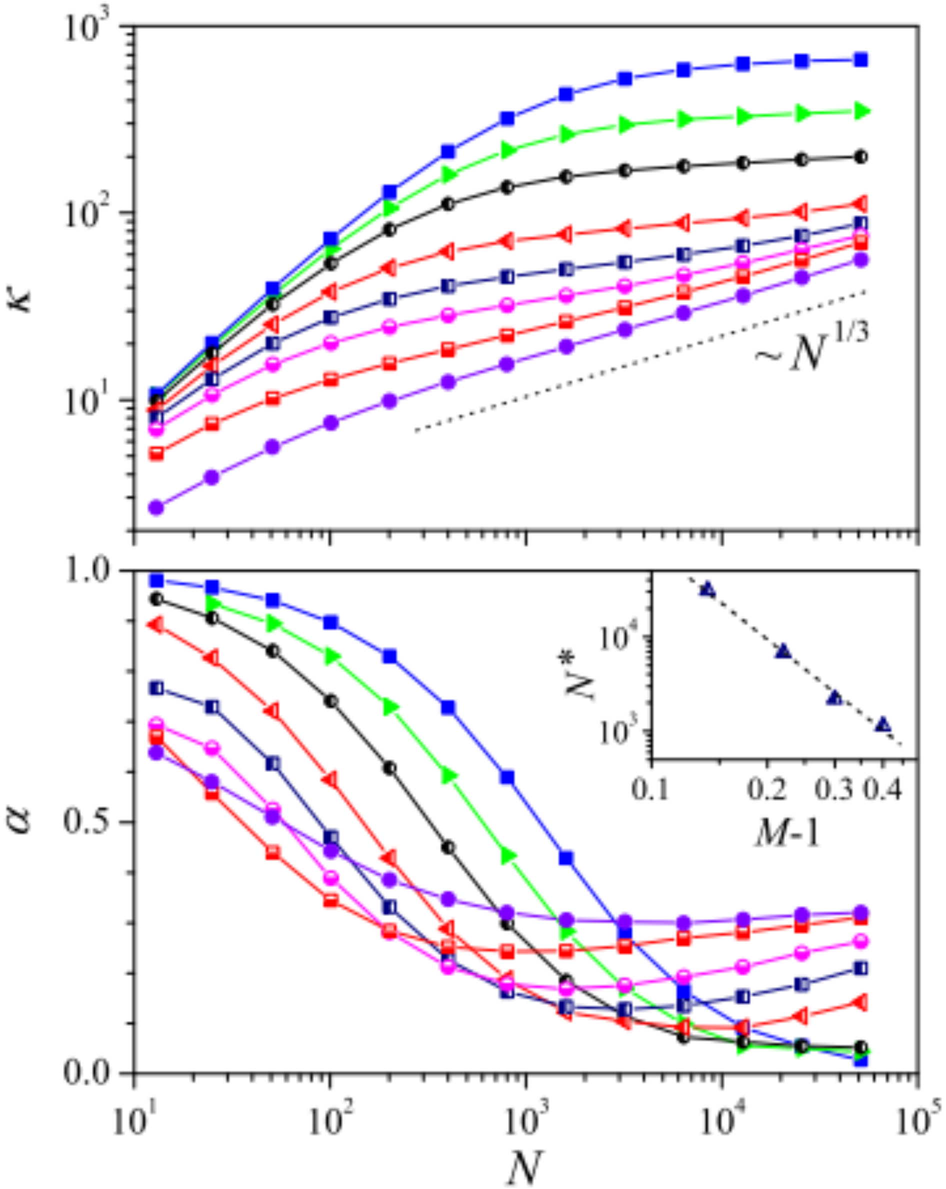
$$\kappa_{GK}(N) = \frac{1}{k_B T^2 N} \int_0^{\tau_{tr}} dt \langle J(0)J(t)\rangle \qquad \tau_{tr} = N/(2v_s)$$

(S. Chen, J. Wang , G. Casati, G.B., PRE **90**, 032134 (2014))

Confirmation of Fourier law close to the integrable limit?



Is the Fourier-like regime asymptotic?

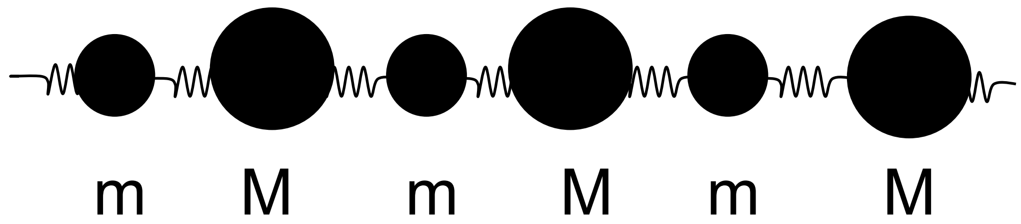


M is, respectively,
1.07, 1.10, 1.14, 1.22, 1.30, 1.40,
the golden mean (≈1.618), and 3
(from top to bottom); (m=1)

The corresponding tangent α
of the κ-N curve is given
with the same symbols

$$N^* = 54/(M-1)^{3.2}$$

1D diatomic Toda lattice



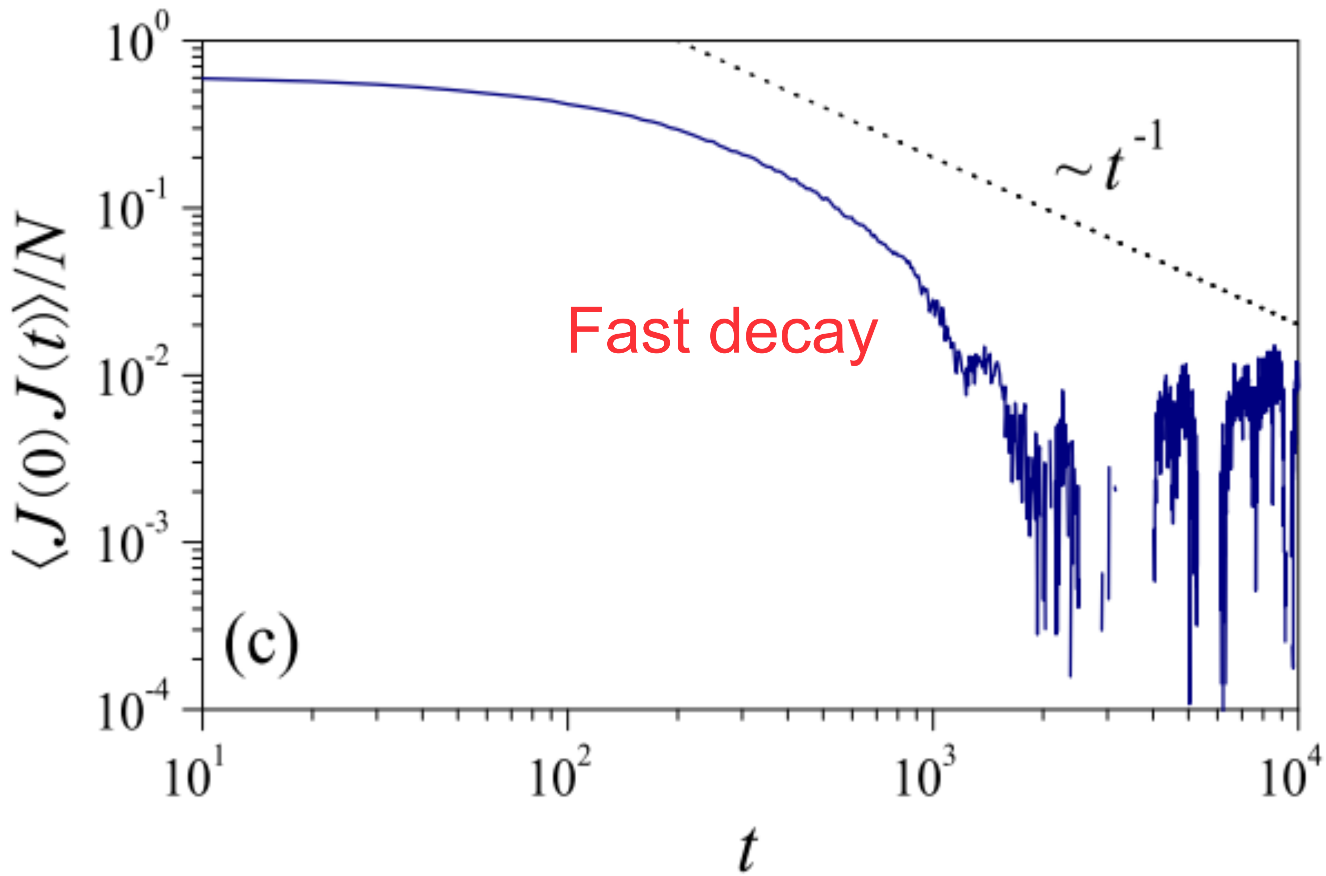
$$H = \sum_i \frac{p_i^2}{2m} + V(x_i - x_{i-1} - 1) \qquad \text{with } V(x) = \exp(-x) + x$$

If M=m, the system is integrable

If M≠m, the system is non-integrable

Heat current correlation function

Results of equilibrium simulations for the diatomic Toda lattice:

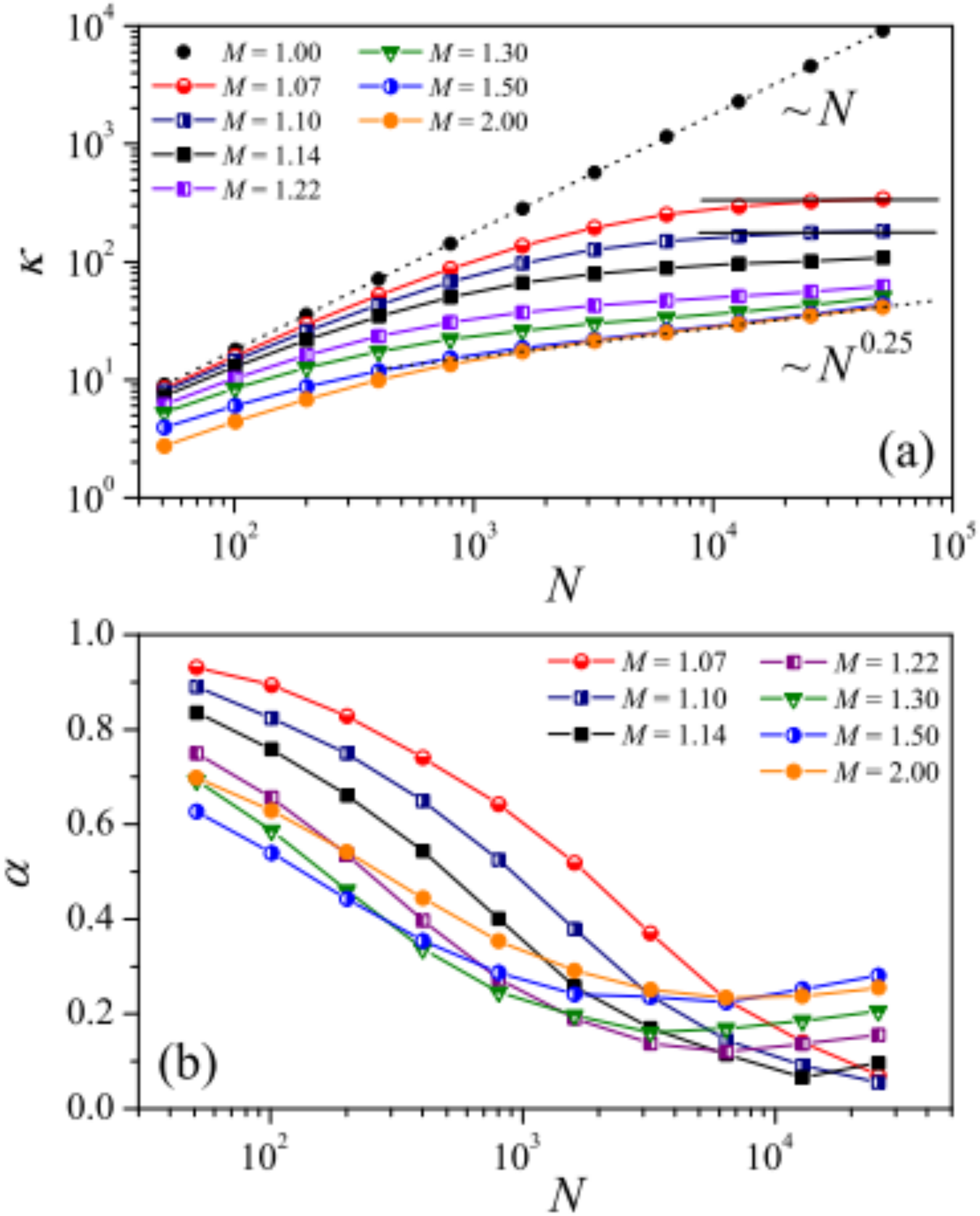


M=1.07

(m=1)

(S. Chen, J. Wang , G. Casati, G.B., PRE **90**, 032134 (2014))

Fourier-like intermediate regime



Results of nonequilibrium simulations for the Toda lattice (Langevin heat baths)

Summary (Part I)

Fourier-like behavior of thermal conductivity for 1D momentum-conserving lattice or gas models close to the integrable limit

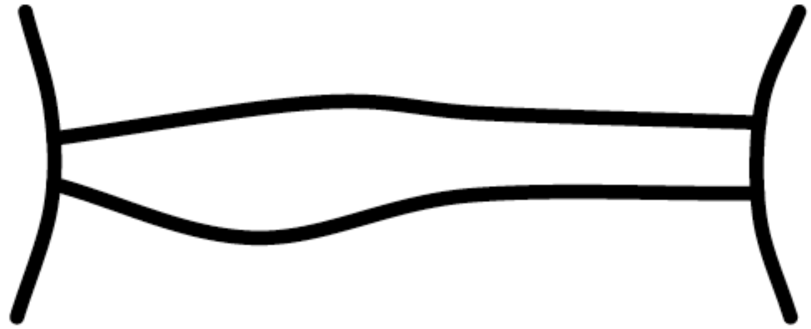
Notwithstanding the agreement between equilibrium and nonequilibrium simulations, the observed Fourier-like behavior might be a finite-size effect

No numerical evidence of a phase transition between anomalous and diffusive behavior when approaching the integrable limit

Coupled 1D particle and heat transport

Stochastic baths: ideal gases at fixed temperature and electrochemical potential

T_L μ_L



T_R μ_R

(we assume $T_L > T_R, \ \mu_L < \mu_R$)

$$\begin{pmatrix} j_\rho \\ j_u \end{pmatrix} = \begin{pmatrix} L_{\rho\rho} & L_{\rho u} \\ L_{u\rho} & L_{uu} \end{pmatrix} \begin{pmatrix} -\nabla(\beta\mu) \\ \nabla\beta \end{pmatrix} \qquad \beta = 1/T$$

Onsager relation:

$$L_{u\rho} = L_{\rho u}$$

Positivity of entropy production:

$$\det \mathbb{L} \geq 0, \ L_{\rho\rho} \geq 0, L_{uu} \geq 0$$

Onsager and transport coefficients

$$\sigma = \frac{e^2}{T} L_{\rho\rho}, \qquad \kappa = \frac{1}{T^2} \frac{\det \mathbb{L}}{L_{\rho\rho}}, \qquad S = \frac{1}{eT} \left(\frac{L_{\rho u}}{L_{\rho\rho}} - \mu \right)$$

$$ZT = \frac{(L_{u\rho} - \mu L_{\rho\rho})^2}{\det \mathbb{L}}$$

Note that the positivity of entropy production implies that the (isothermal) electric conductivity >0 and the thermal conductivity >0

Interacting systems, Green-Kubo formula

The Green-Kubo formula expresses linear response transport coefficients in terms of dynamic correlation functions of the corresponding current operators, calculated at thermodynamic equilibrium

$$L_{ij} = \lim_{\omega \to 0} \mathrm{Re} L_{ij}(\omega)$$

$$L_{ij}(\omega) = \lim_{\epsilon \to 0} \int_0^\infty dt e^{-i(\omega - i\epsilon)t} \lim_{\Lambda \to \infty} \frac{1}{\Lambda} \int_0^\beta d\tau \langle J_i J_j (t + i\tau) \rangle_T$$

$$\mathrm{Re} L_{ij}(\omega) = 2\pi \mathcal{D}_{ij} \delta(\omega) + L_{ij}^{\mathrm{reg}}(\omega)$$

Non-zero generalized Drude weights signature of ballistic transport

Conservation laws and thermoelectric efficiency

Suzuki's formula (which generalizes Mazur's inequality) for finite-size Drude weights

$$D_{ij}(\Lambda) \equiv \frac{1}{2\Lambda} \lim_{t\to\infty} \frac{1}{t} \int_0^t dt' \langle J_i(t') J_j(0) \rangle_T = \frac{1}{2\Lambda} \sum_{n=1}^{M} \frac{\langle J_i Q_n \rangle_T \langle J_j Q_n \rangle_T}{\langle Q_n^2 \rangle_T}$$

Q_n relevant (i.e., non-orthogonal to charge and thermal currents), mutually orthogonal conserved quantities

$$\mathcal{D}_{ij} = \lim_{t\to\infty} \lim_{\Lambda\to\infty} \frac{1}{2\Lambda t} \int_0^t dt' \langle J_i(t') J_j(0) \rangle_T$$

Assuming commutativity of the two limits,

$$\mathcal{D}_{ij} = \lim_{\Lambda\to\infty} D_{ij}(\Lambda)$$

Momentum-conserving systems

Consider systems with a single relevant constant of motion, notably momentum conservation

Ballistic contribution to det*(L)* vanishes as

$$\mathcal{D}_{\rho\rho}\mathcal{D}_{uu} - \mathcal{D}^2_{\rho u} = 0$$

$$k \propto \frac{\det \mathbf{L}}{L_{\rho\rho}} \propto \Lambda^{\alpha}, \quad \alpha < 1$$

$$\sigma \propto L_{\rho\rho} \propto \Lambda$$

$$ZT = \frac{\sigma S^2}{\kappa} T \propto \Lambda^{1-\alpha} \to \infty \text{ when } \Lambda \to \infty$$

$$S \propto \frac{L_{\rho q}}{L_{\rho\rho}} \propto \Lambda^0$$

(G.B., G. Casati, J. Wang, PRL 110, 070604 (2013))

For systems with more than a single relevant constant of motion, for instance for integrable systems, due to the Schwarz inequality

$$D_{\rho\rho}D_{uu} - D_{\rho u}^2 = \| \boldsymbol{x}_\rho \|^2 \| \boldsymbol{x}_u \|^2 - \langle \boldsymbol{x}_\rho, \boldsymbol{x}_u \rangle^2 \geqslant 0$$

$$\boldsymbol{x}_i = (x_{i1}, \ldots, x_{iM}) = \frac{1}{2\Lambda}\left(\frac{\langle J_i Q_1 \rangle_T}{\sqrt{\langle Q_1^2 \rangle_T}}, \ldots, \frac{\langle J_i Q_M \rangle_T}{\sqrt{\langle Q_M^2 \rangle_T}} \right)$$

$$\langle \boldsymbol{x}_\rho, \boldsymbol{x}_u \rangle = \sum_{k=1}^{M} x_{\rho k} x_{uk}$$

Equality arises only in the exceptional case when the two vectors are parallel; in general

$$\det \mathbf{L} \propto L^2, \ \kappa \propto \Lambda, \ ZT \propto \Lambda^0$$

Example: 1D interacting classical gas

Consider a one dimensional gas of hard-point elastically colliding particles with unequal masses: m, M

For $M = m$

(integrable model)

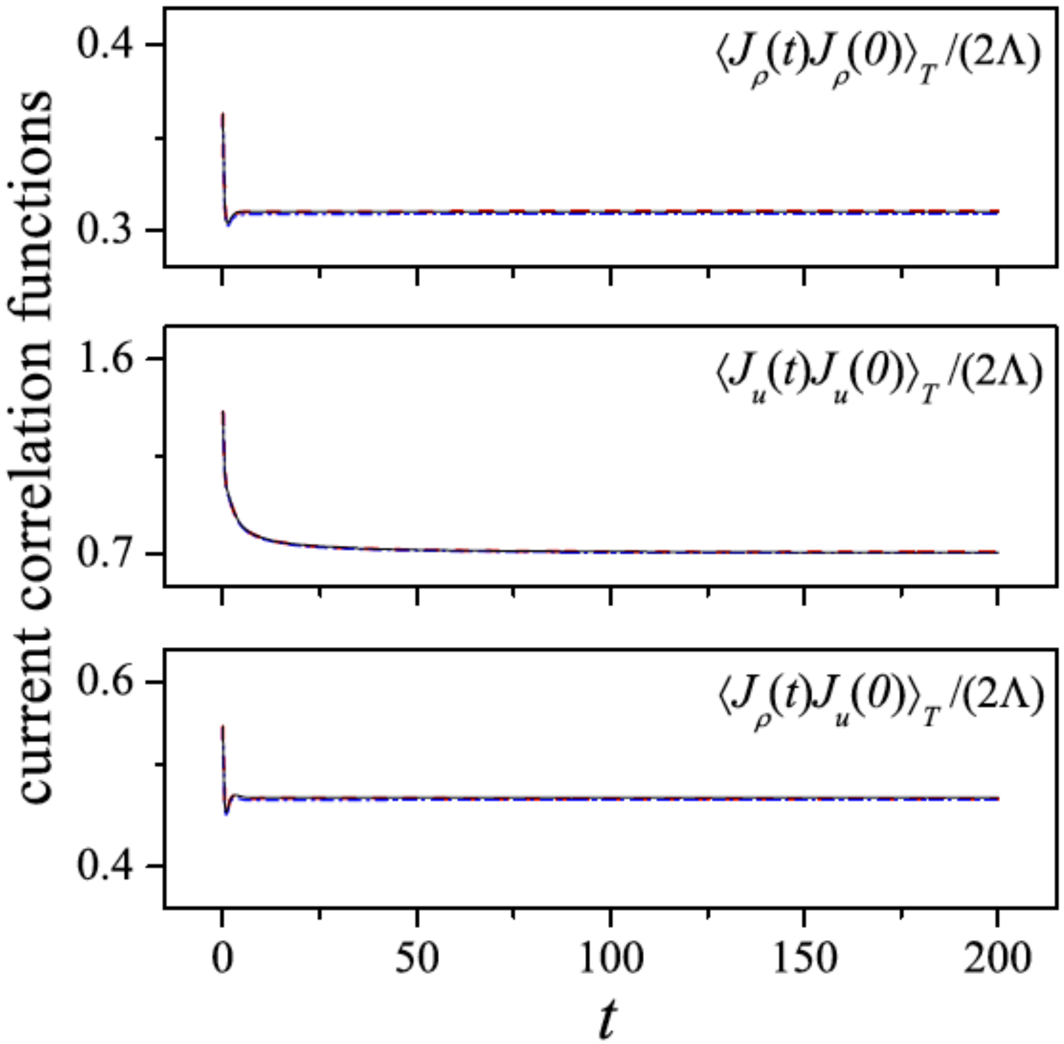
$$J_u = T_L\gamma_L - T_R\gamma_R \qquad (J_u = J_q + \mu J_\rho)$$

$$J_\rho = \gamma_L - \gamma_R. \qquad ZT = 1 \ (\text{at } \mu = 0)$$

$$\gamma_\alpha = \frac{1}{h\beta_\alpha} e^{\beta_\alpha \mu_\alpha}$$ injection rates

For $M \neq m$ ZT depends on the system size

Non-decaying correlation functions



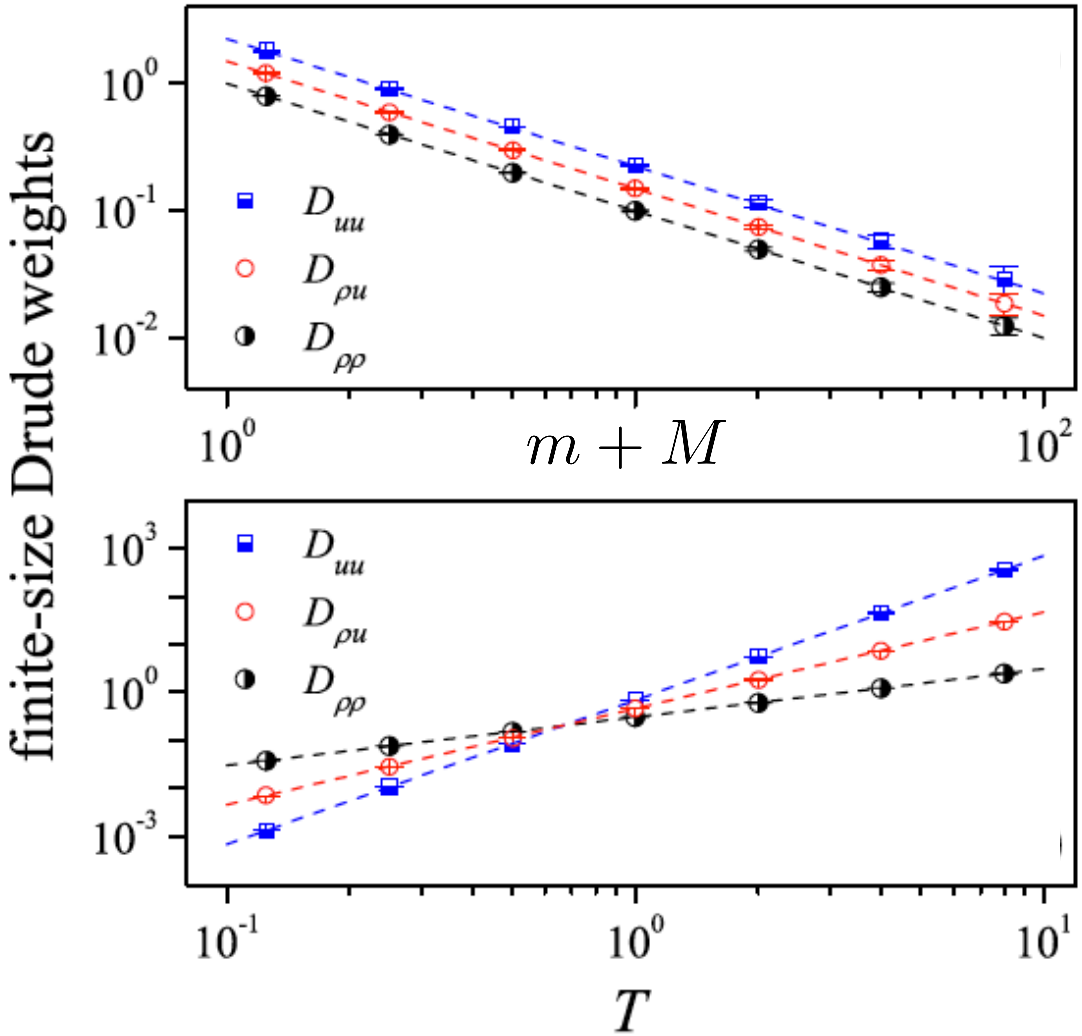
$\Lambda = 256$ (red dashed curve), 512 (blue dash-dotted curve), and 1024 (black solid curve)

Finite-size Drude weights: analytical results vs. numerics

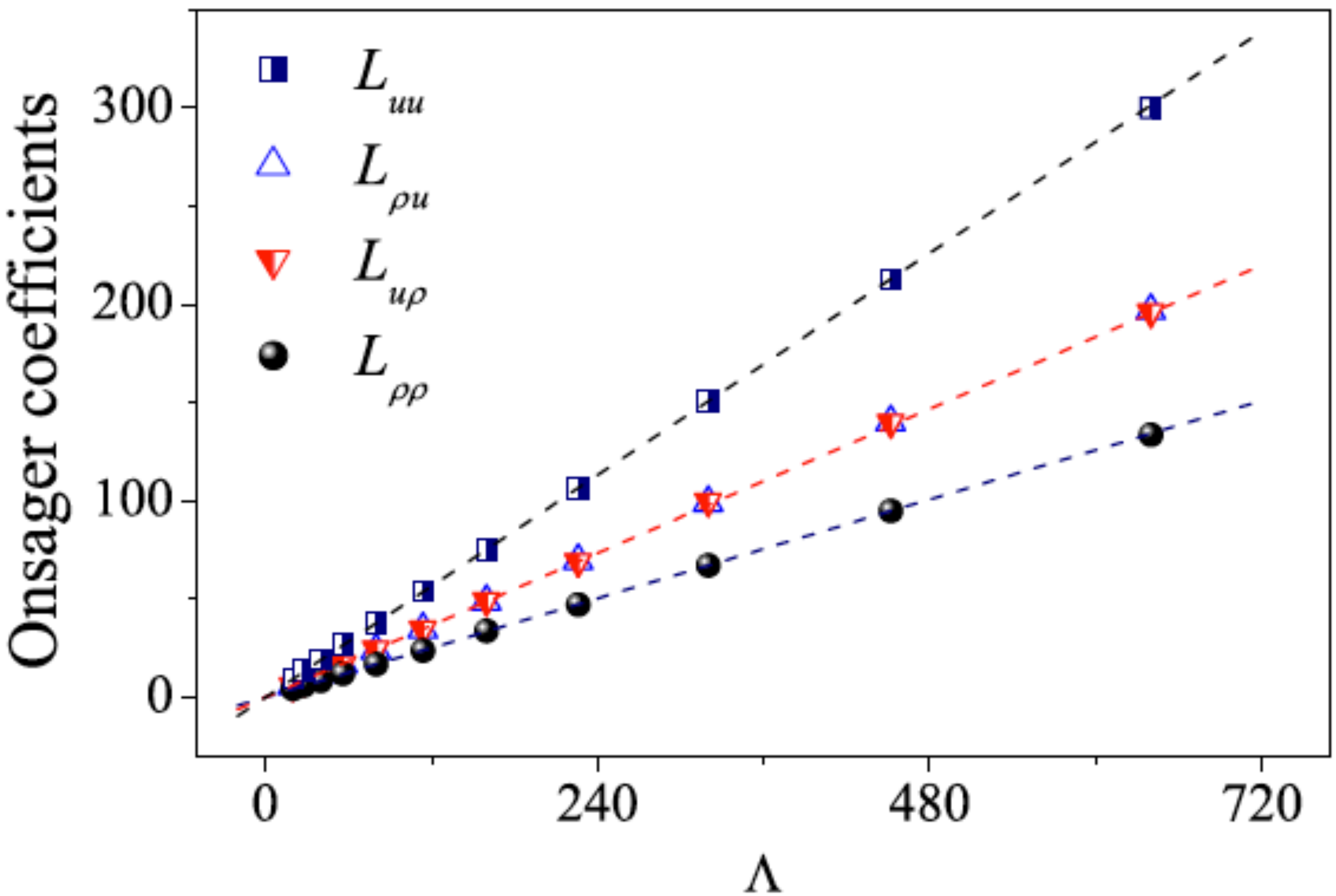
$$D_{\rho\rho}(\Lambda) = \frac{TN^2}{2\Lambda(mN_1 + MN_2)},$$

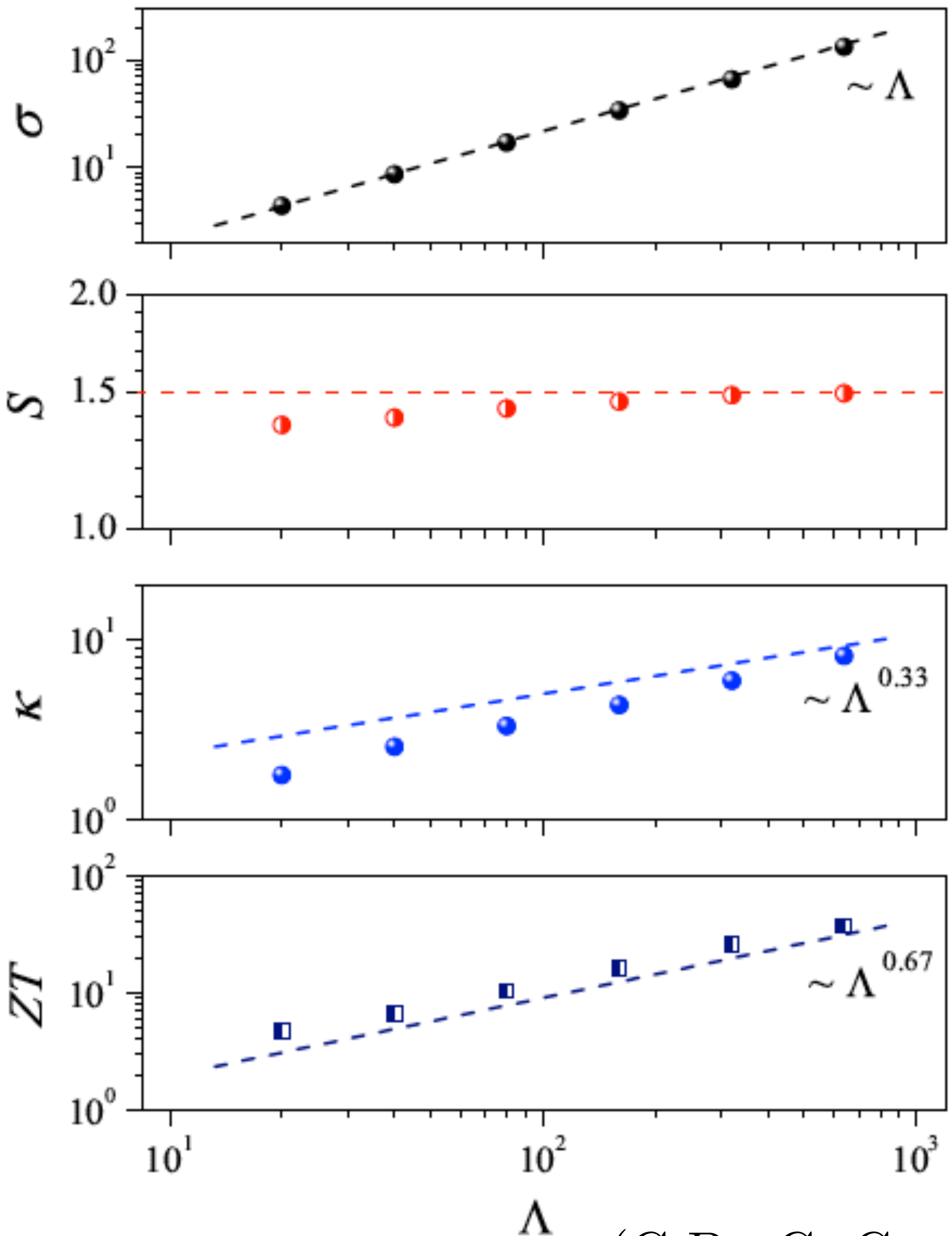
$$D_{uu}(\Lambda) = \frac{9T^3N^2}{8\Lambda(mN_1 + MN_2)},$$

$$D_{\rho u}(\Lambda) = \frac{3T^2N^2}{4\Lambda(mN_1 + MN_2)}.$$



Ballistic behavior of Onsager coefficients





Anomalous thermal transport

$$ZT = \frac{\sigma S^2}{k} T$$

ZT diverges
increasing the systems size

(G.B., G. Casati, J. Wang, PRL 110, 070604 (2013))

1D Coulomb (screened) gas model

$$H = \sum_i \left[\frac{p_i^2}{2m_i} + U(x_i - x_{i-1}) \right], \qquad U(x) = a/x$$

Finite range of interactions: Problem with electrochemical baths: huge unphysical interaction energy when an injected particle (from an indeal-gas reservoir) is too close to a system particle

However, the Seebeck coefficient is measured under open circuit conditions: no need to exchange particles with the reservoir to compute it

Grand-canonical Monte-Carlo method

Sampling the grand-canonical distribution:

$$f_{\mu LT}(\mathbf{x}^N; N) \propto \frac{L^N \exp(\beta\mu N)}{N!\,\lambda^N} \exp[-\beta\mathcal{U}(\mathbf{x}^N)]$$

λ de Broglie thermal wave length $\lambda = h/\sqrt{2\pi m k_B T}$

$\mathcal{U}$ potential energy

N-particle configuration $X^N = (x_1, ..., x_N)$

1. Start from an initial state with random position of particles

2. Random displacement accepted with probability

$$\min\{1, \exp[-\beta(\mathcal{U}_{\text{new}} - \mathcal{U}_{\text{old}})]\}$$

3. Creation of a new particle accepted with probability

$$\min\left\{1, \frac{L}{\lambda(N_{\text{old}}+1)} \exp[-\beta(\mathcal{U}_{\text{new}} - \mathcal{U}_{\text{old}})]\right\}$$

4. Removal of a particle accepted with probability

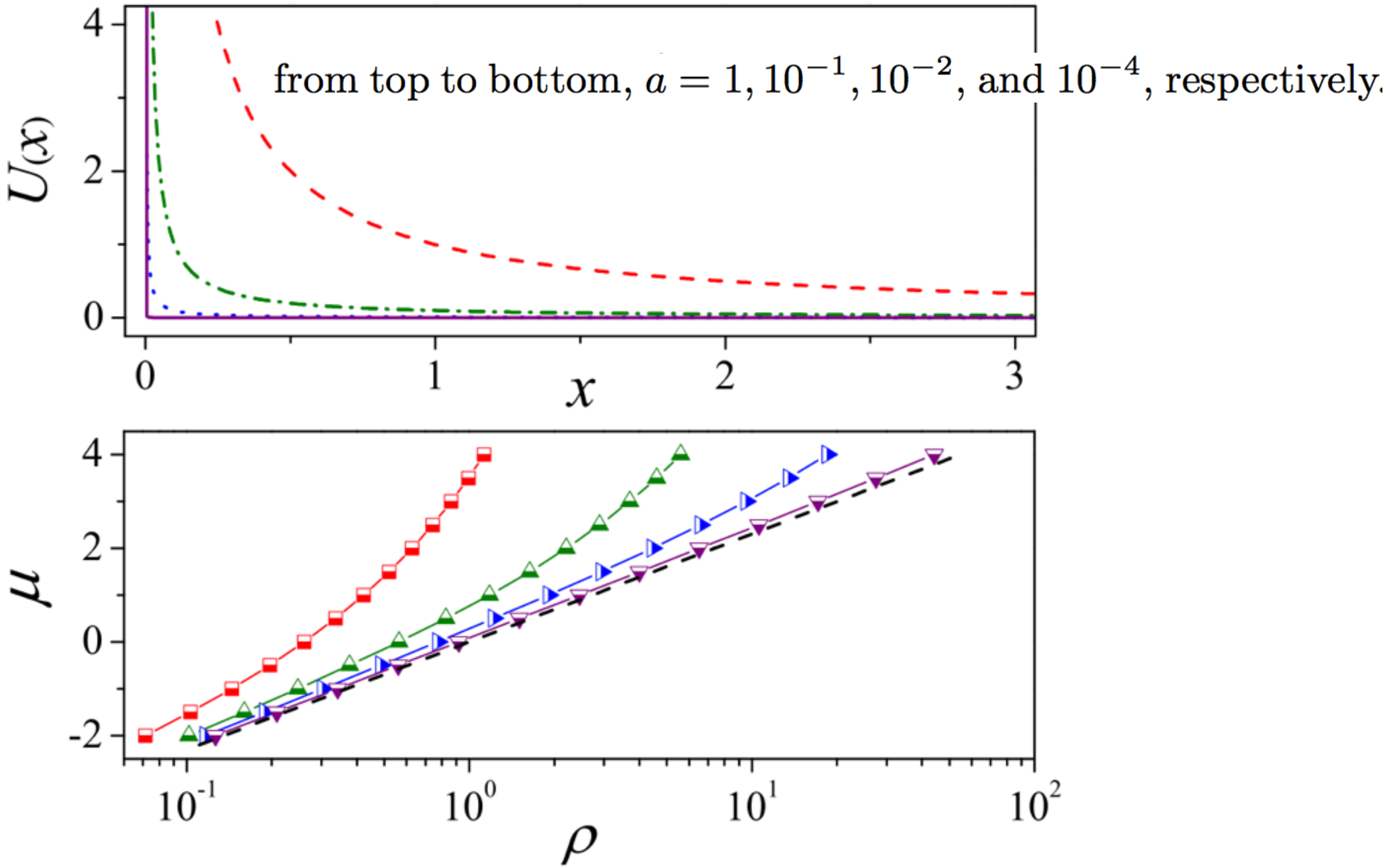
$$\min\left\{1, \frac{\lambda N_{\text{old}}}{L} \exp[-\beta(\mathcal{U}_{\text{new}} - \mathcal{U}_{\text{old}})]\right\}$$

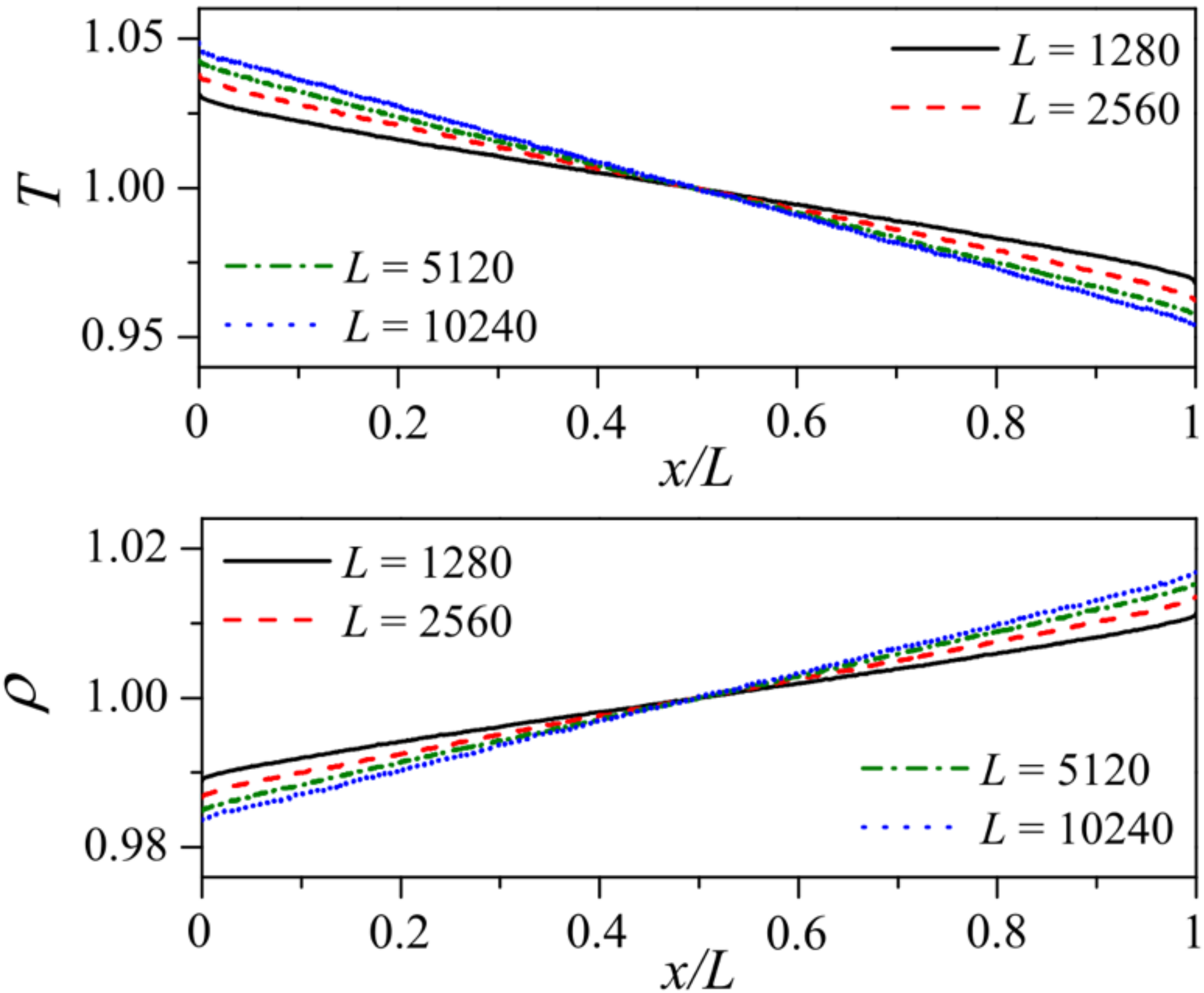
5. Repeat steps 2 to 4, for a long enough time to reach the equilibrium state

6. Repeat steps 2 to 4, to have a sufficient number of microstates to compute the average number of particles and the density with good accuracy

$$\rho = \langle N \rangle / L$$

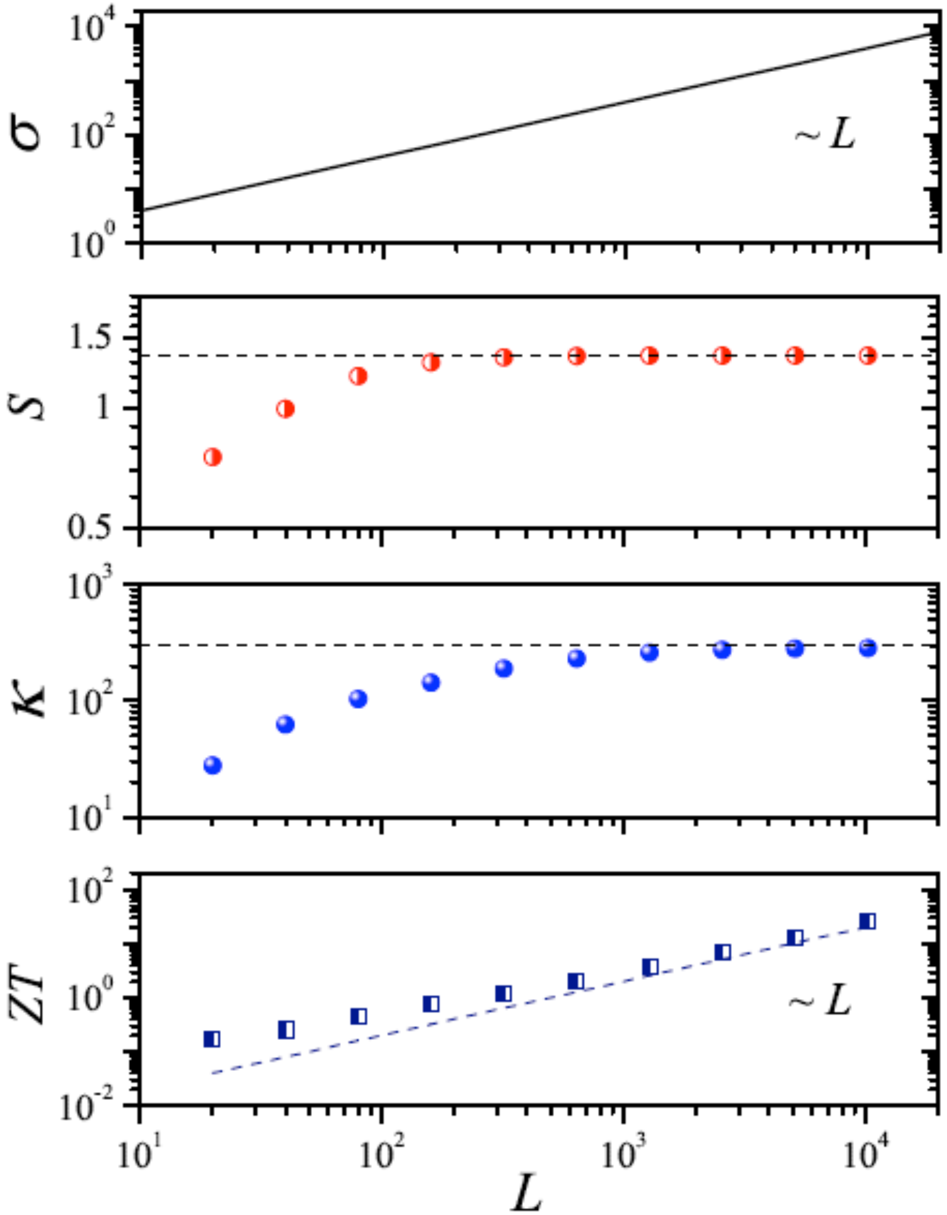
Mapping between electrochemical potential and density for the 1D Coulomb gas model





1.05
1.00
0.95
T
L = 1280
L = 2560
L = 5120
L = 10240
0
0.2
0.4
0.6
0.8
1
x/L
1.02
1.00
0.98
ρ
L = 1280
L = 2560
L = 5120
L = 10240
0
0.2
0.4
0.6
0.8
1
x/L

Transport coefficients for the Coulomb gas model



Fourier-like behavior

(S. Chen, J. Wang , G. Casati, G.B., PRE **92**, 032139 (2015))

Summary (Part II)

New mechanism for achieving Carnot efficiency in extended interacting systems, provided:

1) Overall momentum is the only relevant constant of motion (translational invariance of interactions, absence of on-site pinning potential)

2) Absence of dissipative channels

The Fourier-like regime is more favorable than the hydrodynamic regime for thermoelectric conversion