First-Principle Validation of Fourier's Law: One-Dimensional Classical Inertial Heisenberg Model

H.S. Lima, C. Tsallis, and F.D. Nobre

CBPF

Z. Phys. B – Condensed Matter 59, 207–211 (1985)

Condensed Matter
Zeitschrift für Physik B

Simple and Multiple Scattering in Disordered One-Dimensional Media: Renormalisation Group Approach

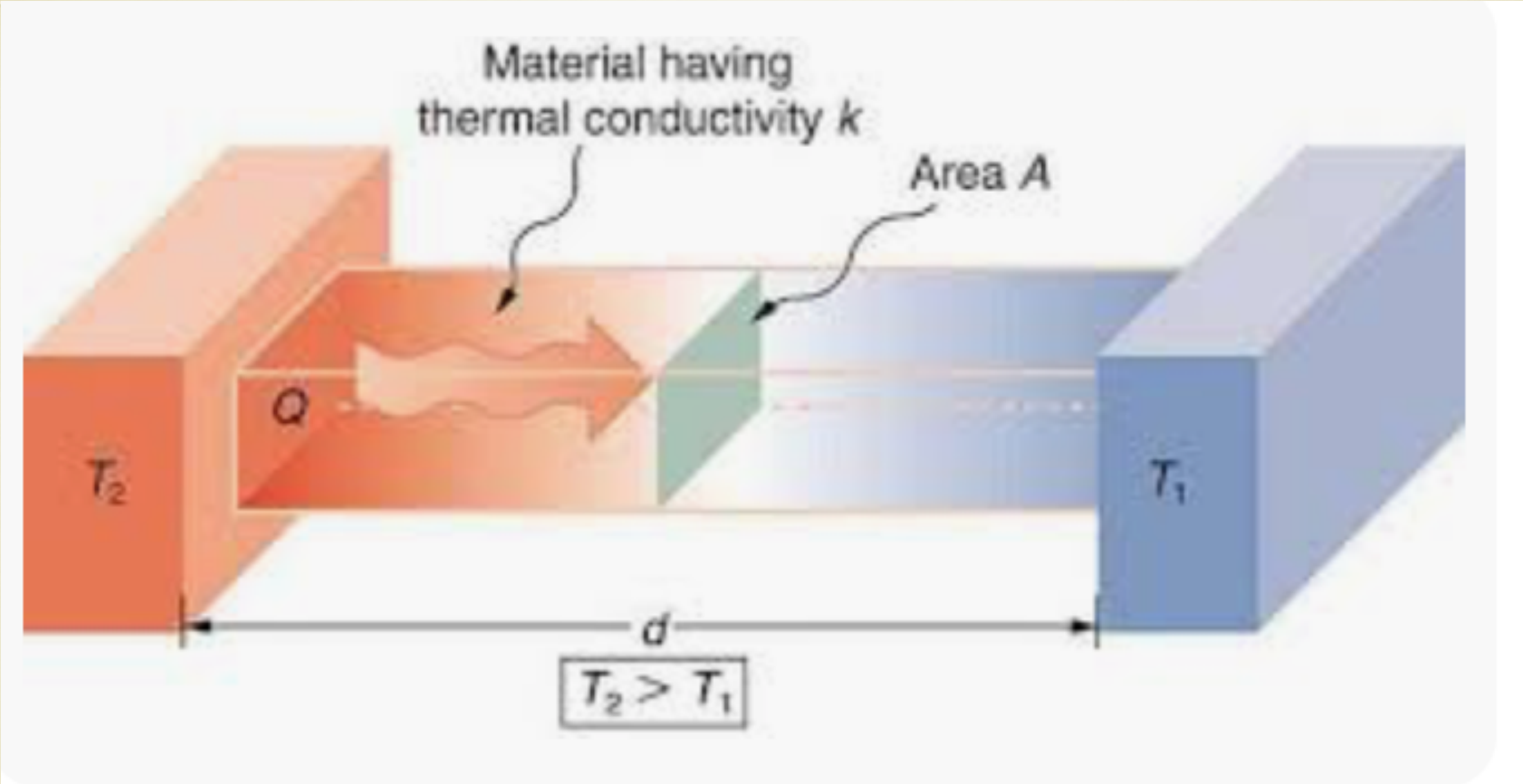
L.S. Lucena, F.D. Nobre, C. Tsallis*, and L.R. da Silva*

Departamento de Fisica, Universidade Federal do Rio Grande do Norte, Natal, RN, Brazil

Received October 10, 1984

The exact characteristic penetration length ξ associated with both simple and multiple incoherent elastic scattering in semi-infinite one-dimensional disordered media is established as a function of p (concentration of scattering centers) and f_0 (transmission coefficient of a single center). Then we exhibit how these phenomena can be seen as critical ones, and the corresponding ξ are reobtained within convenient real space renormalisation group frameworks. Finally we discuss a generalized model where the single center transmission coefficient f can randomly take two different values f_1 and f_2.

→ The first one we never forget!!



Heat Flux: $\mathbf{J} \propto -\nabla T$ (rate of heat per unit area)

J. B. J. Fourier, Théorie Analytique de La Chaleur (1822)

$d = 1: \quad \mathbf{J} = J\mathbf{x}$

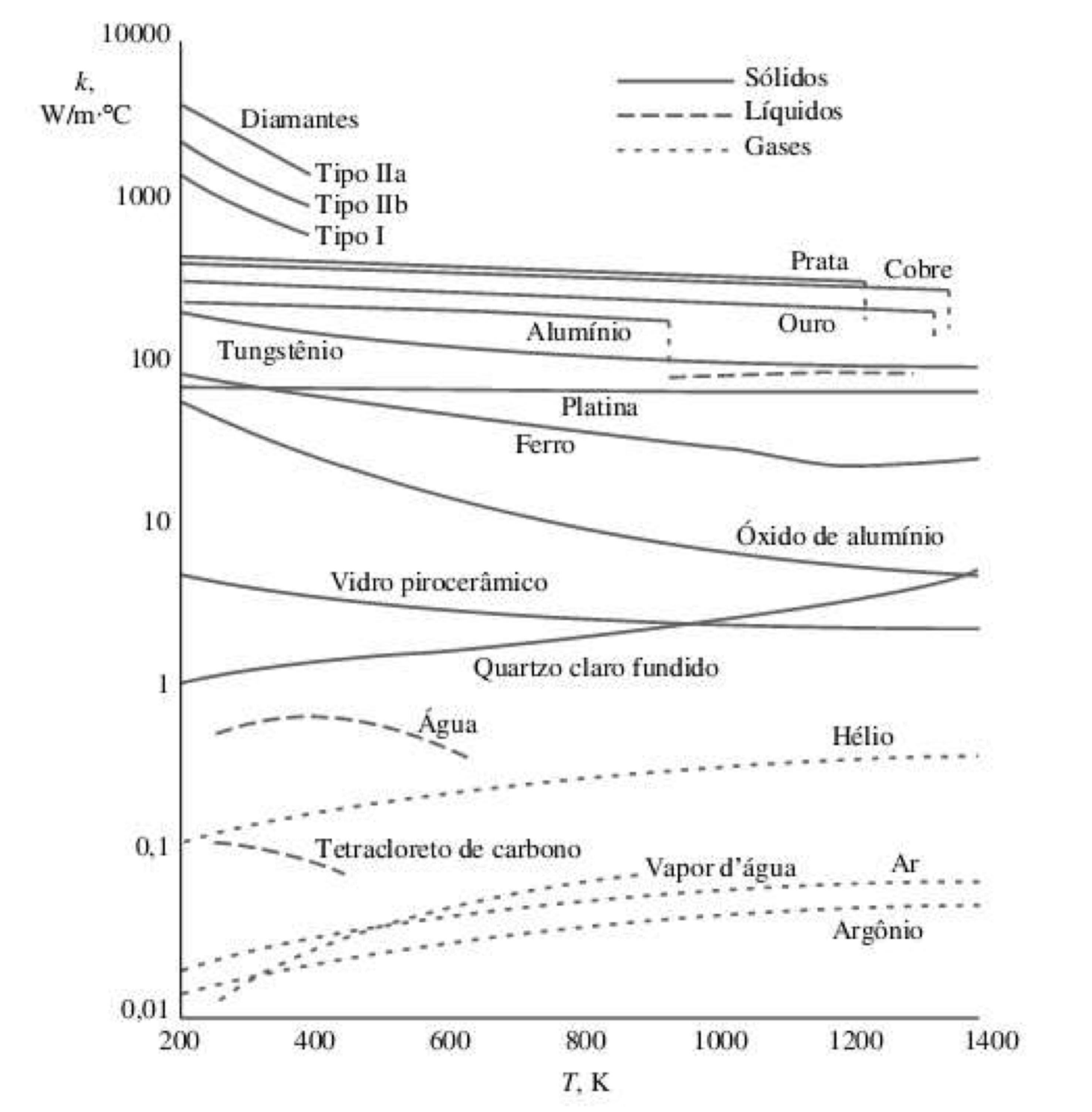
$$J = -\kappa \frac{dT}{dx}$$ → Fourier's Law

$\kappa \equiv \kappa(T):$ Thermal Conductivity

One-dimensional system of size L:

$\sigma(T, L) \equiv \kappa(T)/L:$ Thermal Conductance

Thermal conductivity of typical materials (versus temperature)



- 200 years after J. Fourier

- Fourier’s law holds for a variety of systems:

Coal, rocks from coalfields, 2d materials, …

- Fourier’s law is violated for:

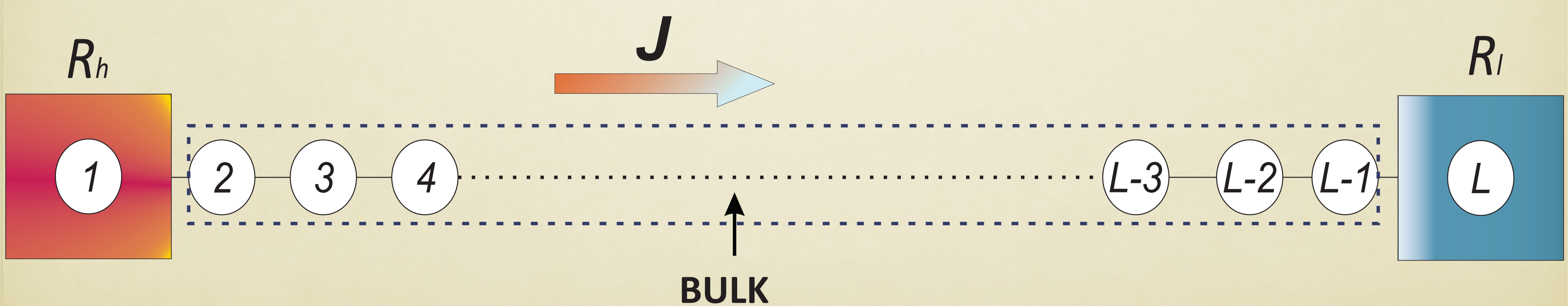
Silicon nanowires, carbon nanotubes, low-dimensional nanoscale systems, …

→ Theoretical and computational investigations in many-particle systems

System of microscopic constituents: classical nearest-neighbour-interacting Heisenberg rotators

$$\mathcal{H} = \frac{1}{2}\sum_{i=1}^{L}\mathbf{L}_i^2 + \frac{1}{2}\sum_{\langle ij\rangle}(1-\mathbf{S}_i\cdot\mathbf{S}_j)$$

$$\mathbf{L}_i \equiv (L_{ix}, L_{iy}, L_{iz}) \;;\quad \mathbf{S}_i \equiv (S_{ix}, S_{iy}, S_{iz})$$



Equations of motion $(i = 2, 3, \cdots L-1)$:

$$\dot{\mathbf{S}}_i = \mathbf{L}_i \times \mathbf{S}_i$$

$$\dot{\mathbf{L}}_i = \mathbf{S}_i \times (\mathbf{S}_{i+1} + \mathbf{S}_{i-1})$$

Rotators at extremities (Langevin dynamics):

$$\dot{\mathbf{L}}_1 = -\mathbf{L}_1 + \mathbf{S}_1 \times \mathbf{S}_2 + \mathbf{e}_h$$

$$\dot{\mathbf{L}}_L = -\mathbf{L}_L + \mathbf{S}_L \times \mathbf{S}_{L-1} + \mathbf{e}_l$$

Gaussian white noise for each Cartesian component:

$$\mathbf{e}_h \equiv (e_{hx}, e_{hy}, e_{hz}) \ ; \quad \mathbf{e}_l \equiv (e_{lx}, e_{ly}, e_{lz})$$

$$\langle e_{h\mu}(t) \rangle = \langle e_{l\mu}(t) \rangle = 0$$

$$\langle e_{h\mu}(t) e_{h\nu}(t') \rangle = 2\delta_{\mu\nu} T_h \delta(t-t') \ ; \quad \langle e_{l\mu}(t) e_{l\nu}(t') \rangle = 2\delta_{\mu\nu} T_l \delta(t-t')$$

Continuity equation:

$$\frac{dE_i}{dt} = -(J_i - J_{i-1})$$

$$E_i = \frac{1}{2}\mathbf{L}_i^2 + \frac{1}{2}\sum_{j=i\pm 1}(1 - \mathbf{S}_i \cdot \mathbf{S}_j)$$

$$J_i = \frac{1}{2}\left(\mathbf{S}_i \cdot \dot{\mathbf{S}}_{i+1} - \mathbf{S}_{i+1} \cdot \dot{\mathbf{S}}_i\right)$$

Stationary state:

$$(dE_i/dt) = 0 \quad \Rightarrow \quad J_i = J_{i-1}$$

Details of simulations

Temperatures of reservoirs:

$$T_h = T(1+\varepsilon)\ ; \quad T_l = T(1-\varepsilon) \quad \Rightarrow \quad T = \frac{T_h + T_l}{2}$$

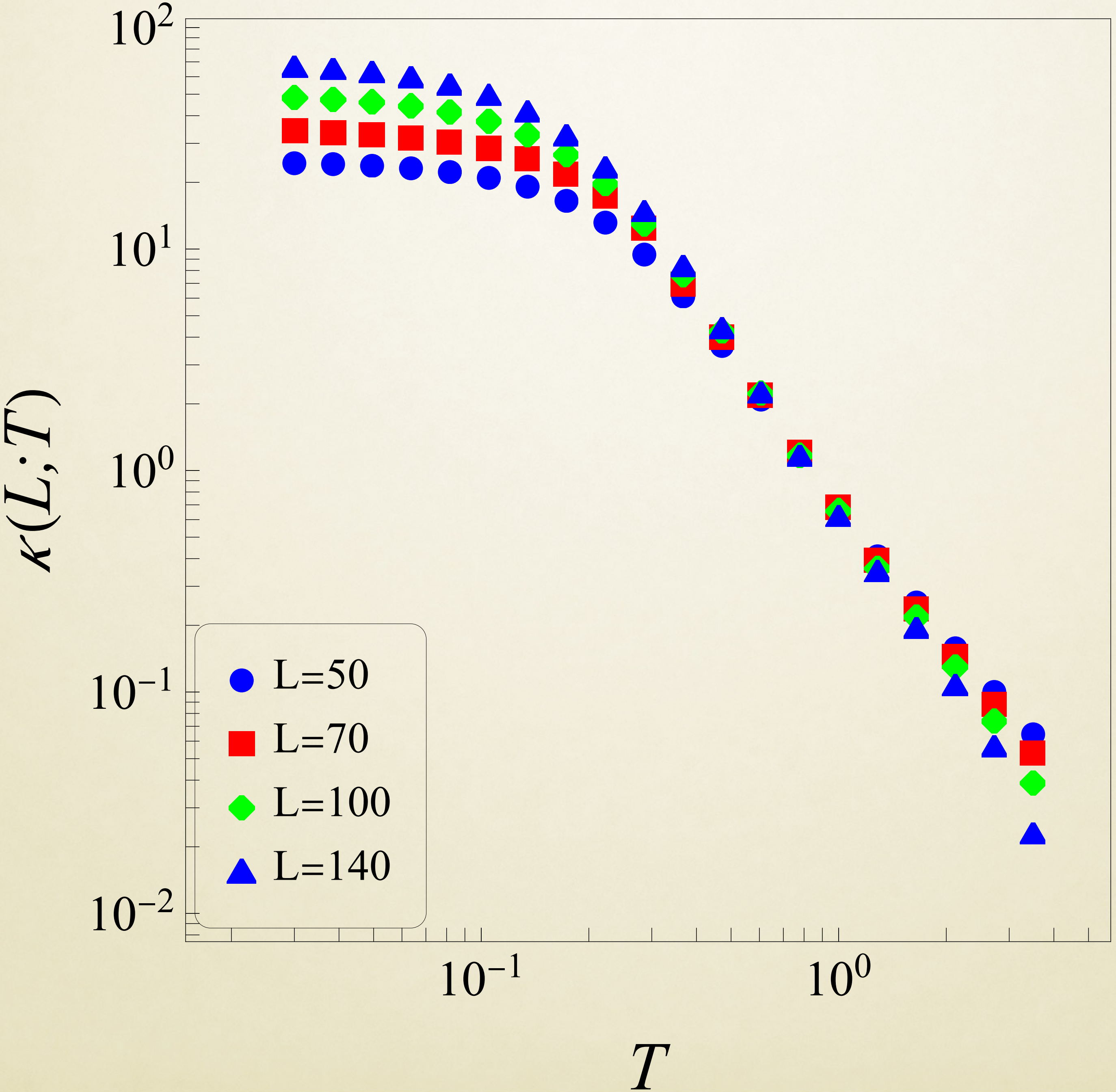
$$\varepsilon = 0.125\ ; \quad 0 < T \leq 3.5$$

Integration time step: $dt = 0.005$

Transient time: 5×10^7 time units

→ $J_i = J_{i-1}$ (within 3 decimal digits at least)

Thermal conductivity:



- Remarks:

Crossover between two regimes: $T \simeq 0.3$

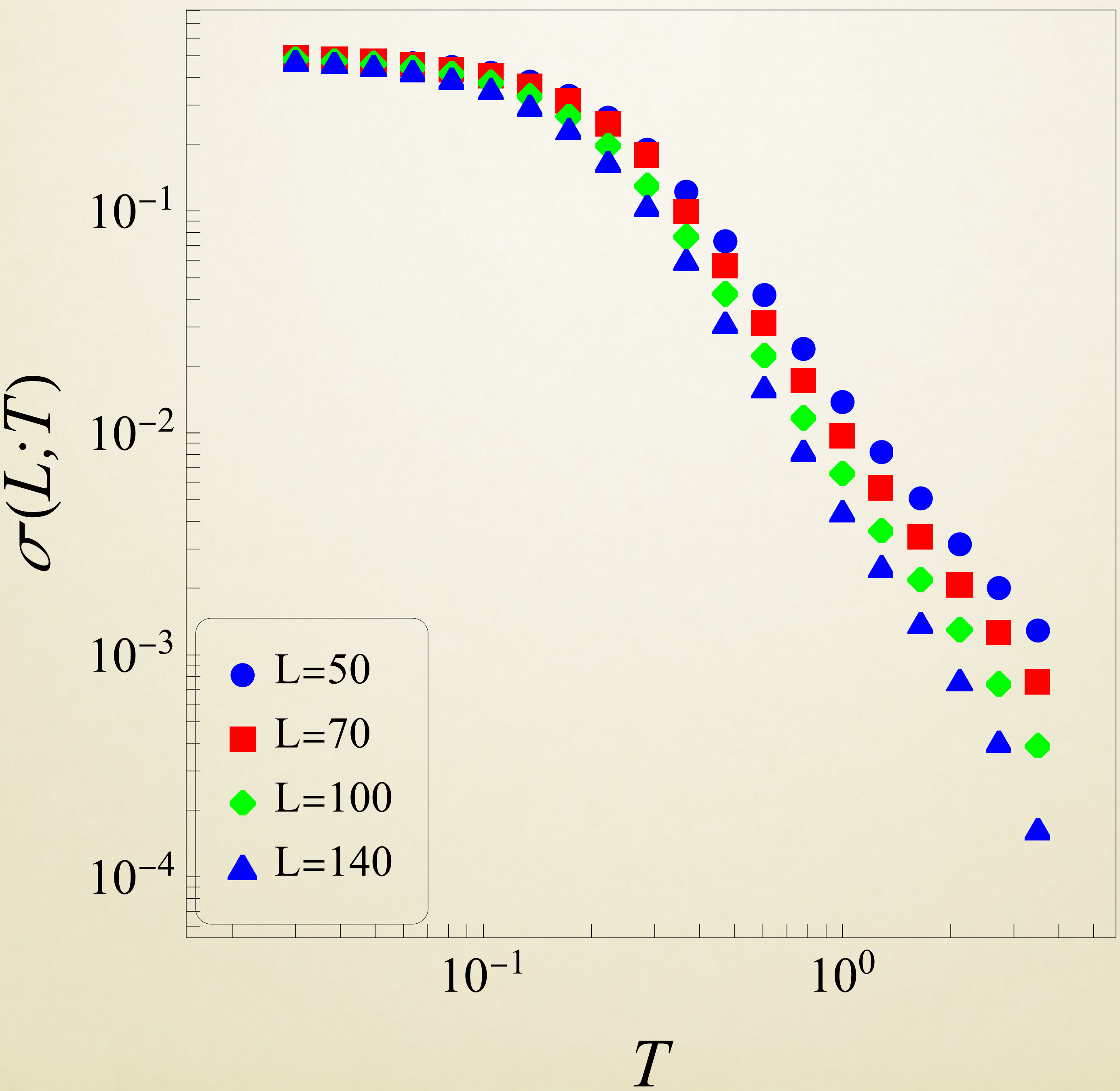
i) Low-temperature regime:

$$\kappa(L,0) \equiv \lim_{T\to 0} \kappa(L,T) \sim L$$

→ Classical model

ii) High-temperature regime: $\kappa(T) \sim T^{-2.25}$

Thermal conductance: $\sigma(L,T) \equiv \kappa(T)/L$



q-exponential:

$$\exp_q(u) = [1 + (1-q)u]_+^{1/(1-q)} \ ; \quad (\exp_1(u) = \exp(u))$$

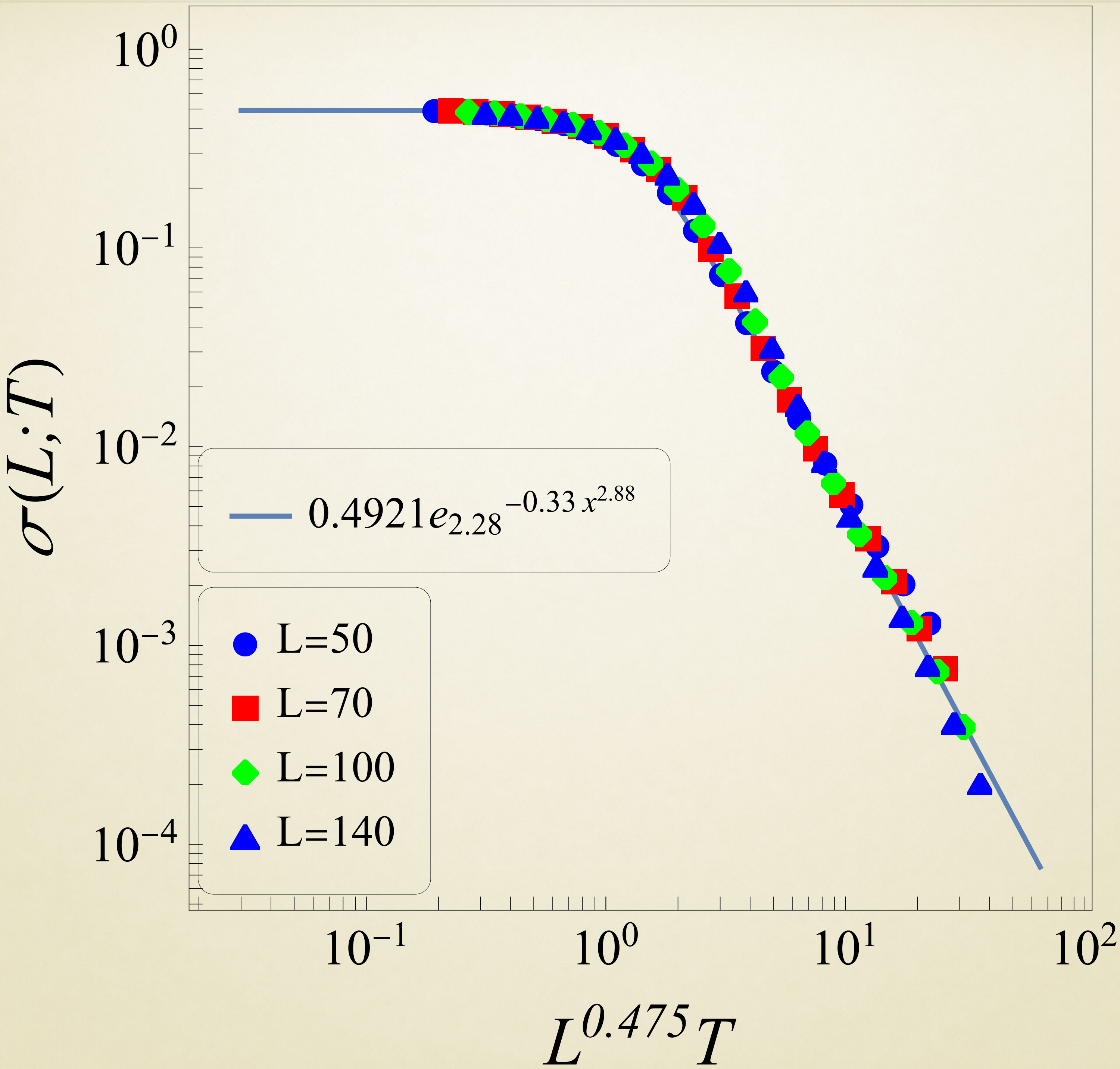
$$[y]_+ = y, \text{ for } y > 0 \text{ (zero otherwise)}$$

Stretched q-exponential distribution:

$$P_q(u) = P_0 \exp_q(-\beta |u|^\eta) \quad (0 < \eta \leq 1)$$

"Shrinked" q-exponential distribution:

$$P_q(u) = P_0 \exp_q(-\beta |u|^\eta) \quad (\eta > 1)$$



$0.4921e_{2.28}{}^{-0.33\,x^{2.88}}$
L=50
L=70
L=100
L=140
$\sigma(L;T)$
$L^{0.475}T$

- Remarks:

$$\sigma(L,T) = A\exp_q(-Bx^\eta)$$

$$x = L^{0.475}T, \;\; q = 2.28 \pm 0.04, \;\; \eta = 2.88 \pm 0.04,$$

$$A = 0.492 \pm 0.002, \;\; B = 0.33 \pm 0.04$$

Defining $x = L^\gamma T$

→ $\sigma(L,T)$ scales with L^{-1} at high temperatures (for $L \to \infty$) if

$\dfrac{\eta\gamma}{q-1} = 1$ → Criterion for validation of Fourier's law

Conclusions

- Fourier's law validated for a system of Heisenberg (n=3) rotators in d=1
- Nonextensive statistical mechanics: also applicable to out-of-equilibrium regimes
- Previous works have validated Fourier's law for a system of XY (n=2) rotators in d=1,2,3
- General condition for Fourier's law:

$$\frac{\eta(n,d)\gamma(n,d)}{q(n,d)-1} = 1$$

Temperatures of reservoirs:

$$T_h = T(1+\varepsilon) \ ; \quad T_l = T(1-\varepsilon) \quad \Rightarrow \quad T = \frac{T_h + T_l}{2}$$

Continuity equation:

$$\frac{dE_i}{dt} = -(J_i - J_{i-1})$$

$$E_i = \frac{1}{2}\,\mathbf{L}_i^2 + \frac{1}{2}\sum_{j=i\pm 1}(1 - \mathbf{S}_i \cdot \mathbf{S}_j)$$

Stationary state:

$$(dE_i/dt) = 0 \quad \Rightarrow \quad J_i = J_{i-1}$$

a) FPE Associated with BG Entropy

- Nonlinear Fokker-Planck Equation:

Spins:

- Remark:

J. B. J. Fourier, Théorie Analytique de La Chaleur

- Critical phenomenon: collective effect in a many-particle system, associated with significant changes
  - Appropriate description, critical point, critical quantities
  - Phase transitions
  - Self-organized criticality
  - Critical phenomena in biological systems

Conclusions

- Critical Phenomenon:

- $t_{\mathrm{QSS}} \propto (U_C - U)^{-\xi} \qquad (U \to U_C \text{ from below})$

- $\xi \simeq 5/3 \quad (\mathrm{XY};\ 0 \leq \alpha/d \leq 1)$

$\xi \simeq 3/2 \quad (\mathrm{Heisenberg};\ 0 \leq \alpha/d \leq 1)\ (\text{in progress})$

➡ Conjecture:

$$\xi = \frac{n+3}{n+1} \quad (n\text{−component rotators})$$

- References:

1) L.J.L. Cirto, A. Rodríguez, F.D. Nobre, C. Tsallis, Europhys. Lett. 123, 30003 (2018).

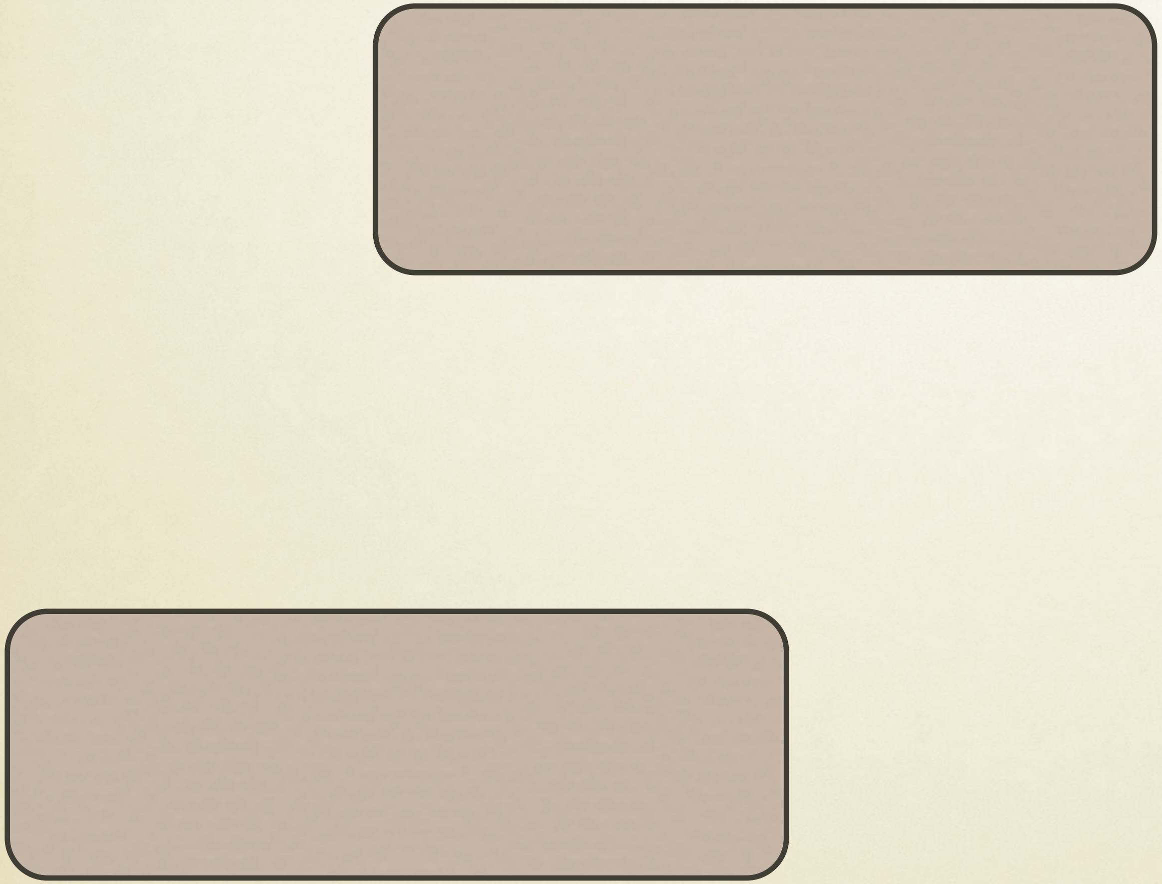
2) A. Rodríguez, F.D. Nobre, C. Tsallis, Entropy 21, 31 (2019).

3) A. Rodríguez, F.D. Nobre, C. Tsallis, Phys. Rev. Research 2, 023153 (2020).

4) A. Rodríguez, F.D. Nobre, C. Tsallis, Phys. Rev. E 103, 042110 (2021).

5) A. Rodríguez, F.D. Nobre, C. Tsallis, Phys. Rev. E 104, 014144 (2021).

6) A. Rodríguez, F.D. Nobre, C. Tsallis, Phys. Rev. E 105, 044111 (2022).



a) FPE Associated with BG Entropy

- Nonlinear Fokker-Planck Equation:
- Remark: