INSTITUTO CARLOS I
FÍSICA TEÓRICA Y COMPUTACIONAL

Universidad de Granada

VIOLATION OF UNIVERSALITY IN ANOMALOUS FOURIER'S LAW ?

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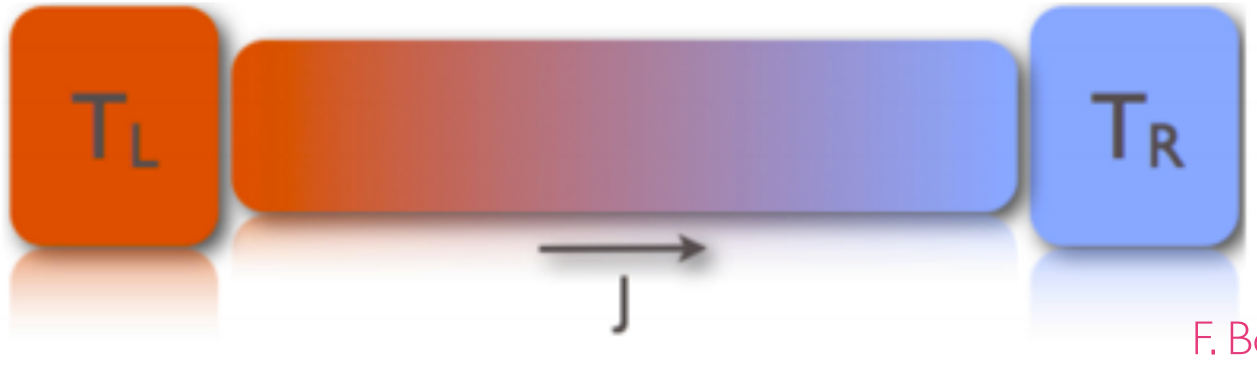
FOURIER'S LAW: A CHALLENGE TO THEORISTS

- Describes **heat transport** in a temperature gradient



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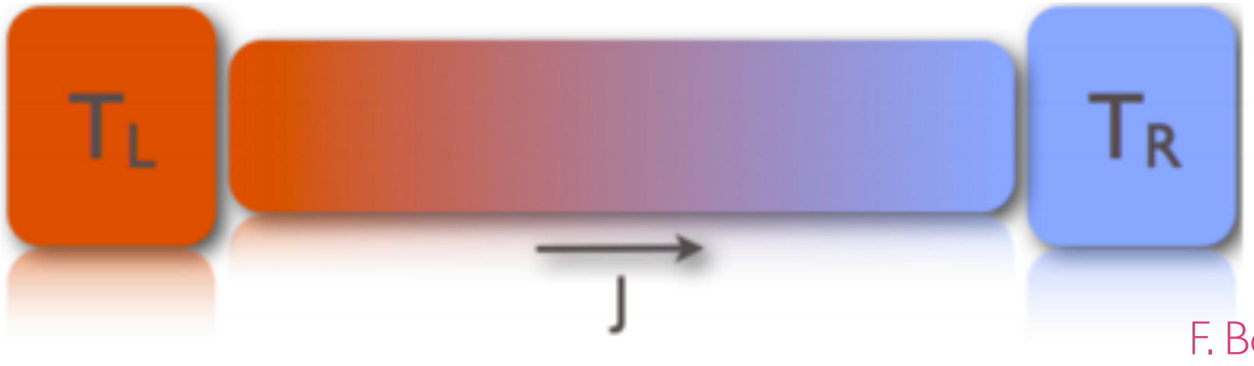

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- No first principles derivation of Fourier's law !!!!! (1822-2015 ...)

- **In low dimensions, anomalous heat transport: $\kappa(\rho,T)$ depends on L!!!**
  In 1d momentum-conserving systems, $\kappa(\rho,T) \sim L^{\alpha}$

- Many **open questions**:
  - ☑ Does Fourier's law just break down in 1d or rather there exists an anomalous FL?
  - ☑ Does Fourier's law remains valid for **strong temperature gradients**?
  - ☑ Is the anomaly in 1d Fourier's law universal?

FOURIER'S LAW: STATE OF THE ART

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C.B. Mendl & H. Spohn, PRL (2013)

- Recent **theoretical breakthrough**: **nonlinear fluctuating hydrodynamics** predicts **universal behavior** of 1d heat conductivity: **Kardar-Parisi-Zhang (KPZ) universality class**

$$\kappa_L(\rho, T) \sim L^{1/3}$$

- Other universality class with **α**=1/2 predicted under special conditions (e.g. zero pressure)

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- **Numerically**, a large number of results seem to support asymptotically the overall picture. All based on linear response, depend on N→∞ limit

$$\kappa(N) = \frac{JN}{\Delta T}$$

Small gradient limit

$$\kappa_{GK}(N) = \frac{1}{k_B T^2 N} \int_0^{\tau^*} \langle J(0) J(t) \rangle$$

Green-Kubo formula

Models: Fermi-Pasta-Ulam, hard particles, Lennard-Jones, double-well, Toda, ϕ^4, rotors, harmonic, disorder, quantum, ...

Authors: Aoki, Basile, Benenti, Bernardin, Casati, Cipriani, Chen, Das, Delfini, Denisov, Deutsch, Dhar, Eckmann, Garrido, Gendelman, Giardina, Grassberger, Gray, Hatano, Hu, Kipnis, Kusnezov, Lebowitz, Lee-Dadswell, Lepri, Li, Liu, Livi, Lukkarinen, Mai, Marchioro, Mendl, Mohanty, Nadler, Narayan, Nickel, Olla, Politi, Presutti, Prosen, Roy, Ruffo, Saito, Savin, Spohn, Stolz, Tsironis, Van Beijeren, Vasali, Wang, Xie, Xu, Yang, Zhang, Zolotaryuk, ...

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- **No conclusive results though ...**

SCALING LAWS IN FOURIER'S LAW

- The two following statements are equivalent

$$J = -\kappa_L(\rho,T)\frac{dT(x)}{dx}$$

Fourier's law

$$P = \rho(x)T(x)$$

Local equilibrium

$$\kappa_L(\rho,T) = L^\alpha\sqrt{T/m}k(\rho)$$

Anomalous conductivity

$$\rho(x) = F\left(\frac{\psi x}{L^\alpha} + \zeta\right) \quad ; \quad \frac{T(x)}{P} = \frac{1}{F\left(\frac{\psi x}{L^\alpha} + \zeta\right)}$$

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Fourier's law — Local equilibrium — Anomalous conductivity

Write Fourier's law in terms of ρ(x)

$$\frac{J\sqrt{m}}{P^{3/2}}L^{-\alpha} = G'(\rho)\frac{d\rho}{dx} = \frac{dG(\rho)}{dx}$$

$$G'(\rho) \equiv k(\rho)\rho^{-5/2}$$

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- There exists an **universal master curve F(u)** ($\forall\ \eta, T_0, T_L, \mu, L$) from which any steady state profile follows after a **linear spatial scaling** $x=L^\alpha(u-\zeta)/\psi$

- Alternatively, **any measured steady profile can be collapsed onto the universal master curve** by scaling space by $L^{-\alpha}\psi$ and shifting the resulting profile by ζ

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OBJECTIVES

- Test scaling picture and use it to **measure the anomaly exponent**
- High precission: Scaling expected to be **very sensitive to the anomaly exponent**
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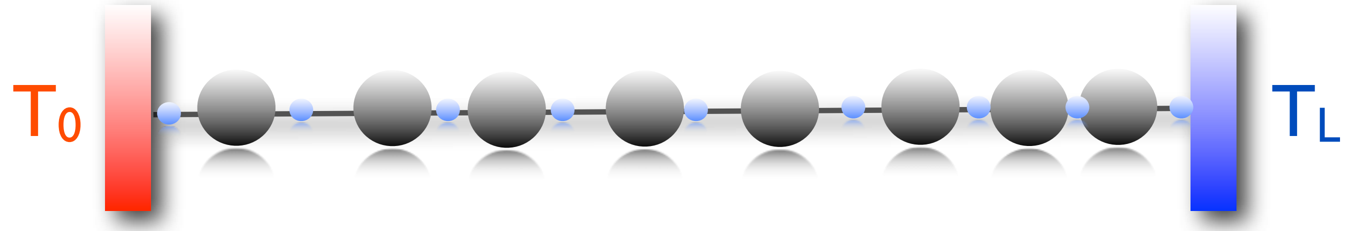
MODEL: DIATOMIC HARD-POINT GAS

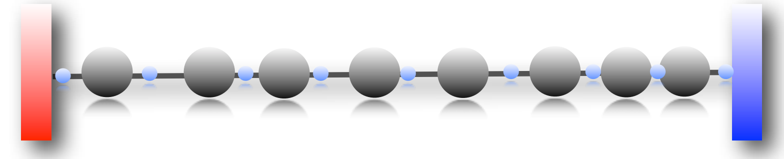
- Model: **diatomic hard-point gas** characterized by **mass ratio $\mu=M/m > 1$**

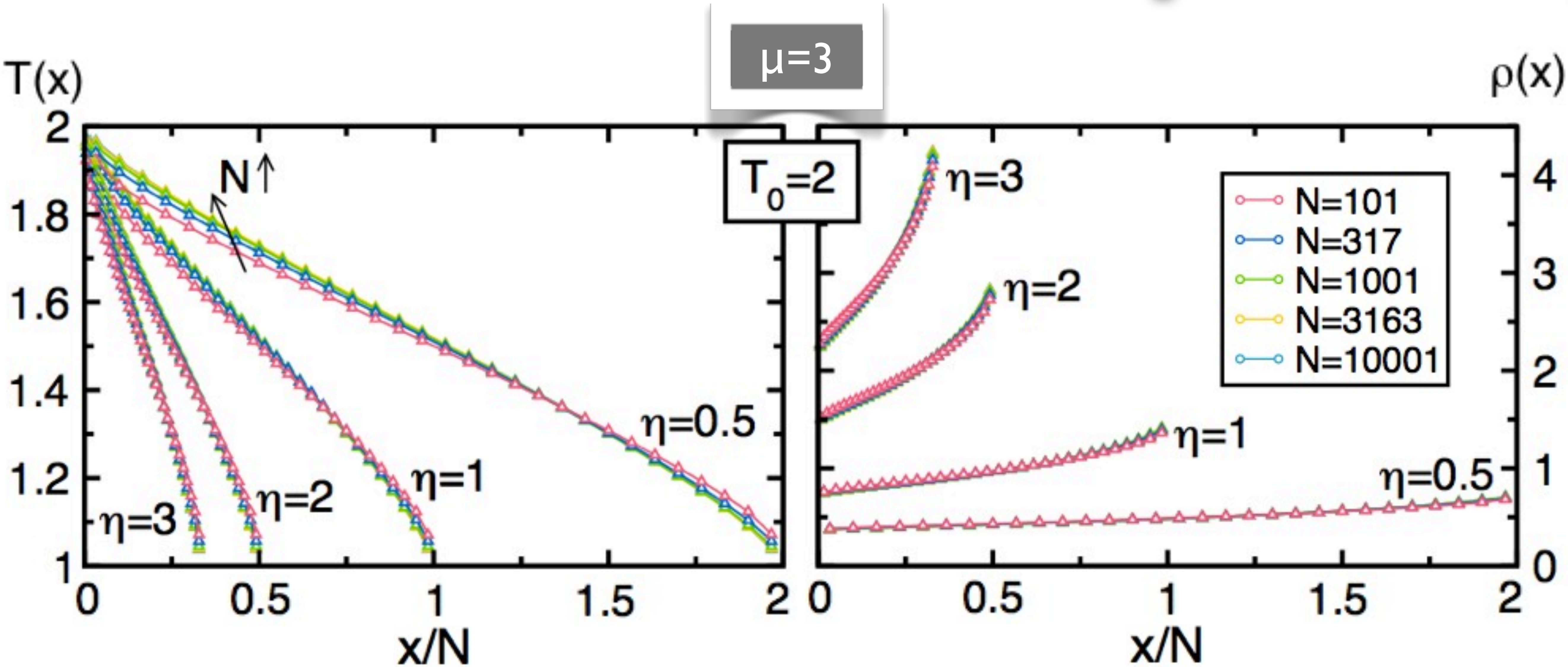


N particles
System of length L ($\eta=N/L$)
Stochastic thermal walls
Bath temperatures T_0 and T_L
Mass ratio $\mu=M/m>1$
Momentum and energy conservation

- **Advantages:**
  - ☑ Simple dynamical rules (ballistic motion in between elastic collisions)
  - ☑ Efficient computer algorithm: event driven simulation + stochastic heat baths
  - ☑ Density-temperature separability and simple equation of state

TEMPERATURE AND DENSITY PROFILES





640 simulations

- 5 different $N \in [101, 10001]$
- 4 different ΔT with $T_0 \in [1,20]$
- 4 densities $\eta \in [0.5,3]$
- 8 different mass rations $\mu \in [1.3,100]$
- Time unit $t_0 = [M/(2T_L\eta^2)]^{1/2}$
- Measurements every $10t_0$ for $(10^8\text{-}10^9)t_0$
- Observables: $T(x)$, $\rho(x)$, $P(x)$, $J(x)$, P_{wall}, J_{wall}, ...

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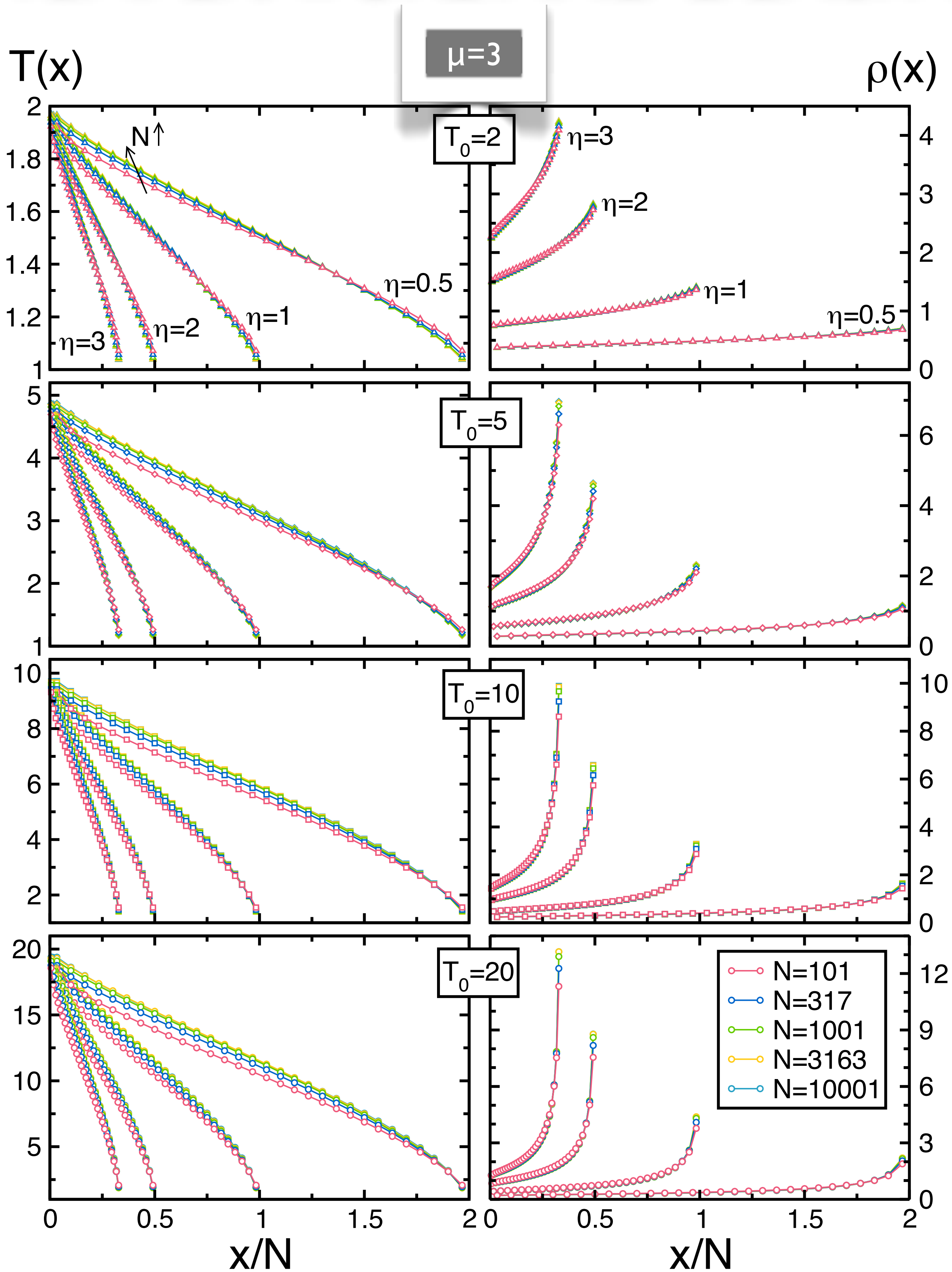

- **Nonlinear** temperature and density profiles
- **Strong finite-size effects!!**

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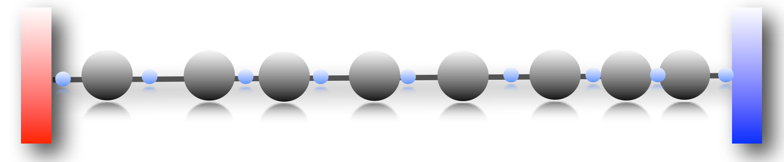

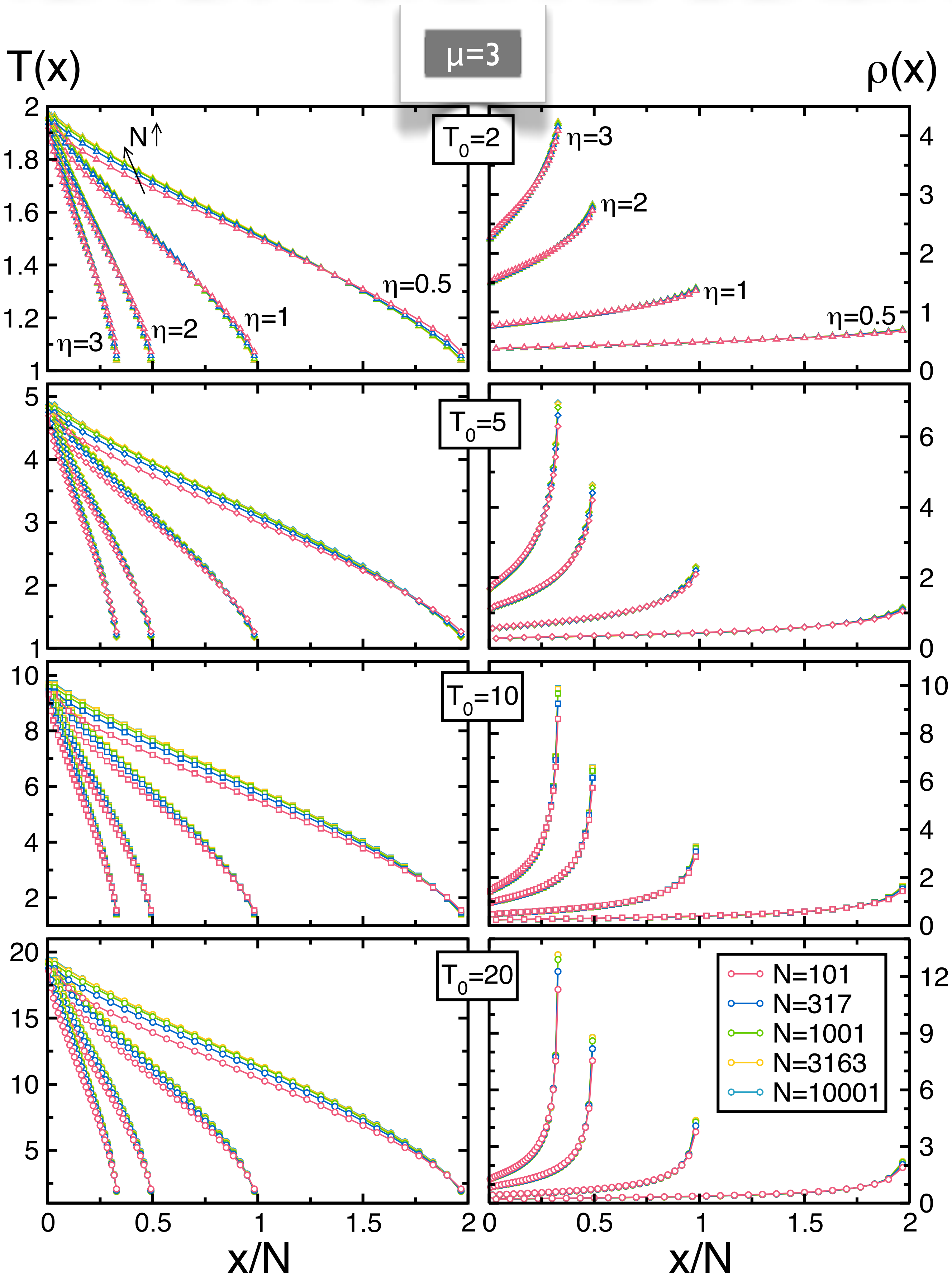

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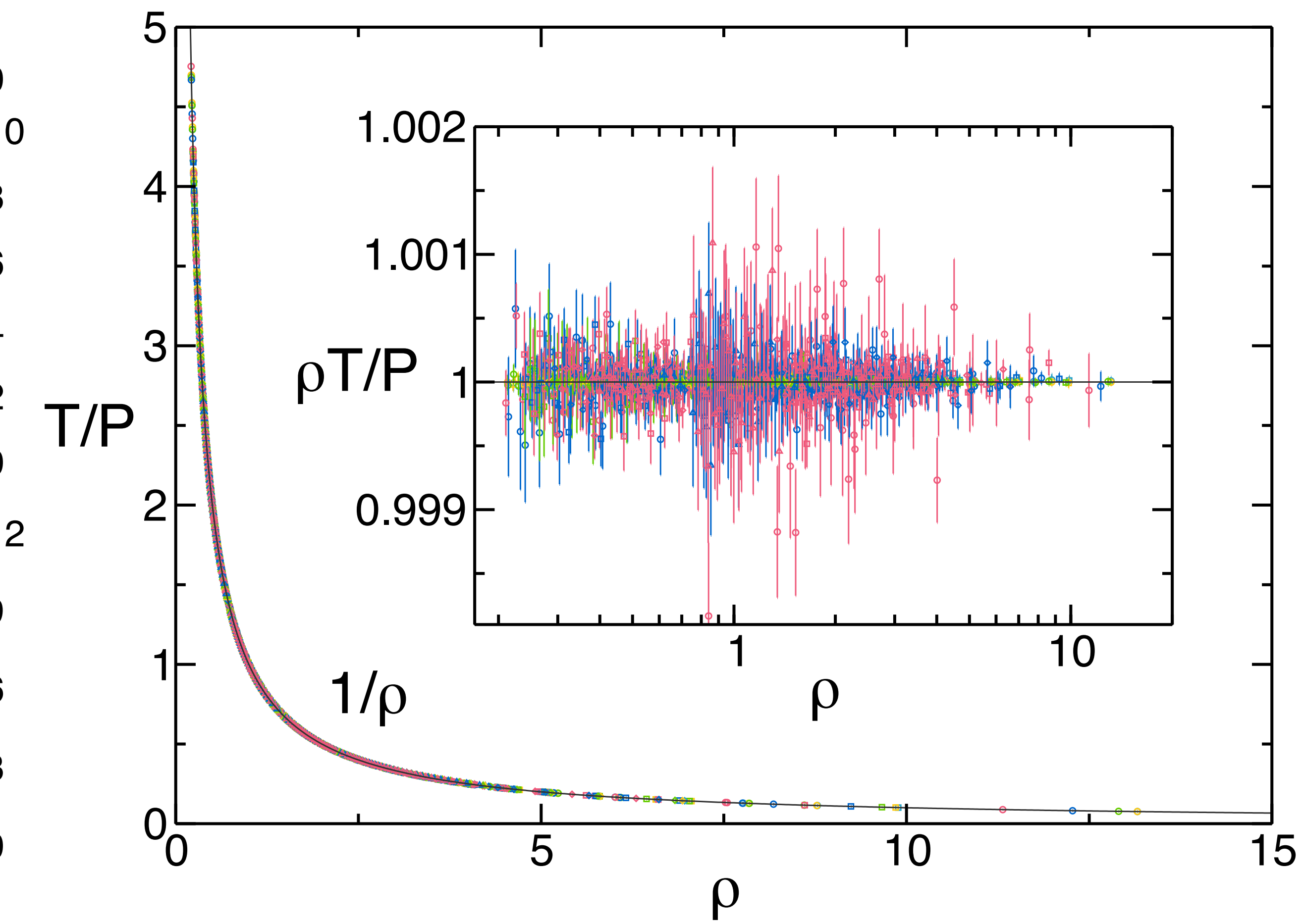
- **Strong finite-size effects!!**
- However, **macroscopic local equilibrium** is very robust



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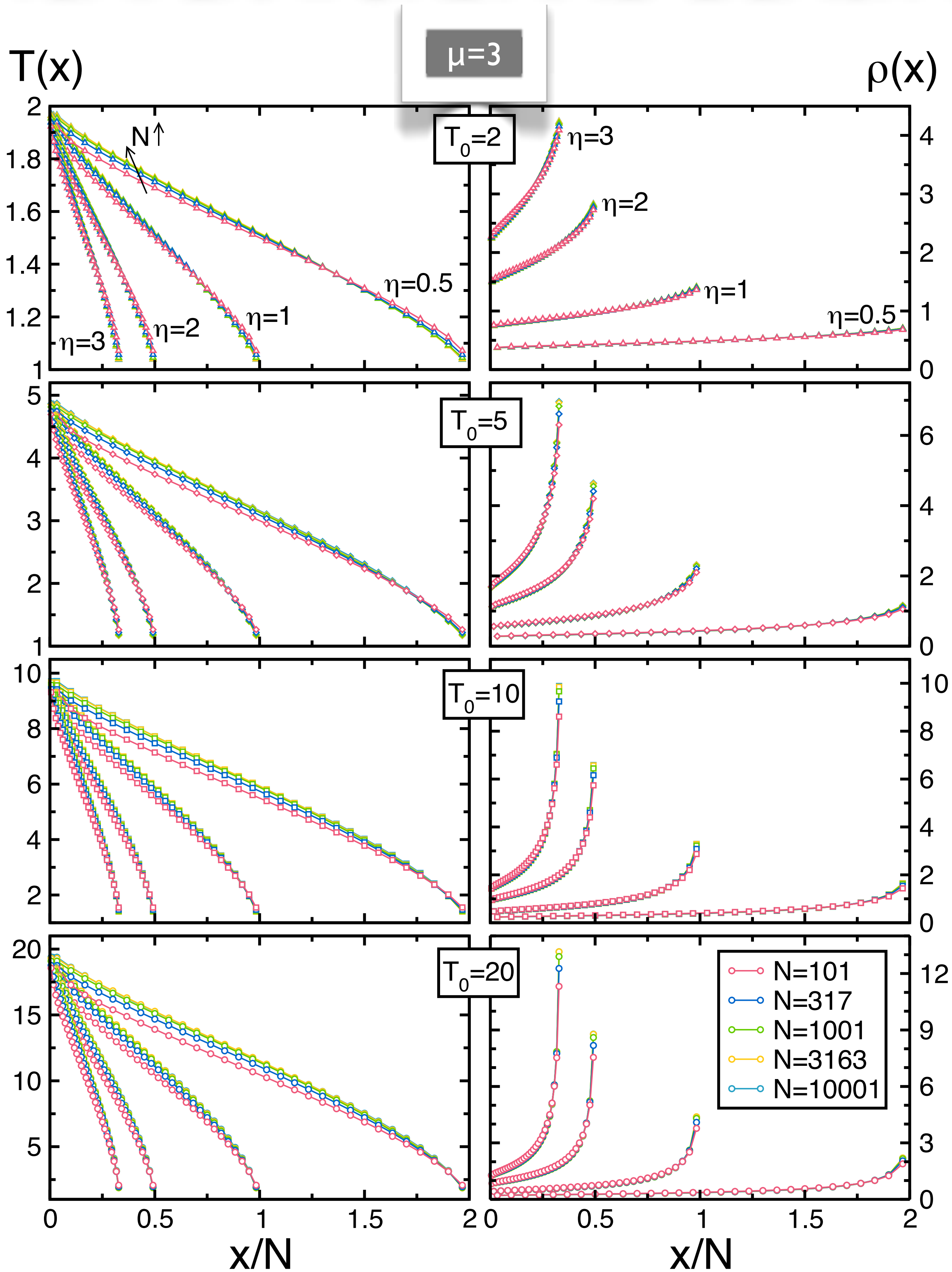

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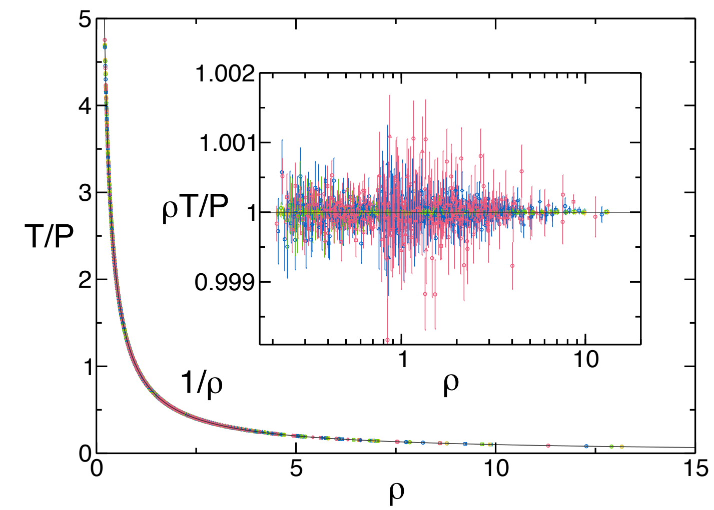
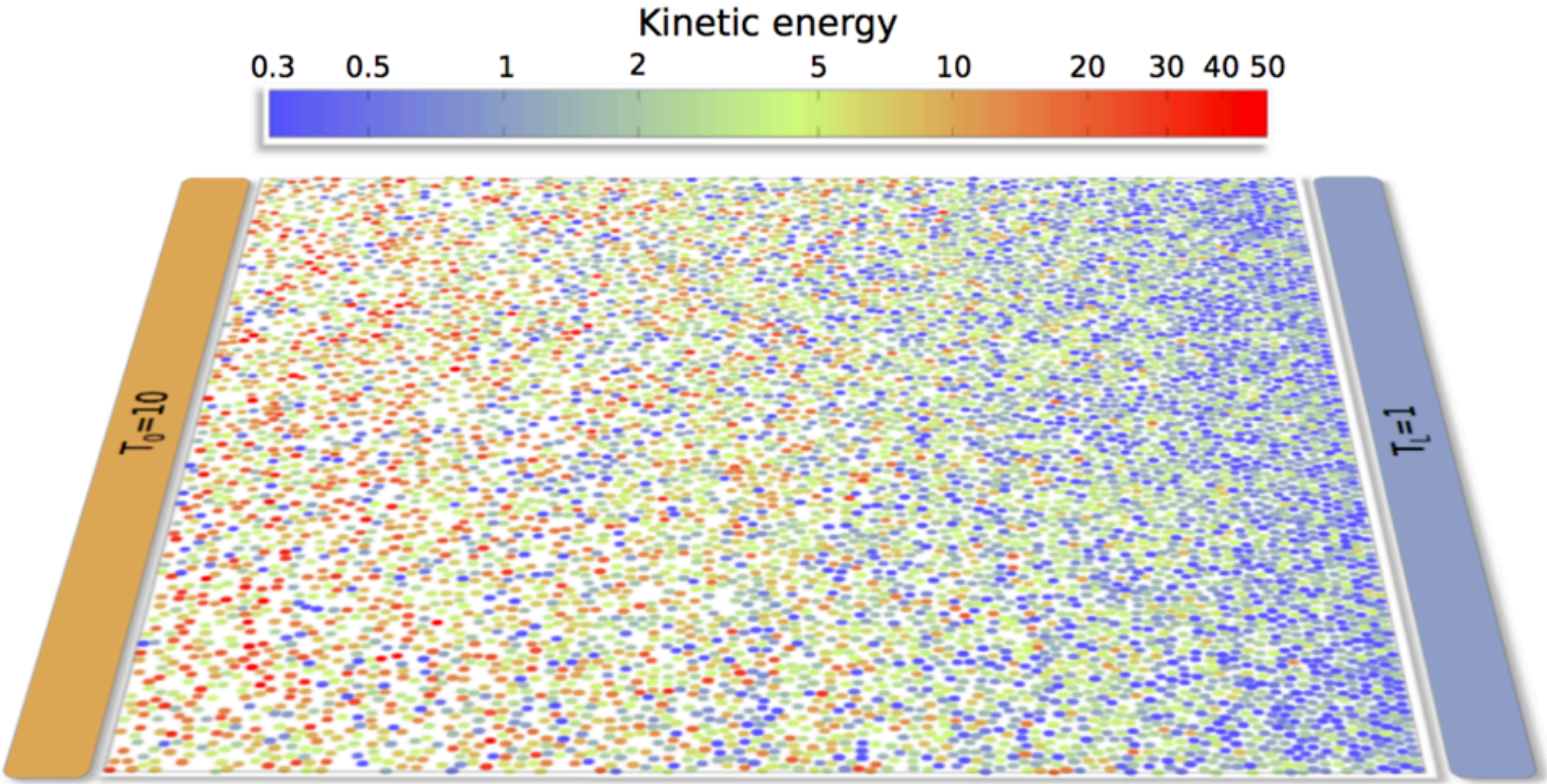


- Thermal walls disrupt the surrounding fluid: **boundary layers**
- **Bulk behavior: For scaling analysis, remove boundary layers**

EXAMPLE: COLLAPSE IN HARD DISKS

$$\rho(x) = F\left(\frac{\psi x}{L^{\alpha}} + \zeta\right)$$



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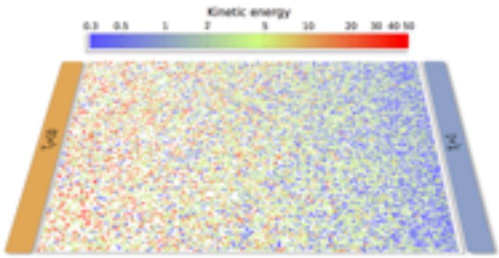

Case 1

Constant mean Packing Fraction ; Variable Gradient

$$N_{Bulk} = 8878$$

$$\bar{\eta} = 0.5$$

$$\nabla T = [1,2,\ldots,18,19]$$

SCALING AND COLLAPSE OF PROFILES

$$\rho(x) = F\left(\frac{\psi x}{L^\alpha} + \zeta\right)$$

- For fixed α, we **plot the kth bulk density profile vs $L^{-\alpha} J_k m^{1/2} x / P_k^{3/2}$**, with J_k and P_k measured in each case, and **shift the profile by ζ_k along the x-axis for optimal overlap**

$$\psi = \frac{J\sqrt{m}}{P^{3/2}}$$

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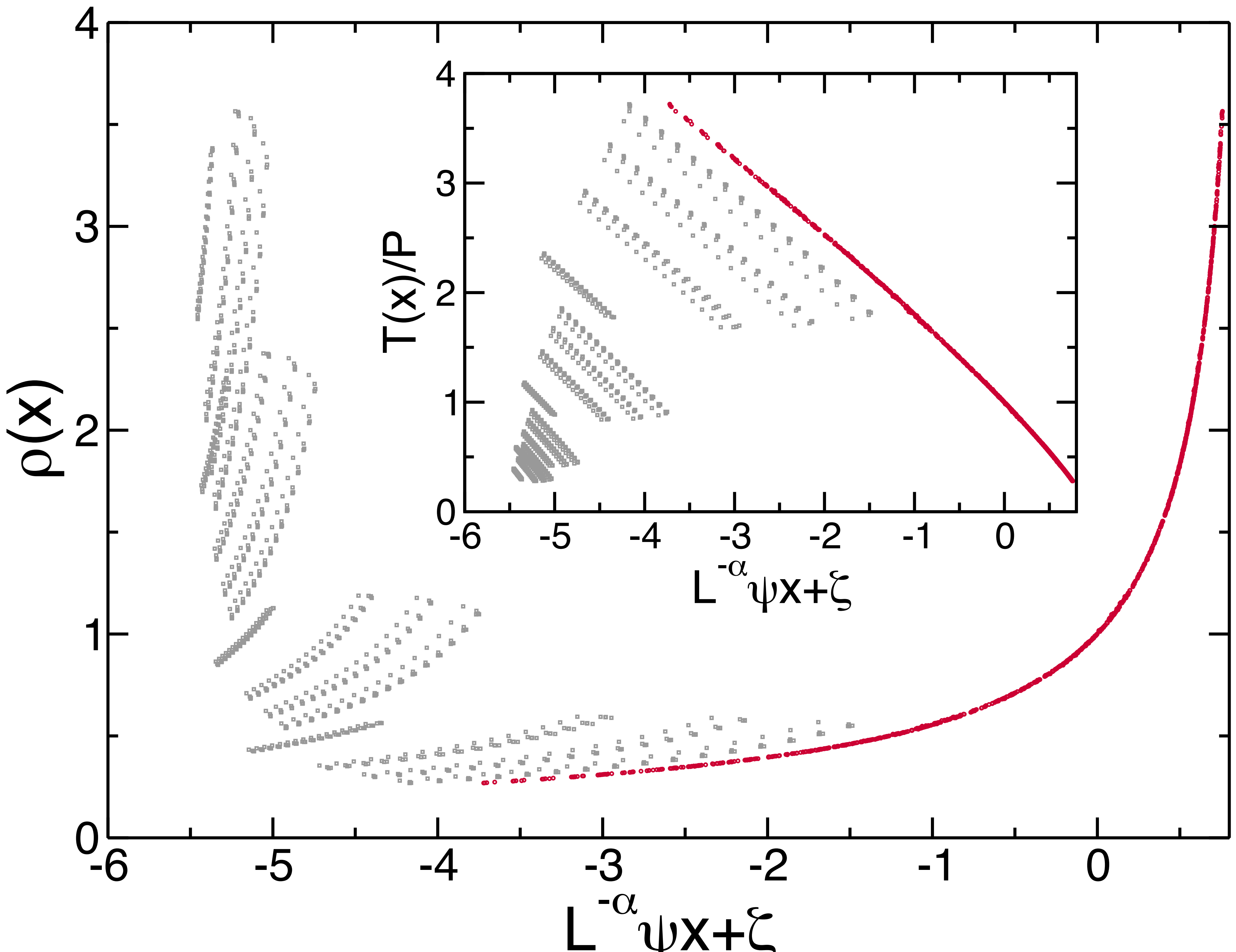

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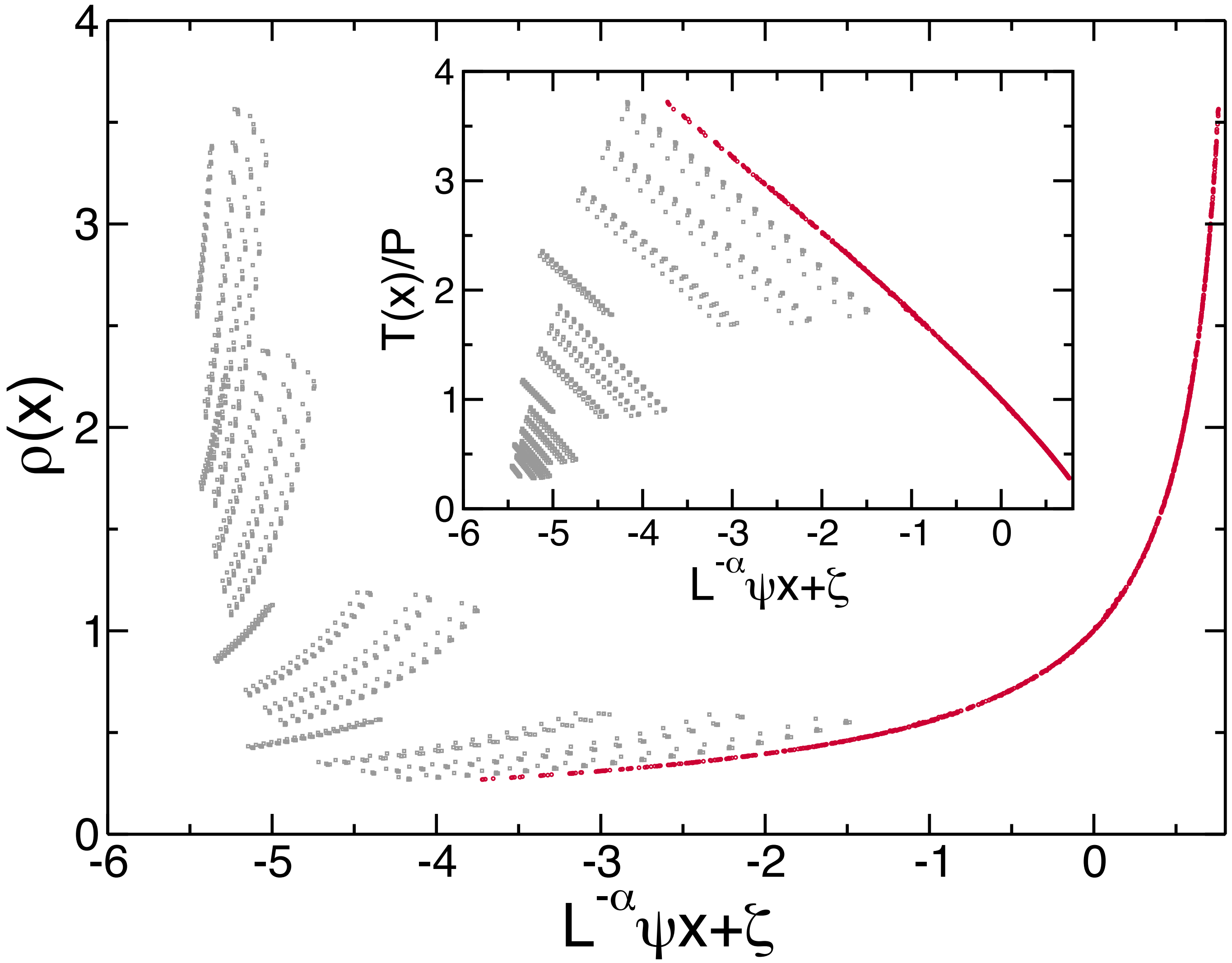


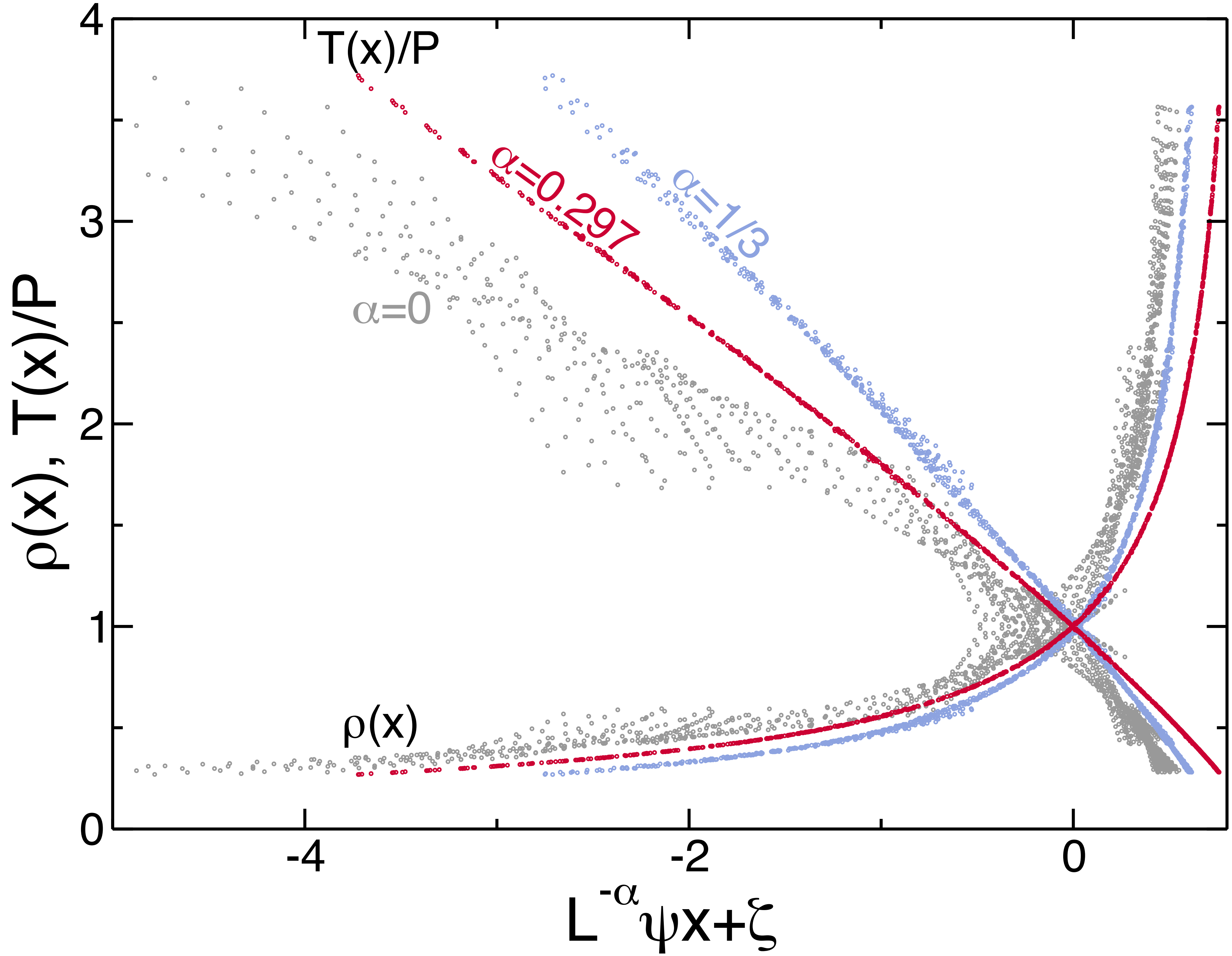
$$\frac{T(x)}{P} = \frac{1}{F\left(\frac{\psi x}{L^\alpha} + \zeta\right)}$$

- **Vector of optimal shifts $\{\zeta_k\}_0$** obtained by **minimizing an standard collapse metric $D(\{\zeta_k\};\alpha,\mu)$** that measures distance between pairs of curves

- The **same shifts $\{\zeta_k\}_0$** obtained from bulk density profiles are used to **collapse bulk temperature profiles**

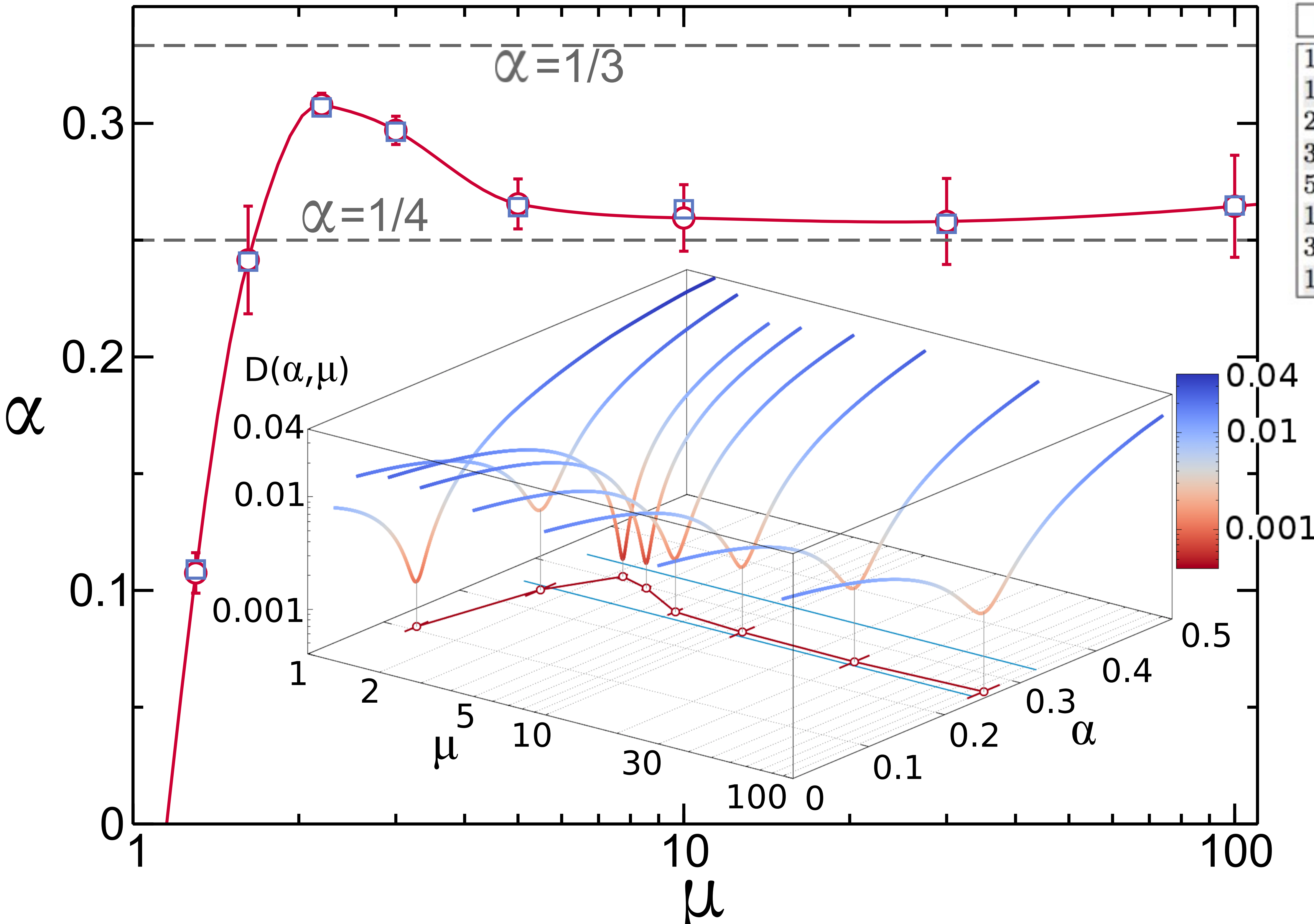
SENSITIVITY OF COLLAPSE TO ANOMALY EXPONENT

- The resulting **collapse is very sensitive to the value of the anomaly exponent.** Offers a **high-precission measurement of α**



ANOMALY EXPONENT IS NON-UNIVERSAL

- To compute the true anomaly exponent, we **minimize the distance $D(\alpha,\mu)\equiv D(\{\zeta_k\}_0;\alpha,\mu)$ vs α for each μ:** deep minimum



μ	α
1.3	0.108 (9)
1.618	0.242 (23)
2.2	0.308 (5)
3	0.297 (6)
5	0.266 (11)
10	0.260 (14)
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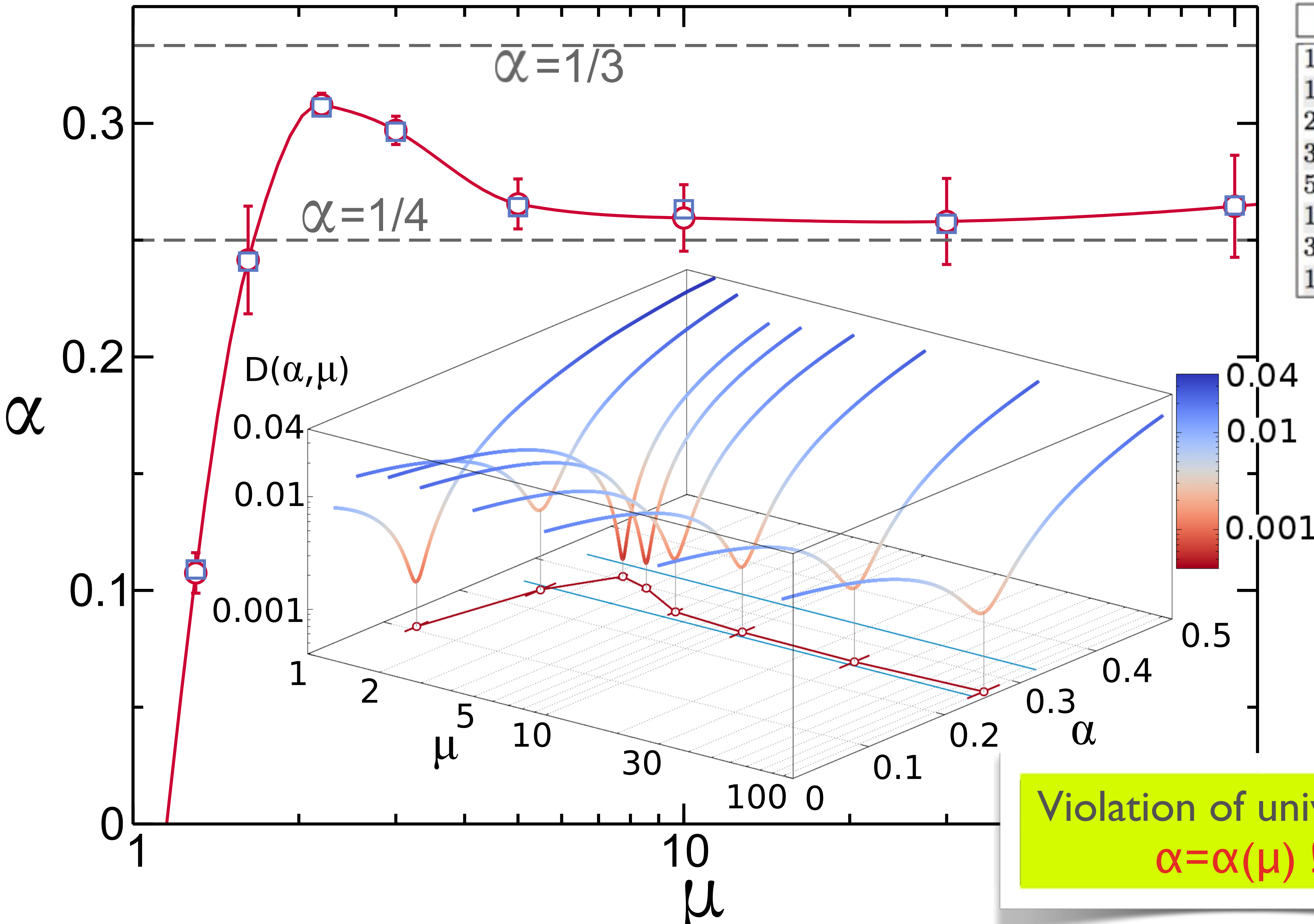

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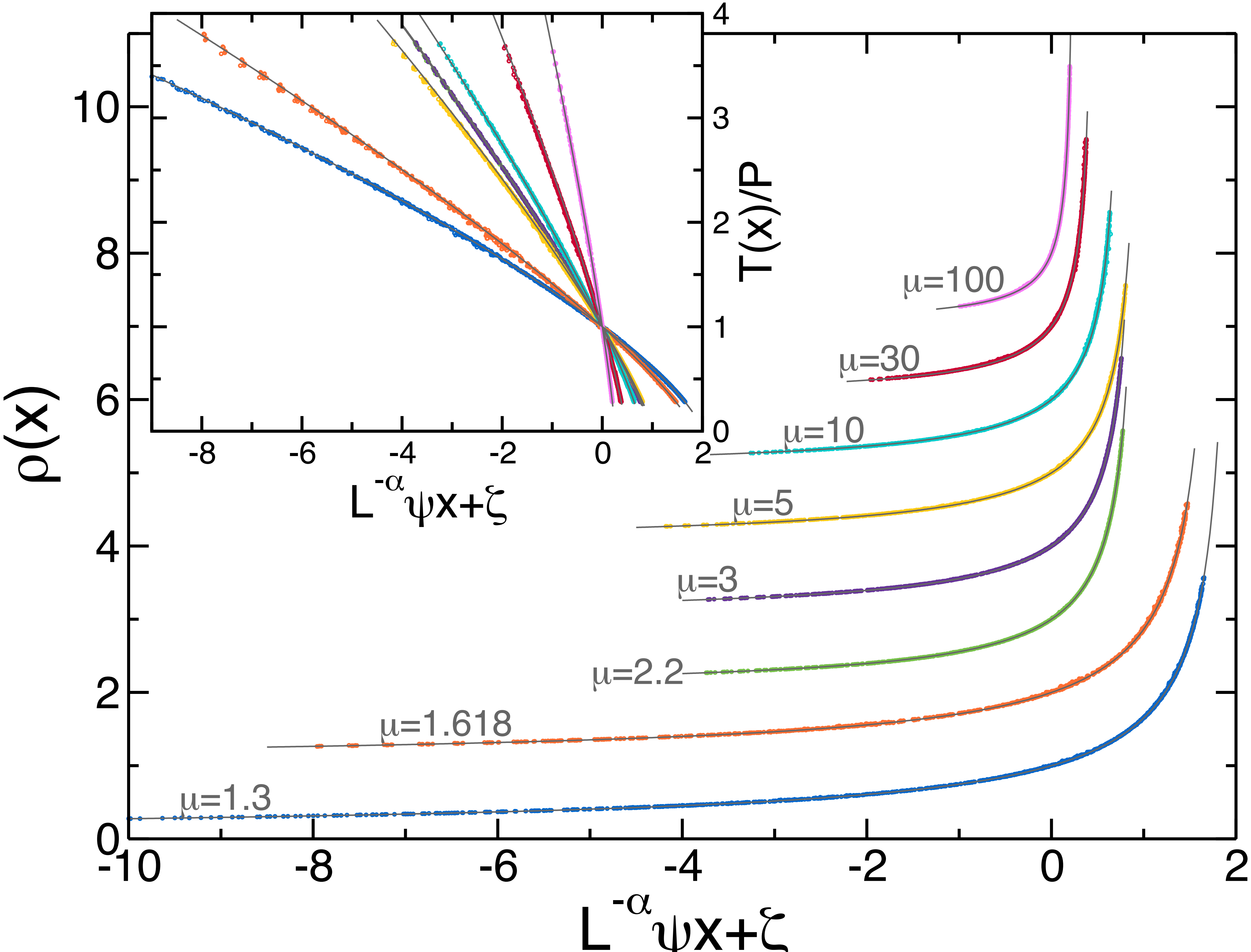
Violation of universality:
$\alpha=\alpha(\mu)$!!!

MASTER CURVES FOR DIFFERENT MASS RATIOS

- **Each curve** for fixed **μ** contains **1280 data points** measured in 80 simulations for 5 different $N \in [10^2, 10^4]$, 4 gradients $T_0 \in [2,20]$, and 4 densities $\eta \in [0.5,3]$



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DENSITY DEPENDENCE OF HEAT CONDUCTIVITY

- It can be shown rigorously that $\kappa_L(\rho,T)=T^{1/2} f(N,\mu)$, **with N and μ adimensional parameters**. But we just showed that $\kappa_L(\rho,T)=L^{\alpha}T^{1/2}k(\rho)$, so **necessarily** $k(\rho)=a\rho^{\alpha}$ with "a" some constant. Let's check it ...

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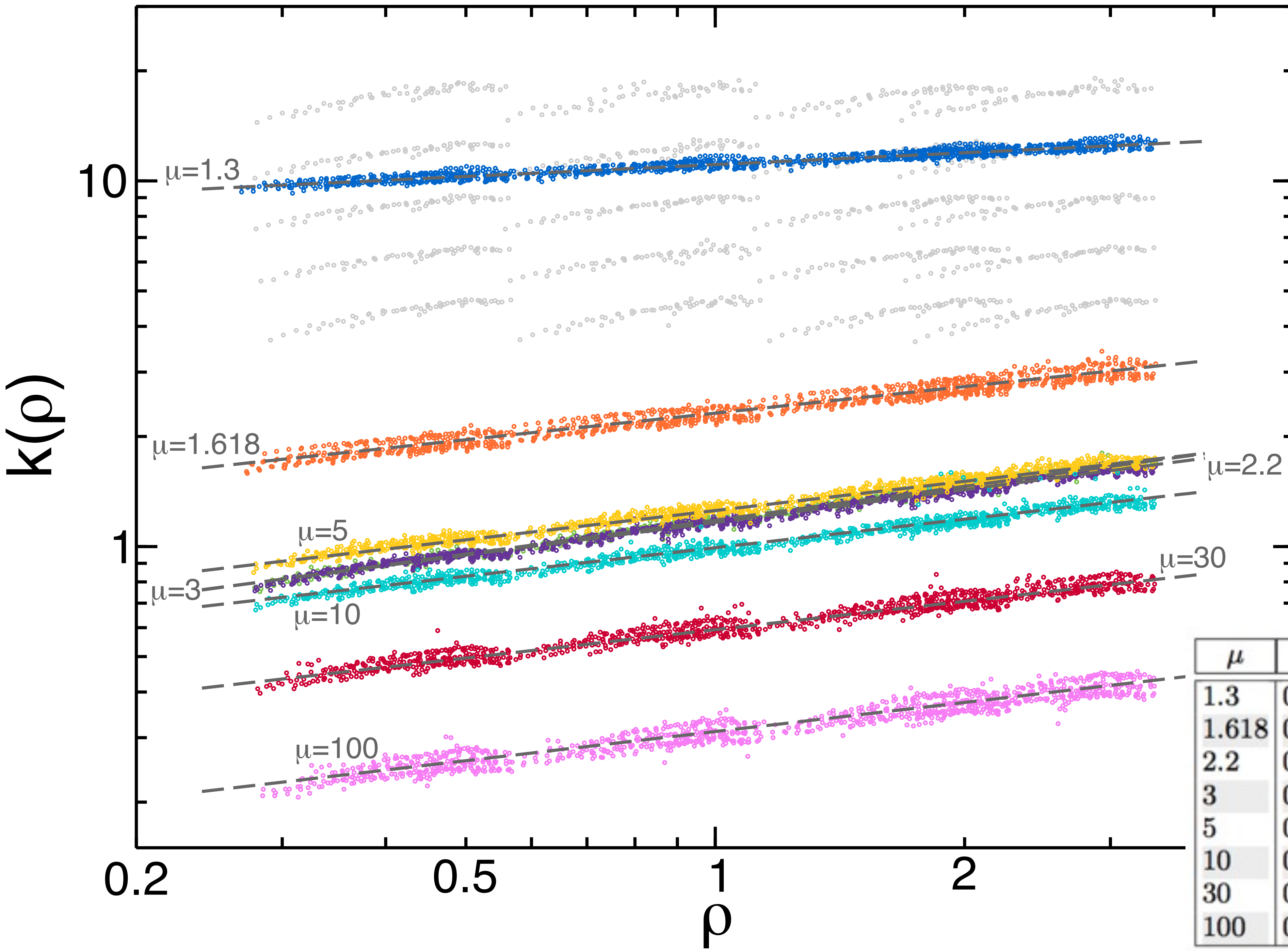
$$k(\rho) = \frac{JL^{-\alpha}}{\sqrt{T(x)}|T'(x)|}$$



μ	α	β	a
1.3	0.108 (9)	0.109 (1)	11.105 (8)
1.618	0.242 (23)	0.2408 (18)	2.307 (3)
2.2	0.308 (5)	0.3068 (11)	1.1765 (9)
3	0.297 (6)	0.2964 (11)	1.1633 (9)
5	0.266 (11)	0.2641 (12)	1.2622 (12)
10	0.260 (14)	0.2632 (19)	0.9874 (14)
30	0.258 (18)	0.257 (1)	0.5942 (12)
100	0.265 (22)	0.2648 (23)	0.3095 (5)

SOLUTION OF MACROSCOPIC TRANSPORT PROBLEM

- Using $k(\rho)=a\rho^{\alpha}$ **the macroscopic transport problem can be solved**

$$G'(\rho) = k(\rho)\rho^{-5/2} \Rightarrow G(\rho) = \nu^*(1-\rho^{\alpha-3/2}) \quad \text{with} \quad \nu^* \equiv a/(\frac{3}{2}-\alpha)$$

$$\text{constant chosen such that } F(0) = 1 = G^{-1}(0)$$

- The **master curve $F(u)=G^{-1}(u)$** hence reads $F(u) = (1-\frac{u}{\nu^*})^{\frac{2}{2\alpha-3}}$

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- The **master curve F(u)=G⁻¹(u)** hence reads $F(u) = (1-\frac{u}{\nu^*})^{\frac{2}{2\alpha-3}}$

- **Density and temperature profiles**, pressure and current in terms of control parameters T_0, T_L, η, μ and L

$$T(x) = \left[T_0^{\frac{3}{2}-\alpha} - \frac{J\sqrt{m}}{\nu^* P^\alpha} L^{-\alpha} x\right]^{\frac{2}{3-2\alpha}} \qquad \rho(x) = P/T(x)$$

$$P = \eta \left(\frac{\frac{1}{2}-\alpha}{\frac{3}{2}-\alpha}\right) \left(\frac{T_0^{3/2-\alpha} - T_L^{3/2-\alpha}}{T_0^{1/2-\alpha} - T_L^{1/2-\alpha}}\right) \qquad J = \frac{a\eta^\alpha(\frac{1}{2}-\alpha)^\alpha}{L^{1-\alpha}\sqrt{m}(\frac{3}{2}-\alpha)^{1+\alpha}} \frac{(T_0^{3/2-\alpha} - T_L^{3/2-\alpha})^{1+\alpha}}{(T_0^{1/2-\alpha} - T_L^{1/2-\alpha})^\alpha}$$

SOLUTION OF MACROSCOPIC TRANSPORT PROBLEM

- Using $k(\rho)=a\rho^{\alpha}$ **the macroscopic transport problem can be solved**

$$G'(\rho) = k(\rho)\rho^{-5/2} \Rightarrow G(\rho) = \nu^*(1-\rho^{\alpha-3/2}) \quad \text{with} \quad \nu^* \equiv a/(\frac{3}{2}-\alpha)$$

constant chosen such that $F(0) = 1 = G^{-1}(0)$

- The **master curve $F(u)=G^{-1}(u)$** hence reads $F(u) = (1-\frac{u}{\nu^*})^{\frac{2}{2\alpha-3}}$

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- **Corollary**: the master curve F(u) exhibits a vertical asymptote ⇒ maximal scaled reduced current ψ^* ⇒ **upper bound on current in terms of pressure**

$$L^{1-\alpha}J \le \psi^* P^{3/2} = \nu^* T_0^{3/2-\alpha} P^{\alpha}/\sqrt{m}$$

UNIVERSAL MASTER CURVE: THEORY VS MEASUREMENT

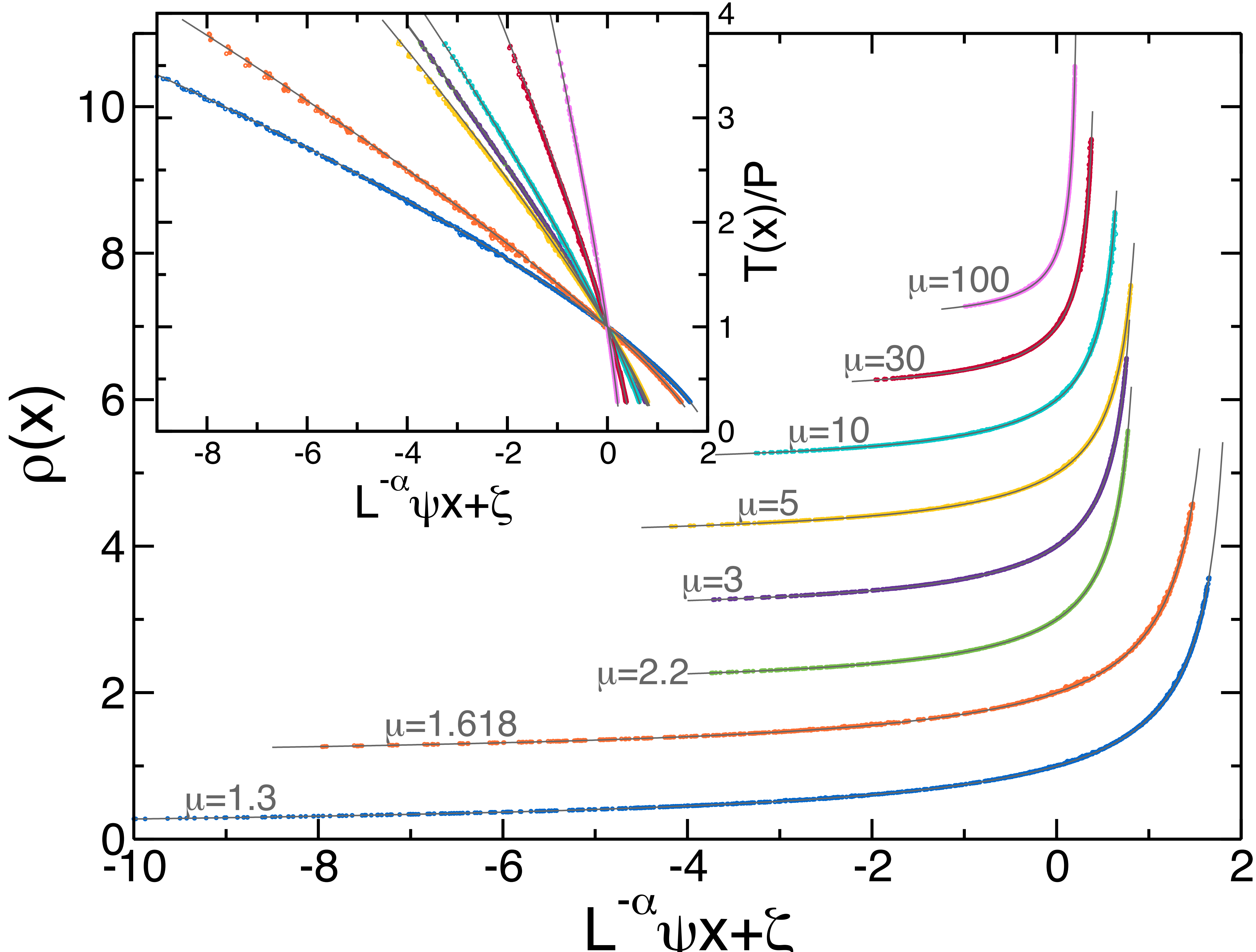
- The **agreement** with collapsed data is **striking in all cases**

$$F(u) = (1 - \frac{u}{\nu^*})^{\frac{2}{2\alpha - 3}}$$

$$\nu^* \equiv \frac{a}{\frac{3}{2} - \alpha}$$

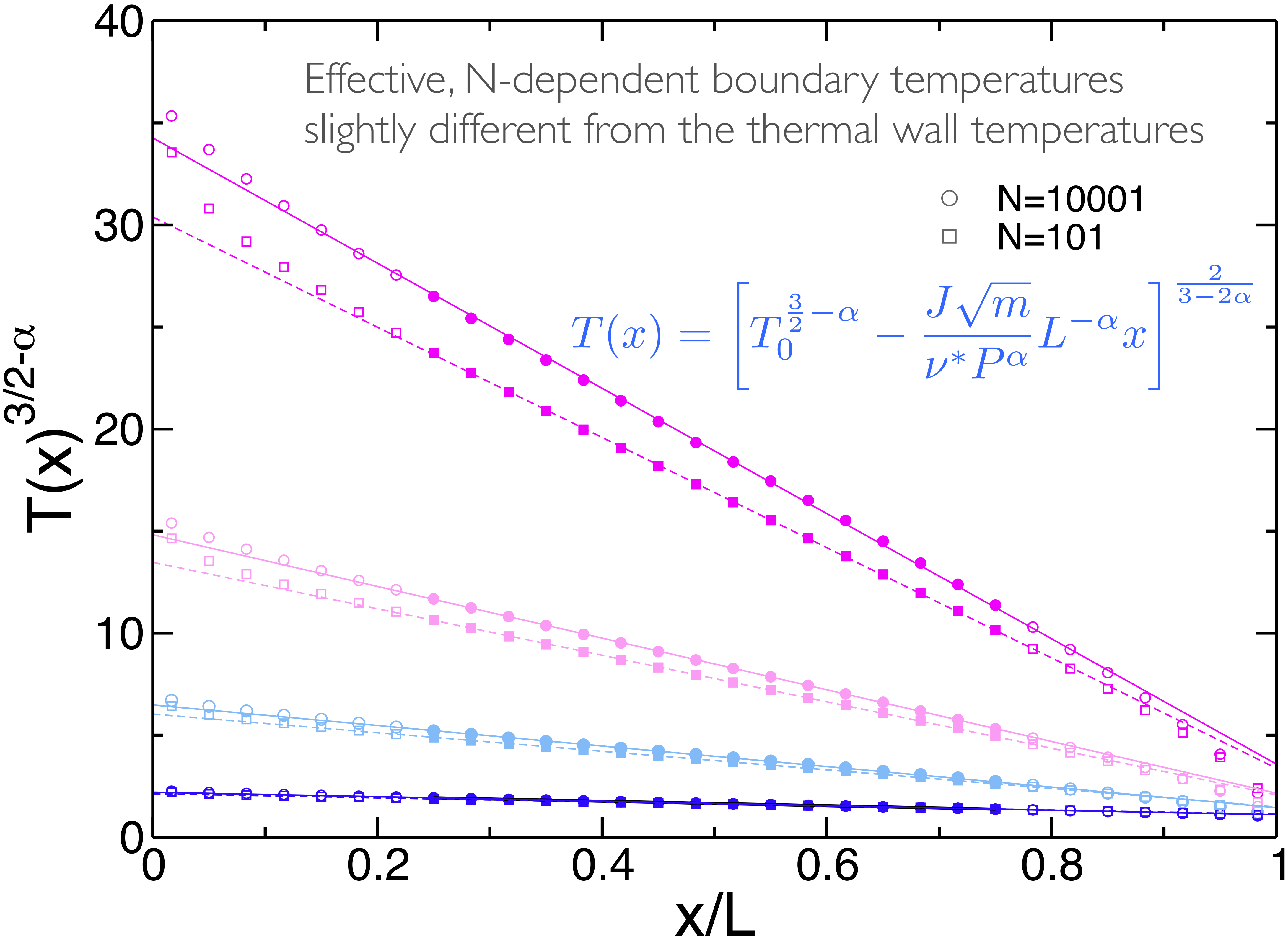
$$\alpha = \alpha(\mu)$$

$$a = a(\mu)$$

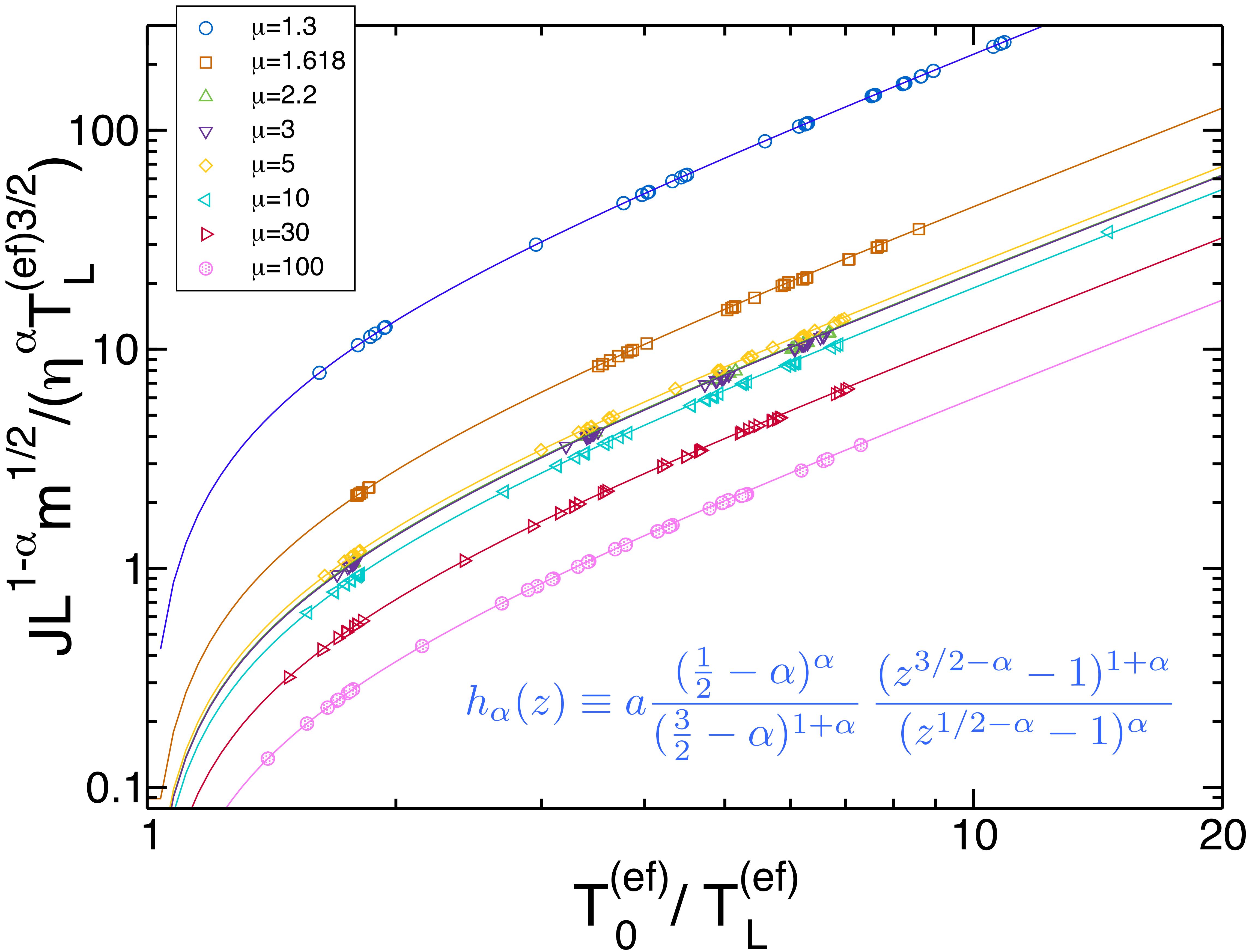


TEMPERATURE PROFILES: THEORY VS MEASUREMENT

- Theory predicts $T(x)^{3/2-\alpha}$ to be linear in x with slope $-JL^{-\alpha}m^{1/2}/(\nu^*P^\alpha)$



CURRENT: THEORY VS MEASUREMENT



INTERESTING IMPLICATIONS

$$J = -\kappa_L(\rho, T)\frac{dT(x)}{dx}$$

$$\kappa_L(\rho, T) = L^{\alpha}\sqrt{T}k(\rho)$$

$$P = \rho T$$

- Anomalous Fourier's law valid for finite systems ($N \sim 10^2$!!!) and deep into the nonlinear regime. No higher-order, Burnett-like corrections to Fourier's law

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- **Anomalous Fourier's law valid** for **finite systems** (N~10^2!!!) and deep into the **nonlinear regime**. **No higher-order, Burnett-like corrections to Fourier's law**
- **Bulk-boundary decoupling:** collapse implies that **bulk profiles for any finite N correspond to profiles of the macroscopic system!!** **Catch**: N-dependent effective boundary conditions (imposed by the boundary layers).

INTERESTING IMPLICATIONS

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- Anomalous Fourier's law valid for finite systems ($N \sim 10^2$!!!) and deep into the nonlinear regime. **No higher-order, Burnett-like corrections to Fourier's law**
- Bulk-boundary decoupling: collapse implies that **bulk profiles for any finite N correspond to profiles of the macroscopic system!!** Catch: N-dependent effective boundary conditions (imposed by the boundary layers).
- Universality breaks down for anomalous heat conduction in 1d
- These results question some predictions of nonlinear fluctuating hydrodynamic for anomalous Fourier's law in 1d.
- Reason? Maybe there are more slowly varying fields in this1d model other than the locally-conserved ones. **This has been already reported (e.g. shock waves)**
- What is the correct nonlinear fluctuating hydrodynamics description? Our data suggest that such a theory may involve an **anomalous, non-diffusive hydrodynamic scaling of microscopic spatiotemporal variables**

$$x \to x/L^{1-\alpha} \qquad\qquad t \to t/L^{2-3\alpha}$$

CHALLENGES AND OUTLOOK

- **Challenge**: How can we make compatible the **local** character of Fourier's law with the very **non-local term L^{α}** in the conductivity?
- **Scaling method completely general**: can be generalized to any d-dimensional fluid with arbitrary potential
- Scaling behavior confirmed in hard disks under temperature gradient. Similar, albeit more complex, **scaling laws hold in sheared fluids** (mixed Couette-Fourier flow)
- **Other 1d models to study**: Fermi-Pasta-Ulam, hard-point particles with shoulders, Lennard-Jones, etc.

Thank you

Backup slides

FOURIER'S LAW: STATE OF THE ART

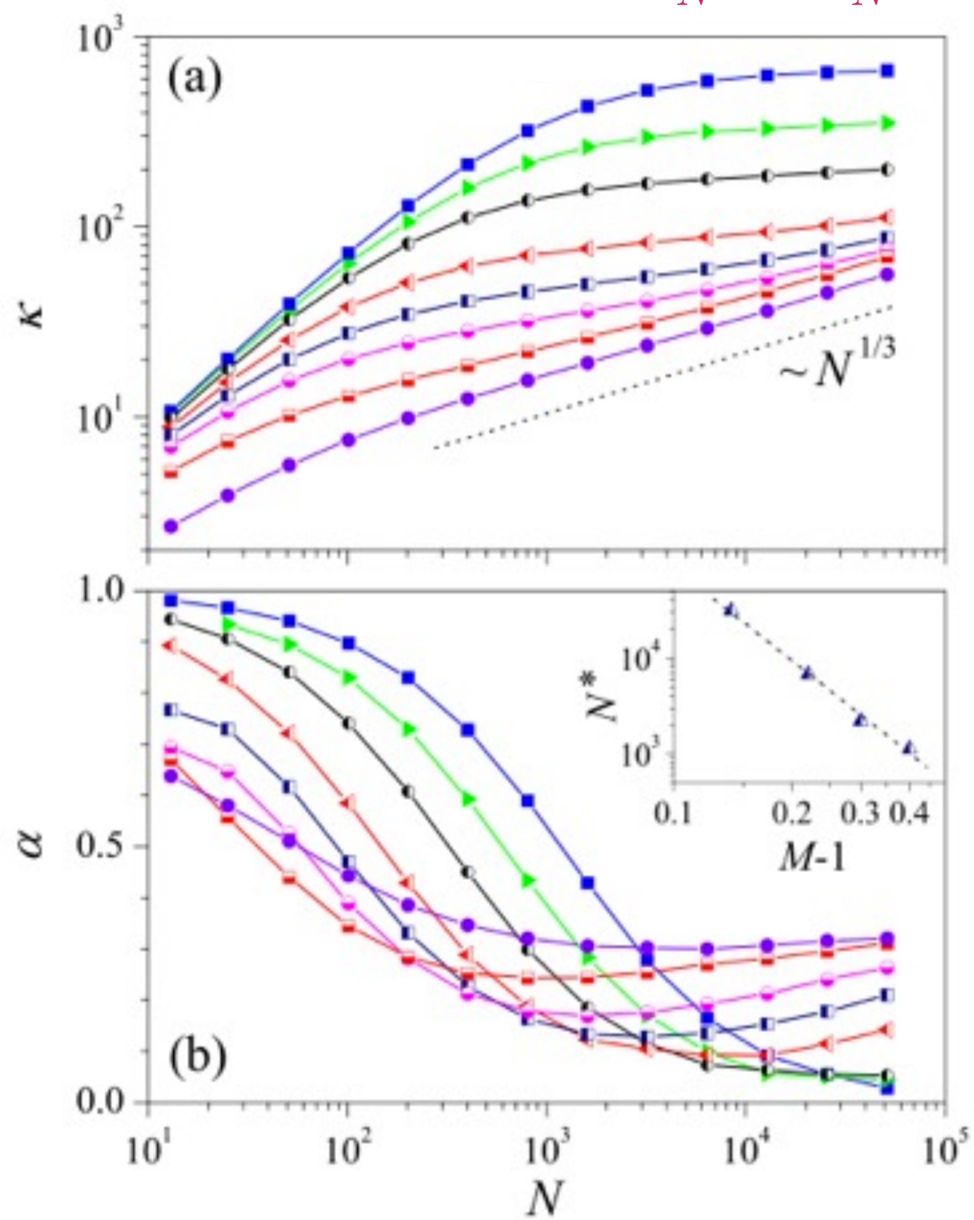
- **Numerical example**: diatomic hard-point gas

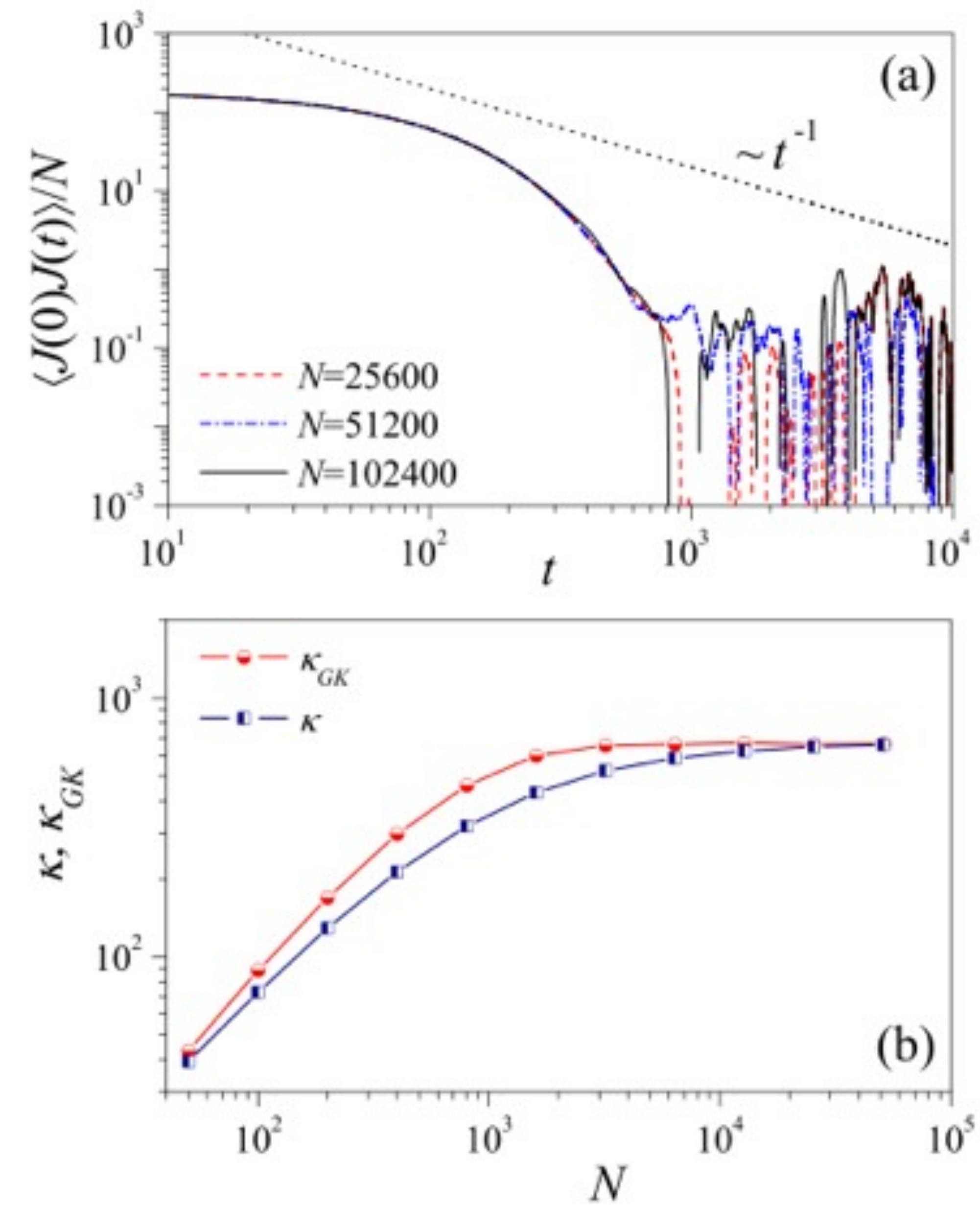
$$\kappa(N) = \frac{JN}{\Delta T}$$

Small gradient limit $\frac{\Delta T}{N} \equiv \frac{T_0 - T_L}{N} \to 0$

$$\kappa_{GK}(N) = \frac{1}{k_B T^2 N} \int_0^{\tau^*} \langle J(0)J(t) \rangle$$

Green-Kubo formula



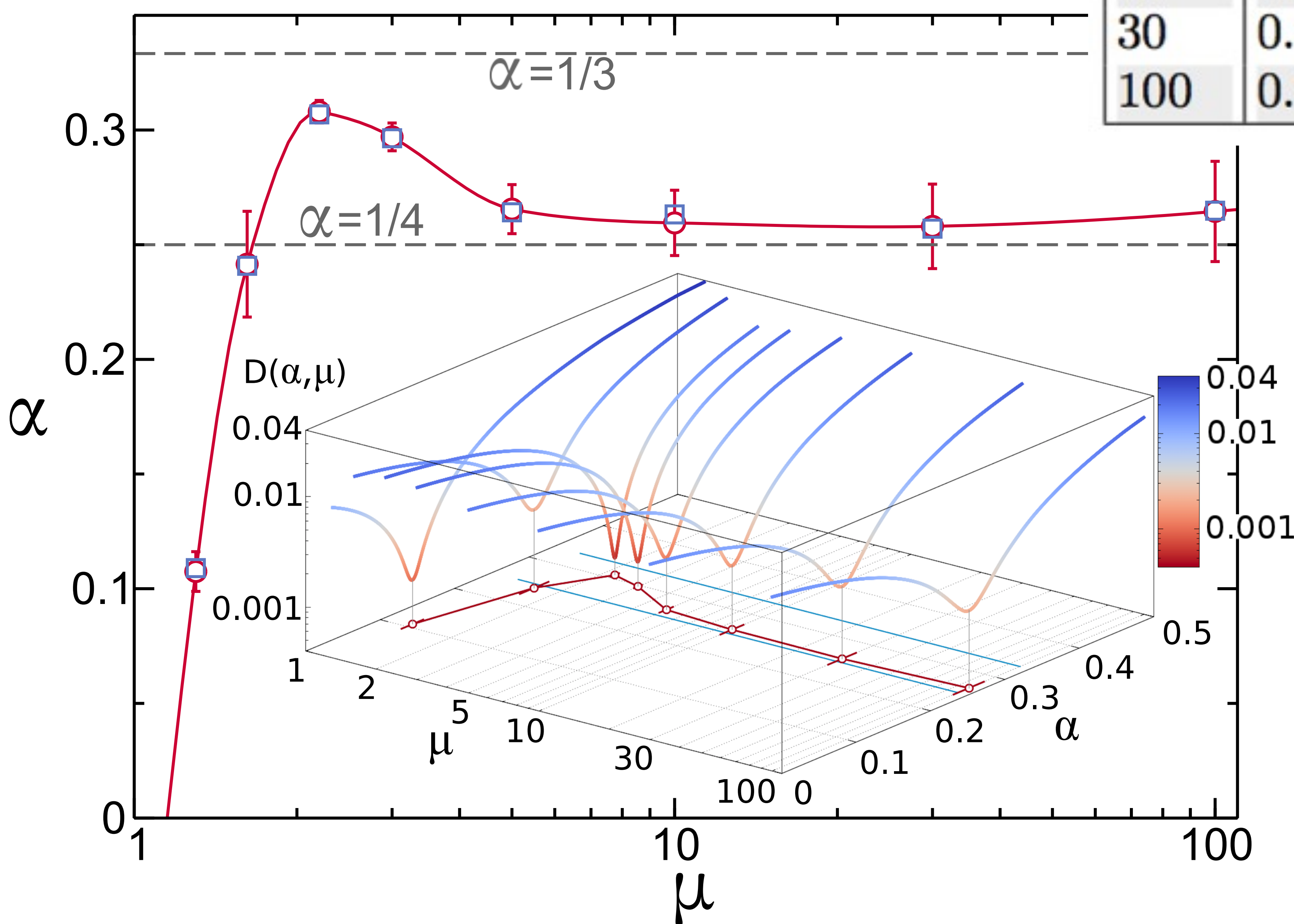


- No conclusive results though ...

S. Chen, J. Wang, G. Casati, G. Benenti, Phys. Rev. E **90**, 032134 (2014)

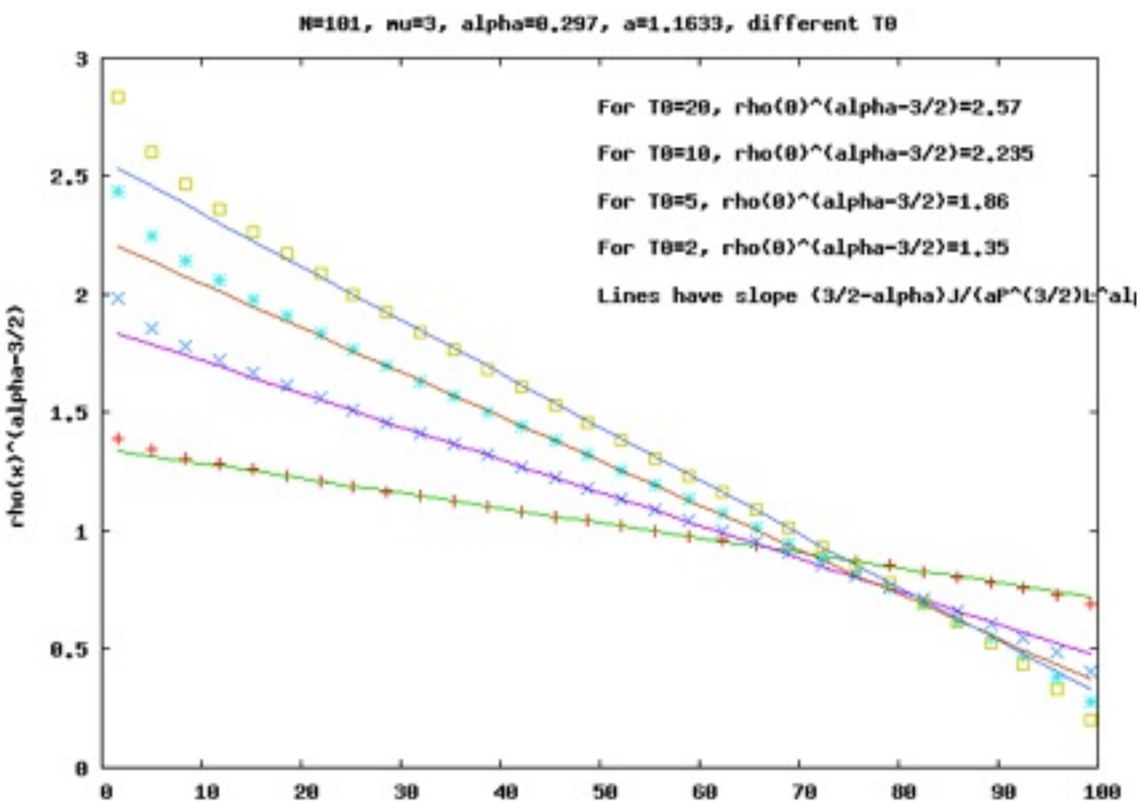
TABLE: ANOMALY EXPONENT

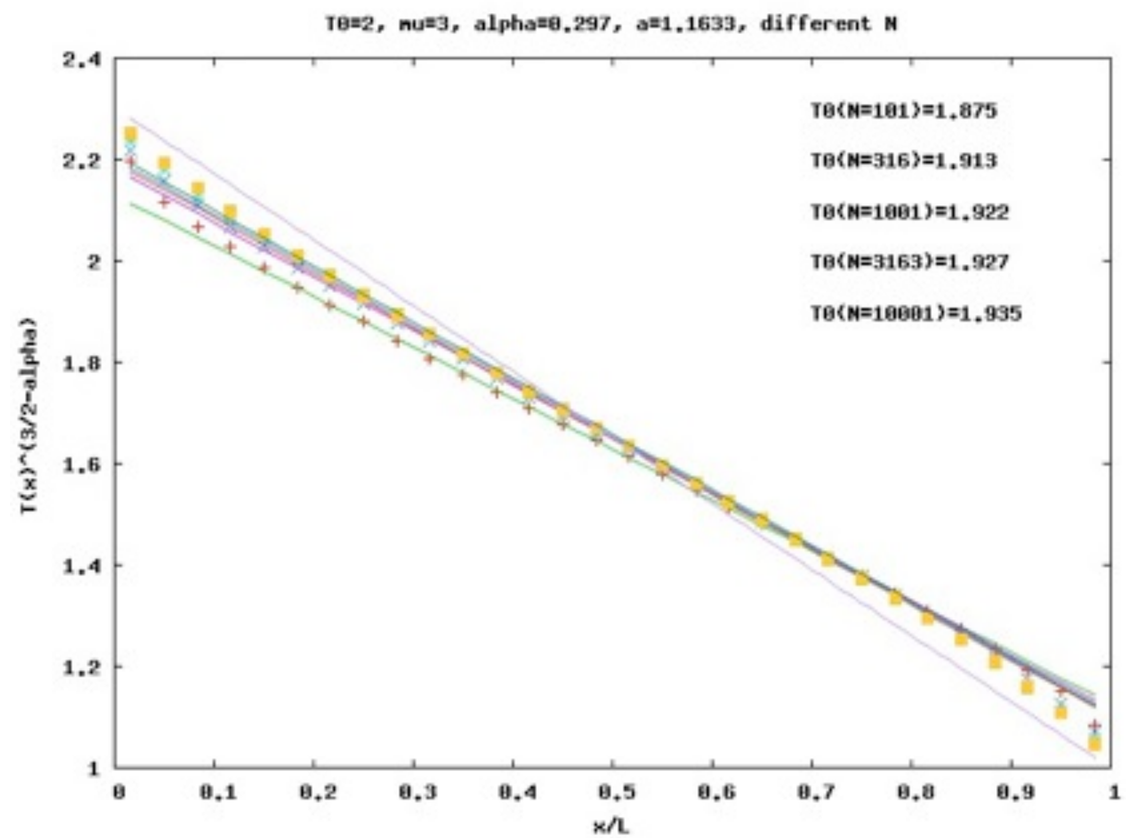
μ	α	β	a
1.3	0.108 (9)	0.109 (1)	11.105 (8)
1.618	0.242 (23)	0.2408 (18)	2.307 (3)
2.2	0.308 (5)	0.3068 (11)	1.1765 (9)
3	0.297 (6)	0.2964 (11)	1.1633 (9)
5	0.266 (11)	0.2641 (12)	1.2622 (12)
10	0.260 (14)	0.2632 (19)	0.9874 (14)
30	0.258 (18)	0.257 (1)	0.5942 (12)
100	0.265 (22)	0.2648 (23)	0.3095 (5)

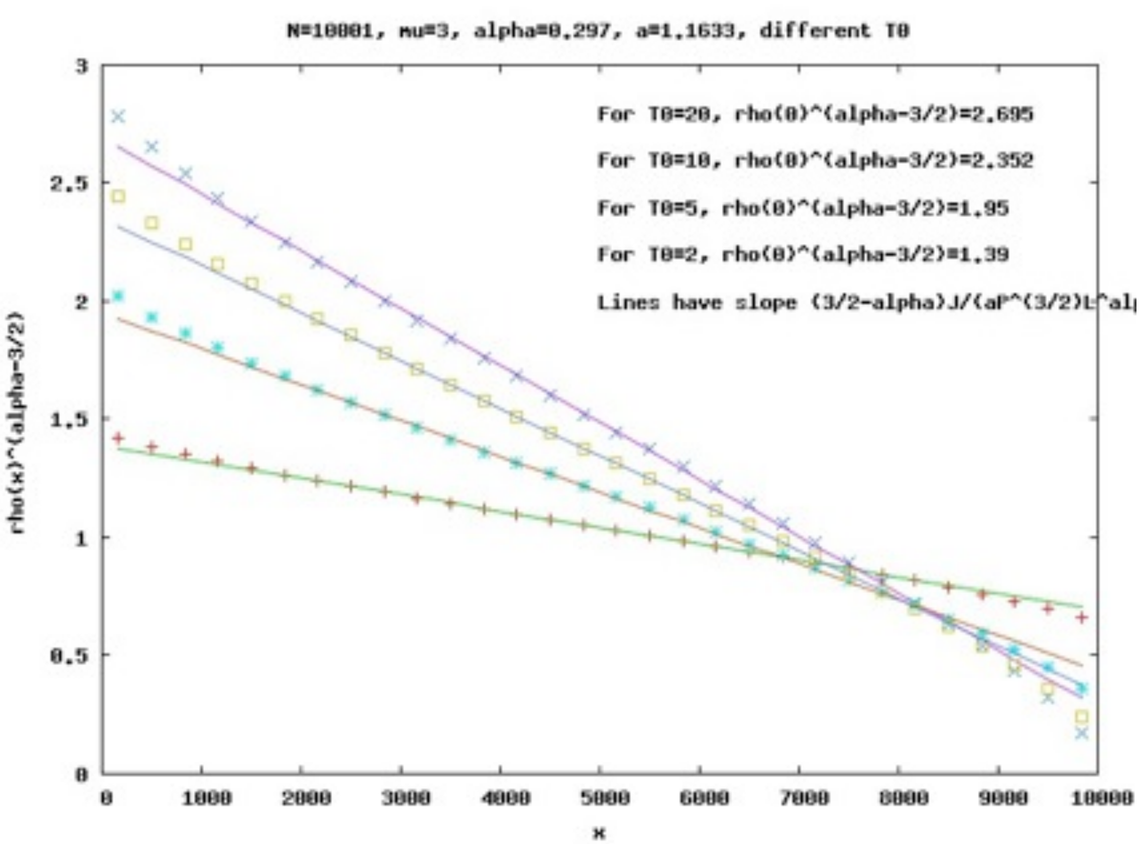


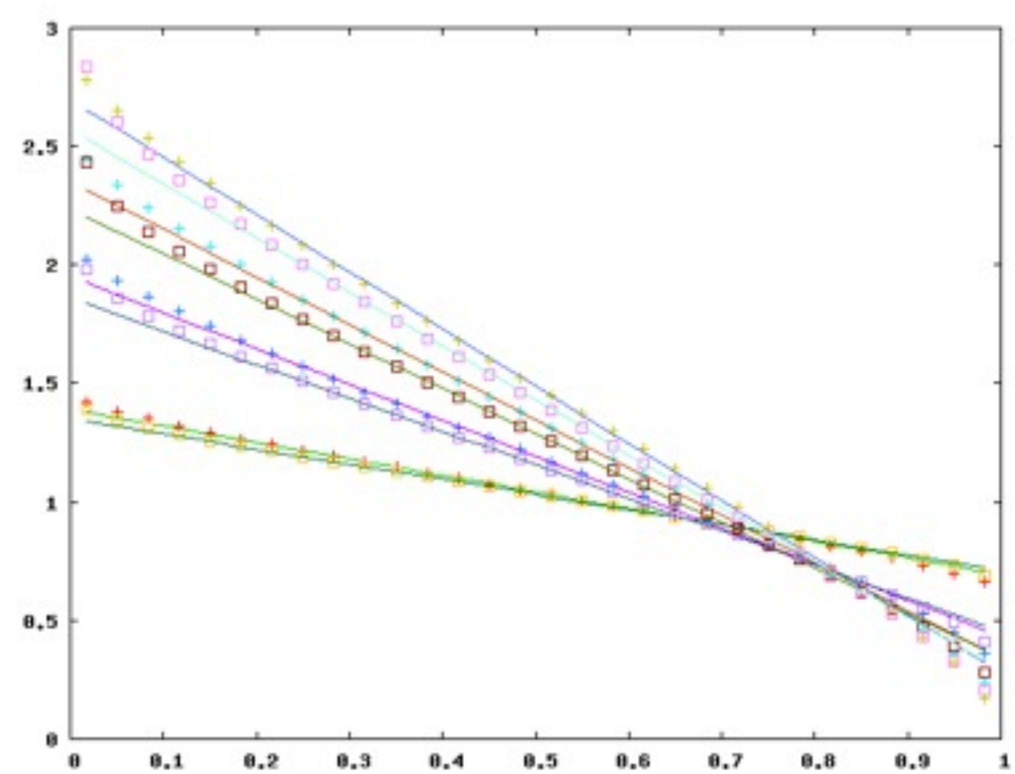
DENSITY AND TEMPERATURE PROFILES: THEORY VS SIMULATION

$$\rho(x) = \left[\rho_0 - \frac{JL^{-\alpha}}{\nu^* P^{3/2}} x\right]^{\frac{2}{2\alpha-3}}$$

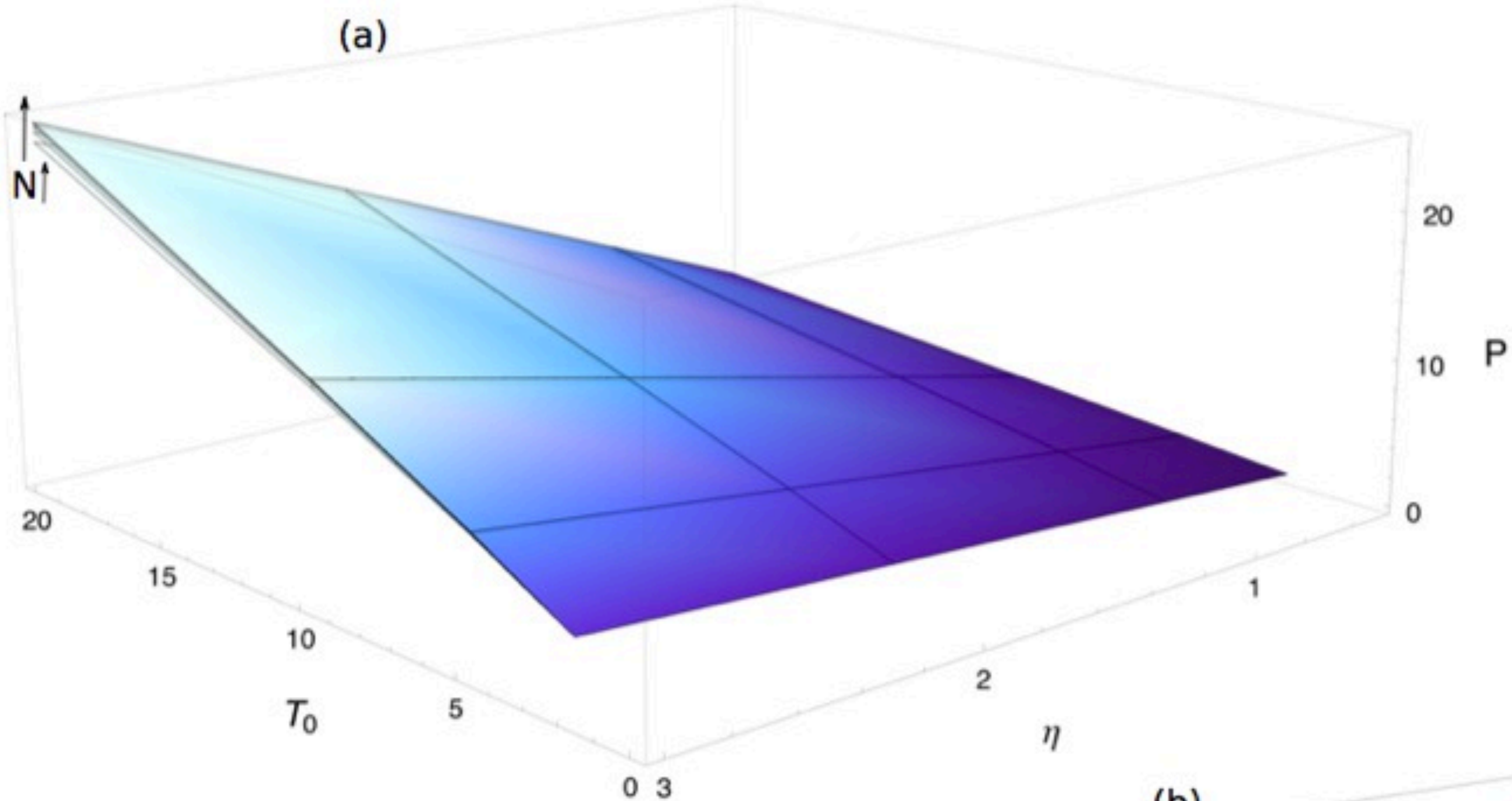




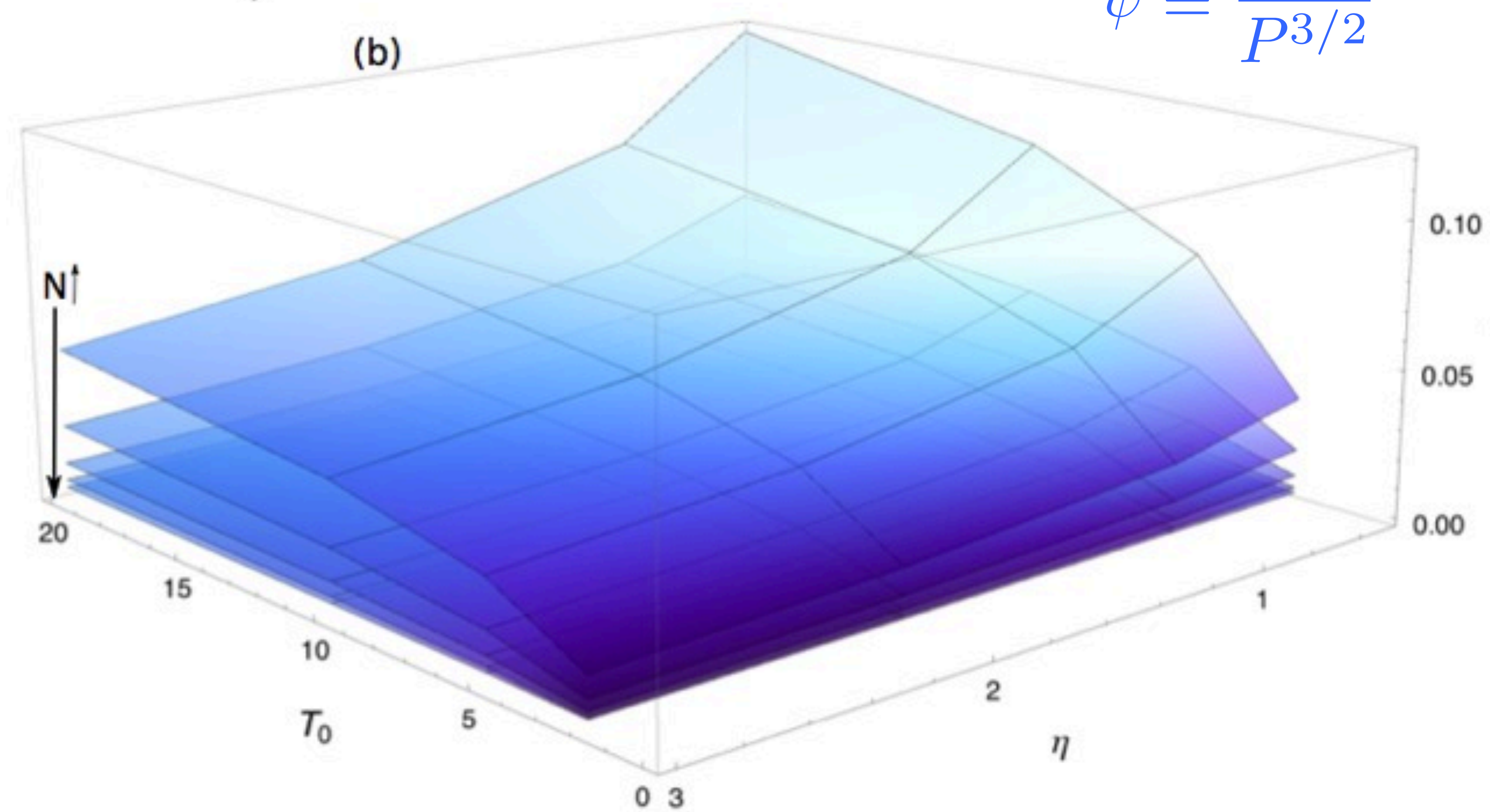




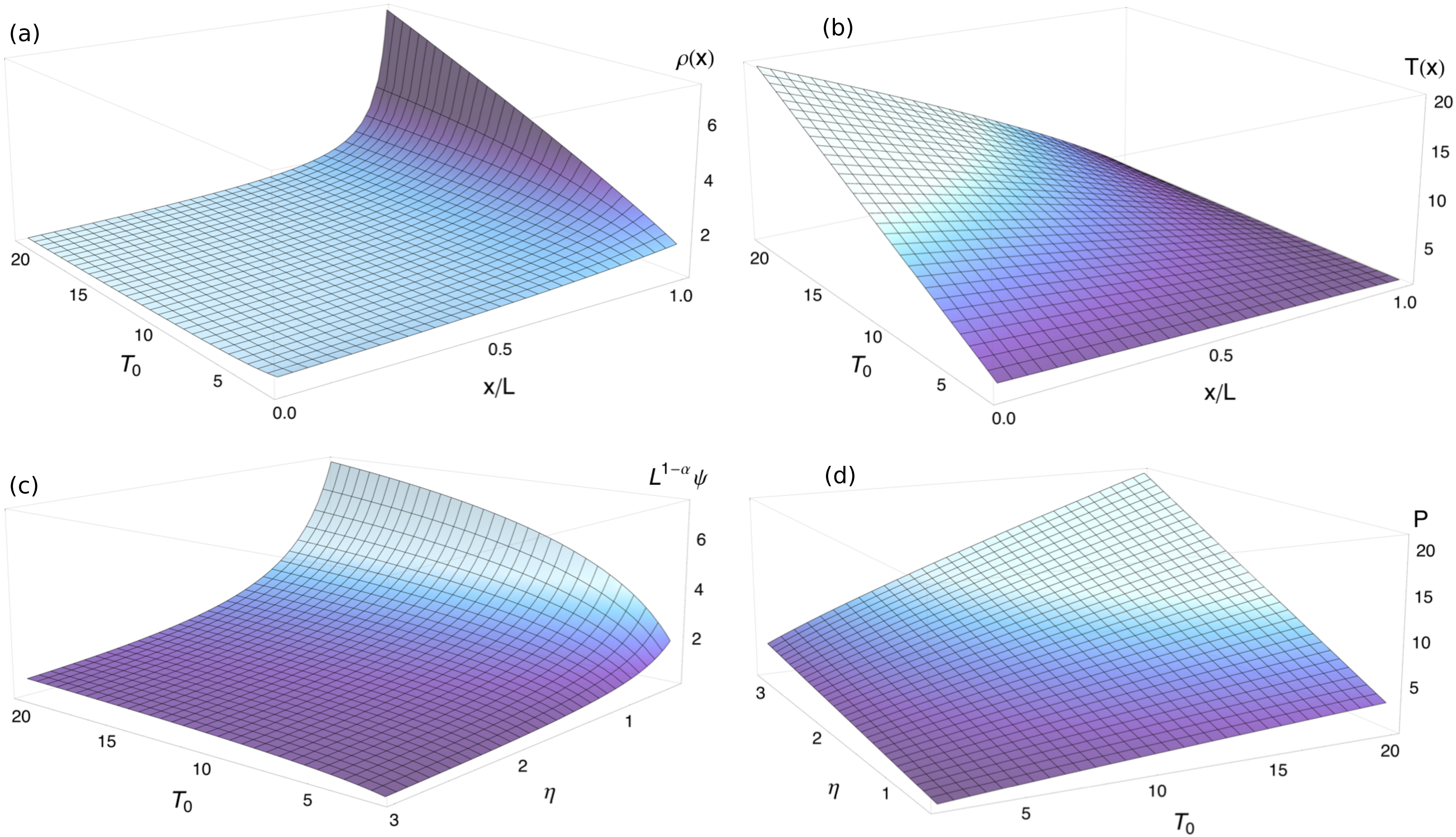
DATA FOR PRESSURE AND REDUCED CURRENT



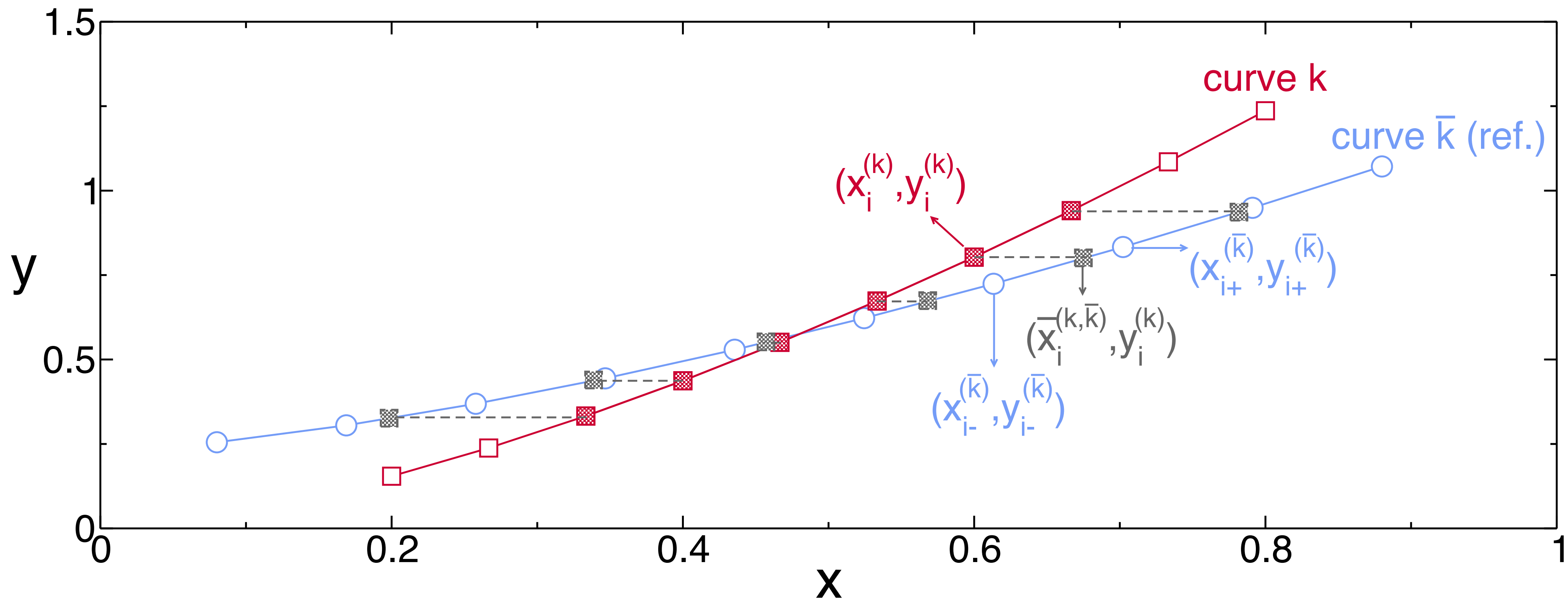
$$\psi \equiv \frac{J}{P^{3/2}}$$



SOLUTION OF MACROSCOPIC TRANSPORT PROBLEM



A METRIC TO QUANTIFY DATA COLLAPSE



$$D \equiv \frac{1}{\ell_{\max}\mathcal{N}_{\mathrm{overl}}} \sum_{\bar{k}=1}^{K} \sum_{\substack{k=1 \\ k\neq\bar{k}}}^{K} \sum_{\substack{i=1 \\ i\ \mathrm{overlap}\ \bar{k}}}^{M} \left| x_i^{(k)} - \bar{x}_i^{(k,\bar{k})} \right| ,$$

$$A_i^{(k,\bar{k})} = \frac{y_{i+}^{(\bar{k})} - y_{i-}^{(\bar{k})}}{x_{i+}^{(\bar{k})} - x_{i-}^{(\bar{k})}}$$

$$\bar{x}_i^{(k,\bar{k})} = \frac{y_i^{(k)} - B_i^{(k,\bar{k})}}{A_i^{(k,\bar{k})}}$$

$$B_i^{(k,\bar{k})} = \frac{y_{i+}^{(\bar{k})} x_{i-}^{(\bar{k})} - y_{i-}^{(\bar{k})} x_{i+}^{(\bar{k})}}{x_{i+}^{(\bar{k})} - x_{i-}^{(\bar{k})}}$$

SCALING: BOUNDARY CONDITIONS FOR DENSITY FIELD AND MACROSCOPIC SOLUTION

- Boundary conditions for the density field can be inferred from the constraints

$$\frac{T_0}{T_L} = \frac{\rho_L}{\rho_0}$$

$$\eta = \frac{1}{L}\int_0^L \rho(x)dx = \frac{\int_{\rho_0}^{\rho_L} \rho\, G'(\rho)d\rho}{G(\rho_L) - G(\rho_0)}$$

- Moreover, we empirically find that k(ρ)=aρ^α, and this results in:

$$G'(\rho) = k(\rho)\rho^{-5/2} \Rightarrow G(\rho) = \nu^*(1-\rho^{\alpha-3/2}) \quad \text{with} \quad \nu^* \equiv a/(\frac{3}{2}-\alpha)$$

constant chosen such that $F(0) = 1 = G^{-1}(0)$

- Hence the master curve $F(u)=G^{-1}(u)$ reads $F(u) = (1-\frac{u}{\nu^*})^{\frac{2}{2\alpha-3}}$

- Density and temperature profiles, pressure and current

$$\rho(x) = \left[\left(\frac{P}{T_0}\right)^{\alpha-\frac{3}{2}} - \frac{\psi}{\nu^*}L^{-\alpha}x\right]^{\frac{2}{2\alpha-3}} \qquad T(x) = P/\rho(x)$$

$$P = \eta\left(\frac{\frac{1}{2}-\alpha}{\frac{3}{2}-\alpha}\right)\left(\frac{T_0^{3/2-\alpha} - T_L^{3/2-\alpha}}{T_0^{1/2-\alpha} - T_L^{1/2-\alpha}}\right) \qquad J = \frac{a\eta^\alpha(\frac{1}{2}-\alpha)^\alpha}{L^{1-\alpha}(\frac{3}{2}-\alpha)^{1+\alpha}}\,\frac{(T_0^{3/2-\alpha} - T_L^{3/2-\alpha})^{1+\alpha}}{(T_0^{1/2-\alpha} - T_L^{1/2-\alpha})^\alpha}$$

INSTITUTO CARLOS I
FÍSICA TEÓRICA Y COMPUTACIONAL

SCALING LAWS AND BULK-BOUNDARY DECOUPLING IN HEAT FLOW

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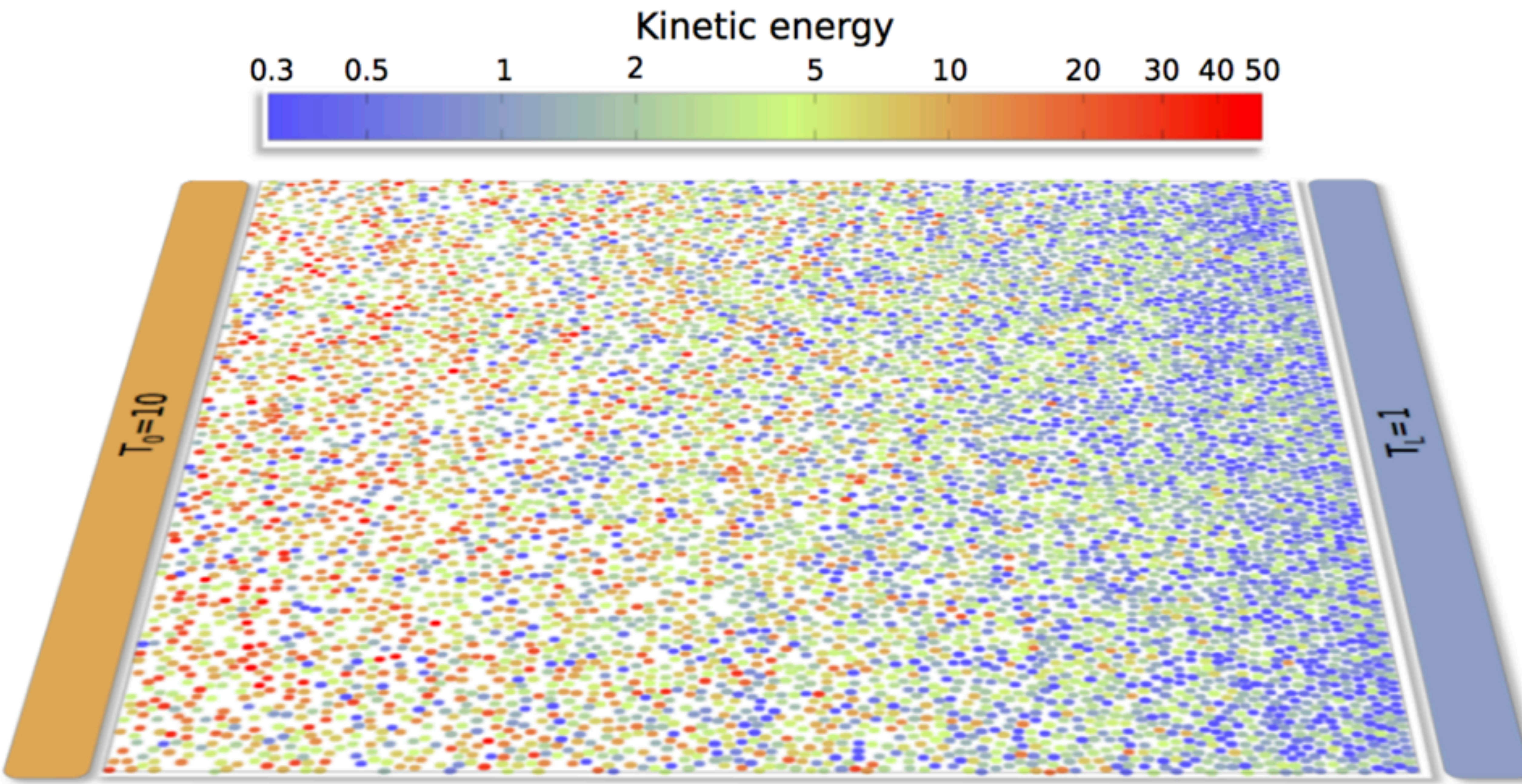
Universidad de Granada (Spain)

in collaboration with
Pedro L. Garrido
Jesús J. del Pozo

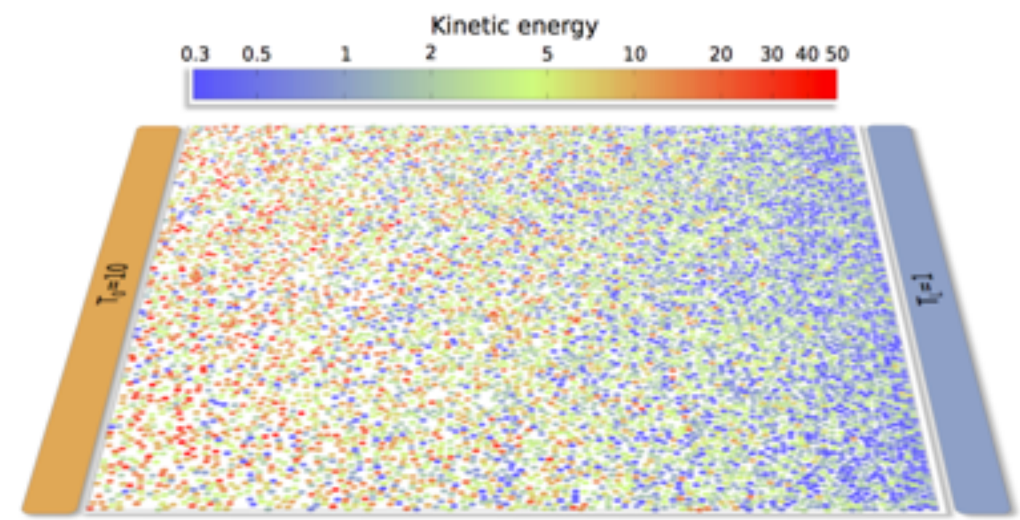
Workshop on Nonequilibrium Statistical Mechanics
ICTS, Bangalore, October 30 (2015)

MODEL: HARD-DISK FLUID OUT OF EQUILIBRIUM



MODEL: HARD-DISK FLUID OUT OF EQUILIBRIUM

- **Advantages:**
  - ☑ Simple dynamical rules (elastic collisions)
  - ☑ Efficient computer algorithm: event driven simulation + stochastic heat baths
  - ☑ Athermal behavior: temperature scales out of thermodynamic/transport quantities



- **Drawbacks/interesting points:**
  - ☑ Divergence of heat conductivity as $N \to \infty$ due to long-time tails
  - ☑ Expected strong finite-size effects

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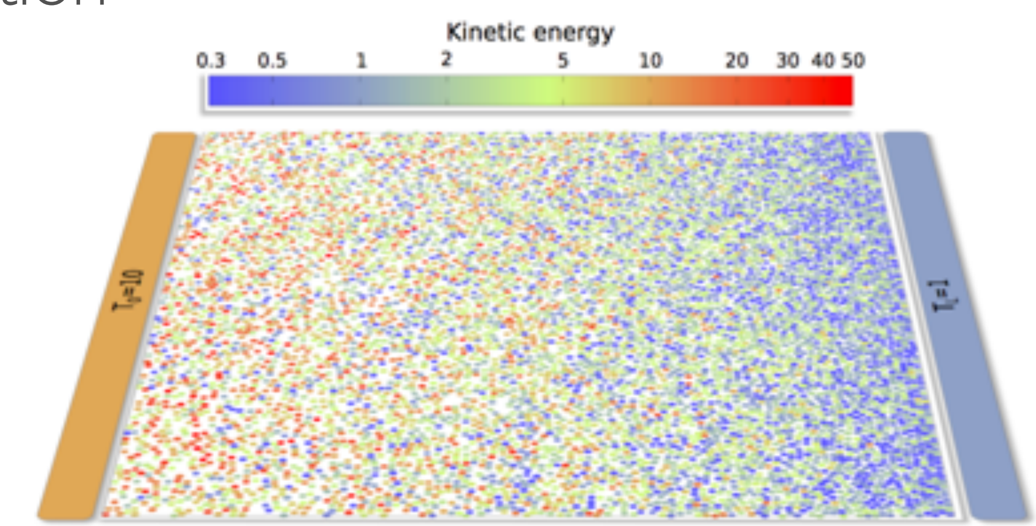


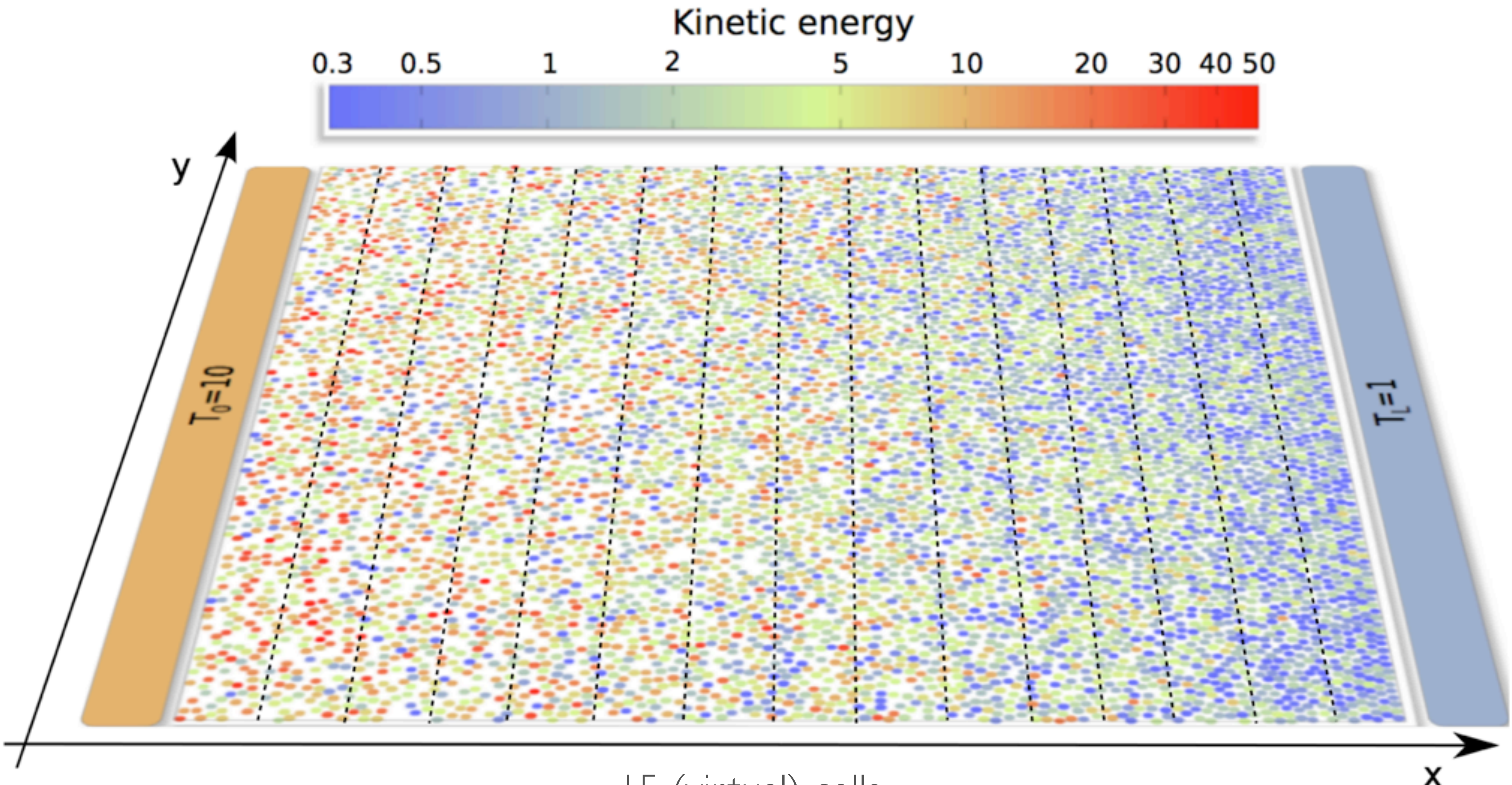
- **Drawbacks/interesting points:**
  - ☑ Divergence of heat conductivity as $N\to\infty$ due to long-time tails
  - ☑ Expected strong finite-size effects

222 simulations

- 10 different $N\in[1500,9000]$
- 20 different ΔT with $T_0\in[1,20]$
- 12 packing fractions $\eta\in[0.05,0.6]$

MEASURED OBSERVABLES

- At the **nonequilibrium steady state**, we measure **LOCAL** magnitudes ...

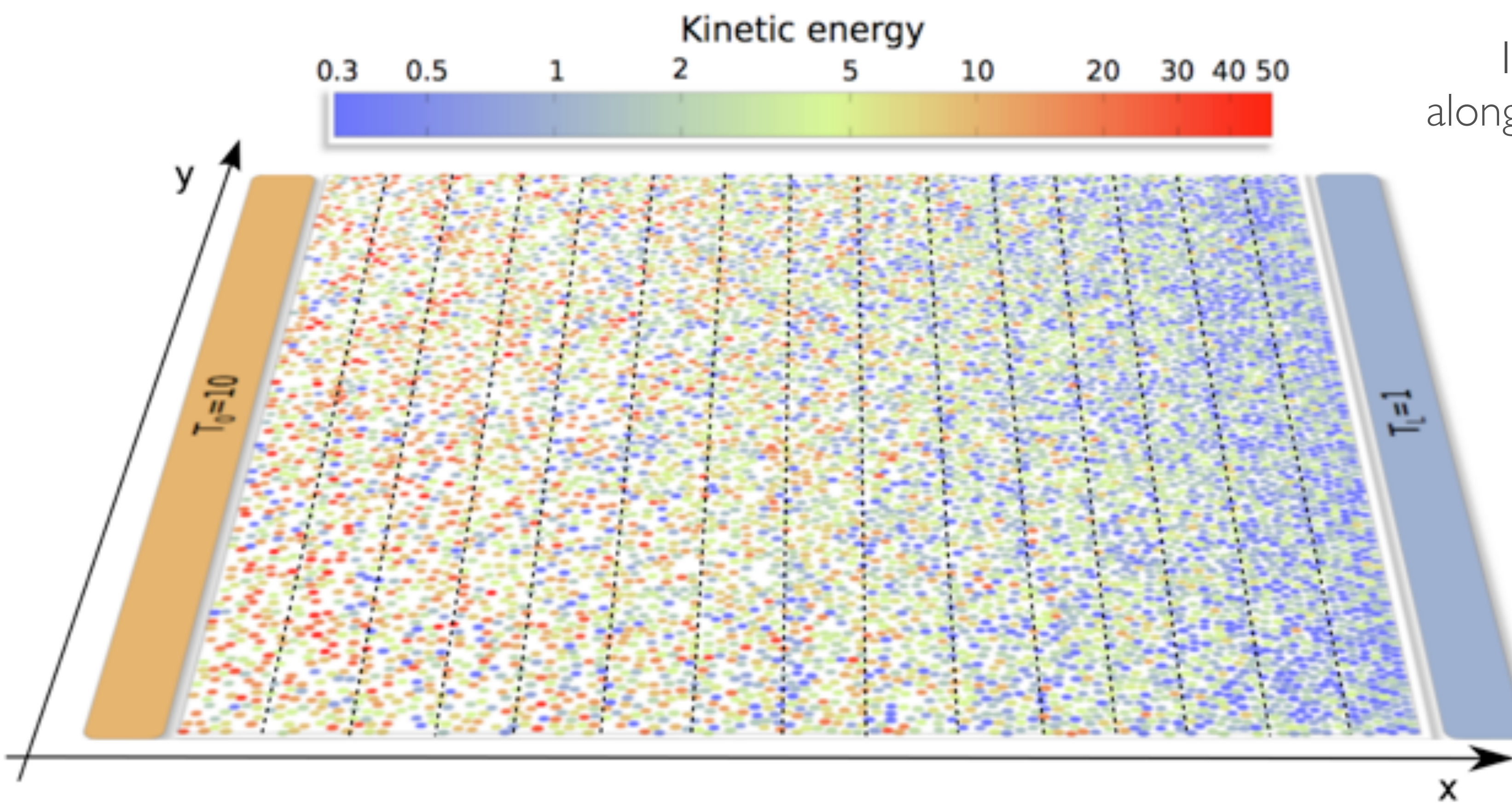


15 (virtual) cells
along gradient direction

MEASURED OBSERVABLES

- At the **nonequilibrium steady state**, we measure **LOCAL** magnitudes ...

  - ☑ Local temperature: $T_x = \frac{1}{N_x} \sum_{i=1}^{N_x} \vec{v}_i^2 \quad (x=1,2,\ldots,15)$
  - ☑ Local density: $\rho_x = \frac{N_x \pi \ell^2}{L^2}$
  - ☑ Local virial pressure: $P_x^{(v)} = N_x T_x + \frac{1}{2\tau_{\rm col}} \sum_{n=1}^{N_{\rm col}} \vec{r}_n^{(x)} \cdot \vec{v}_n^{(x)}$
  - ☑ Wall pressure: $P^{(w)} = \frac{1}{L\tau_{\rm col}} \sum_{n=1}^{N_{\rm col}} \Delta p_x^{(n)}$
  - ☑ Energy current (at walls)
  - ☑ Etc. etc



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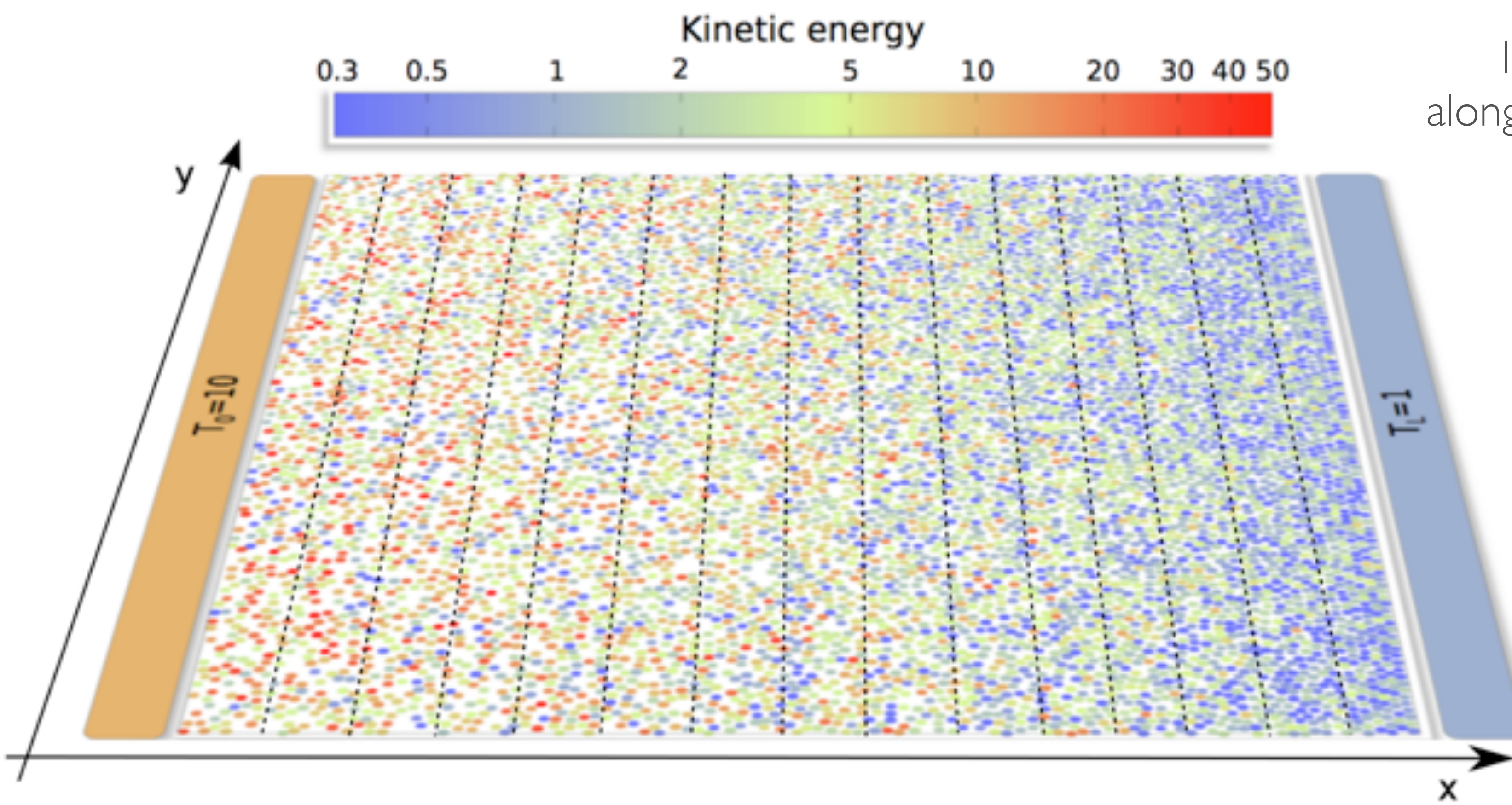
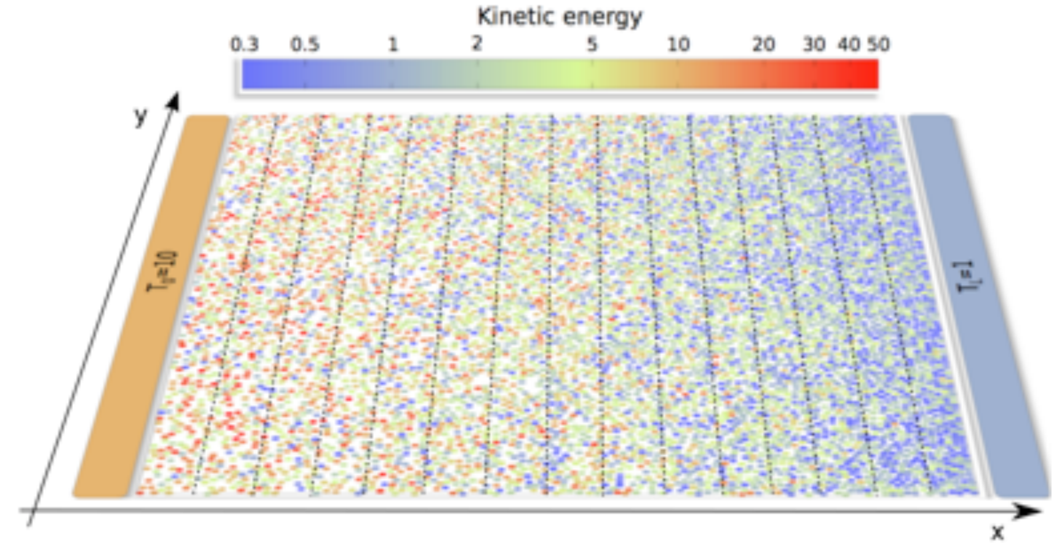


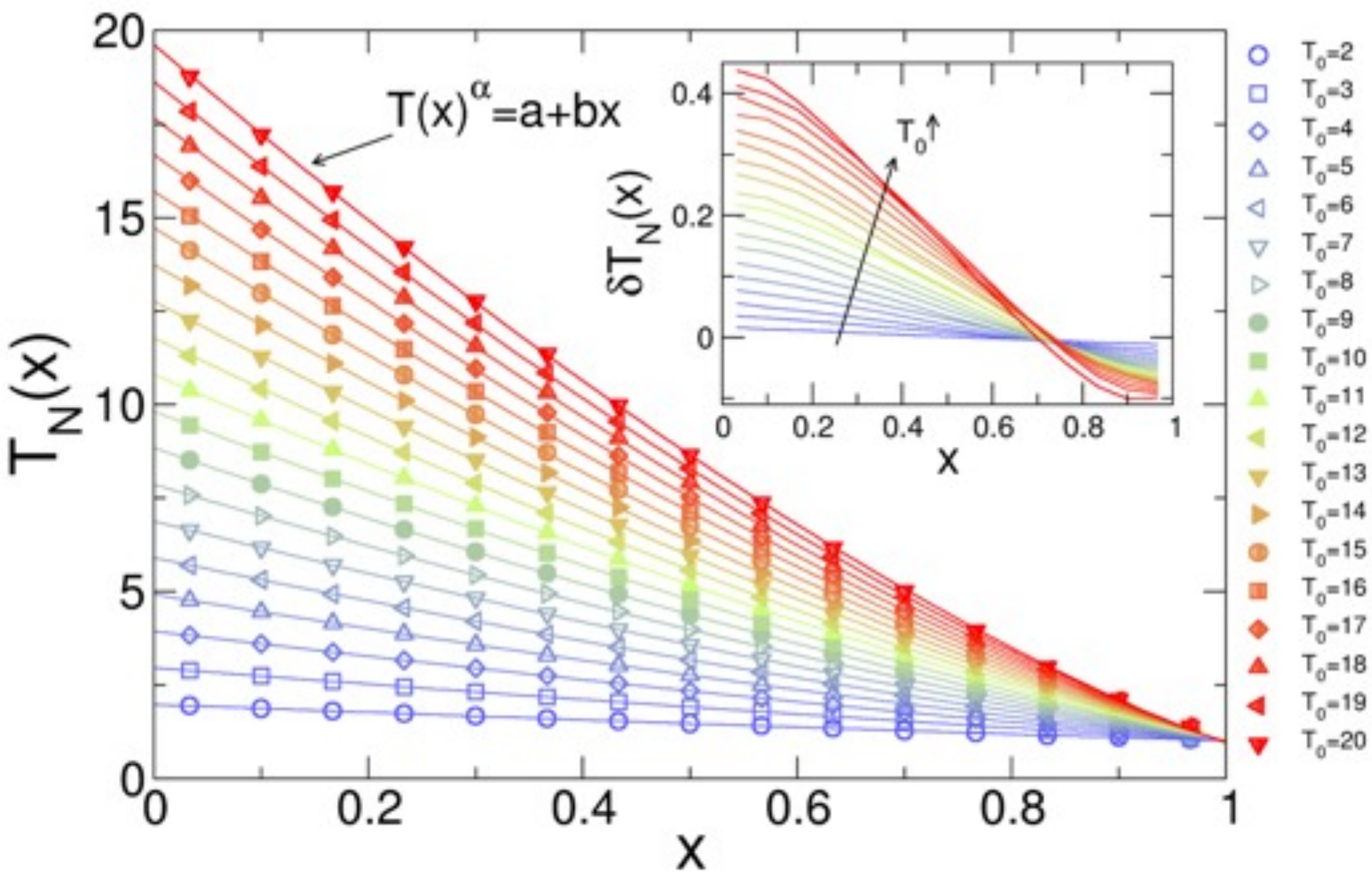
- ... and **GLOBAL** observables:
  - ☑ One-particle velocity distribution and its moments
  - ☑ Total energy per particle distribution and its moments

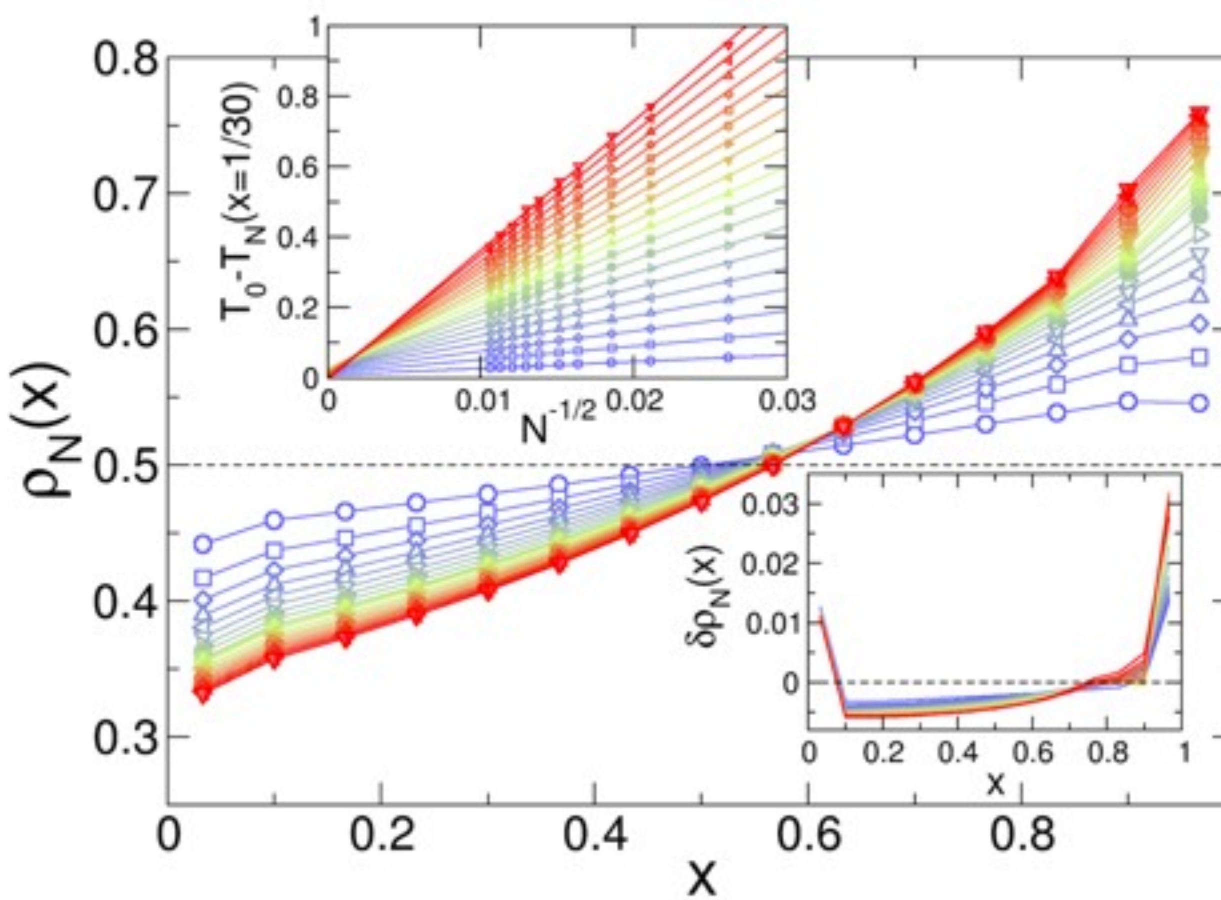
HYDRODYNAMIC PROFILES



- **Nonlinear** temperature and density profiles
- **Strong finite-size effects!!**

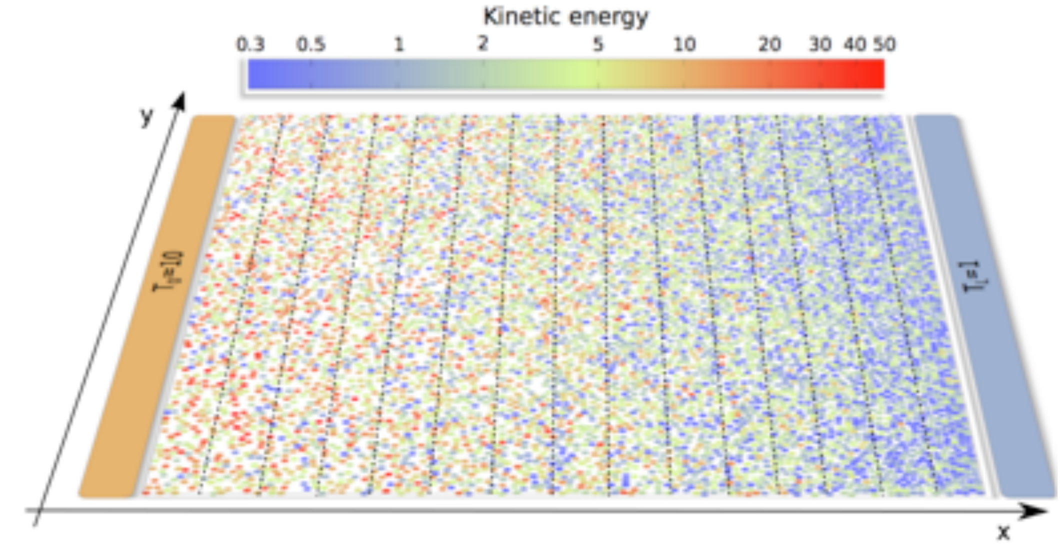
$$\delta f_{\mathrm{N}}(x) = f_{\mathrm{N_{max}}}(x) - f_{\mathrm{N_{min}}}(x)$$





N=8838, **η**=0.5

HYDRODYNAMIC PROFILES

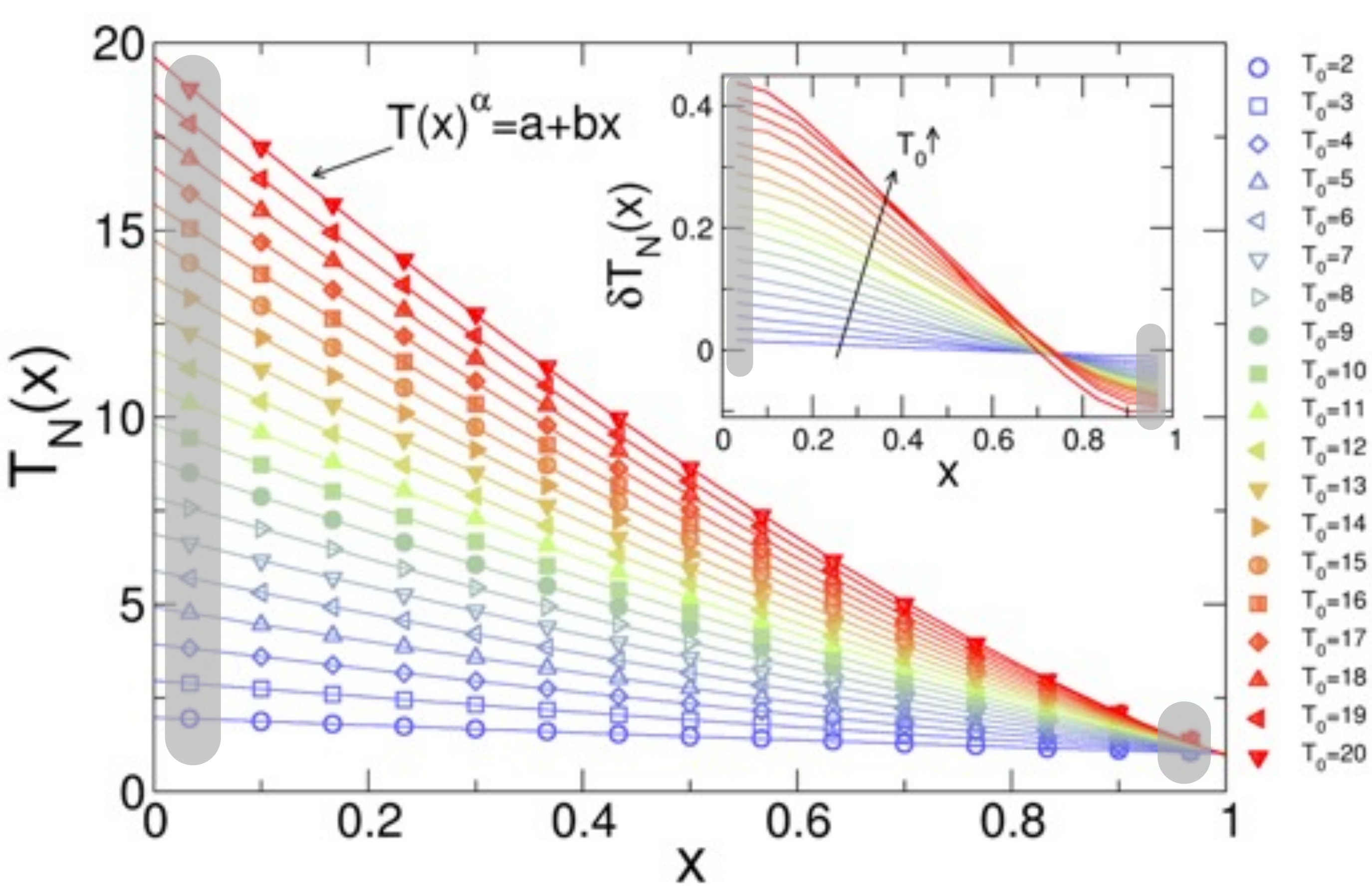


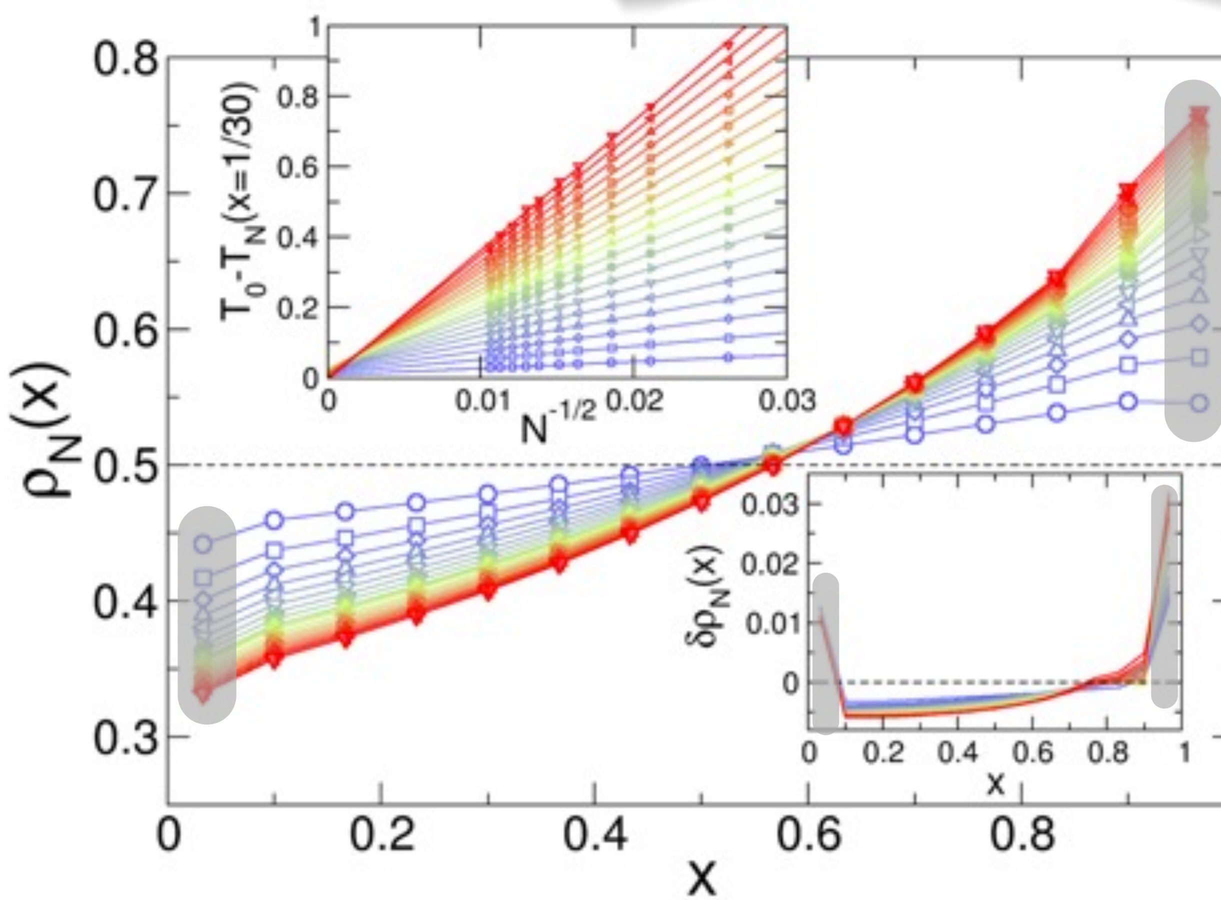
- **Nonlinear** temperature and density profiles
- **Strong finite-size effects!!**

$$\delta f_{\mathrm{N}}(x) = f_{\mathrm{N_{max}}}(x) - f_{\mathrm{N_{min}}}(x)$$

- Thermal walls disrupt the surrounding fluid: **boundary layers**
- Thermal resistance or **temperature gap at walls**

Remove boundary layers



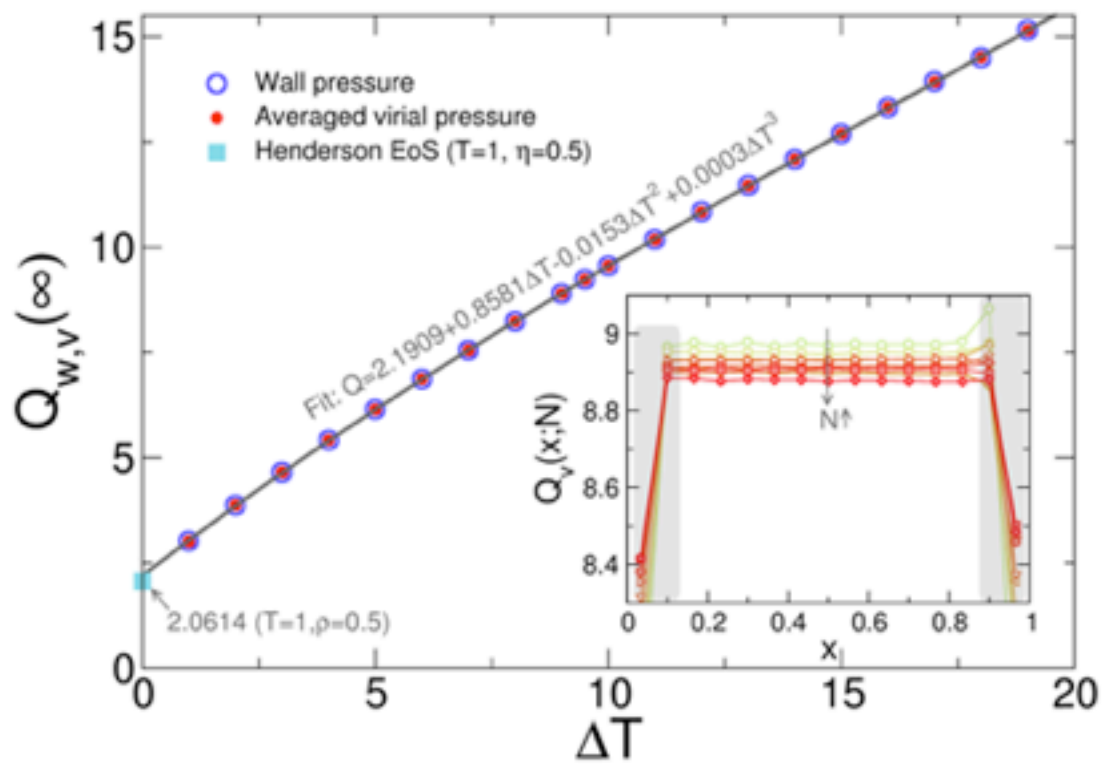


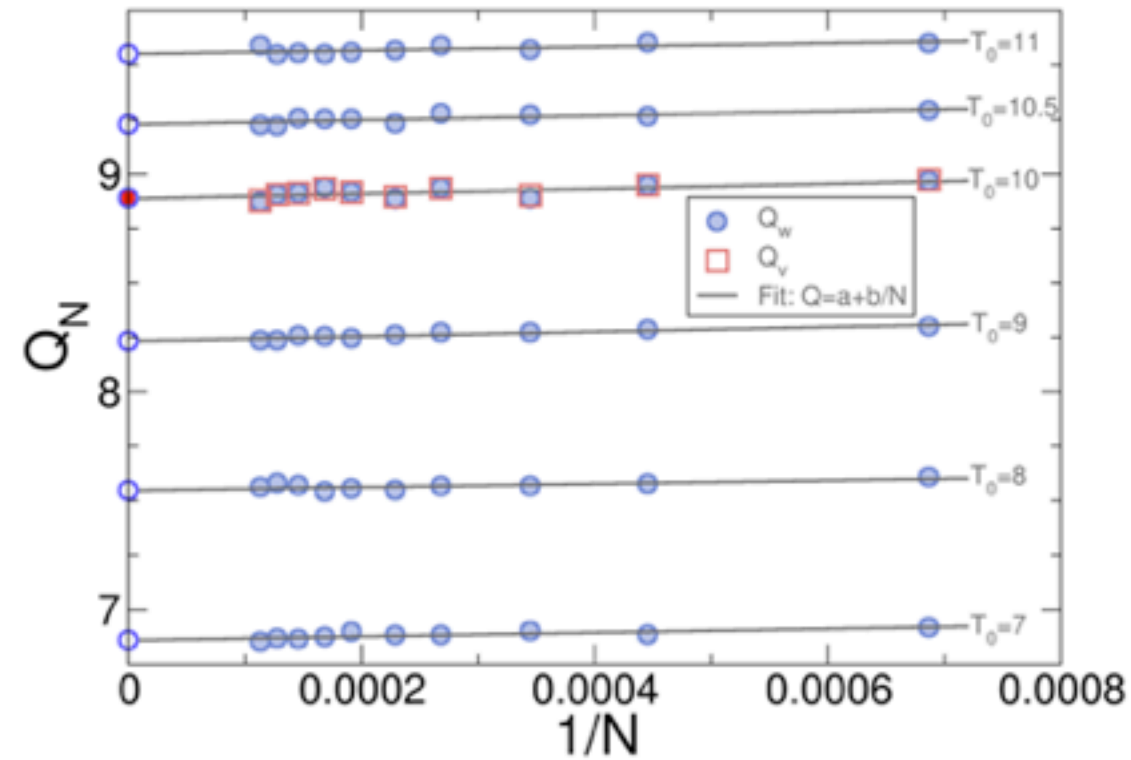
N=8838, η=0.5

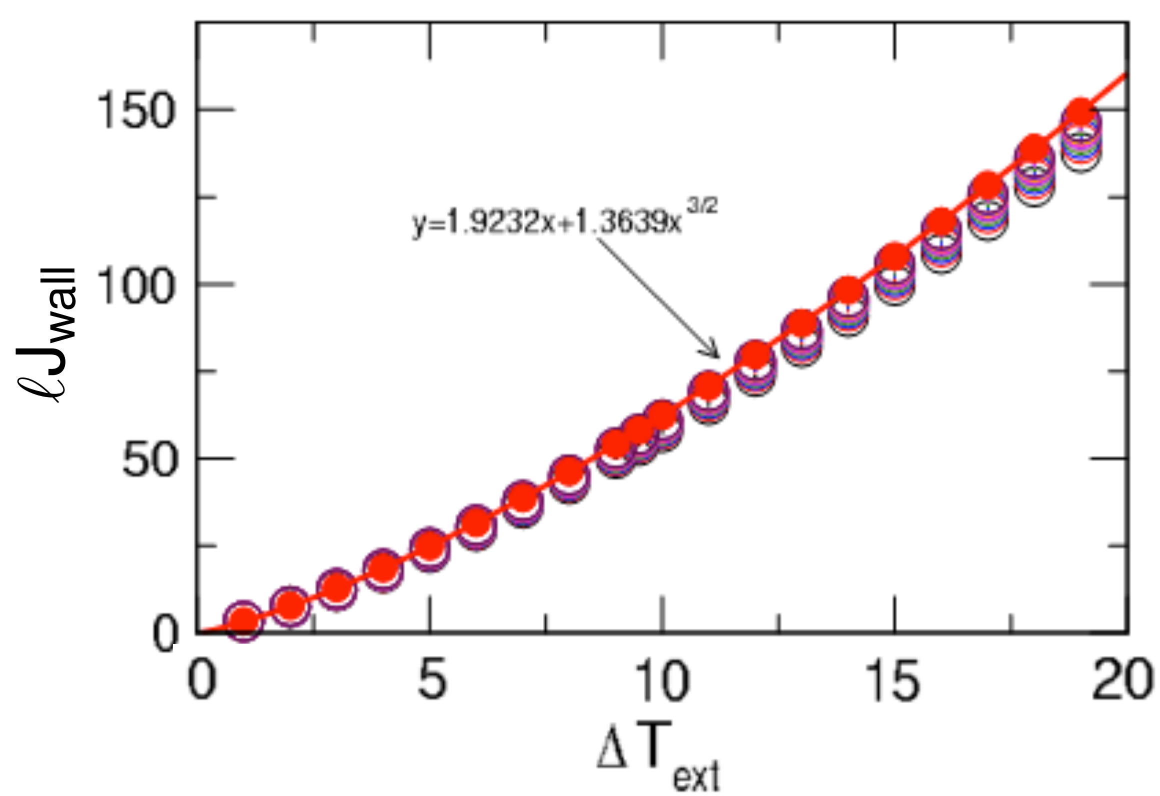
PRESSURE AND CURRENT

- Q and J: also strong finite-size effects!!

Reduced pressure: $Q = P\pi\ell^2$







Heat current: J_{wall}

LOCAL THERMODYNAMIC EQUILIBRIUM

Compressibility factor

- Is there a **local equation of state** (EoS)? $Q = T\rho Z(\rho) \Longrightarrow Z_{\mathrm{N}} \equiv \dfrac{Q_{\mathrm{N}}(\Delta T)}{T_{\mathrm{N}}(x;\Delta T)\rho_{\mathrm{N}}(x;\Delta T)}$

LOCAL THERMODYNAMIC EQUILIBRIUM

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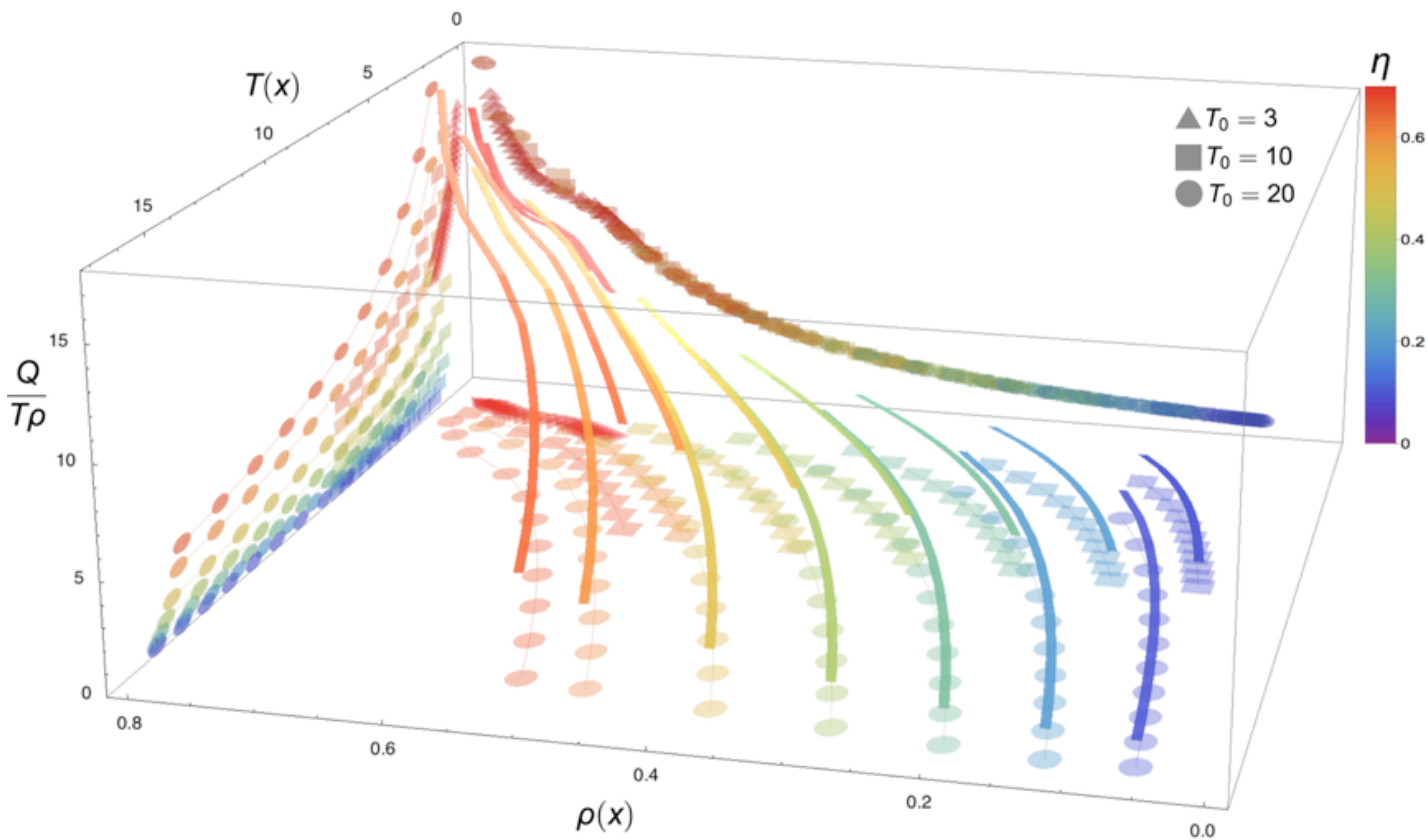
- We plot Z_N vs $\rho_N(x)$ and $T_N(x)$: **EoS surface**



LOCAL THERMODYNAMIC EQUILIBRIUM

- Is there a **local equation of state** (EoS)?

Compressibility factor

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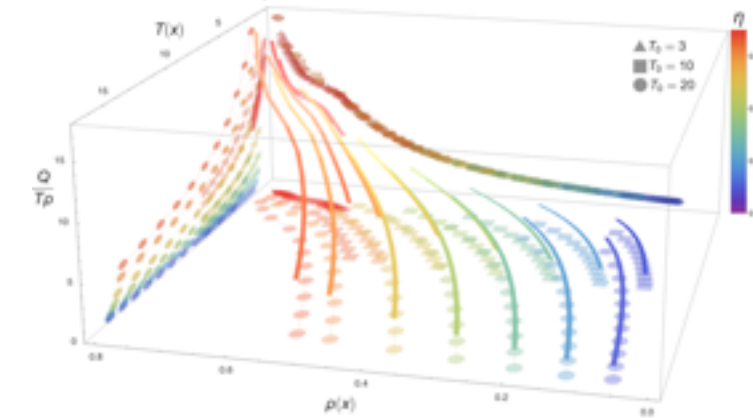
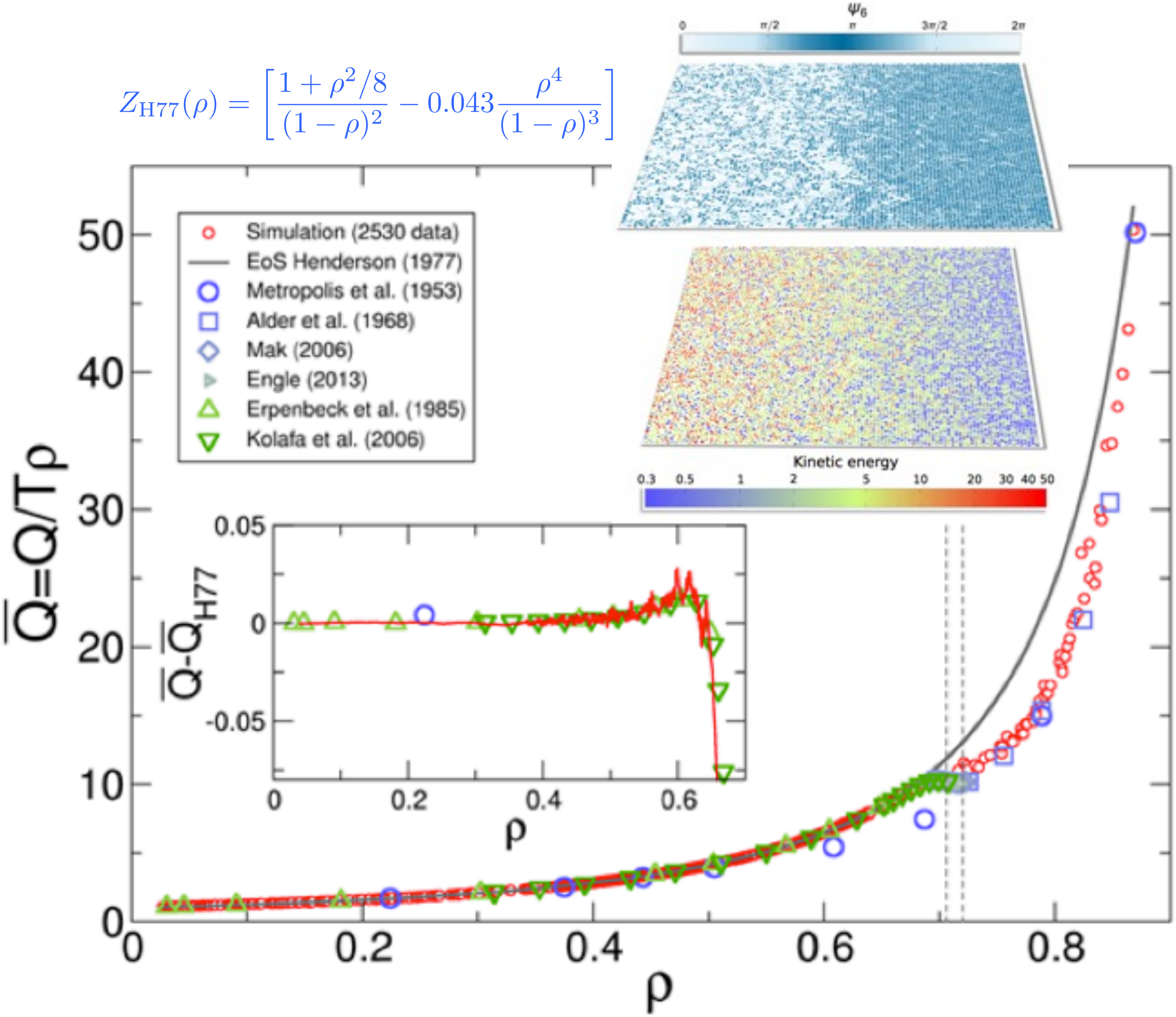
- We plot Z_N vs $\rho_N(x)$ and $T_N(x)$: **EoS surface**



$$Z_{\mathrm{H77}}(\rho) = \left[\frac{1+\rho^2/8}{(1-\rho)^2} - 0.043\frac{\rho^4}{(1-\rho)^3}\right]$$



- Z_N vs $\rho_N(x)$ ∀ N, η, ΔT
- NO finite-size effects!!
- **Recover equilibrium EoS**
- Striking accuracy ~ 1%
- **Nonequilibrium liquid-solid coexistence**

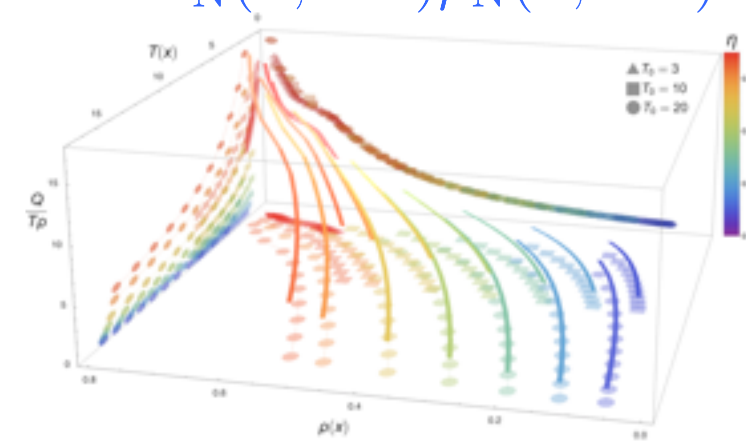
LOCAL THERMODYNAMIC EQUILIBRIUM

- Is there a **local equation of state** (EoS)?

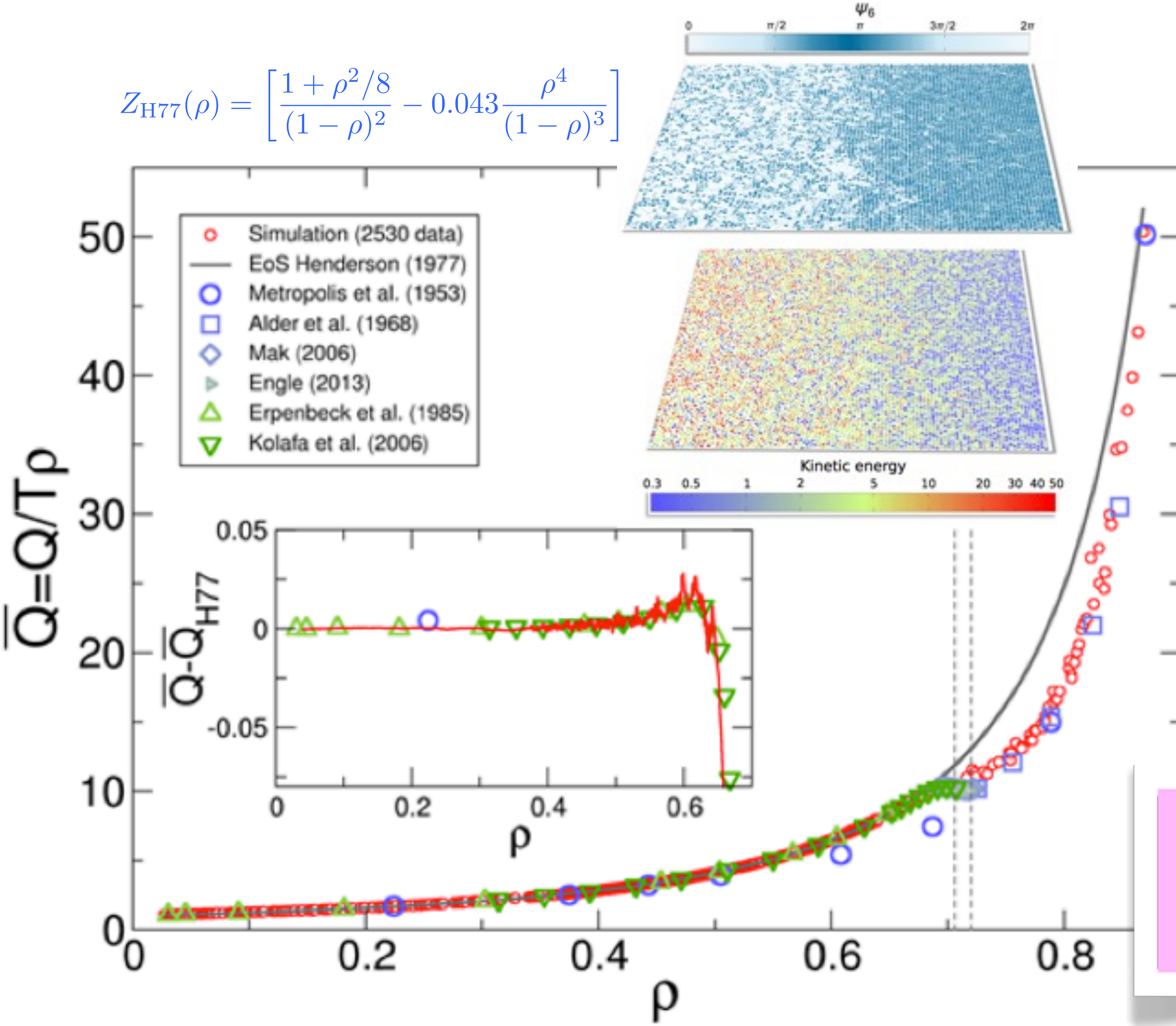
$$Q = T\rho Z(\rho) \Longrightarrow Z_{\mathrm{N}} \equiv \frac{Q_{\mathrm{N}}(\Delta T)}{T_{\mathrm{N}}(x;\Delta T)\rho_{\mathrm{N}}(x;\Delta T)}$$

Compressibility factor

- We plot Z_N vs $\rho_N(x)$ and $T_N(x)$: **EoS surface**



$$Z_{\mathrm{H77}}(\rho) = \left[\frac{1+\rho^2/8}{(1-\rho)^2} - 0.043\frac{\rho^4}{(1-\rho)^3}\right]$$



- Z_N vs $\rho_N(x)$ ∀ N, η, ΔT
- NO finite-size effects!!
- Recover equilibrium EoS
- Striking accuracy ~ 1%
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(macroscopic) Local Equilibrium holds !!

SCALING LAWS IN NONEQUILIBRIUM FLUIDS

- Assume **Fourier's law** and **macroscopic LTE** for hard disks

$$J=-\kappa(\rho,T)\frac{dT(x)}{dx}$$

Fourier's law

$$Q=Tq(\rho)$$

Equation of state (athermal)

$$\kappa(\rho,T)=\sqrt{T}k(\rho)$$

Conductivity (athermal)

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$$\frac{J}{Q^{3/2}} = G'[\rho(x)]\frac{d\rho(x)}{dx} \implies G[\rho(x)] = \frac{J}{Q^{3/2}}x + \xi$$

$$G'(\rho) = k(\rho)q(\rho)^{-5/2}q'(\rho)$$

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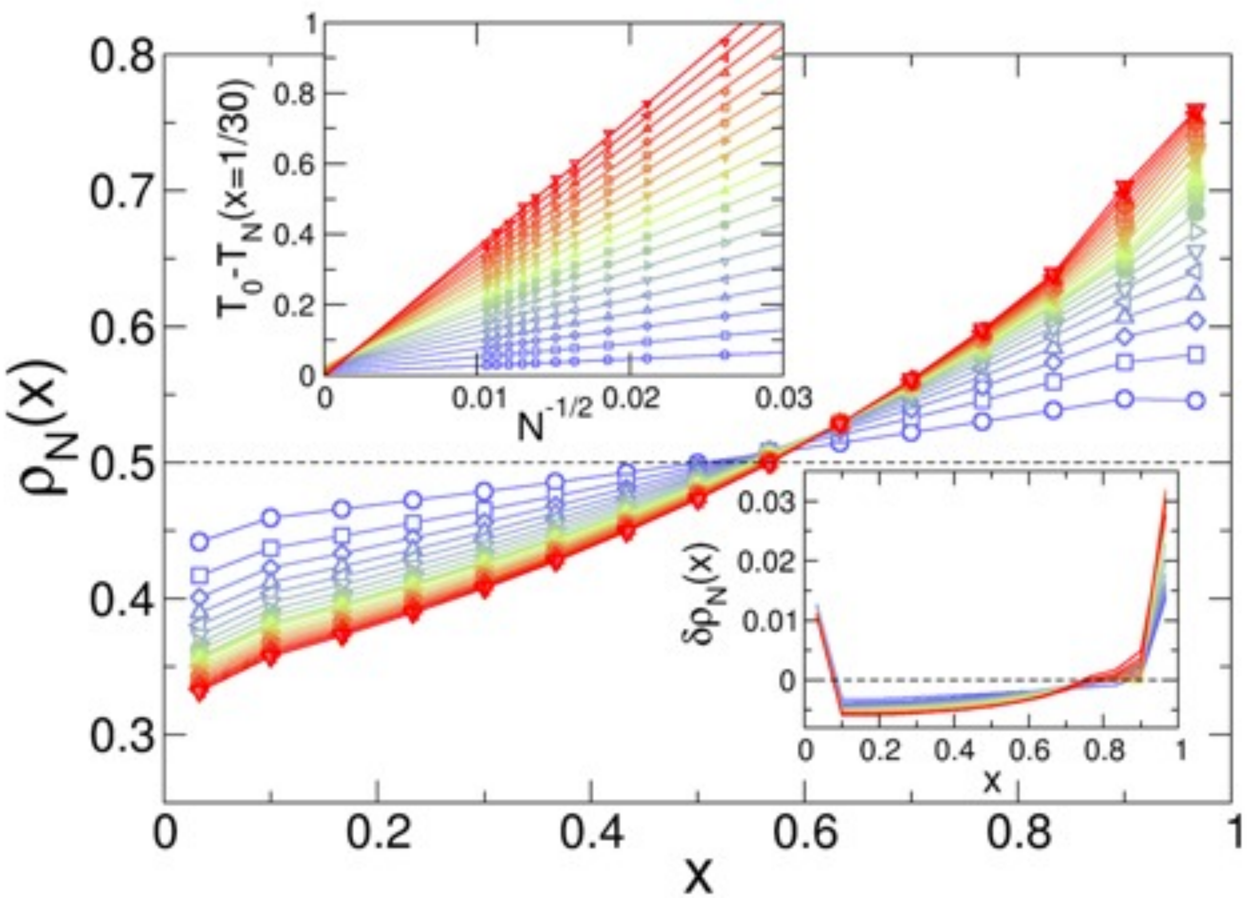
- **Two universal master curves** (∀ η, ΔT) from which any steady state profile follows after a **linear spatial scaling**

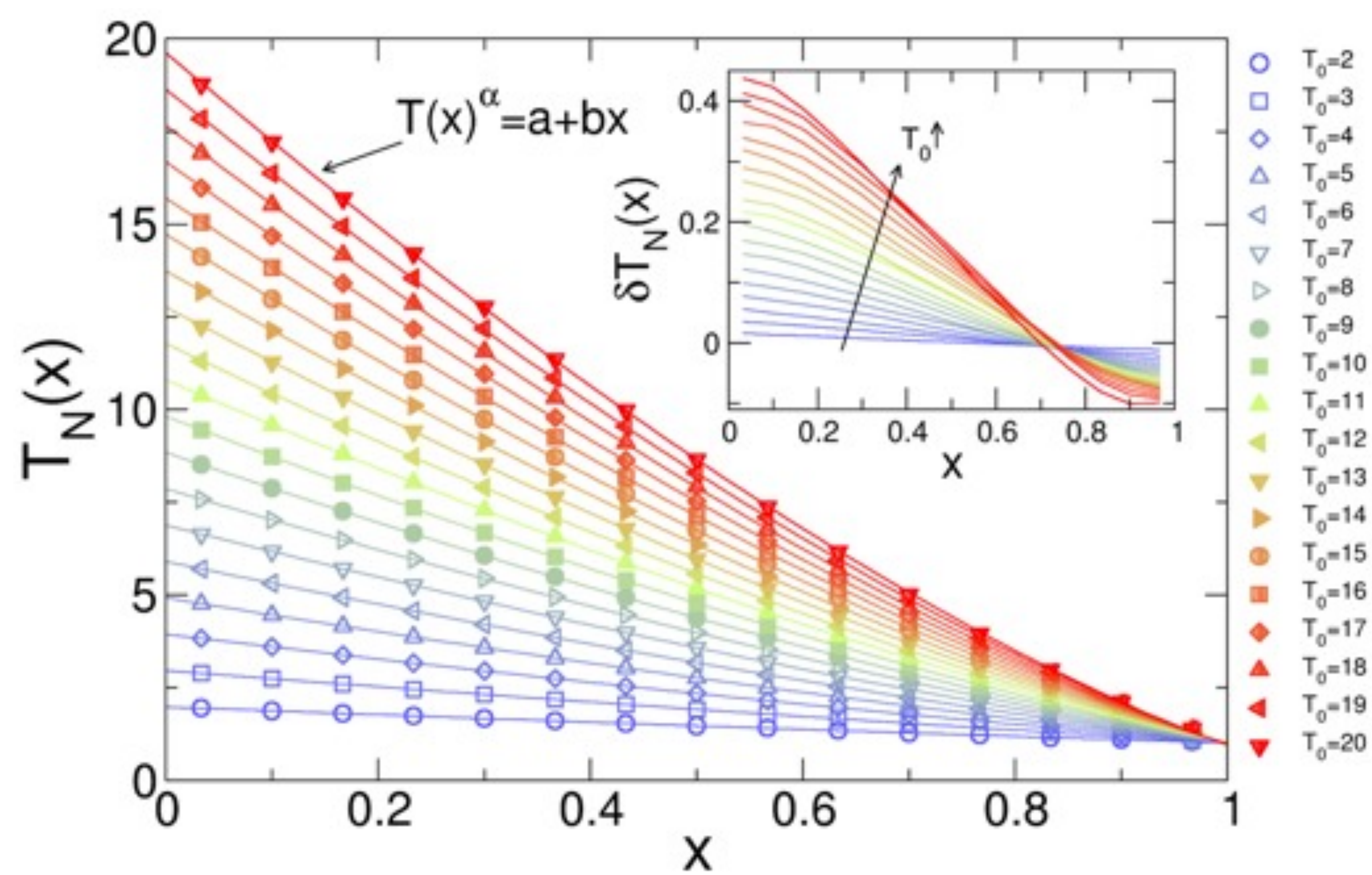
$$\bar{\rho}(y) \qquad \bar{T}(y) \qquad x = \frac{Q^{3/2}}{J}(y - \xi)$$

- Alternatively, any measured steady profile can be collapsed onto the universal master curves by scaling space by $J/Q^{3/2}$ and shifting the resulting profile by ξ

CAN WE OBSERVE THESE UNIVERSAL SCALING LAWS IN OUR DATA FOR HARD DISKS?

$$\rho(x) = G^{-1}\left(\frac{J}{Q^{3/2}}x + \xi\right) \quad , \quad \frac{T(x)}{Q} = F\left(\frac{J}{Q^{3/2}}x + \xi\right)$$





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Case 1

Constant mean Packing Fraction ; Variable Gradient

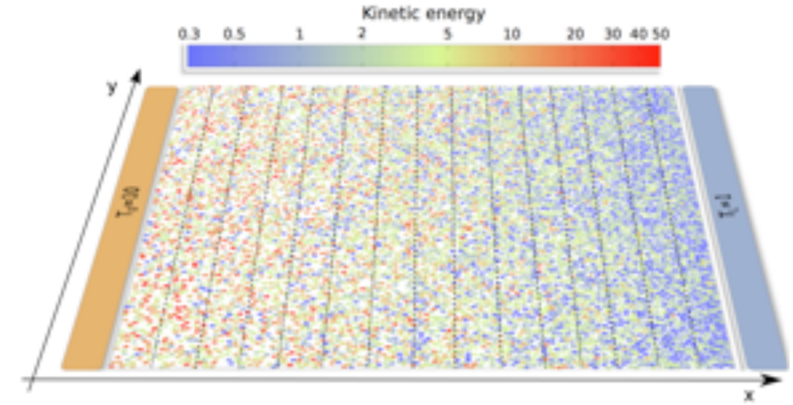
$$N_{Bulk} = 8878$$

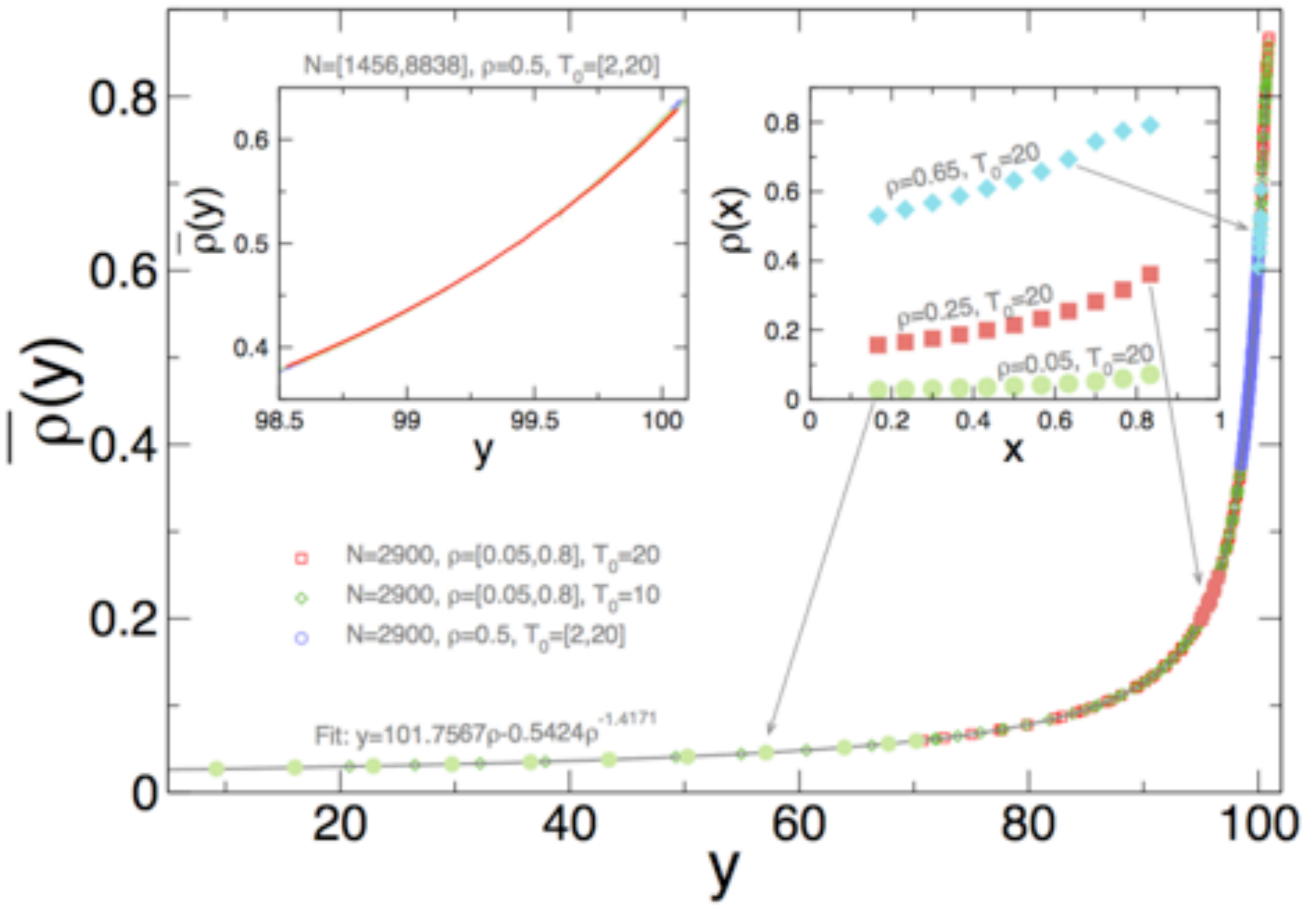
$$\bar{\eta} = 0.5$$

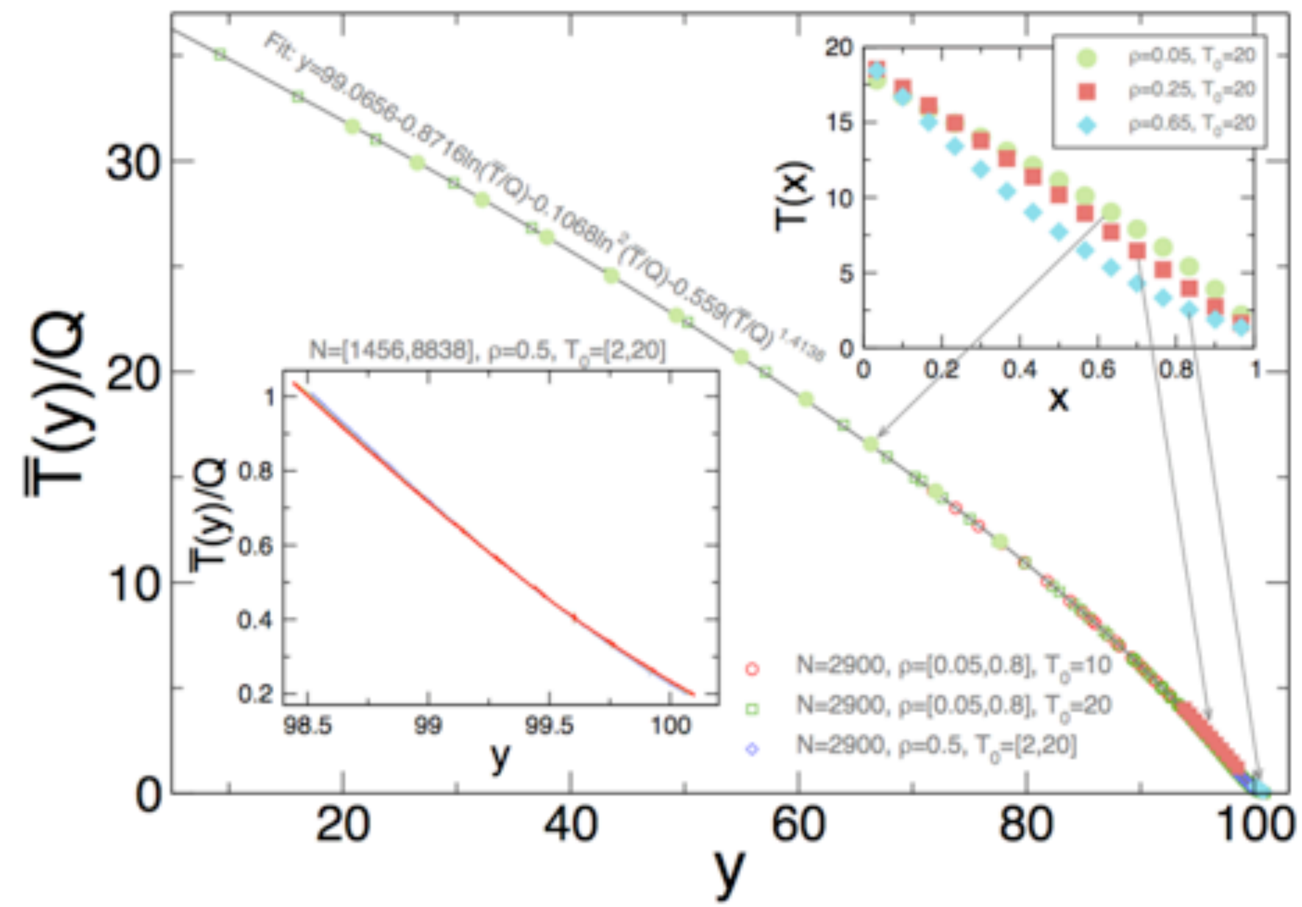
$$\nabla T = [1,2,...,18,19]$$

THE UNIVERSAL MASTER CURVES

$$\rho(x) = G^{-1}\left(\frac{J}{Q^{3/2}}x + \xi\right) \quad , \quad \frac{T(x)}{Q} = F\left(\frac{J}{Q^{3/2}}x + \xi\right)$$







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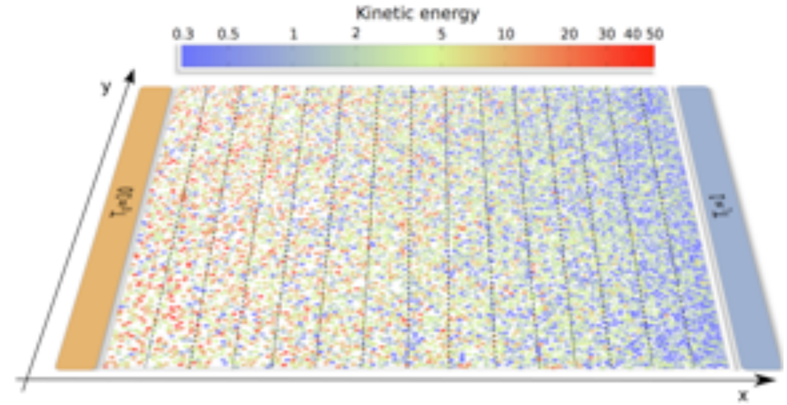
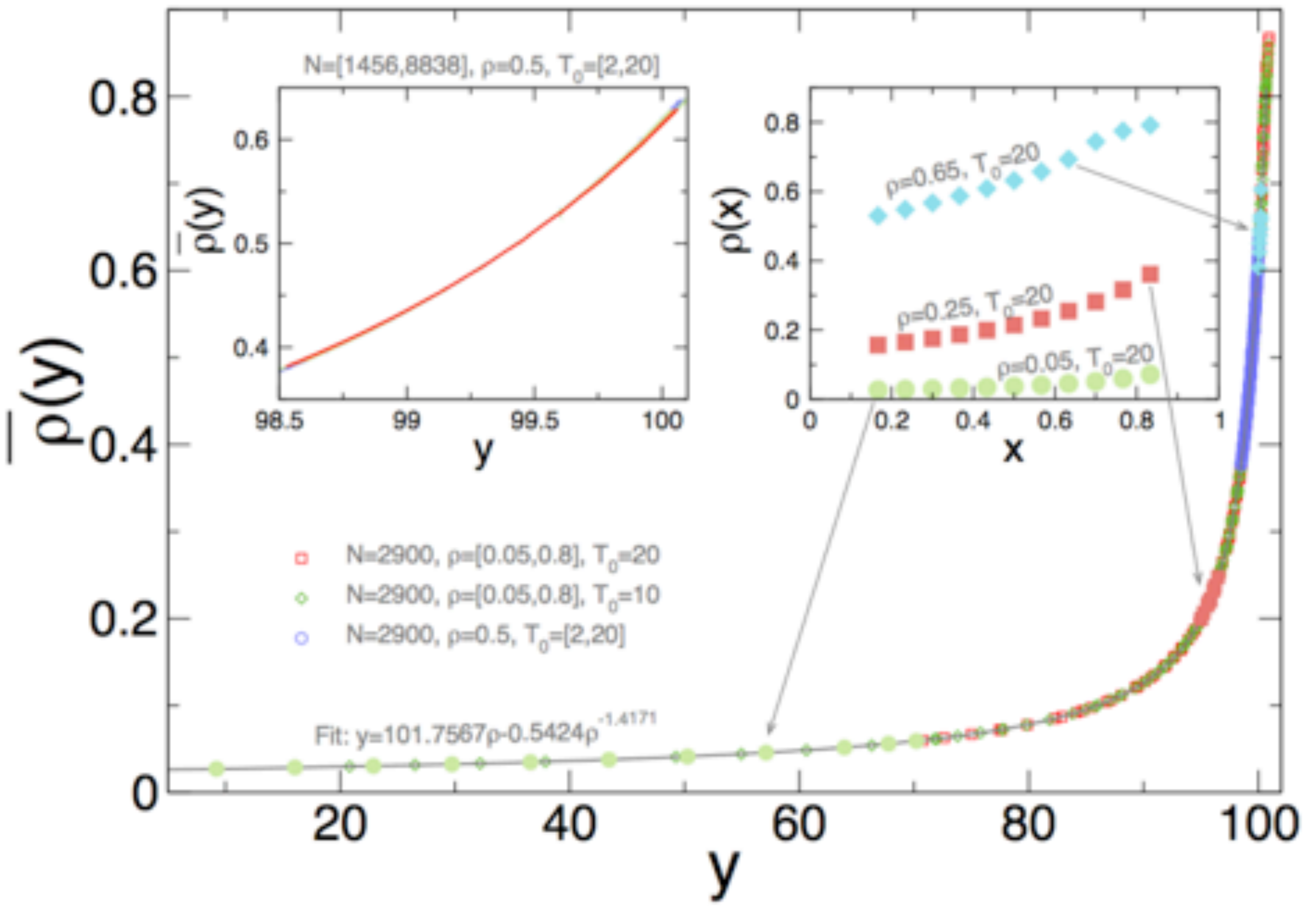
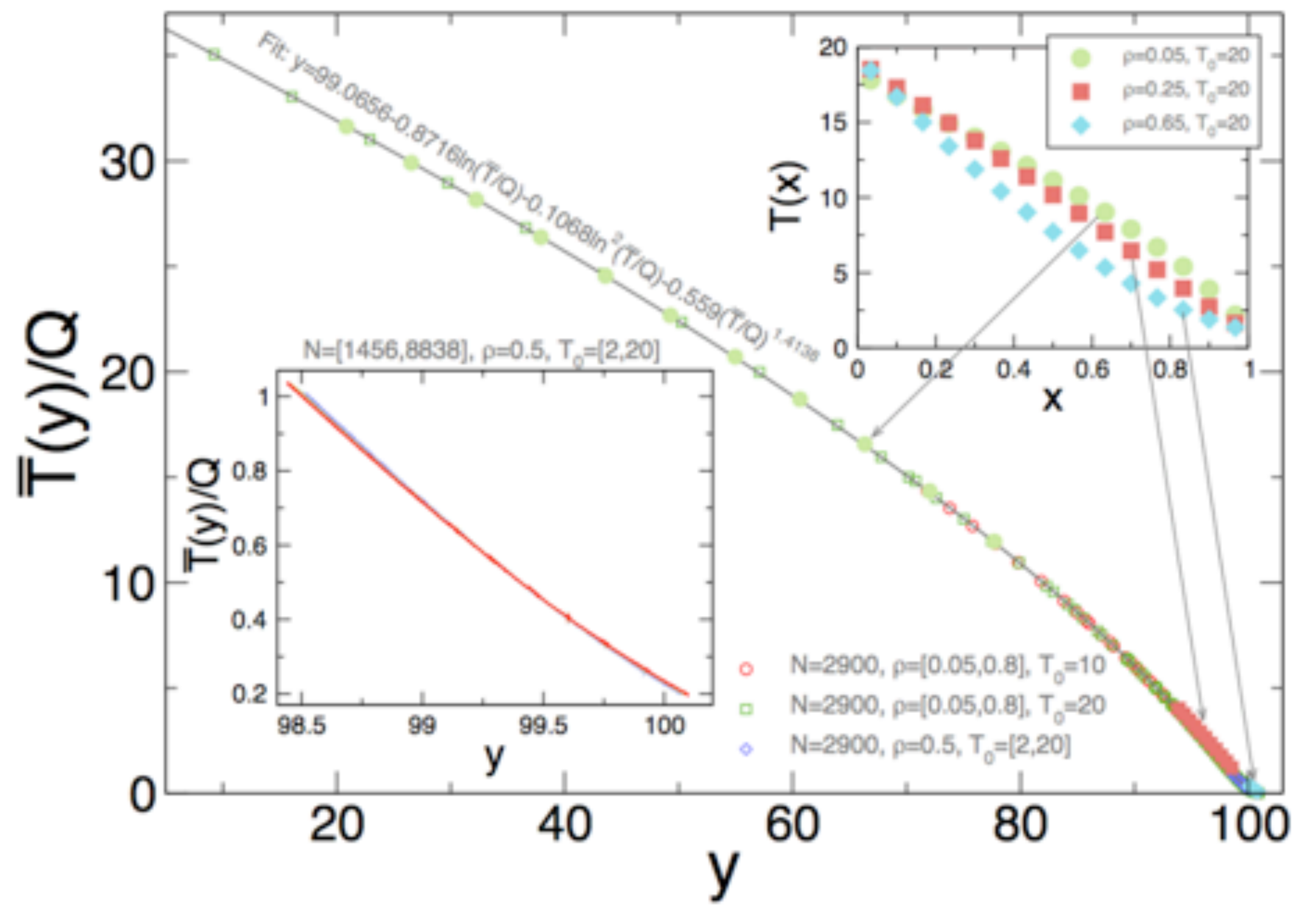






- All measured bulk profiles ∀(N,**η**,ΔT) collapse onto two universal master curves
- No finite-size corrections!!

Bulk-boundary decoupling phenomenon

- **The measured bulk profiles are those of a** macroscopic **hard-disk fluid** subject to to some **renormalized, effective boundary conditions** set by the finite boundary layers, which sum up all sorts of finite-size effects and boundary corrections.

GENERALIZATIONS

- Similar universal scaling laws exist for **d-dimensional hard spheres** (d=1,3,...)

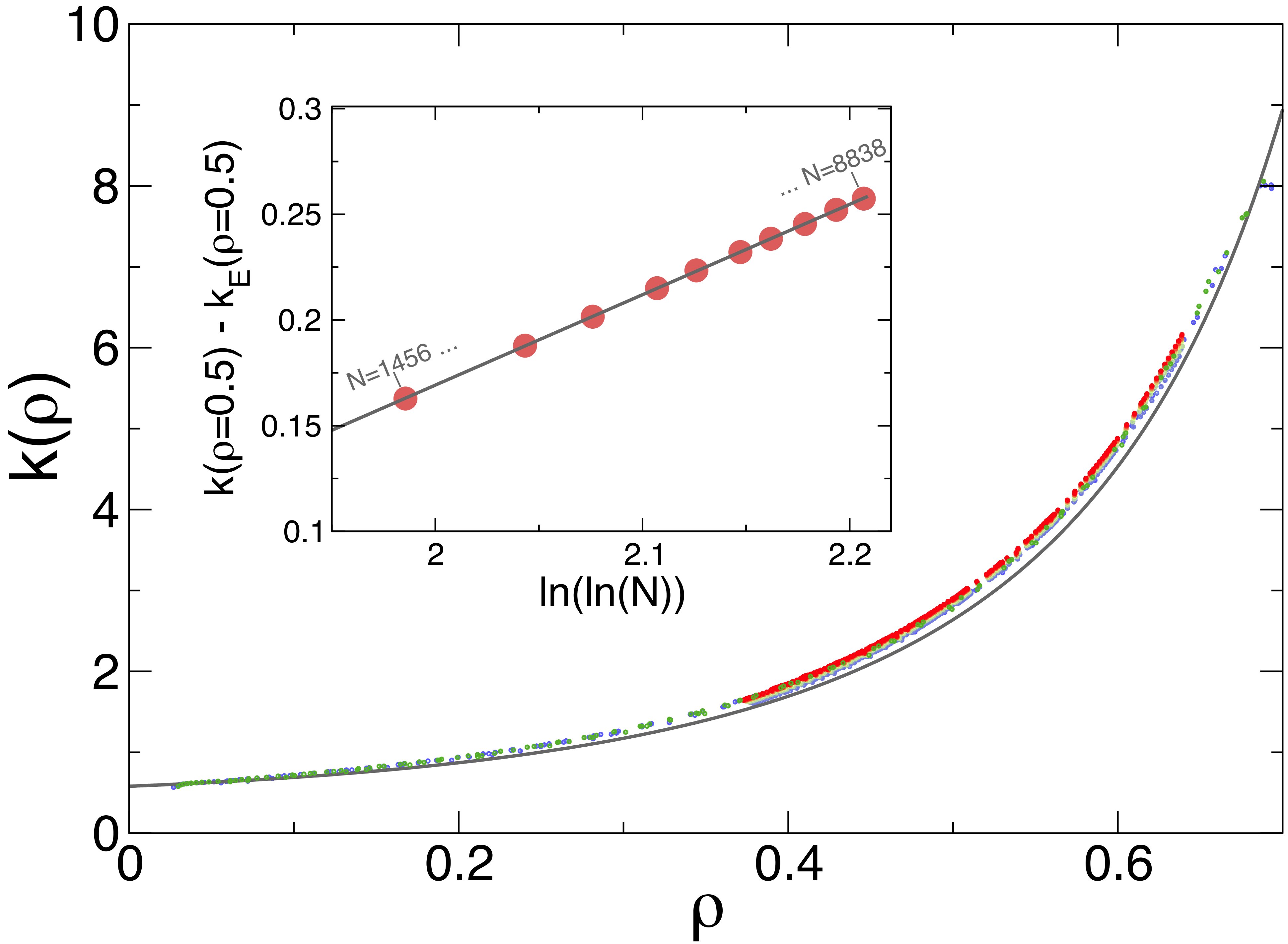
- Scaling laws also predicted for d-dimensional fluids with **homogeneous (or inverse power law - IPL) potentials**

$$V(r) = \epsilon \left(\frac{\sigma}{r} \right)^n$$

- Results likely to remain valid in the much broader family of **strongly correlating fluids** where excluded volume interactions are dominant

HEAT CONDUCTIVITY FROM SCALING

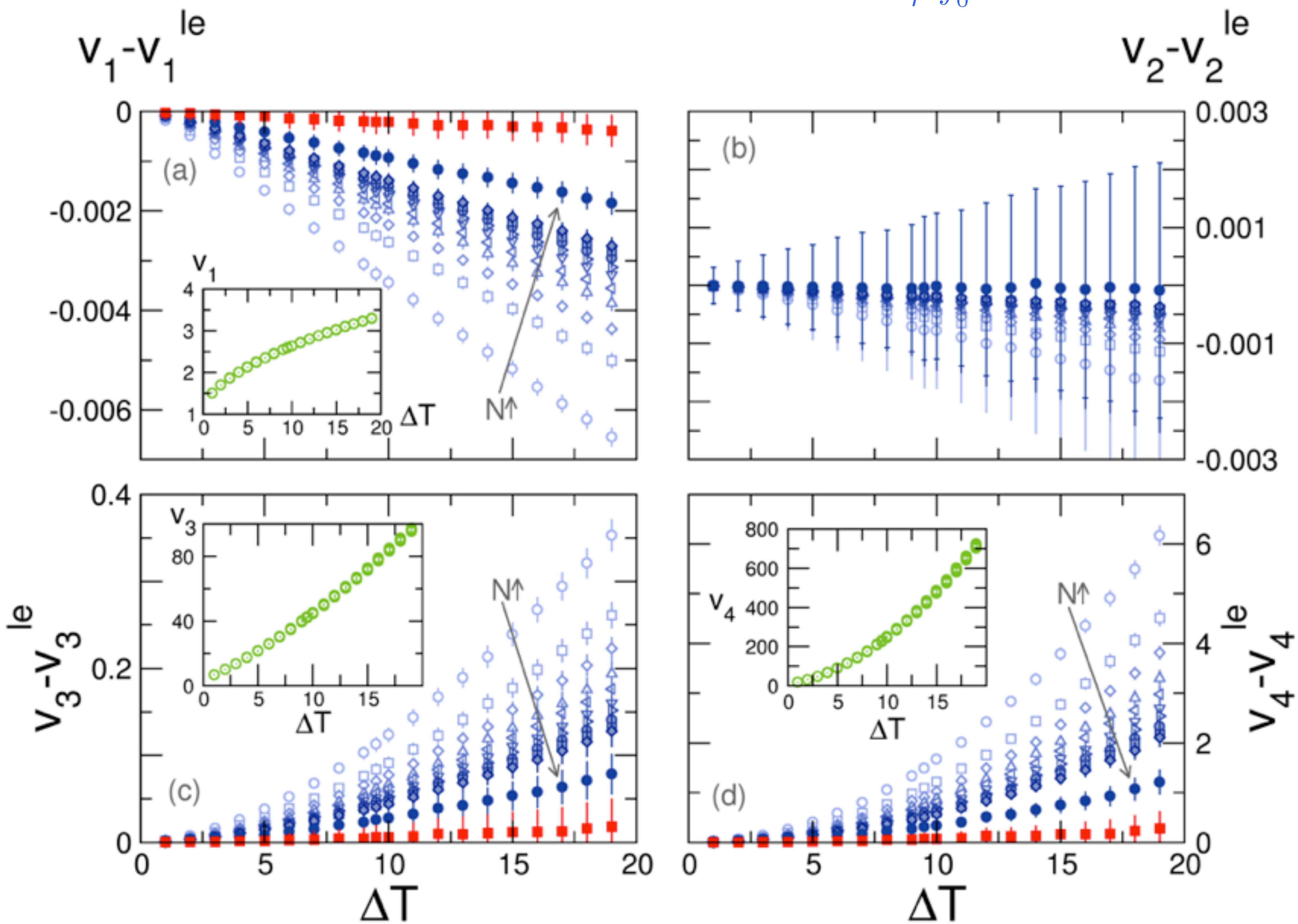
$$\kappa(\rho, T) = \sqrt{T}k(\rho)$$



LTE: VELOCITY MOMENTS

$$v_n \equiv \langle \frac{1}{N} \sum_{i=1}^{N} |\vec{v}_i|^n \rangle \qquad n = 1, 2, 3, 4$$

$$v_n^{\mathrm{le}} \equiv \frac{a_n}{\eta} \int_0^1 dx \rho(x) T(x)^{n/2}$$



LTE: ENERGY MOMENTS

$$u \equiv N^{-1} \sum_{i=1}^{N} \frac{1}{2} m \vec{v}_i^2$$

$$m_n(u) \equiv \langle (u - \langle u \rangle)^n \rangle$$