Heat Conduction in Atomic Systems

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Workshop - Numerical aspects of nonequilibrium dynamics,
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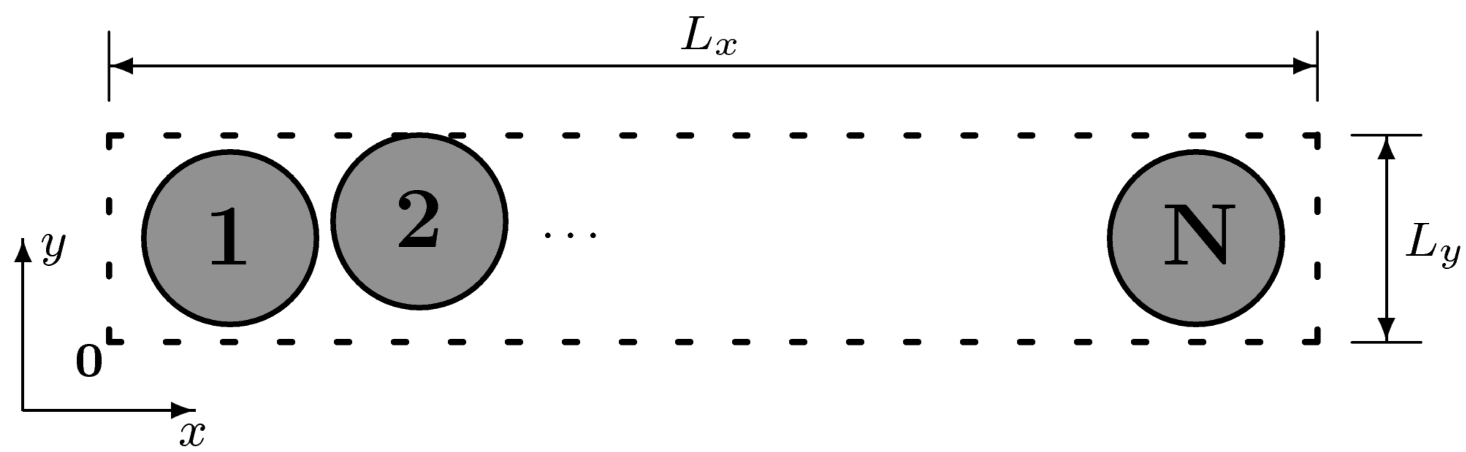
Quasi-One-Dimensional Hard Disks

Quasi-One-Dimensional system



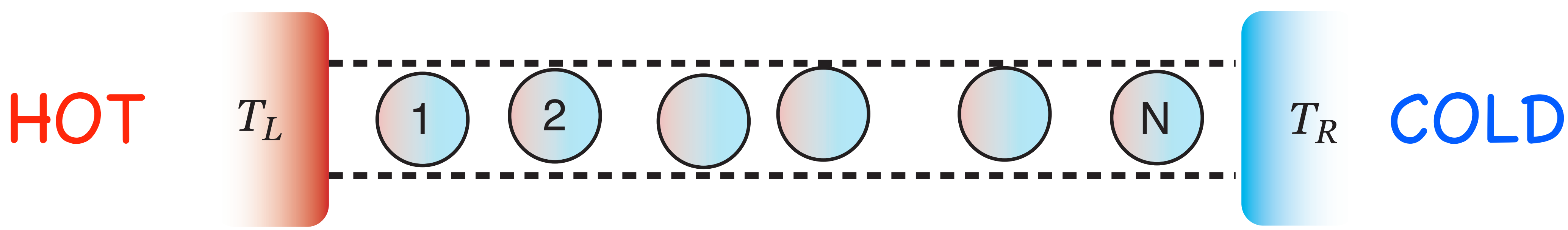
Ly<2

Attach two reservoirs

$L_y = 1.15$

Collisions with the reservoir boundary changed to

$$p'_x = \varepsilon p_I - (1-\varepsilon) p_x \qquad 0 \le \varepsilon \le 1 \qquad \varepsilon = 0 \quad \text{hard wall}$$



Left and Right reservoirs at temperatures T_L and T_R

Reservoir momenta directed outwards - $p_I = \pm\sqrt{2T_I}$

- Typical states: low density 0.03 and high density 0.8

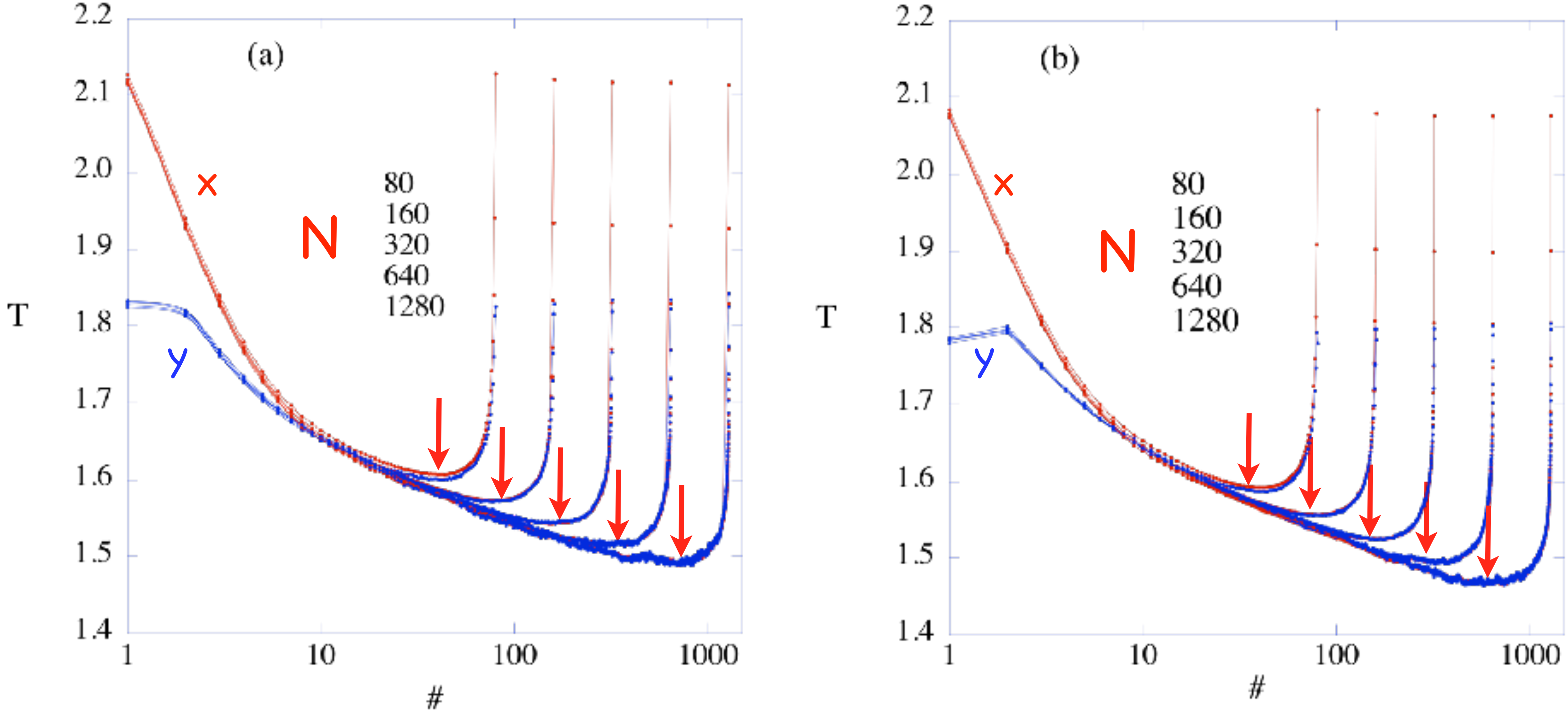
Scaling

Separate bulk effects from boundary effects

Equal Temperature Reservoirs

Equilibrium Temperature Profiles

Tx and Ty as a function of ln(#) for different system sizes
- particle number



$\rho = 0.03$ $\rho = 0.8$

LHS T gradients indep of N, T centre decreases with ln(N)

“Equilibrium” QOD Systems

Temperature

- Centre T decreases with ln(N), characteristic shape.
- Energy input is through x-direction but equilibration with Ty
- Tx-Ty is independent of N and density near reservoirs. Boundary effect involving the first 6 to 8 particles.
- Separate boundary effects from bulk effects.
- Understand scaling with system size.

Micro to Macro

Hydrodynamics - fluid element

Conservation Laws of Hydrodynamics

Mass density

Mass

$$\frac{\partial \rho(\mathbf{r},t)}{\partial t} = -\nabla \cdot \left[\rho(\mathbf{r},t)\mathbf{u}(\mathbf{r},t) \right]$$

Momentum density

Momentum density

Momentum

$$\frac{\partial \left[\rho(\mathbf{r},t)\mathbf{u}(\mathbf{r},t) \right]}{\partial t} = -\nabla \cdot \left[\rho(\mathbf{r},t)\mathbf{u}(\mathbf{r},t)\mathbf{u}(\mathbf{r},t) + \mathbf{P}(\mathbf{r},t) \right]$$

Pressure

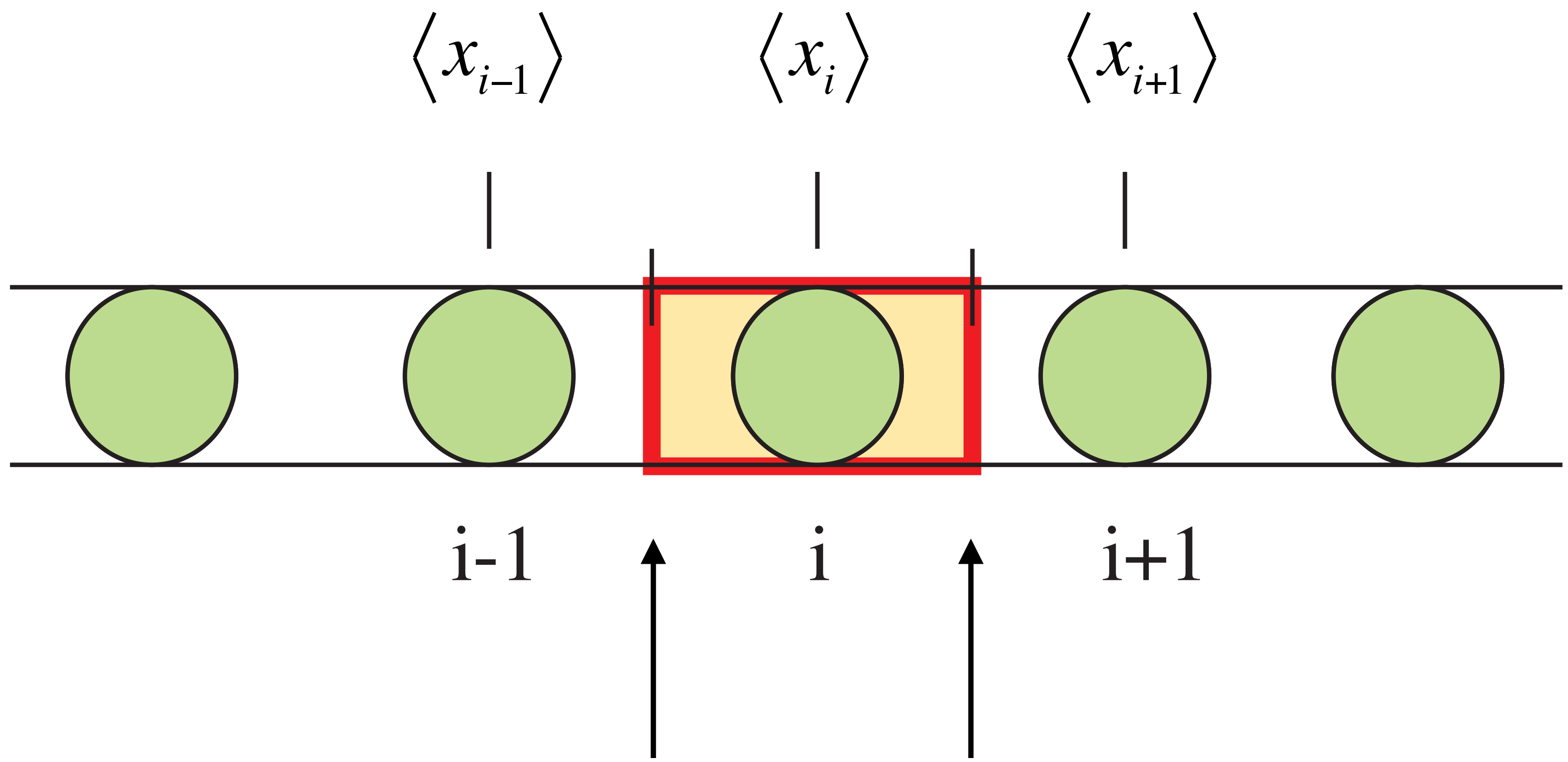
Energy density

Energy

$$\frac{\partial \left[\rho(\mathbf{r},t)e(\mathbf{r},t) \right]}{\partial t} = -\nabla \cdot \left[\rho(\mathbf{r},t)e(\mathbf{r},t)\mathbf{u}(\mathbf{r},t) + \mathbf{J}_Q(\mathbf{r},t) + \mathbf{P}(\mathbf{r},t) \cdot \mathbf{u}(\mathbf{r},t) \right]$$

Heat flux vector

Fluid Element



$$\frac{\langle x_i \rangle + \langle x_{i-1} \rangle}{2} \qquad \frac{\langle x_{i+1} \rangle + \langle x_i \rangle}{2} \qquad L_i = \frac{\langle x_{i+1} \rangle - \langle x_{i-1} \rangle}{2}$$

At the ends $\langle x_0 \rangle = 0$ $\langle x_{N+1} \rangle = L_x$

$V_i = L_y L_i$ **Local density** $\rho_i = 1 / L_y L_i$

Local properties determined by the particle.

Instantaneous microscopic representation of local Fluxes

mass density
$$\rho(\mathbf{r},t) = \sum_i m_i \delta(\mathbf{r} - \mathbf{r}_i(t))$$

Lab velocity = thermal + streaming
$$\dot{\mathbf{r}}_i = \mathbf{v}_i + \mathbf{u}(\mathbf{r}_i, t)$$

Pressure tensor
$$\mathbf{P}(\mathbf{r},t) = \sum_i m_i \mathbf{v}_i \mathbf{v}_i \delta(\mathbf{r} - \mathbf{r}_i) - \tfrac{1}{2}\sum_{i,j} \mathbf{r}_{ij}\mathbf{F}_{ij} \int_0^1 d\lambda\, \delta(\mathbf{r} - \mathbf{r}_i - \lambda \mathbf{r}_{ij})$$

Heat flux vector
$$\mathbf{J}_Q(\mathbf{r},t) = \sum_i U_i \mathbf{v}_i \delta(\mathbf{r} - \mathbf{r}_i) - \tfrac{1}{2}\sum_{i,j} \mathbf{r}_{ij}\mathbf{F}_{ij} \cdot (\mathbf{v}_i + \mathbf{u}(\mathbf{r}_i) - \mathbf{u}(\mathbf{r})) \int_0^1 d\lambda\, \delta(\mathbf{r} - \mathbf{r}_i - \lambda \mathbf{r}_{ij})$$
$$U_i = \tfrac{1}{2} m v_i^2 + \tfrac{1}{2}\sum_j \phi_{ij}$$

Energy Flows

Local heat flux vector

$$J_Q(\mathbf{r},t) = \sum_{i=1}^{N} U_i \mathbf{v}_i \delta(\mathbf{r}-\mathbf{r}_i) - \frac{1}{2}\sum_{i,j}^{N} \hat{\mathbf{r}}_{ij}\left(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{v}}_{ij}\right)\hat{\mathbf{r}}_{ij}\cdot\left(\mathbf{v}_i+\mathbf{v}_j\right)\delta\left(t-t_{ij}\right)\int_0^1 d\lambda\,\delta\left(\mathbf{r}-\mathbf{r}_i-\lambda\mathbf{r}_{ij}\right)$$

Approximate integral $\int_0^1 dx f(x) \approx \frac{1}{2}\left(f(0)+f(1)\right)$

$$J_Q(\mathbf{r},t) = \sum_{i=1}^{N} U_i \mathbf{v}_i \delta(\mathbf{r}-\mathbf{r}_i) - \frac{1}{4}\sum_{i,j}^{N} \hat{\mathbf{r}}_{ij}\left(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{v}}_{ij}\right)\hat{\mathbf{r}}_{ij}\cdot\left(\mathbf{v}_i+\mathbf{v}_j\right)\delta\left(t-t_{ij}\right)\left(\delta\left(\mathbf{r}-\mathbf{r}_i\right)+\delta\left(\mathbf{r}-\mathbf{r}_j\right)\right)$$

kinetic potential

Heat flux per unit volume

$$J_Q(t) = \frac{1}{V}\int_V d\mathbf{r}\, J_Q(\mathbf{r},t)$$

Fixed Temperature Gradient

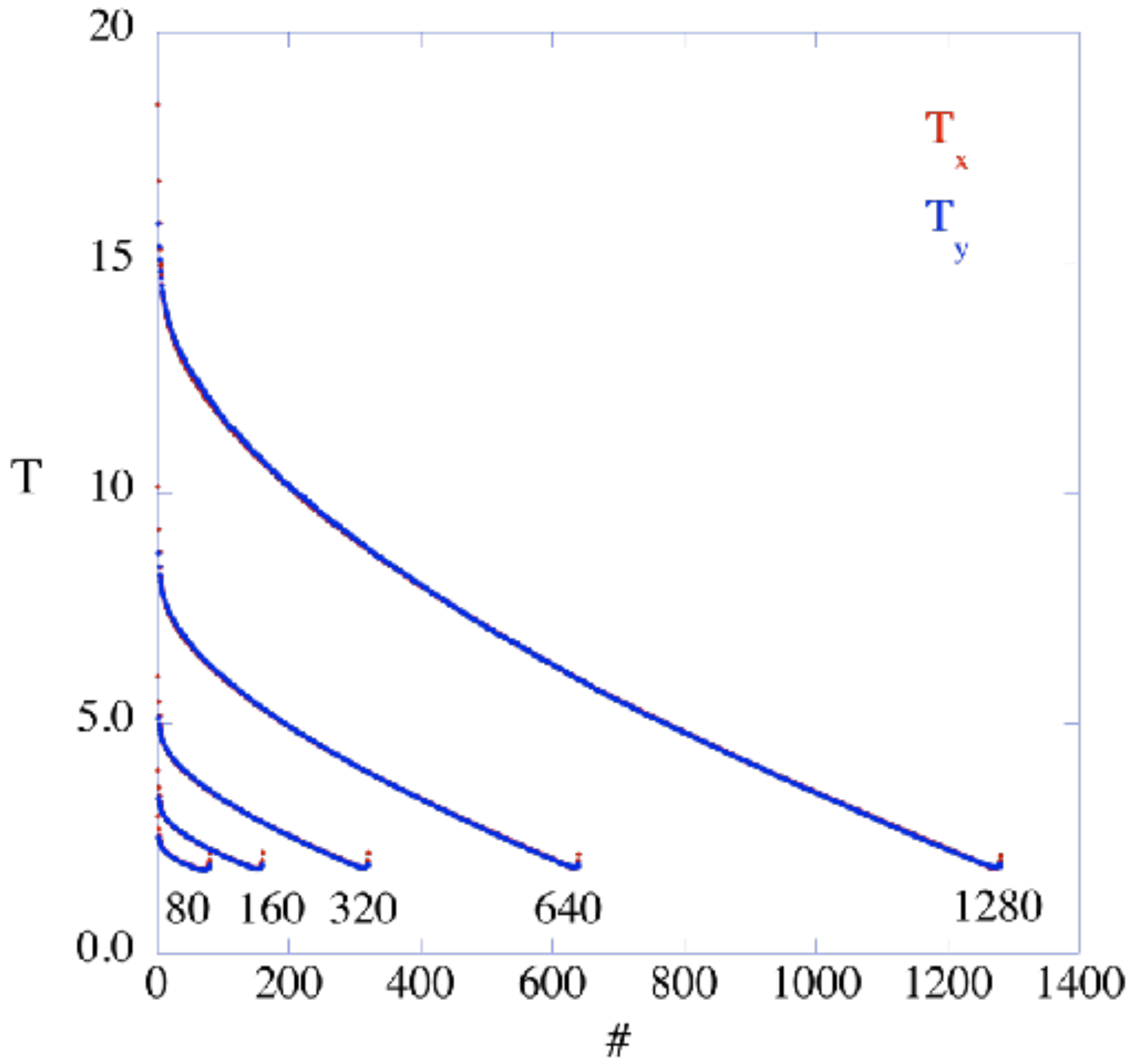
$$\nabla T = \frac{T_R - T_L}{L_x} = \frac{2-3}{86.95652} = -0.01150$$

$$T_L = T_R - \boxed{\frac{\nabla T}{\rho L_y}} N$$

constant

$T_R = 2$ $\quad$ T_L changes with N

Temperature Profiles at fixed external gradient



T_R=2

$$\rho = 0.8$$

Instantaneous microscopic representation of total Fluxes

Integrate over volume

$$\mathbf{J}_Q V = \sum_i U_i \mathbf{v}_i - \tfrac{1}{2}\sum_{i,j} \mathbf{r}_{ij}\mathbf{F}_{ij} \cdot \mathbf{v}_i$$

Energy balance

Energy entering from reservoir I=L,R

$$\Delta e_I = \tfrac{1}{2}\left(p_x'^2 - p_x^2\right) = \tfrac{\varepsilon}{2}\left[\varepsilon p_I^2 + 2(\varepsilon - 1) p_I p_x + (\varepsilon - 2) p_x^2\right]$$

Energy entering from the left is equal and opposite to energy entering from the right

$$\Delta e_L = -\Delta e_R$$

Average heat flux/volume

$$\bar{J}_Q = \frac{1}{T}\int_0^T J_Q(t)dt$$

Energy balance

$$\bar{J}_Q = \frac{\Delta e_L}{L_y} = -\frac{\Delta e_R}{L_y}$$

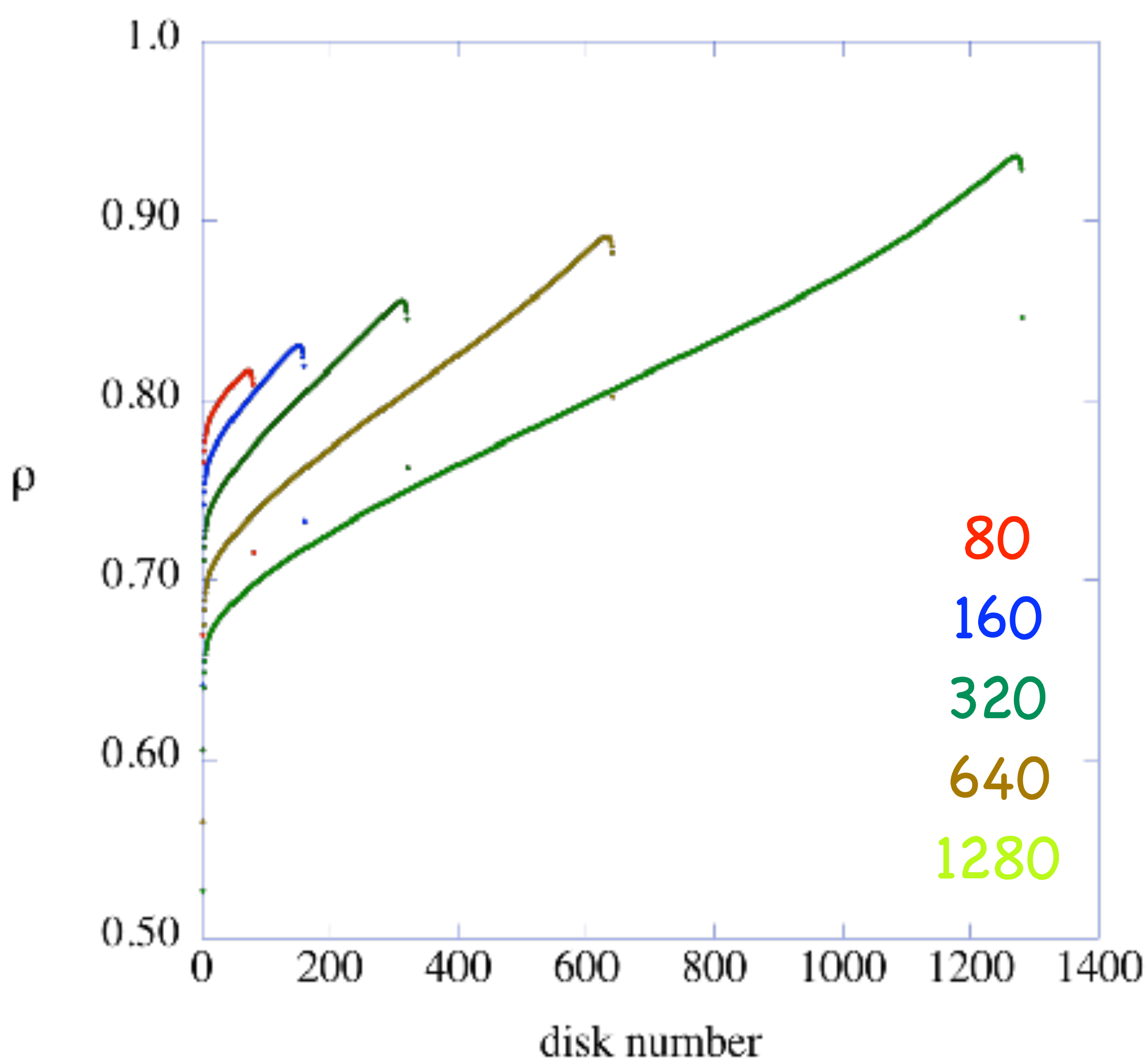
Energy Balance Results - constant gradient

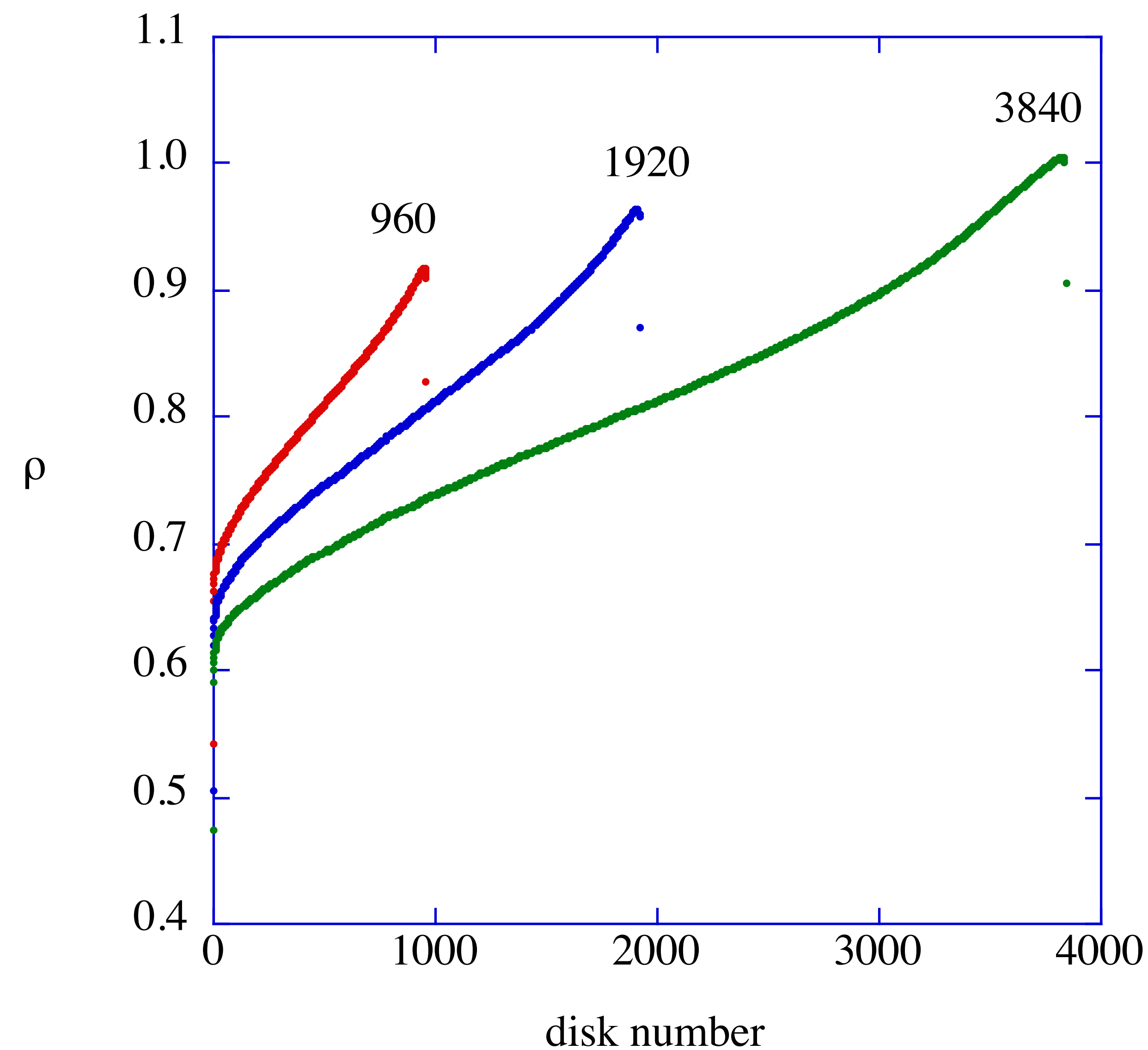
$$\rho = 0.8$$

	Kinetic	Potential	Total	Left	Right
N	JQx(K)	JQx(P)	JQx	$\Delta e_L / L_y$	$\Delta e_R / L_y$
80	0.037981	0.208039	0.24602	0.24888	0.24888
160	0.053149	0.289119	0.34227	0.34425	0.34424
320	0.075735	0.407122	0.48286	0.48426	0.48425
640	0.11193	0.59120	0.70313	0.70413	0.70413
1280	0.17402	0.89712	1.07114	1.07174	1.07217
2560	0.27940	1.40366	1.68306	1.68335	1.68349

Both kinetic and potential contributions are significant

Density profiles



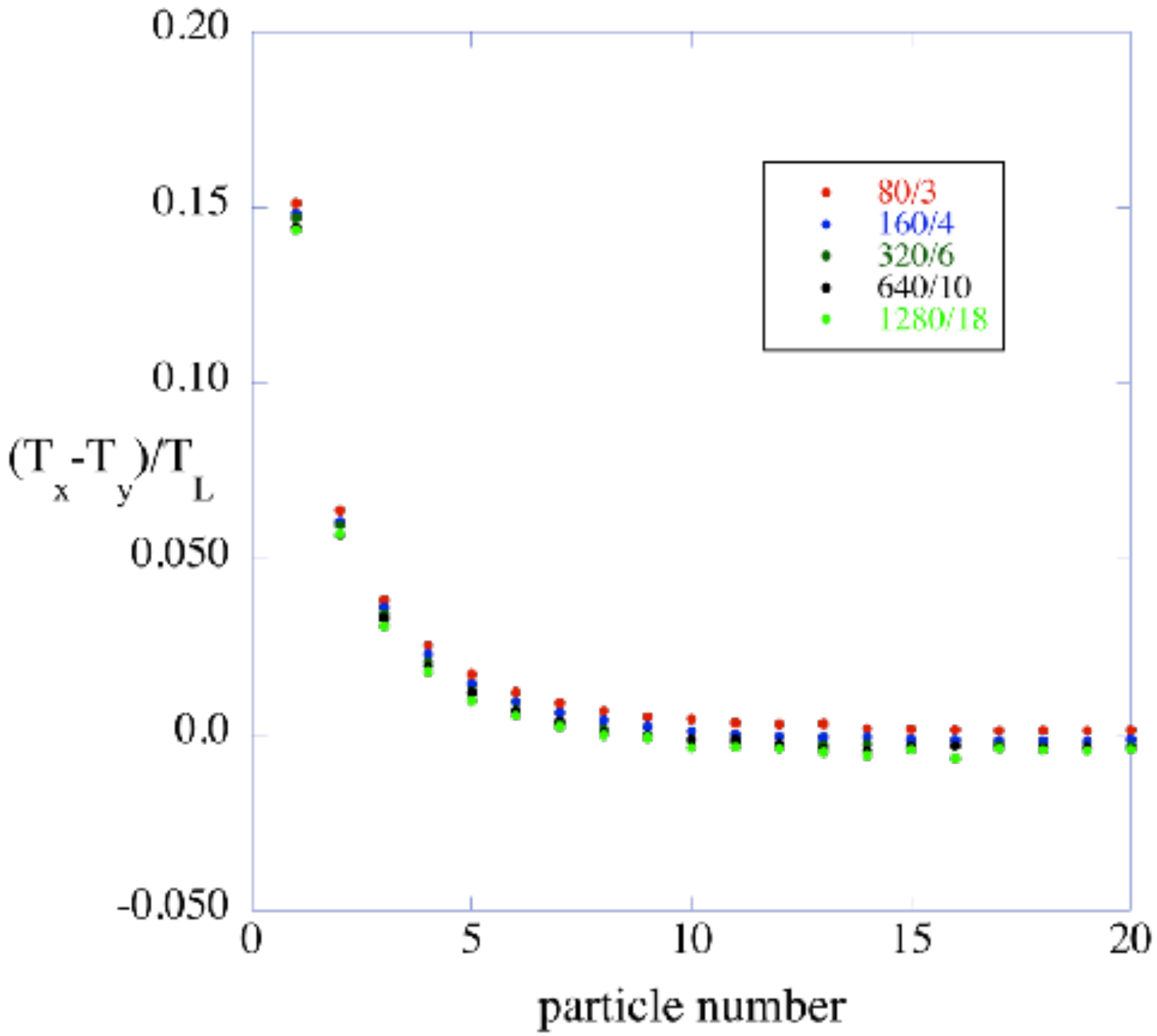


$$\rho = 0.8$$

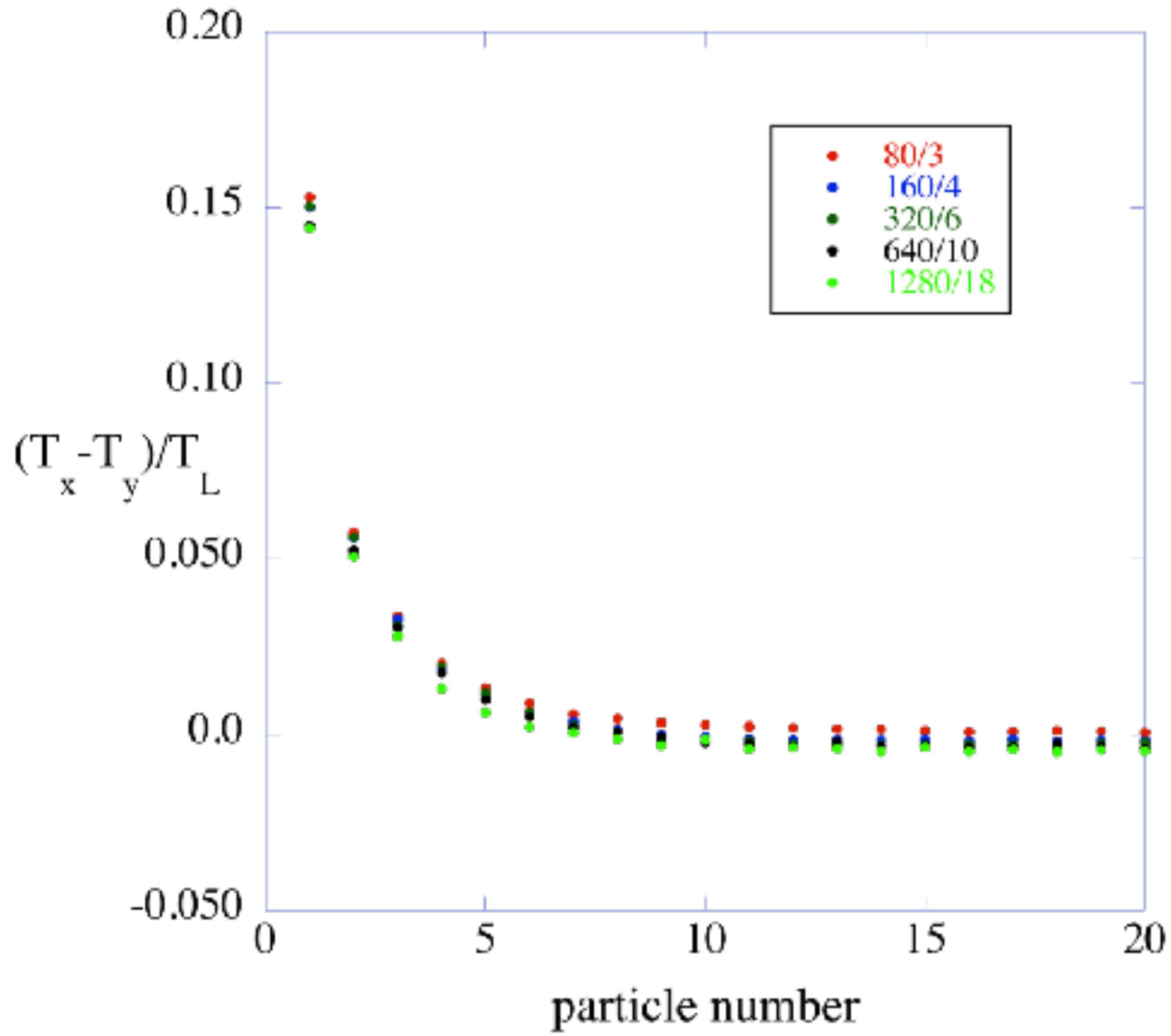
maximum density 1.0628

solidification at cold end for larger N ?

Temperature Difference Profiles



$\rho = 0.03$



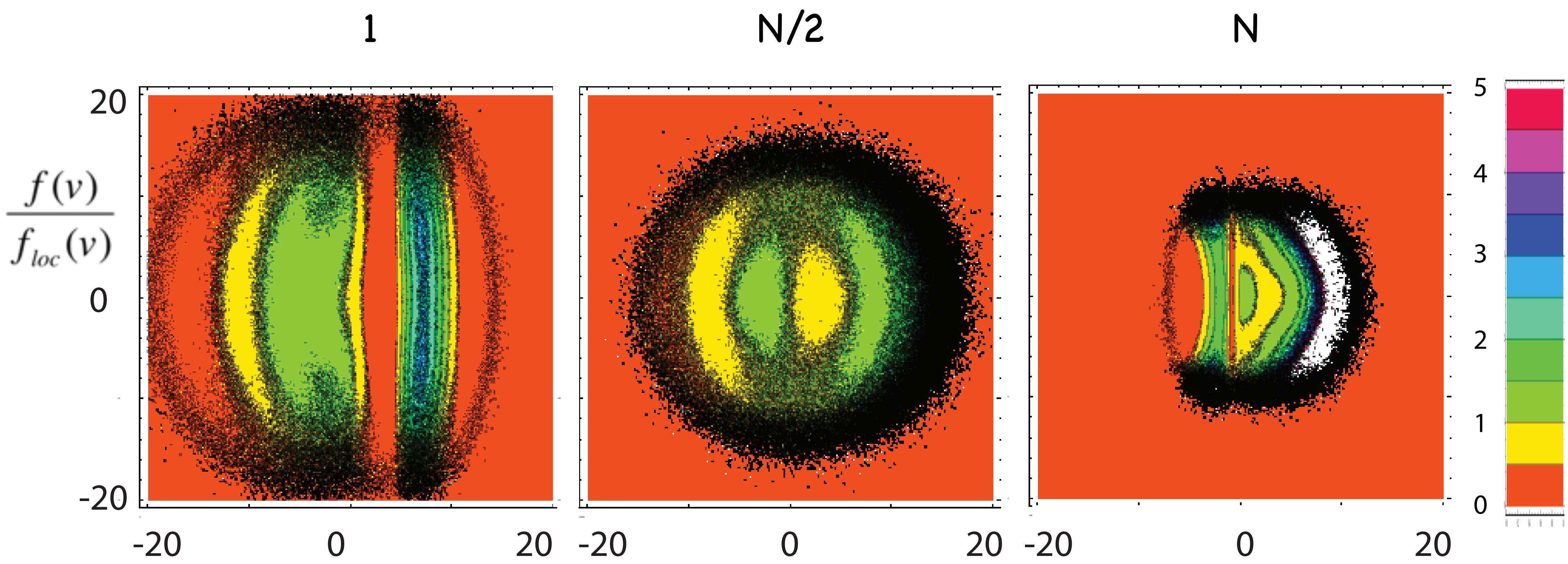
$\rho = 0.8$

Scales with particle number - independent of density

Same as equal reservoir scaling!

N=80 TL=34 TR=2 rho=0.8

Velocity probability density divided by local equilibrium density
for particle 1, N/2 and N in a QOD system of N disks
connected to two reservoirs with different temperatures



Halo region is where statistics are poor and probabilities vary wildly from point-to-point,
Orange is less than one half. White is off scale, greater than 5.

Kinetic Entropy

Entropy Changes

Change in Entropy density

$$s(\mathbf{r},t) = -k\int d\mathbf{v} f \ln f$$

$$\frac{\partial}{\partial t} s(r,t) = -k\frac{\partial}{\partial t}\int d\mathbf{v} f \ln f = -k\int d\mathbf{v}\frac{\partial f}{\partial t}(1+\ln f)$$

Use Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} = \left(\frac{\partial f}{\partial t}\right)_{coll} = J[f]$$

Collision operator

$$\frac{\partial}{\partial t} s(r,t) = -k\int d\mathbf{v}\left(-\mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} + J[f]\right)(1+\ln f)$$

$$= k\frac{\partial}{\partial \mathbf{r}}\cdot\int d\mathbf{v}\mathbf{v} f(1+\ln f) - k\int d\mathbf{v} J[f](1+\ln f)$$

Entropy Changes

$$\frac{\partial}{\partial t}s(r,t) = k\frac{\partial}{\partial \mathbf{r}}\cdot \int d\mathbf{v}\mathbf{v}f\left(1+\ln f\right) - k\int d\mathbf{v}J\left[f\right]\left(1+\ln f\right)$$

$$k\int d\mathbf{v}\mathbf{v}f\left(1+\ln f\right) = k\int d\mathbf{v}\mathbf{v}f + k\int d\mathbf{v}\mathbf{v}f\ln f = k\mathbf{u} - \mathbf{j}_s$$

Local fluid velocity

$$\mathbf{u} = \int d\mathbf{v}\mathbf{v}f$$

Entropy flux

$$\mathbf{j}_S = -k\int d\mathbf{v}\mathbf{v}f\ln f$$

$$\frac{\partial}{\partial t}s + \frac{\partial}{\partial \mathbf{r}}\cdot \mathbf{j}_s = -k\int d\mathbf{v}\left(1+\ln f\right)J\left[f\right] = \sigma_{ent}$$

BGK Approximation

Collision operator

$$J[f] = -\frac{1}{\tau}\left(f - f_{loc}\right)$$

τ relaxation time

f_{loc} has the same moments as f

$$\int d\mathbf{v}\left(f - f_{loc}\right) = 0$$

$$\int d\mathbf{v}\left(f - f_{loc}\right)\ln f_{loc} = 0$$

$$\sigma_{ent} = \frac{k}{\tau}\int d\mathbf{v}\left(1+\ln f\right)\left(f - f_{loc}\right) = \frac{k}{\tau}\int d\mathbf{v}\left(f - f_{loc}\right)\ln f$$

$$\sigma_{ent} = \frac{k}{\tau}\left\{\int d\mathbf{v}\left(f - f_{loc}\right)\ln f - \int d\mathbf{v}\left(f - f_{loc}\right)\ln f_{loc}\right\}$$

$$= \frac{k}{\tau}\int dv\left(f - f_{loc}\right)\left(\ln f - \ln f_{loc}\right)$$

$$\left(x-y\right)\left(\ln x - \ln y\right) \geq 0 \qquad \sigma_{ent} \geq 0$$

Changes in Entropy

$$\frac{\partial s}{\partial t} + \nabla \cdot \mathbf{j}_s = \sigma_{ent}$$

LHS conservation equation

RHS source terms

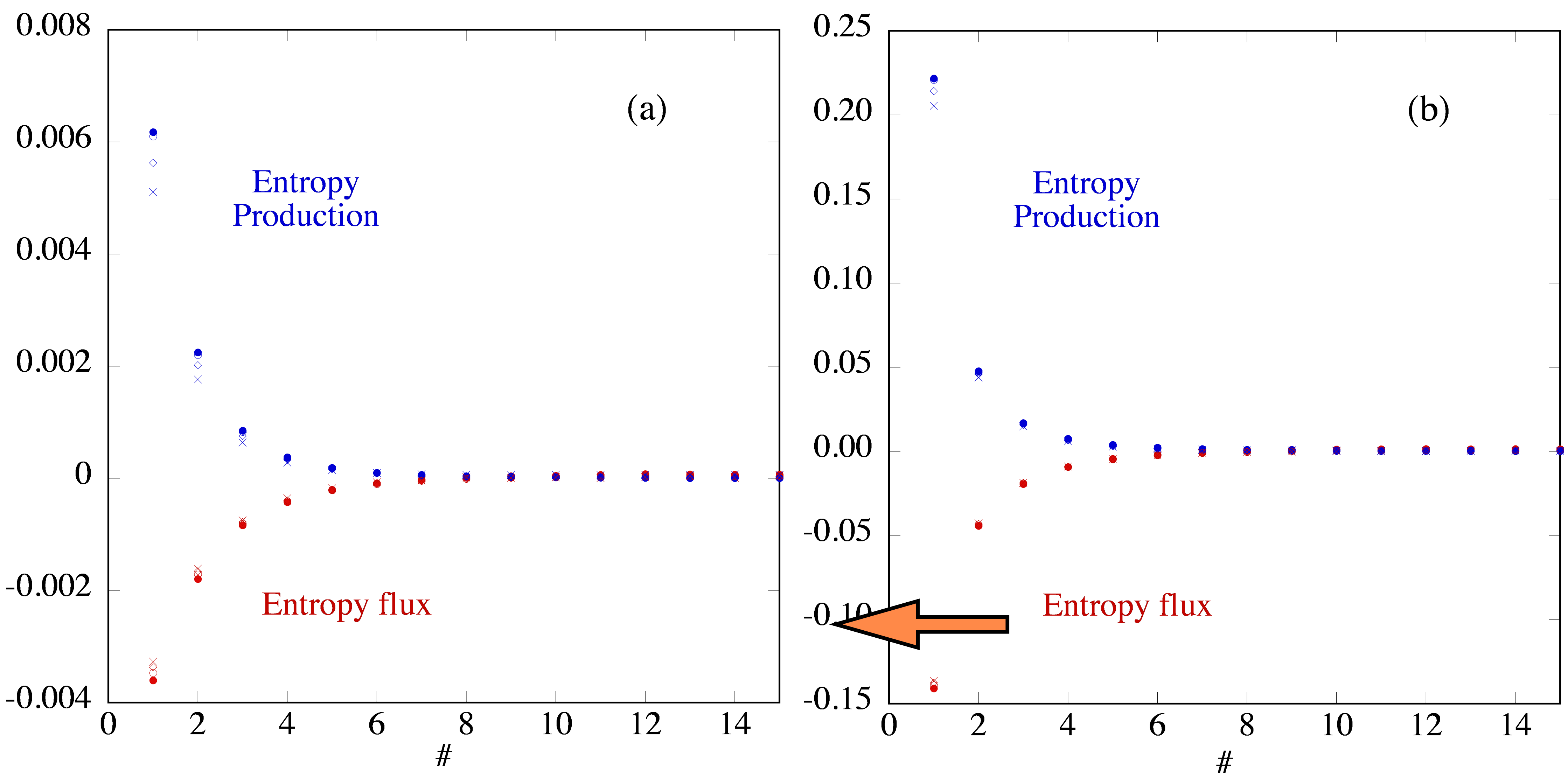
Steady state $\frac{\partial s}{\partial t} = 0$

QOD system

$$\frac{\partial}{\partial x} j_s(x) = \sigma_{ent}(x)$$

Entropy Production and Entropy Flux

Independent of system size - depends on particle #



$\rho = 0.03$ $\rho = 0.8$

Simulations Constant external gradient $\rho = 0.8$

N	TL	TR	Lx	B
80	3	2	86.95652	8
160	4	2	173.91304	8
320	6	2	347.82609	8
640	10	2	695.65218	18
960	14	2	1043.47827	20
1280	18	2	1391.30436	16
1920	26	2	2086.95654	16
2560	34	2	2782.60871	18
3840	50	2	4173.91308	16
5120	66	2	5565.21742	24
10240	130	2	11130.43484	24

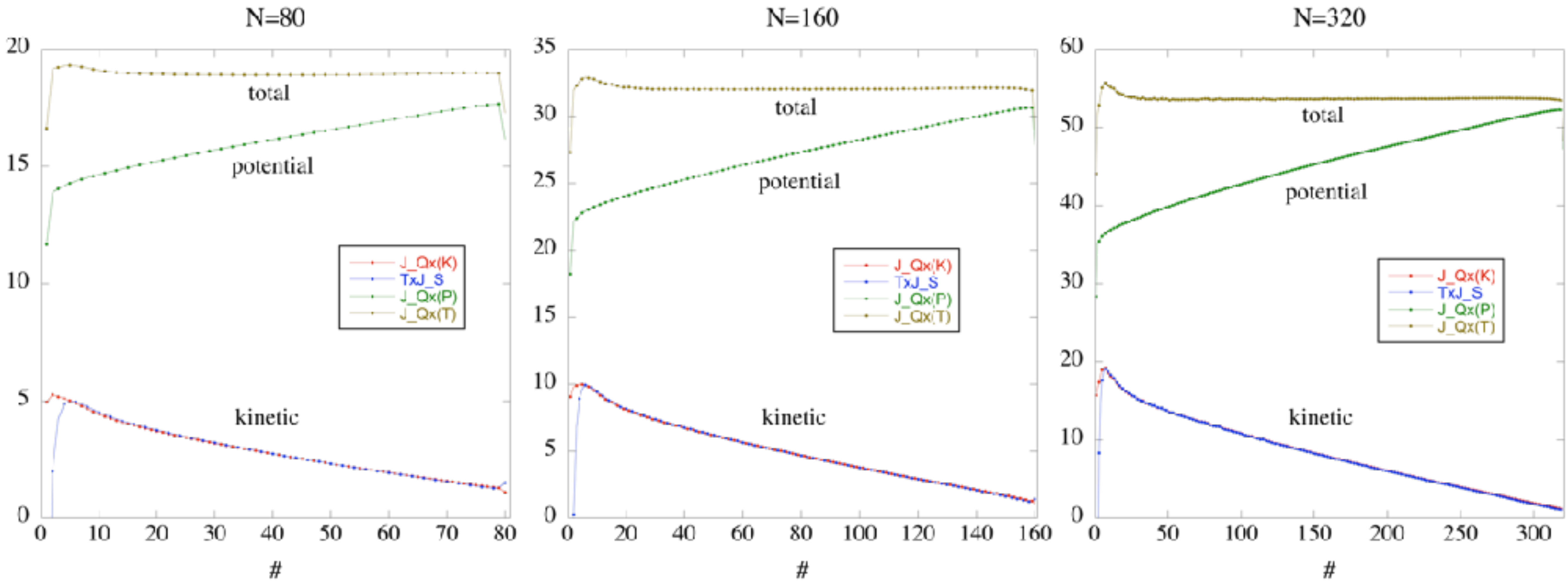
$$\nabla T = \frac{T_R - T_L}{L_x} = \frac{2-3}{86.95652} = -0.01150$$

B blocks of 10^9 collisions

Heat Flux vector

- Continuity
- Anomalous thermal conductivity

Local Heat Flux   same ∇T



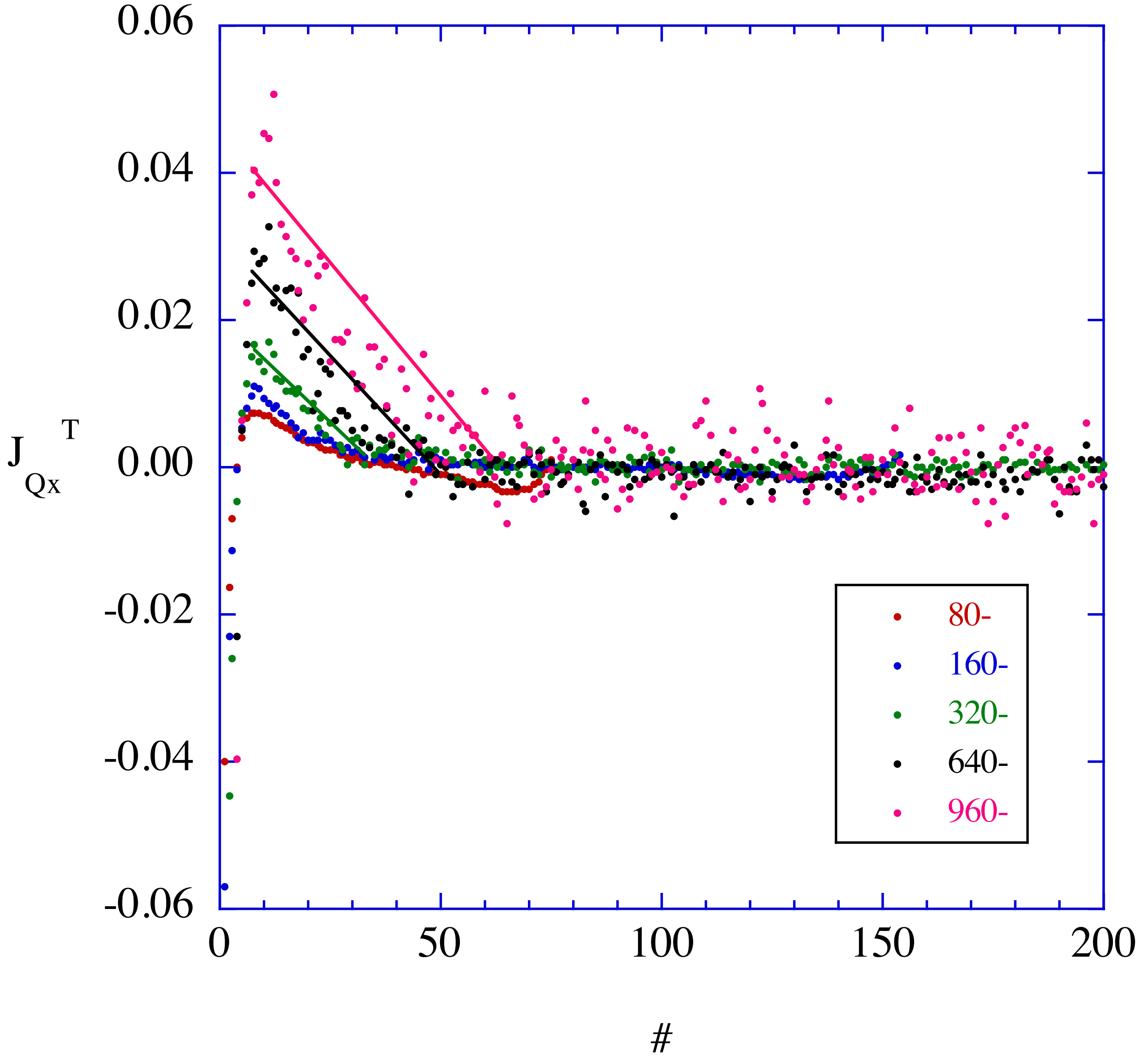
$\rho = 0.8$

Kinetic heat flux vector = T x kinetic Entropy flux $\quad J_Q^K = T j_s$

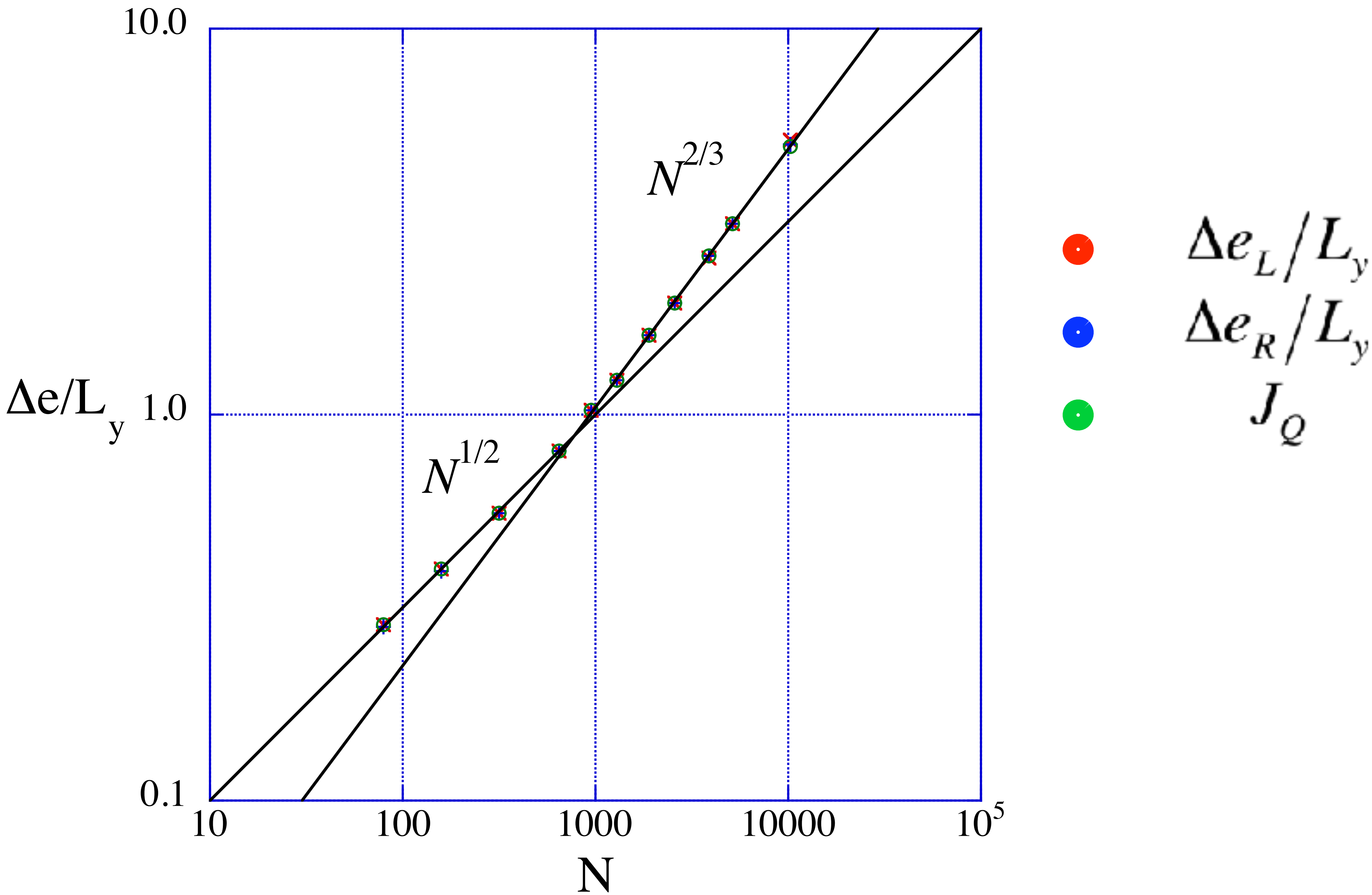
Total heat flux vector = kinetic + potential $\quad J_Q = J_Q^K + J_Q^P$

Total heat flux vector is constant across the system $\quad J_Q = \text{constant}$

Energy continuity anomaly



N dependence of Heat Flux



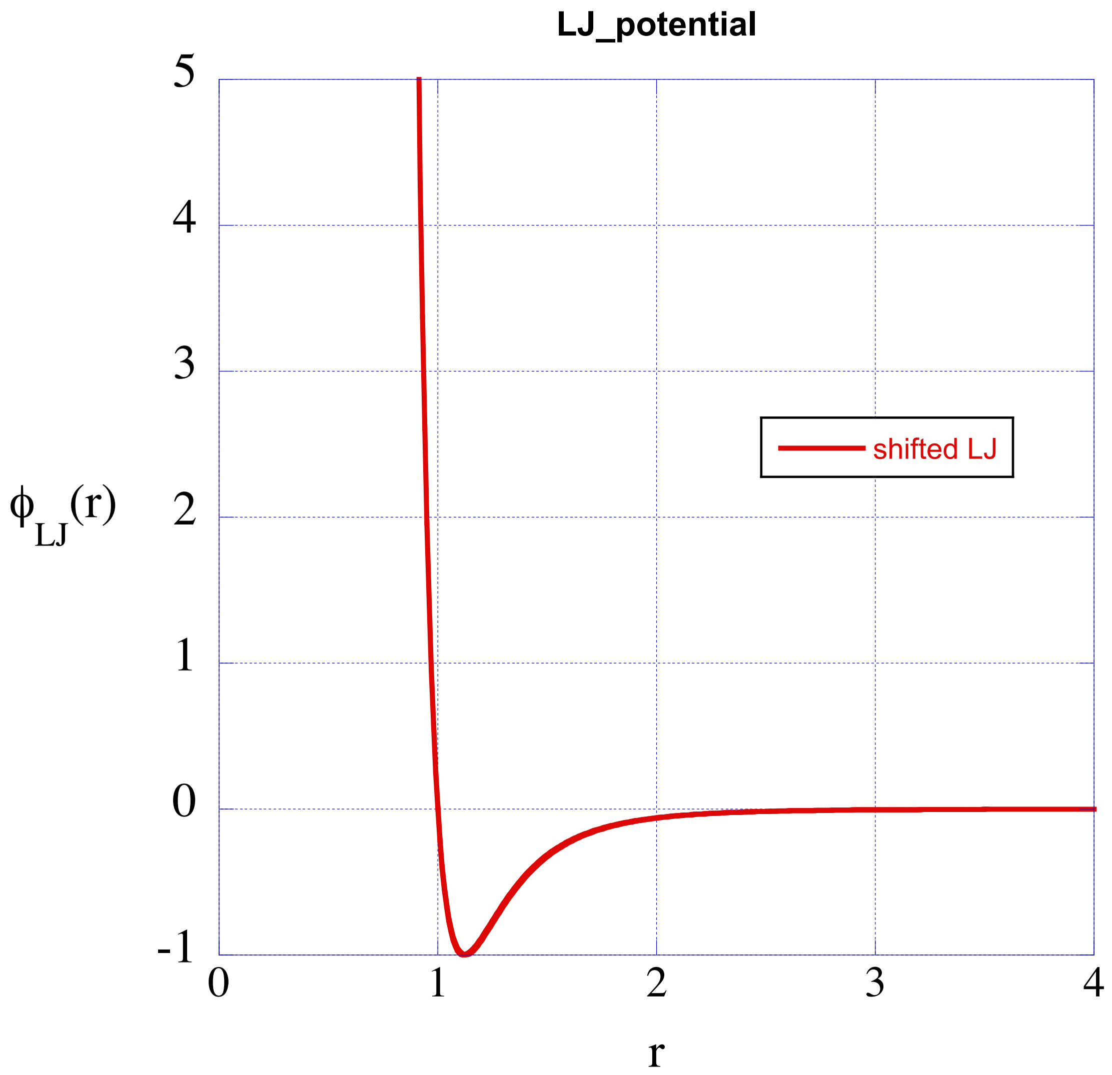
Fixed external gradient $\nabla T = \frac{T_R - T_L}{L_x} = -0.01150$

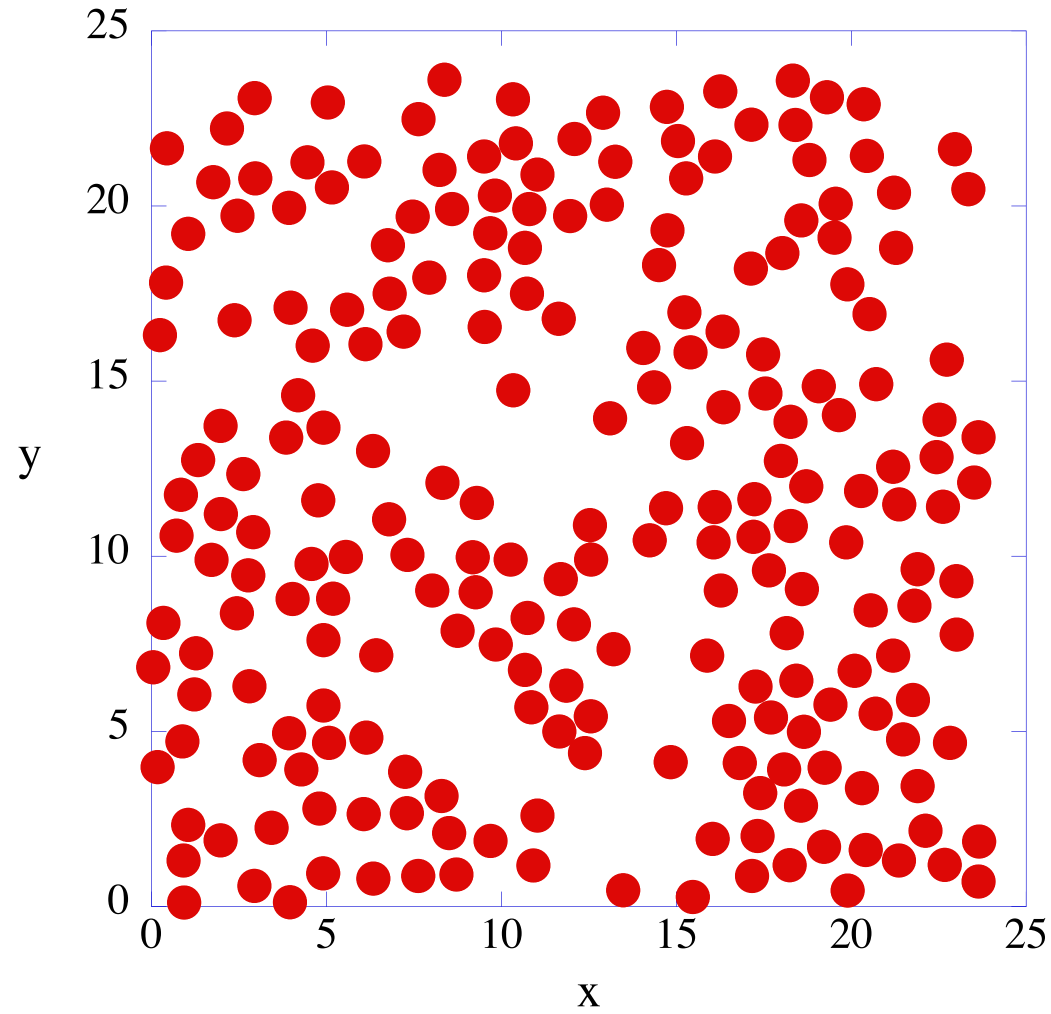
QOD Summary

- Local heat flux vector
- Mechanical energy transfer from a reservoir
- Separation of boundary and bulk effects
- Some nice scaling relations
- No potential contributions to local flux or production entropy .....

Soft Discs Thermal Conductivity

Constant Heat Flux





Thermal Conductivity

Define 2nd rank quantity Ω_i

$$\Omega_i = e_i\mathbf{I} - \tfrac{1}{2}\sum_j \mathbf{F}_{ij}\mathbf{r}_{ij}$$

$$\bar{\Omega} = \frac{1}{N}\sum_i \Omega_i = \frac{1}{N}\sum_i \left(e_i\mathbf{I} - \tfrac{1}{2}\sum_j \mathbf{F}_{ij}\mathbf{r}_{ij}\right) = \bar{e}\mathbf{I} - \tfrac{1}{2}\overline{\mathbf{Fq}}$$

Heat flux vector is

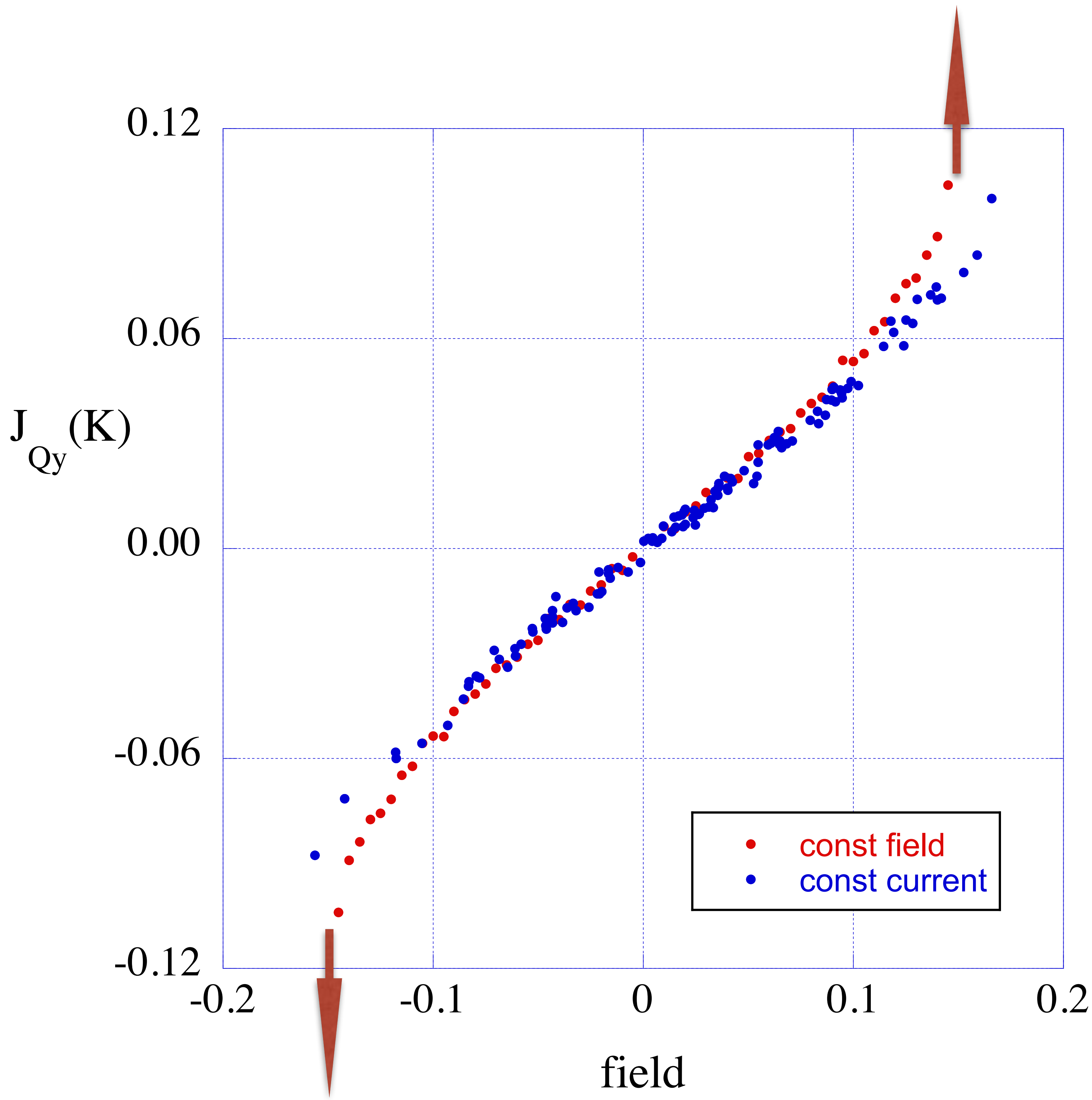
$$\mathbf{J}_Q(t)V = \sum_i e_i\mathbf{v}_i - \tfrac{1}{2}\sum_{i,j}\mathbf{v}_i \cdot \mathbf{F}_{ij}\mathbf{r}_{ij} = \sum_i \mathbf{v}_i \cdot \Omega_i$$

Isokinetic equations of motion

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$

$$m\dot{\mathbf{v}}_i = \mathbf{F}_i + \left(\Omega_i - \bar{\Omega}\right)\cdot \lambda(t) - \alpha m\mathbf{v}_i$$

Kinetic Heat Flux Vector



2D LJ

$r_{cut} = 3.5$

$\rho = 0.4$

T=1