Isolated Non-Equilibrium Systems in Contact

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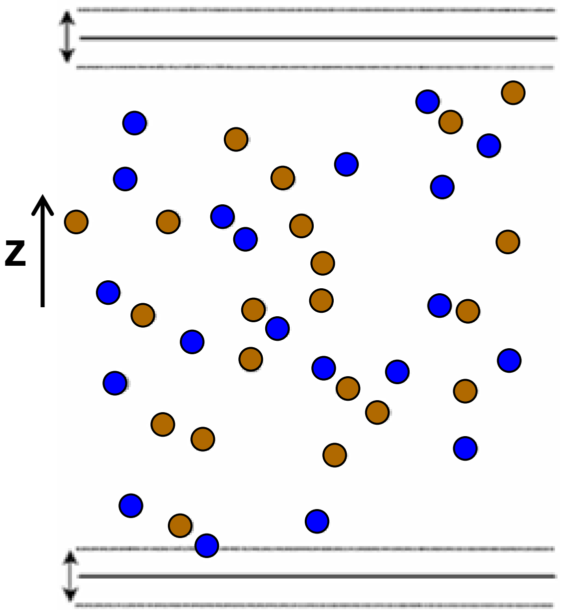
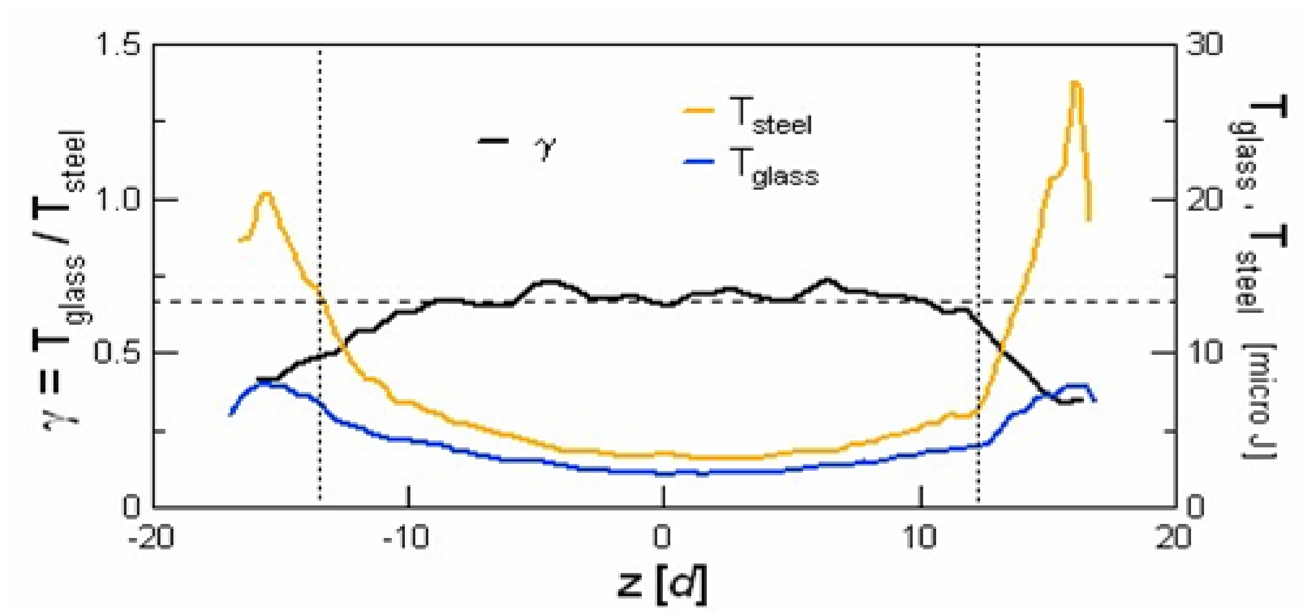
Isolated Non-Equilibrium Systems in Contact



- Shake a box with 2 types of grains
- Measure: T_G = average energy per particle
- Energy not equipartitioned



Wildman & Parker 2002
Feitosa & Menon 2002
Barrat & Trizac 2002

Isolated Non-Equilibrium Systems in Contact

- Shake a box with 2 types of grains
- Measure: T_G = average energy per particle
- Energy not equipartitioned
- Not that surprising:
  restitution coefficient
  → energy dissipation rate
  → steady-state energy
- Maybe fluctuation-dissipation relations encode deeper meaning of temperature ?

Isolated Non-Equilibrium Systems in Contact

- Shake a box with 2 types of grains
- Measure:
  - Fluctuation (diffusion)
  - Response (mobility)
- Define: $T_{FD} = \frac{\text{Fluctuation}}{\text{Response}}$
- Simulations: $T_{FD}(A) \approx T_G(A) \neq T_{FD}(B) \approx T_G(B)$
- Maybe fluctuation-dissipation relations encode deeper meaning of temperature ?

? ? ?

Puglisi, Baldassarri, Loreto 2002
Barrat, Loreto, Puglisi 2004

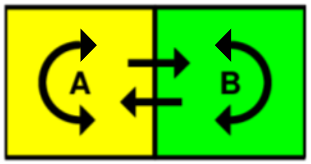
Isolated Non-Equilibrium Systems in Contact

- Entropy, S, maximized
- Energy, E, conserved

$$\Downarrow$$

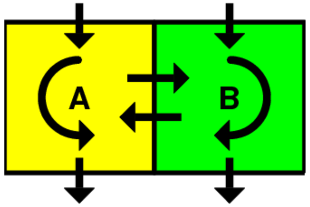
- Temperature, $T = \left(\frac{\partial S}{\partial E}\right)^{-1}$ equalizes

Isolated Non-Equilibrium Systems in Contact



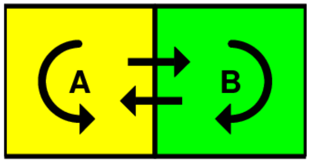
Equilibrium (isolated & detailed balance)

E=const. , max(S) $\Rightarrow$ T(A)=T(B)



Driven Dissipative (open & no detailed balance)

E≠const. , S ? , $T_{eff}(A) \stackrel{?}{=} T_{eff}(B)$

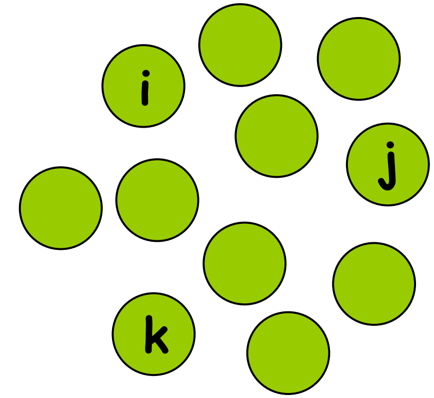


Isolated & no detailed balance

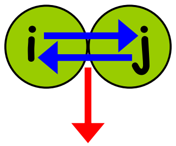
Non-equilibrium , Simpler

Shokef, Shulkind, Levine 2007

Minimal Modeling



- Particles $1 \le i \le N$ have energies $\{e_i > 0\}$
- Mean-field interactions (randomly chose i , j , k)
- Energy



- exchanged
- lost

$$e_i \longrightarrow z\alpha(e_i+e_j)$$

$$e_j \longrightarrow (1-z)\alpha(e_i+e_j)$$

$$(1-\alpha)(e_i+e_j)$$

$0 \le z \le 1$ random (uniform dist.)
$0 \le \alpha \le 1$ restitution coefficient

- **$\alpha=1$** (Ulam 1980) → system equilibrates (H-theorem)
- Dissipation ($\alpha < 1$) → system cools to $e_i=0$
- Connect to thermostat → (open) non-equilibrium steady state

Srebro & Levine 2004

Isolated non-equilibrium model:

- Give dissipated energy to 3rd particle

$$e_k \longrightarrow e_k+(1-\alpha)(e_i+e_j)$$

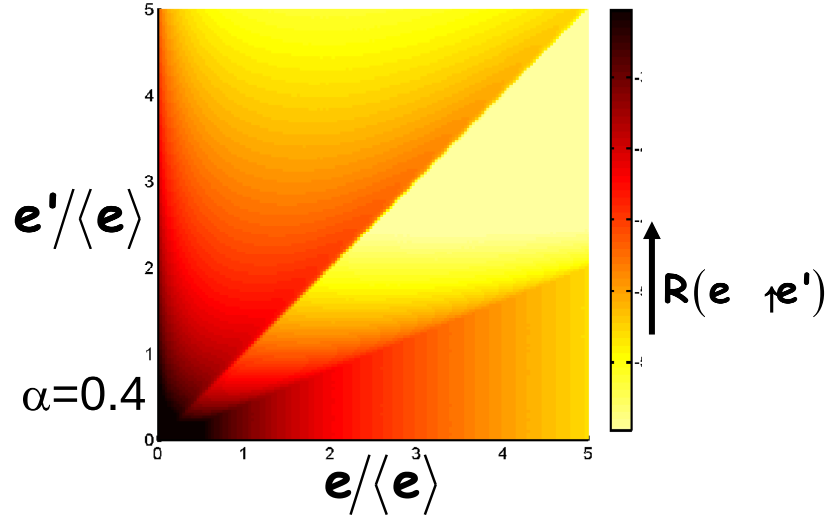
Shokef, Shulkind, Levine 2007

Isolated System is Far from Equilibrium

- Consider subsystem of 1 particle in large isolated system
- Measure rates of transitions between its states

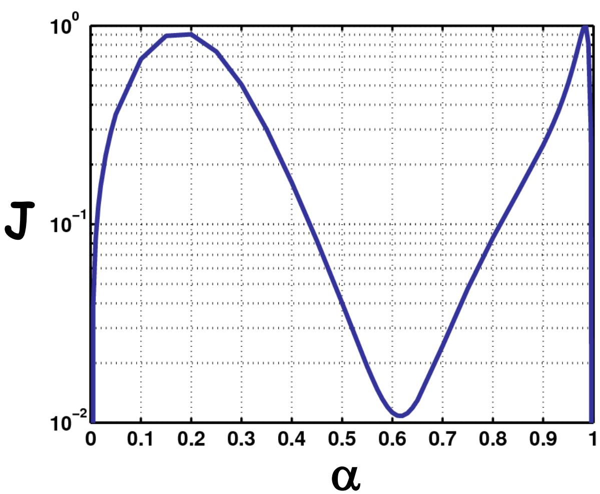
$$R(e \to e') = W(e \to e' | e) P(e)$$

Rate at which transition occur — Probability for transition, given e



- Microscopic irreversibility
  → **Detailed-balance violation**:

$$R(e \to e') \neq R(e \to e')$$



Quantify distance from equilibrium with net probability current:

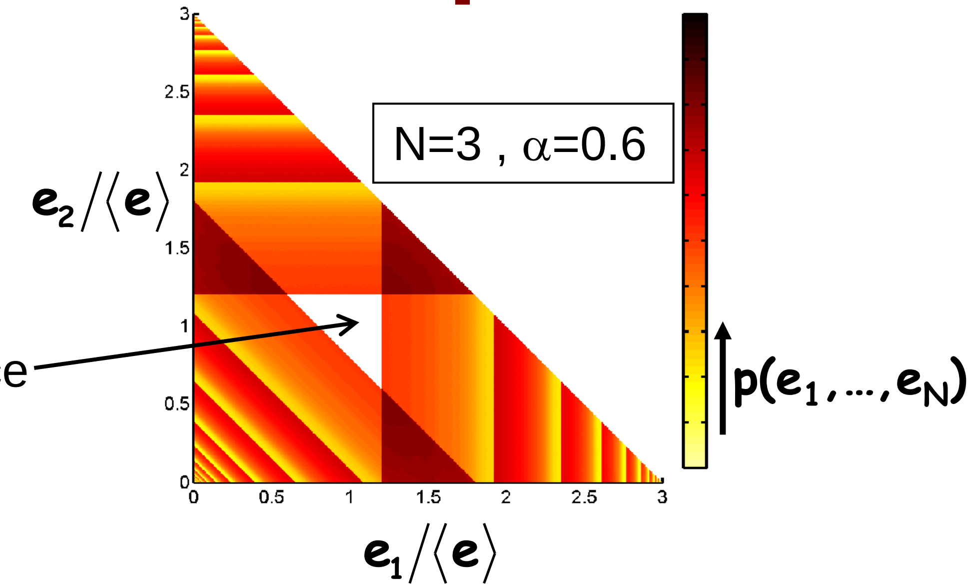
Zia & Schmittmann 2006

$$J \equiv \int \left[R(e \to e') - R(e' \to e) \right]^2 de\, de'$$

$$e_i \longrightarrow z\alpha(e_i + e_j)$$
$$e_j \longrightarrow (1-z)\alpha(e_i + e_j)$$
$$e_k \longrightarrow e_k + (1-\alpha)(e_i + e_j)$$

Isolated System is Far from Equilibrium

- Microscopic irreversibility
  → **Ergodicity breaking**



inaccessible region in configuration space

- Microscopic irreversibility
  → **Detailed-balance violation**

Ask what transition brings the system to $e_1=e_2=\ldots=e_N=E/N$

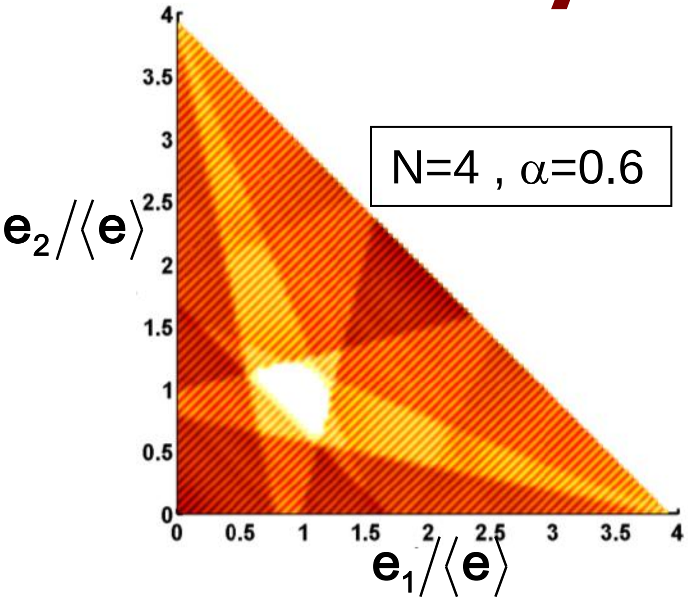
$$\left.\begin{aligned} e_i &\rightarrow z\alpha(e_i+e_j) = E/N \\ e_j &\rightarrow (1-z)\alpha(e_i+e_j) = E/N \\ e_k &\rightarrow e_k+(1-\alpha)(e_i+e_j) = E/N \end{aligned}\right] \longrightarrow e_k = \left(3-\frac{2}{\alpha}\right)\frac{E}{N} > 0 \longrightarrow \alpha > \frac{2}{3}$$

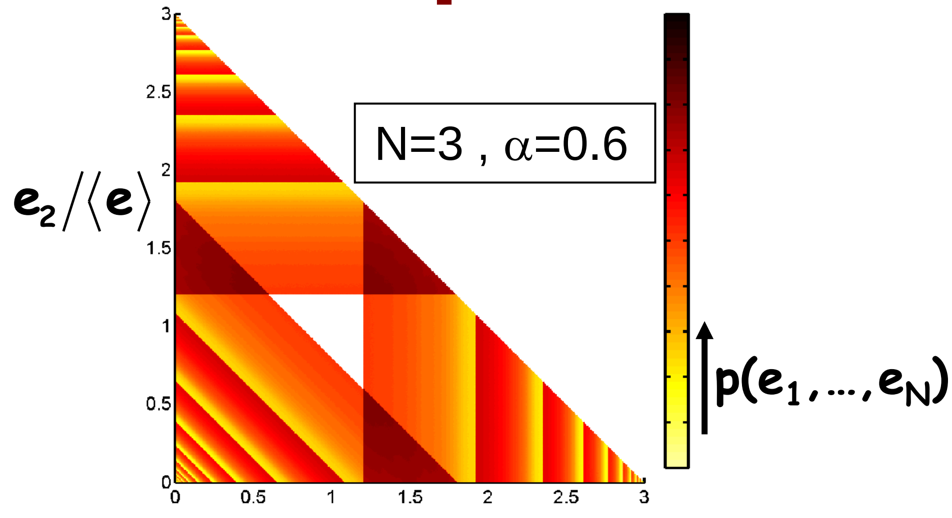
- For $\alpha < \frac{2}{3}$ the dynamics can't bring the system to $e_1=e_2=\ldots=e_N$

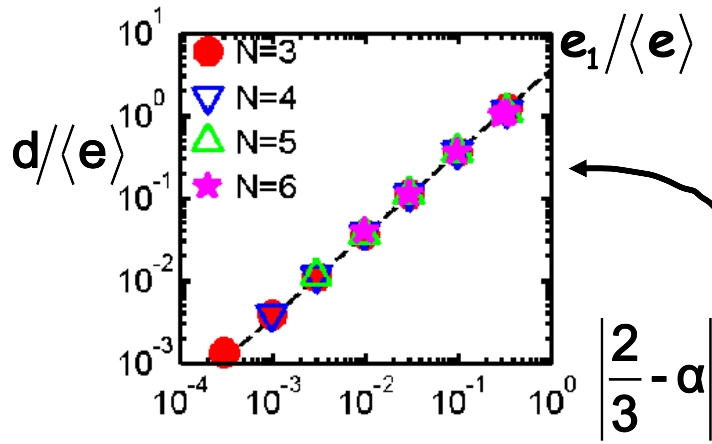
- Diameter of "hole" shrinks linearly with α :

$$d \equiv \left(\sum_{i=1}^{N}(e_i-\langle e\rangle)^2\right)^{1/2} = \sqrt{\frac{3}{2}}\left(\frac{2}{3}-\alpha\right)\langle e\rangle$$

Isolated System is Far from Equilibrium







- Non-ergodicity disappears when system thermostated → ensemble inequivalence (like long-range interactions?)

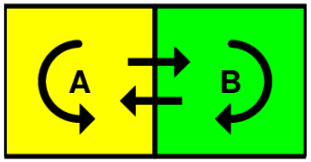
e.g. Mukamel, Ruffo, Schreiber 2005

- For $\alpha < \frac{2}{3}$ the dynamics can't bring the system to $e_1=e_2=\dots=e_N$

- Diameter of "hole" shrinks linearly with α :

$$d \equiv \left(\sum_{i=1}^{N}(e_i-\langle e\rangle)^2\right)^{1/2} = \sqrt{\frac{3}{2}}\left(\frac{2}{3}-\alpha\right)\langle e\rangle$$

Contact between Isolated Systems



- Different types of particles (A≠B)
- Intra-system (α_{AA},α_{BB}) & inter-system (α_{AB}) interactions

Average energy change in each type of interaction:

i j k	$\Delta\langle e_A\rangle$
A A A	0
B B B	0
A A B	$-2(1-\alpha_{AA})\langle e_A\rangle$
B B A	$2(1-\alpha_{BB})\langle e_B\rangle$
A B A	$\langle e_B\rangle-\alpha_{AB}(\langle e_A\rangle+\langle e_B\rangle)/2$
B A A	
A B B	$-\langle e_A\rangle+\alpha_{AB}(\langle e_A\rangle+\langle e_B\rangle)/2$
B A B	

$$\longrightarrow \quad \frac{d\langle e_A\rangle}{dt}=2\left[(2-\alpha_{BB})\langle e_B\rangle-(2-\alpha_{AA})\langle e_A\rangle\right]$$

1) Steady state → no equipartition:

$$T_G(A)=\langle e_A\rangle\neq\langle e_B\rangle=T_G(B)$$

2) Identify operational temperature:

$$T_{op}=(2-\alpha)\langle e\rangle$$

- controls energy flow
- equalizes in steady state
- obeys 0th law (transitivity)
- coincides with equilibrium temperature at $\alpha=1$

(Fluctuation-Dissipation Relations)

$$T_{FD} \equiv \frac{\text{Correlation}}{\text{Response}} = \cdots = \frac{\langle e^2 \rangle}{2\langle e \rangle} = \frac{9 - 12\alpha + 5\alpha^2}{12\alpha - 10\alpha^2} \langle e \rangle$$

Isolated System

- In principle $T_{FD} \neq T_G = \langle e \rangle$, but for $\alpha > 0.5$, deviations <20%
- This may explain $T_{FD} \approx T_G$ in granular gas simulations
- Isolated non-equilibrium systems in contact:

Weak coupling → $\frac{T_{FD}}{T_G} = \frac{\langle e^2 \rangle}{2\langle e \rangle^2}$ not affected → $T_{FD}(A) \neq T_{FD}(B)$

Srebro, Levine 2004
Shokef, Levine 2006
Shokef, Bunin, Levine 2006

Entropy may Decrease due to Contact

- **Isolated System**

Single-particle energy distribution: $$p(e) = \frac{1}{E}\varphi\left(\frac{e}{E};\alpha\right)$$

↖ dimensionless function

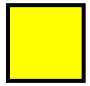
$$s = -\int p(e)\log\left(p(e)\right)de = \log(E)\int p(e)\,de - \int \varphi\left(\frac{e}{E};\alpha\right)\log\left(\varphi\left(\frac{e}{E};\alpha\right)\right)\frac{de}{E} = \log(E) + s_0(\alpha)$$

Phase-space distribution: $$P(e_1,\ldots,e_N) = \frac{1}{E^N}\varphi\left(\frac{e_1}{E},\ldots,\frac{e_N}{E};\alpha\right)$$

↓

$$S = -\int P\cdot\log(P)\,de_1\cdots de_N = \ldots = N\cdot\log(E) + S_0(\alpha)$$

Entropy may Decrease due to Contact

- **Isolated System** 

$$S(E;\alpha)=N\cdot\log(E)+S_0(\alpha)$$

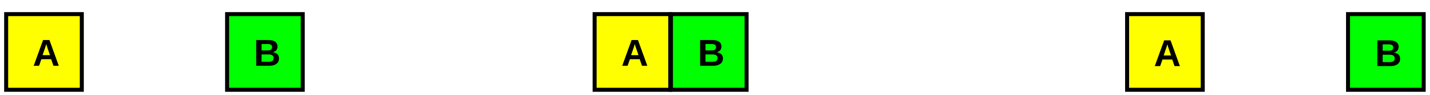
- **Disconnected systems**

$$S=S_A+S_B=N\cdot\log(E_A)+N\cdot\log(E_B)+\text{const.}$$

$$\downarrow$$

$$\max(S)\ \Leftrightarrow\ E_A=E_B$$

- **Start with $E_A=E_B$, connect systems , then disconnect**



Dynamics lead to $E_A\neq E_B$ which has lower entropy ???

Why define S as $-\int p \cdot \log(p)$?

Why not assume $\frac{\partial S}{\partial E} = \frac{1}{T_{op}}$

and integrate to find S ?

Isolated System:

$$\frac{\partial S}{\partial E} = \frac{1}{T_{op}} = \frac{N}{(2-\alpha)E} \longrightarrow dS = \frac{N}{2-\alpha} \cdot \frac{dE}{E} \longrightarrow S = \frac{N}{2-\alpha}\log(E) + const.$$

Two Systems:

$$S = \frac{N}{2-\alpha_{AA}}\log(E_A) + \frac{N}{2-\alpha_{BB}}\log(E_B) + const.$$

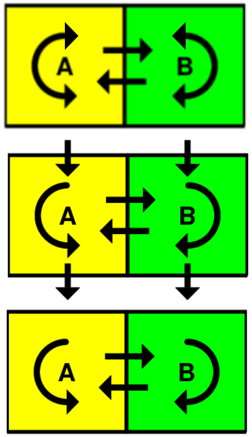
$$\downarrow$$

$$\max(S) \Leftrightarrow \frac{E_A}{E_B} = \frac{2-\alpha_{BB}}{2-\alpha_{AA}}$$

This is the energy partition reached by the dynamics

Entropy is maximized !!!

Isolated Non-Equilibrium Systems in Contact



1) To study contact between non-equilibrium steady states, better disconnect the systems from the environment

2) Simple model:

$$\begin{aligned} e_i &\longrightarrow z\alpha(e_i+e_j) \\ e_j &\longrightarrow (1-z)\alpha(e_i+e_j) \\ e_k &\longrightarrow e_k+(1-\alpha)(e_i+e_j) \end{aligned}$$

Microscopic irreversibility → Detailed-balance violation + Ergodicity breaking

3) Upon contact: - customarily used T_{eff}'s don't equilibrate
- but we identified T_{op}

4) $S=-\int p\cdot\log(p)$ may increase, but $S=\int\frac{dE}{T_{op}}$ is maximized

Details: Y. Shokef, G. Shulkind, D. Levine, Phys. Rev. E **76**, 030101(R) (2007)