4th KIAS Conference on Statistical Physics 2010.07.26

Convection Cells without Shear or Gravity

Surprises from a Simple Model in Non-equilibrium Statistical Mechanics

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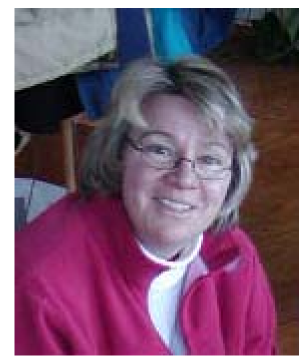

Michel Pleimling   Beate Schmittmann

Siddharth Venkat

Thanks to Alexander von Humboldt Stiftung/Foundation, NSF

Outline

- Motivations
  - Current loops in non-equilibrium steady states
  - Convection cells in real life
- Model specifications
- Simulation studies
  - How currents are measured and displayed: $\boldsymbol{j}$, ψ, and ω
  - Non-trivial steady currents *vs.* fluctuations around zero
- Theoretical considerations
  - An "absolutely minimal" (exactly solvable) system
  - Mesoscopic approach (mean-field, continuum, hydrodynamics)
- What else? (Surprises even above T_c and in 1-D)

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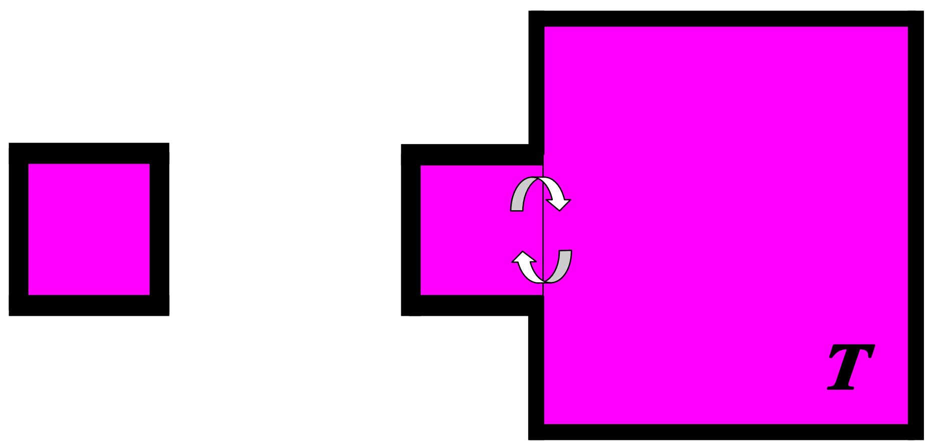
Equilibrium *vs.* Non-equilibrium SM

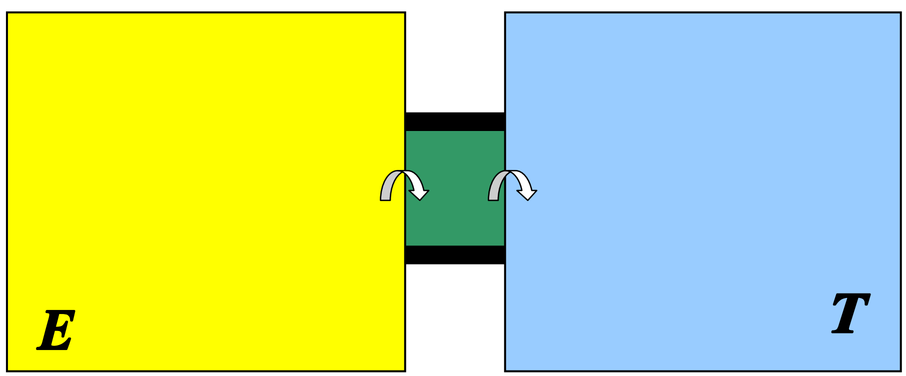
- Interacting many-particle systems – *Statistical Mechanics*
- 3-step program for a system in thermal equilibrium:
  - Specify configurations of system: $\{C\}$
  - Specify internal energy for each configuration: $H[C]$
  - Exploit Boltzmann/Gibbs framework
  - Known $P[C]$; hard part is to compute averages of observables



$P[C] \propto \delta(E - H[C])$ $\quad$ $P[C] \propto exp\{-H[C]/kT\}$

Equilibrium *vs.* Non-equilibrium SM

- Interacting many-particle systems – *Statistical Mechanics*
- How do systems (in steady state) far-from-equilibrium differ?
  - Systems *neither* totally isolated *nor* in contact with just **one** bath
  - "Open systems," coupled to many reservoirs
  - Specify rules for ***evolution*** for $P[C,t]$; may or may not have $H[C]$
  - Rules typically violate t reversal (no detailed balance) $\Rightarrow$
    - *probability* currents can exist in ***stationary*** state: $K^*[C,C']$
    - similar to *magnetostatics*



$P^* = ???$

$K^* = ???$

Non-Equilibrium Statistical Mechanics

- Many examples of systems far from equilibrium:
- Common features:
  - Interacting many-particle systems
  - Subject to external forces and/or open boundaries
  - Non-zero transport of mass, energy, etc.
  - Dynamics breaks detailed balance (microscopic time reversal)
  - Even steady states (from simple microscopics) are typically…

COMPLEX !!

Non-Equilibrium Statistical Mechanics

- Many examples of systems far from equilibrium:
- Common features… ***COMPLEX!!***
- How to proceed ?
  - Biologist approach: one particular system at a time
  - Physicist/mathematician approach:

Study simple models

and

Look for essential, universal properties!

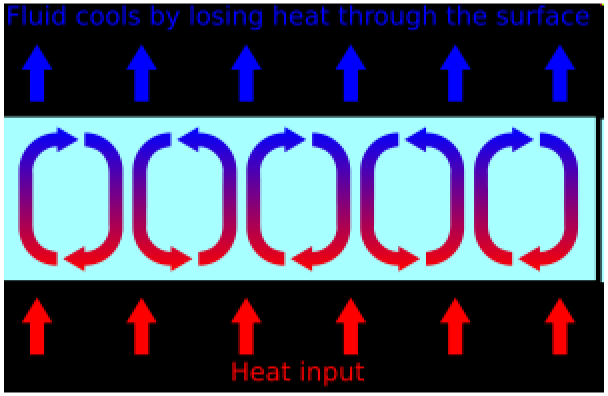
Non-Equilibrium Statistical Mechanics

- Many examples of systems far from equilibrium:
- Common features… ***COMPLEX!!***
- How to proceed ? seek *essential features* in *simple* models
- Physical manifestations of K^* 's
  - energy flux ***through*** the system
  - particle currents (especially loops in steady states!)

Convection Cells

Convection cells in daily life

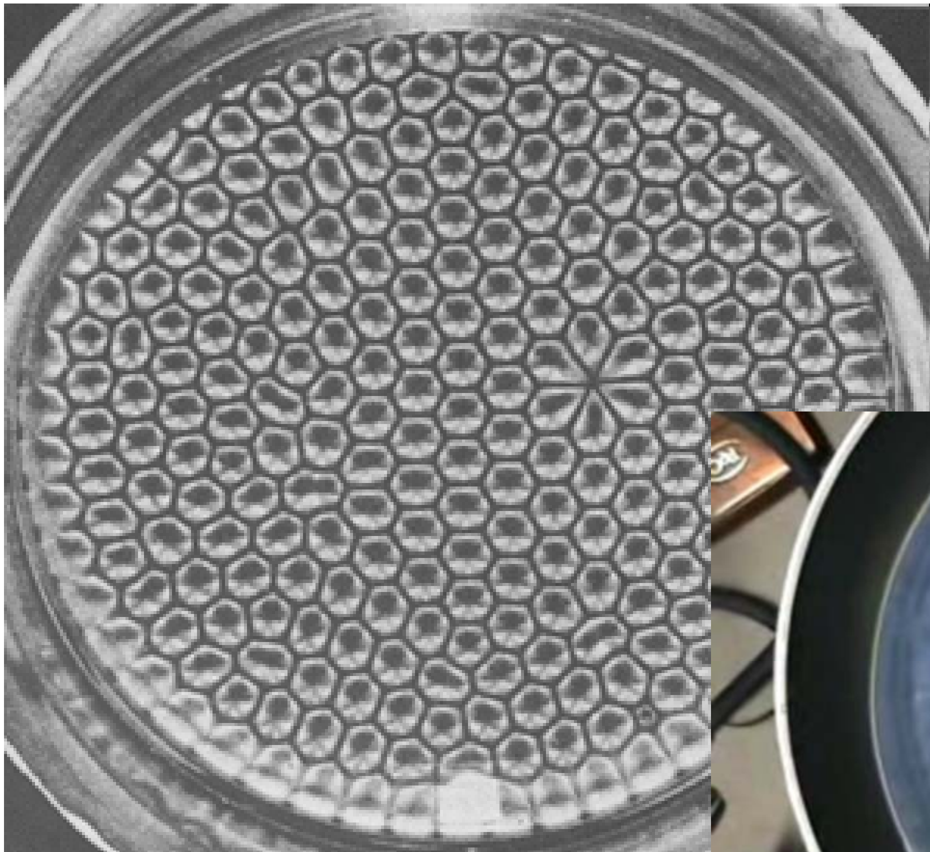
- Rayleigh-Benard

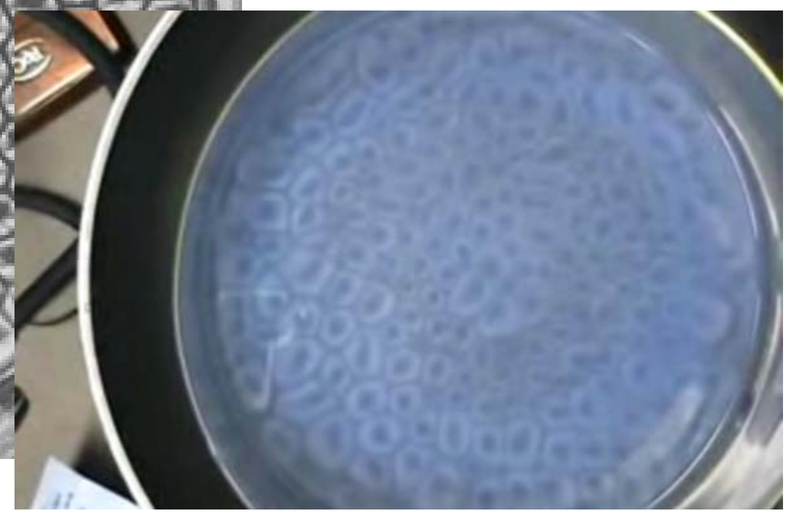


Rayleigh-Bernard convection in cooking oil

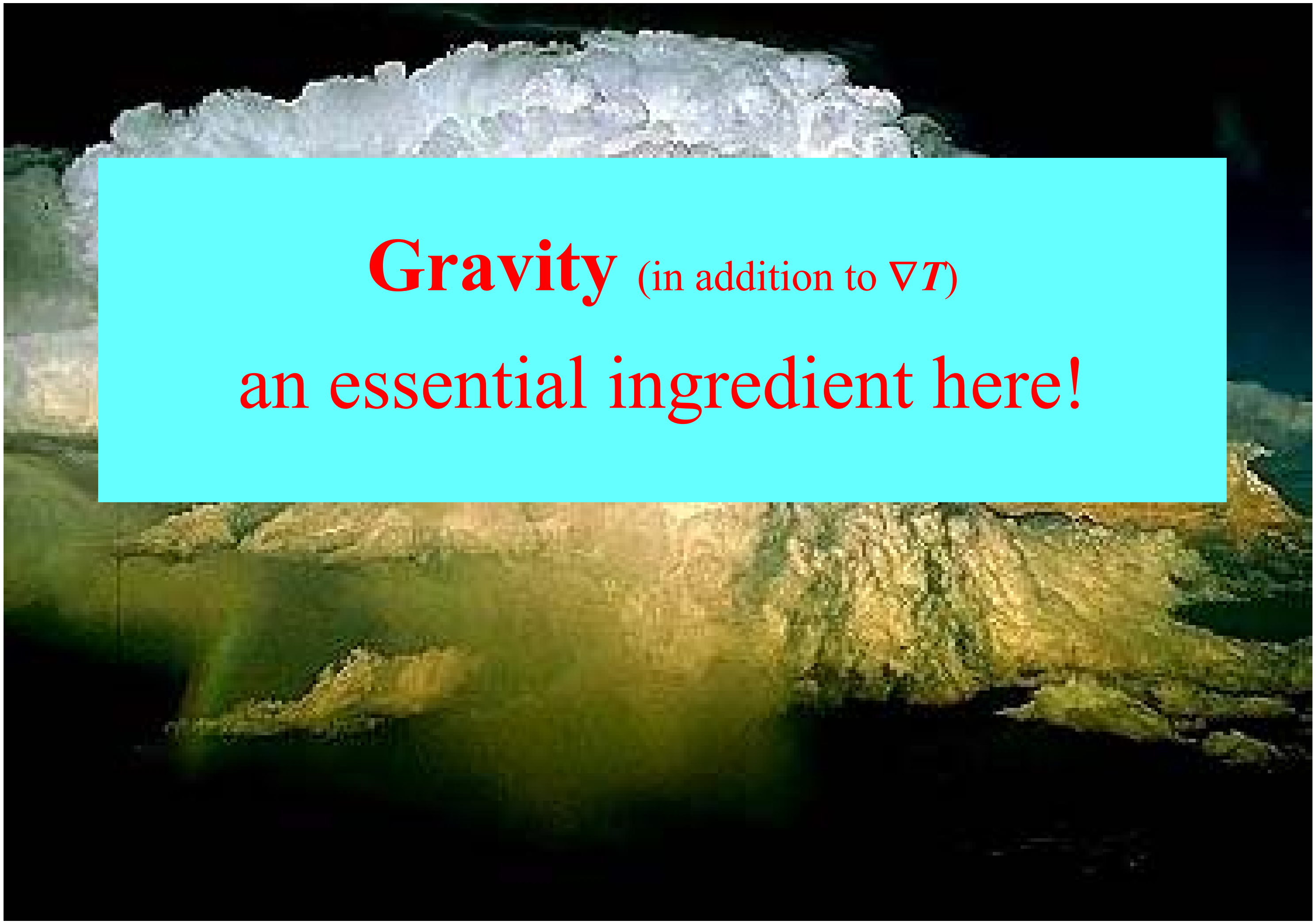
(photo by Ben Schultz April 2009)

http://www.aep.cornell.edu/eng10_student_course.cfm?function=detail&courseID=86





http://www.catea.gatech.edu/grade/mecheng/mod8/mod8.html



Gravity (in addition to $\nabla \boldsymbol{T}$)

an essential ingredient here!

http://www.airphotona.com/image.asp?imageid=712

Convection cells in daily life

- Kelvin-Helmholtz

http://en.wikipedia.org/wiki/File:Wavecloudsduval.jpg

“Kelvin-Helmholtz clouds”

Benjamin Foster; http://www.ucar.edu/news/events/moreclouds.shtm

Shear

an essential ingredient here!

http://en.wikipedia.org/wiki/File:Kelvin_Helmholz_wave_clouds.jpg

Convection cells in daily life

- Rayleigh-Benard
- Kelvin-Helmholtz
- ⋮

Both rely on the presence of "external" driving forces

Both rely on the presence of density fields as well as velocity fields

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Are there *minimal* conditions for convection cells to exist?

- Temperature gradient
  (external – drive into non-equilibrium steady state)
- Density gradient
  (“internal” – from spontaneous sym. breaking)

no gravity, no shear, no (independent) velocity fields

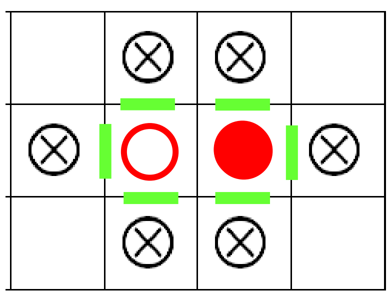
M. Pleimling, B. Schmittmann, and R. K. P. Zia, EPL 89, 50001 (2010)

Ising lattice gas (equilibrium)

- d - dimensional lattice (square in d=2)
- particle or hole at each site ($\mathbf{x} \equiv (x,y)$)
- C : $\{n(\mathbf{x})\}$; $n = 1$ or 0 ; $\Sigma\, n(\mathbf{x}) = N$
- $H(C) = -J \Sigma\, n(\mathbf{x})\, n(\mathbf{x}')$ $\mathbf{x},\mathbf{x}'$ n.n. pairs; ***PBC***; $J > 0$.
- $P(C)$ known : $exp\{-H(C)/k_B T\}$
- displays phase transitions if $d > 1$

Ising lattice gas (equilibrium)

- evolves by Kawasaki dynamics:
  - chose random n.n. pair
  - exchange with prob. ***min*{1, $e^{-\Delta H(C)/kT}$ }** (Metropolis rates)
  - preserves *N*, total particle number (magnetization)
  - system settles into thermal equilibrium…



In general, **6 bonds** can change

Ising lattice gas (equilibrium)

- evolves by Kawasaki dynamics:
  - chose random n.n. pair
  - exchange with prob. $min\{1, e^{-\Delta H(C)/kT}\}$ (Metropolis rates)
  - preserves N, total particle number (magnetization)
  - system settles into thermal equilibrium…
- d=2: $\{ L_x , L_y \}$; half-filled: $N = L_x L_y / 2$
- $T > T_{Onsager} \approx 0.5673 J/k_B$: **homogeneous**
- $T < T_O$: **inhomogeneous**…
  - co-existence of high- and low-density regions
  - separated by microscopically thin interfaces
  - regions are strips aligned with $min\{L_x, L_y\}$

- $T \approx T_O$: **non-trivial critical behavior**

Ising lattice gas (NON-equilibrium)

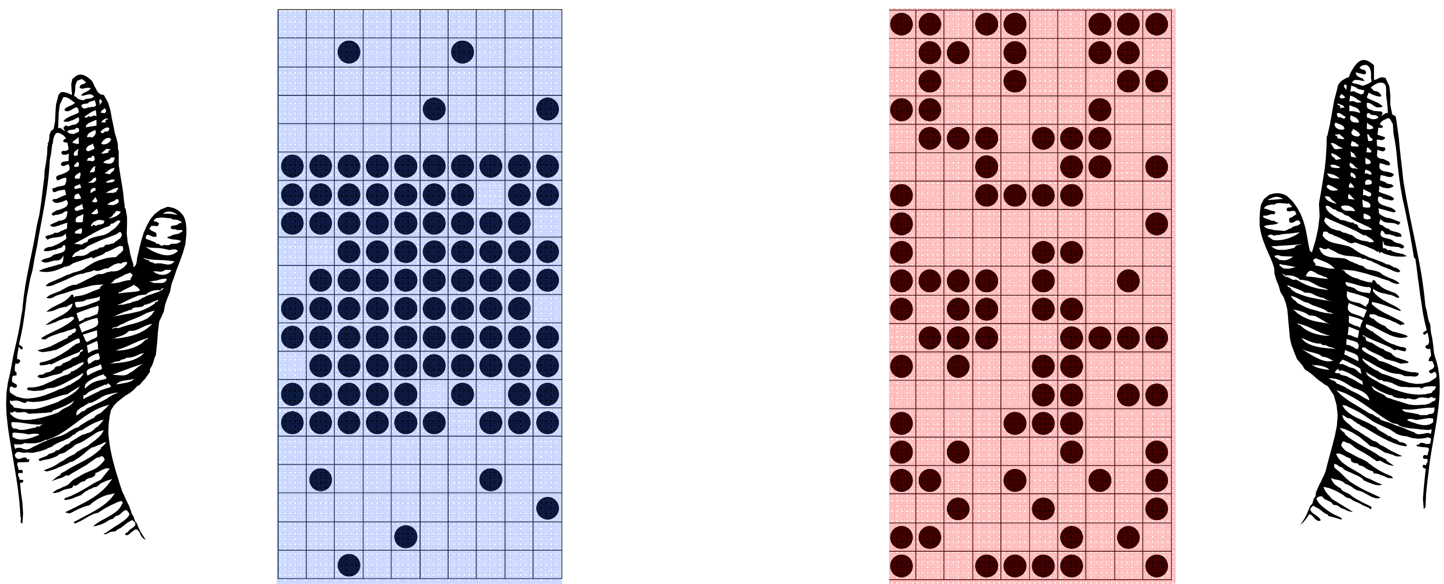
- Take two such systems, identical except for being coupled to two different thermal baths

$$T \text{ and } T'$$

- Put them side by side and change BC's
- … to allow particle exchange

  across a common boundary - "***defect line***"

Ising lattice gas (NON-equilibrium)

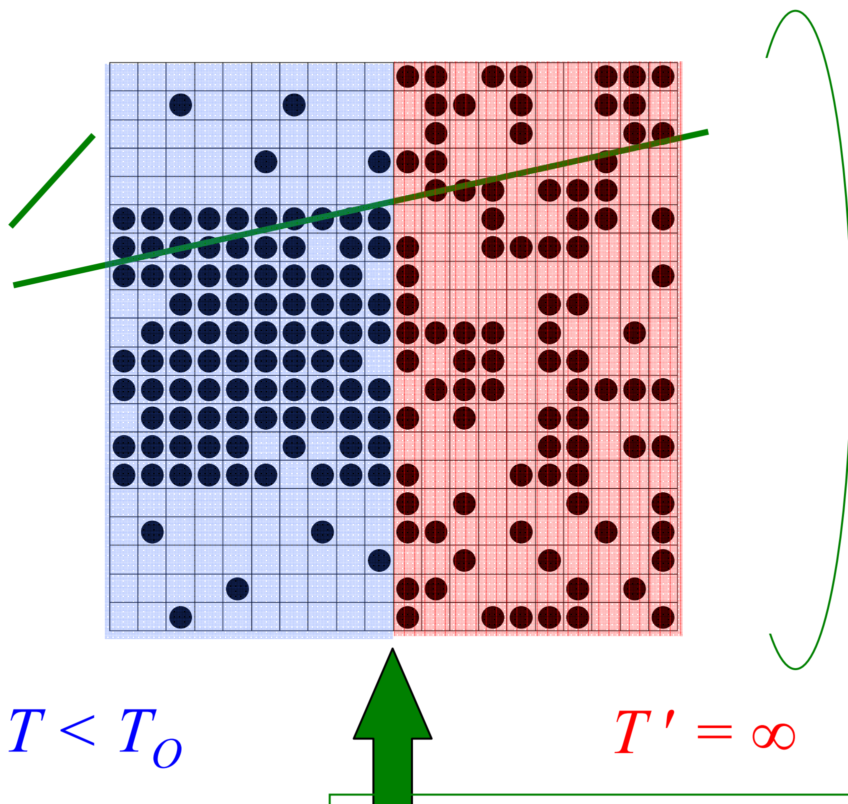


cold T
below T_O

hot T'
say, ∞

Ising lattice gas (NON-equilibrium)

can impose full PBC
(i.e., 2 defects lines)
or Free BC,
or **some others** (later)



PBC
in y

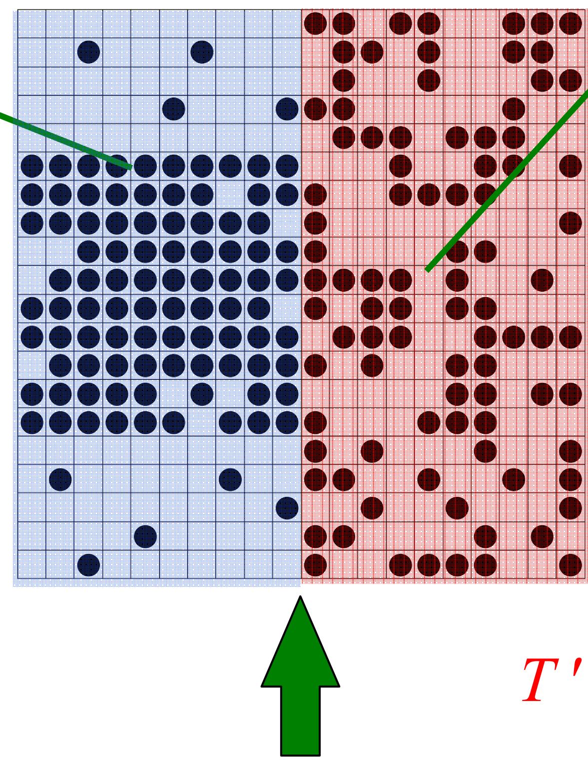
$T < T_O$

$T' = \infty$

- "***defect line***" (of combined system)
- allow p-h exchange across it
- using, say, T' in the rates

Ising lattice gas (NON-equilibrium)

update this side with Metropolis rates using various T's



$T' = \infty$ on this side means ***free diffusion***, just like $J = 0$!

$T' = \infty$

Metropolis rates: $min\{1, e^{-\Delta H(C)/kT}\}$

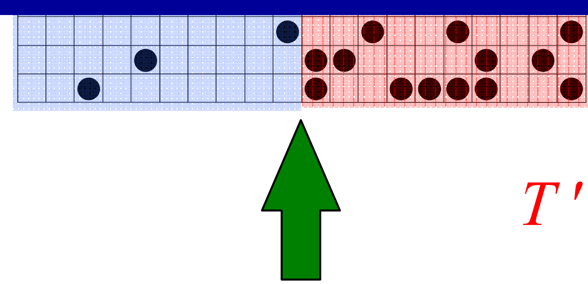
Ising lattice gas (NON-equilibrium)

$T' = \infty$ on this side

ion,

upd

How does this differ from
an Ising model with $J = 0$ on the right,
in contact with a bath at a *single* T ?



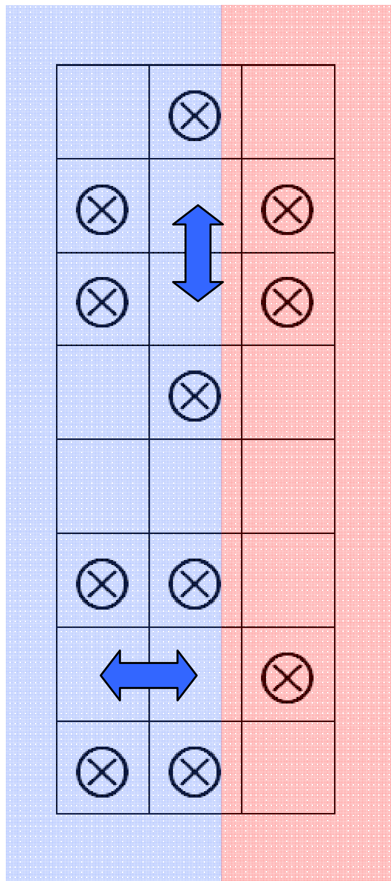
$T' = \infty$

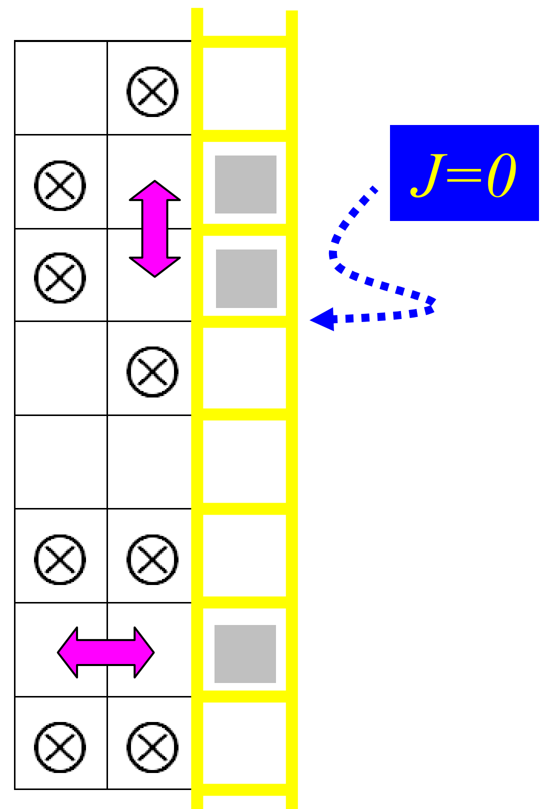
Metropolis rates: $min\{1, e^{-\Delta H(C)/kT}\}$

Model Specs

Ising lattice gases

Non-equilibrium, two *T*'s   Equilibrium, two *J*'s

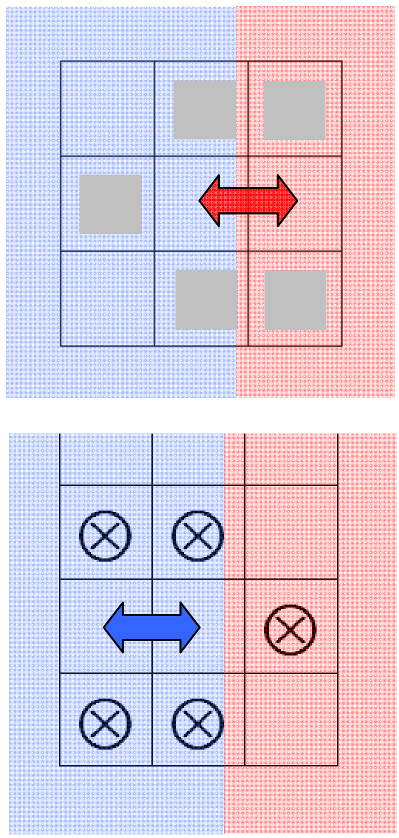




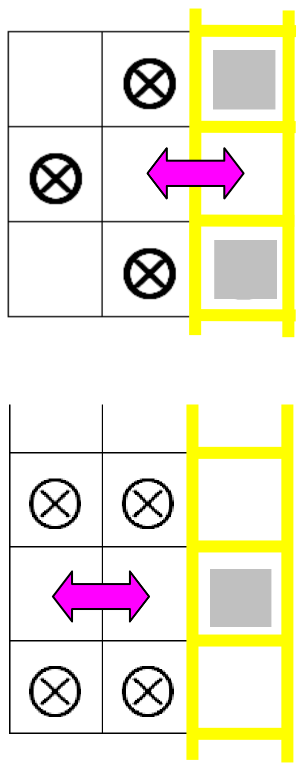
Model Specs

Ising lattice gases

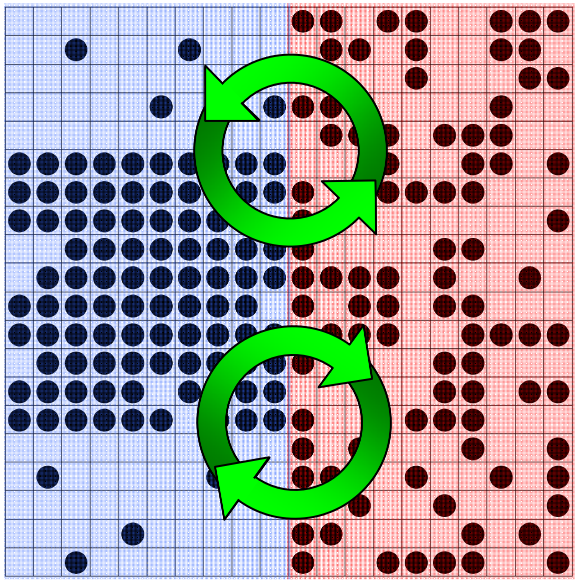
Non-equilibrium, two T's



Equilibrium, two J's



Ising lattice gas (NON-equilibrium)



- dynamics is ***local*** and
- ***homogeneous*** (apart from defect)
- ∇T is localized…
  to defect line, in the sense of ***dynamics***
- density gradients induce net
  particle currents
- …unlike in equilibrium !!
  where density gradients are balanced by attractive interactions
- in steady state, ***currents*** form loops and so, ***convection cells***

Ising lattice gas (NON-equilibrium)

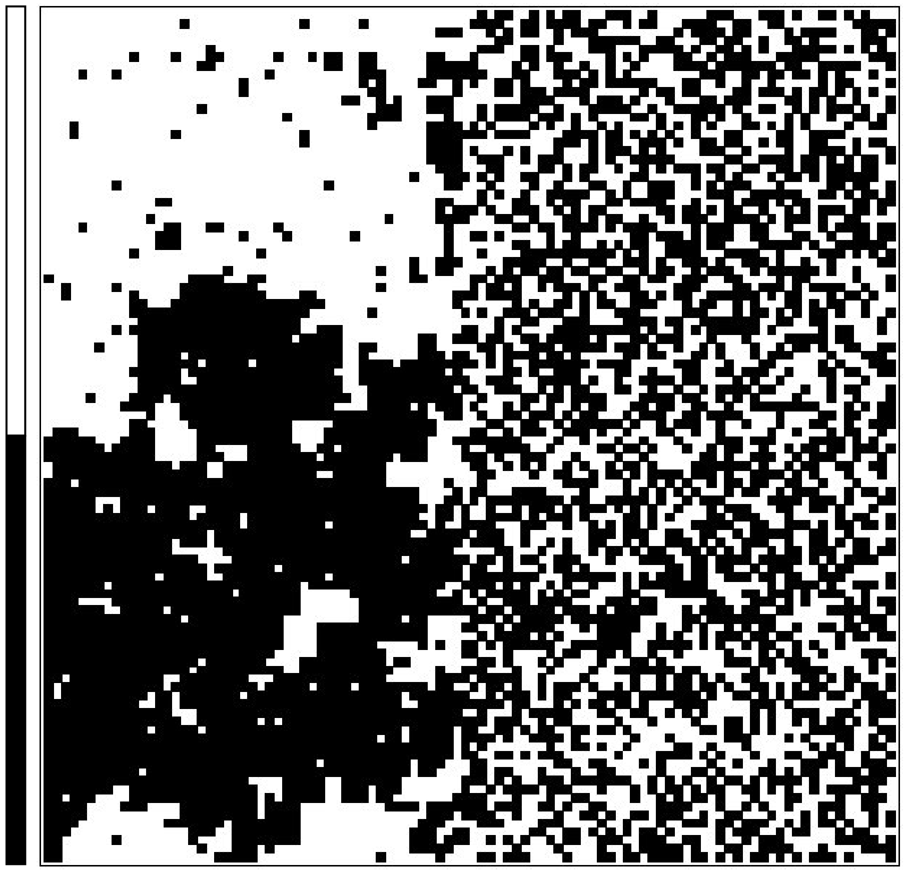
- Other ***cold*** temperatures: T (e.g., > T_O)
- Other fractions (f) of L_x at $T' = \infty$
- Other filling densities: $\rho \equiv N/L_xL_y$
- Other BC's, e.g., Free and ***Pinned***

PinBC (see later) for convenience in MC…

like in equilibrium Ising magnets, for measuring $\langle M \rangle$.

Simulations

a pinned column



$T \sim 0.88\, T_O$; $T' = \infty$

$L_x = L_y = 100$

PinBC + PBC

$f = ½$

$\rho = ½$

A “run” :

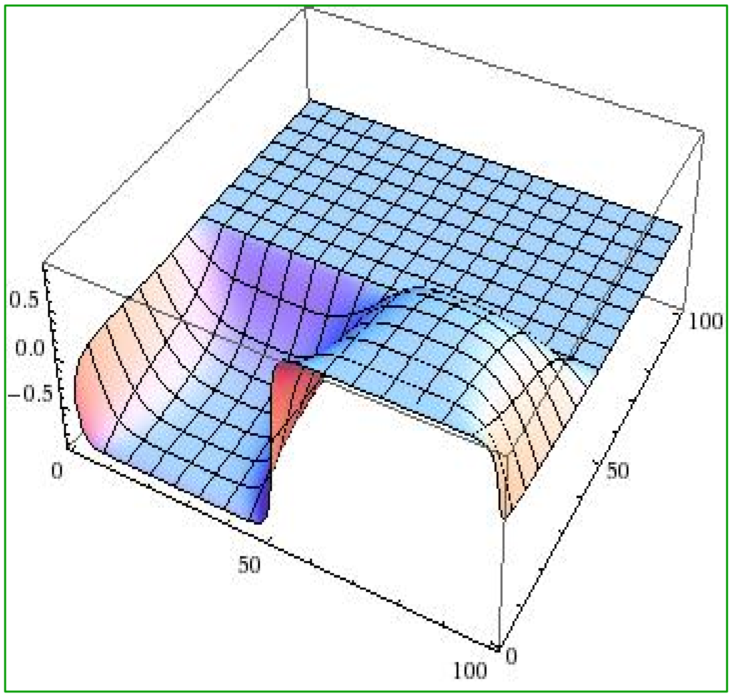
discard 1.6×10^6 MCS

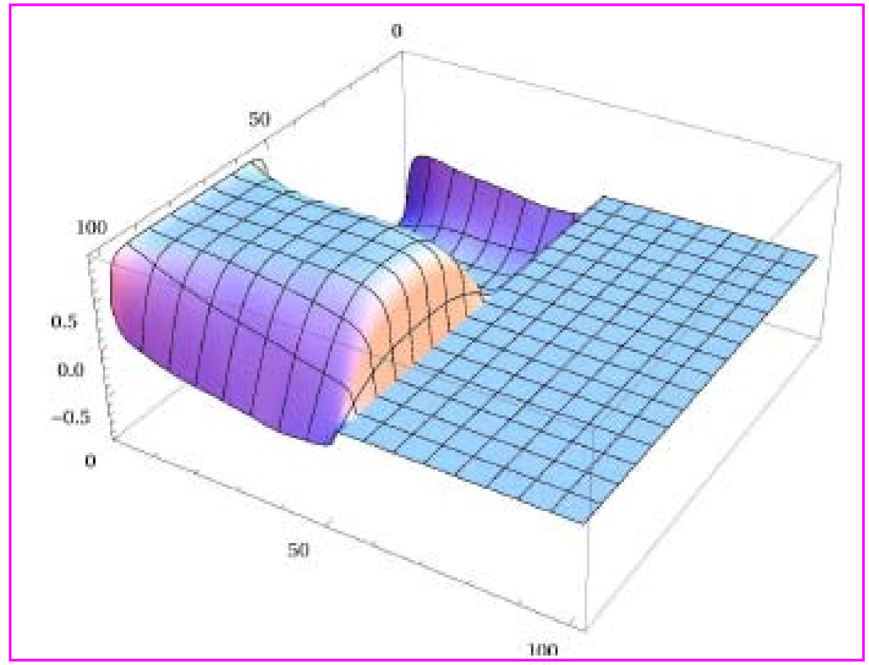
measure in 3×10^7 MCS

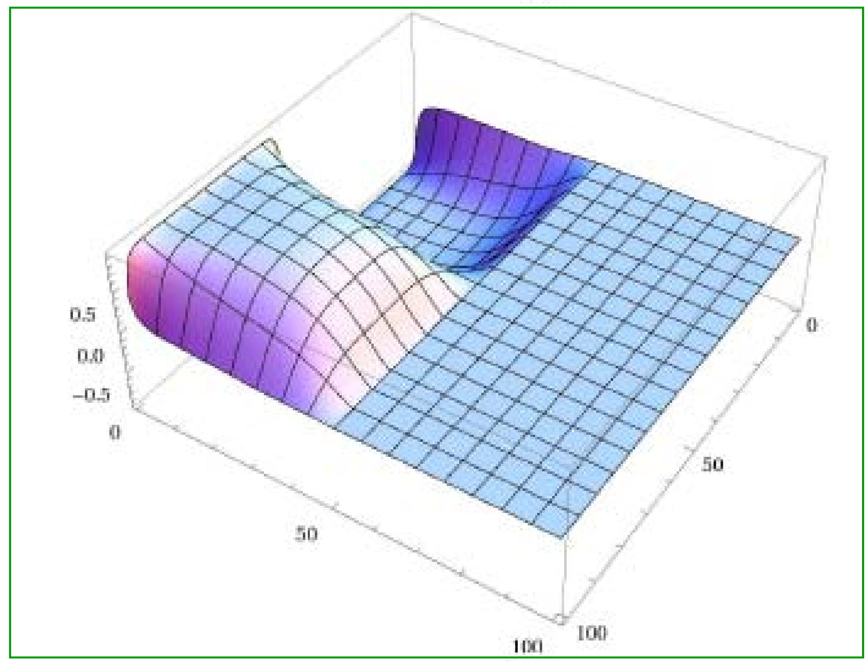
average over 80 runs

Simulations

Non-equilibrium, two *T*'s







Measuring currents $\boldsymbol{j}(\mathbf{x})$

- Keep track of every exchange on every bond, in each direction – $4L_xL_y$ of these!
- The total over the run, $\boldsymbol{Q}$, divided by MCS, is a current across that bond, in that direction.
- *NET* current, $\boldsymbol{j}$, across a bond is the *difference*.
- For systems in equilibrium, $\langle \boldsymbol{j} \rangle = 0$

  Net Q performs unbiased RW and $P(\boldsymbol{Q}) \sim \exp[-c\boldsymbol{Q}^2/\text{MCS}]$
- For ***NESS***, $\langle \boldsymbol{j} \rangle$ non-trivial, but must be divergence free!

Currents and Curls

Drop ⟨…⟩ for simplicity!

- $\nabla\cdot \boldsymbol{j} = 0 \;\Rightarrow\; \boldsymbol{j} = \nabla\times$ ***something***
- In 2-D, this has only z component …
- …known as the *stream function:* ψ
- Also, $\nabla\times \boldsymbol{j} =$ ***something*** … also only z component
- …known as the *vorticity:* ω
- Clearly, $\nabla^2\psi = -\omega$ (~ potential-charge density in electrostatics)

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Currents and Curls

Drop ( ) for simplicity!

- $\nabla \cdot \boldsymbol{j} = ($

ψ allows you to *"see"* the currents

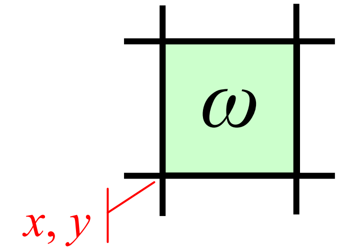
- In 2-D, this has only z component …
- ψ

ω tells you their *"essence"*

much like the "sources" of a magnetic field

- omponent
- Clearly, $\nabla^2 \psi = -\,\omega$ (~ potential-charge density in electrostatics)

Currents and Curls

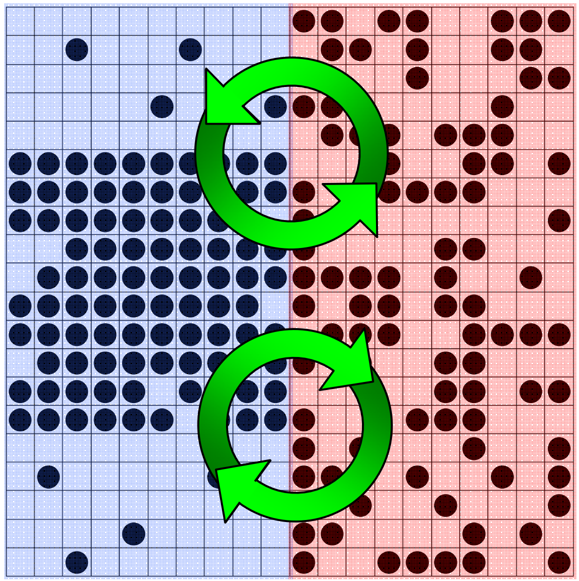


Vorticity and curl $\vec{j}$. By contrast, there is no such constraint on the vorticity $\omega \equiv curl\,\vec{j}$ (a scalar in 2D). On the lattice, $\omega(x,y)$ can be associated with the plaquette centered at $\left(x+\frac{1}{2}, y+\frac{1}{2}\right)$. A discrete version of $\oint \vec{j}\cdot d\vec{\ell}$ around the square,

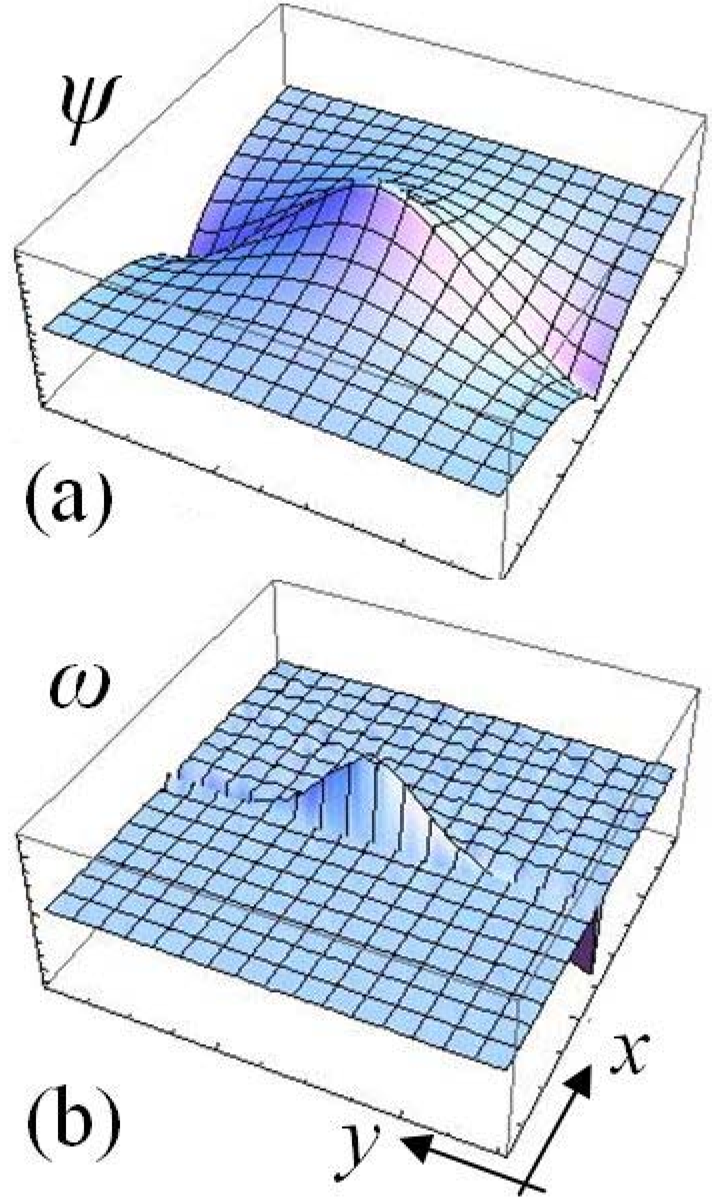
$$\omega(x,y) \equiv j_x(x,y) + j_y(x+1,y) - j_x(x,y+1) - j_y(x,y)$$

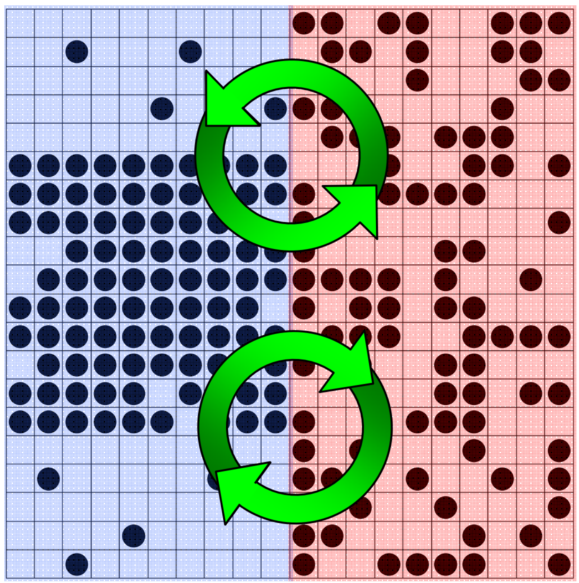
- …known as the *vorticity:* ω
- Clearly, $\nabla^2\psi = -\omega$ (~ potential-charge density in electrostatics)

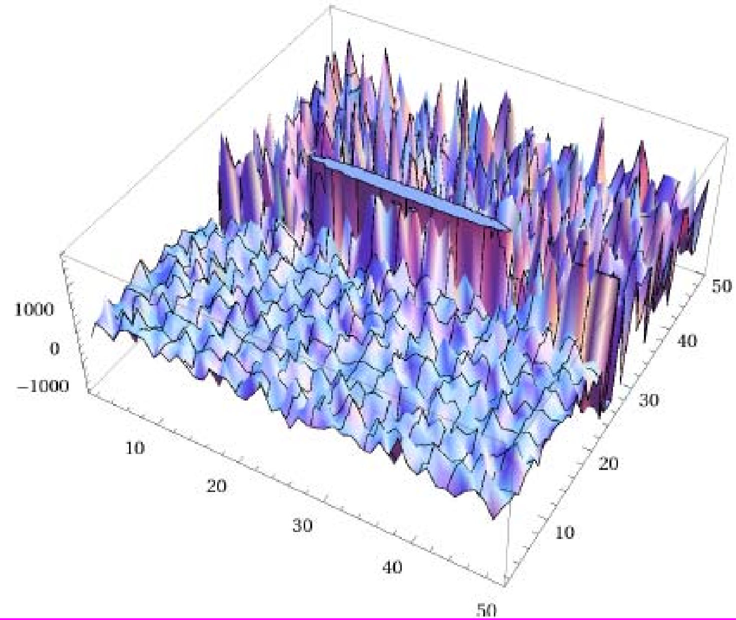
Simulations



Schematic of a 20x20

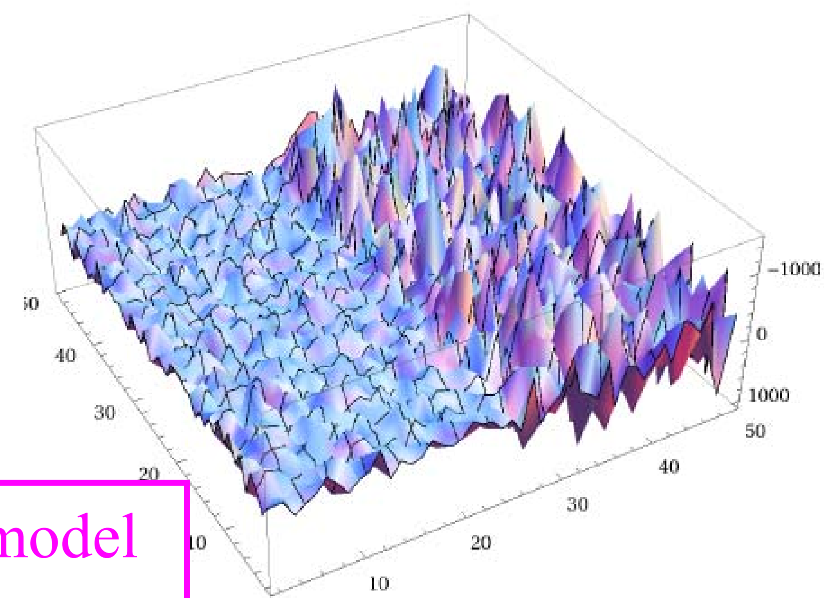






Schematic of a 20x20

Stream function and vorticity in a 50x50



ω for the two J Ising model in **equilibrium**

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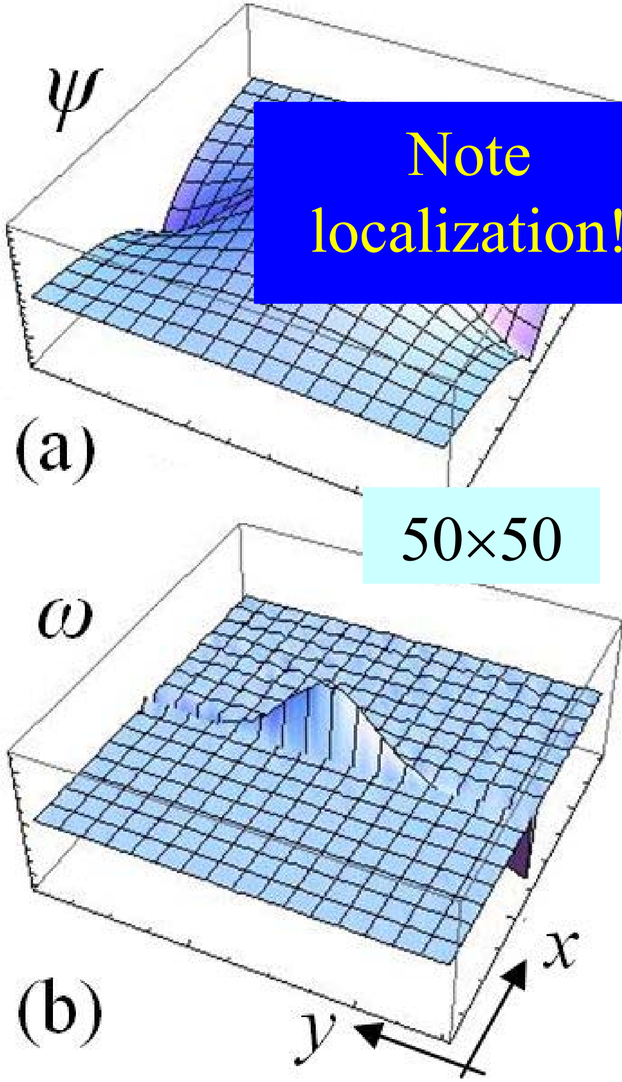
Currents and Curls

- ***j*** is "everywhere"; ω is localized!
- To probe the structure of ω, we studied a variety of L_x , L_y
- ...*e.g.*, 20×400; 20×200; 50×200…
- … finding secondary, anti-vortices!

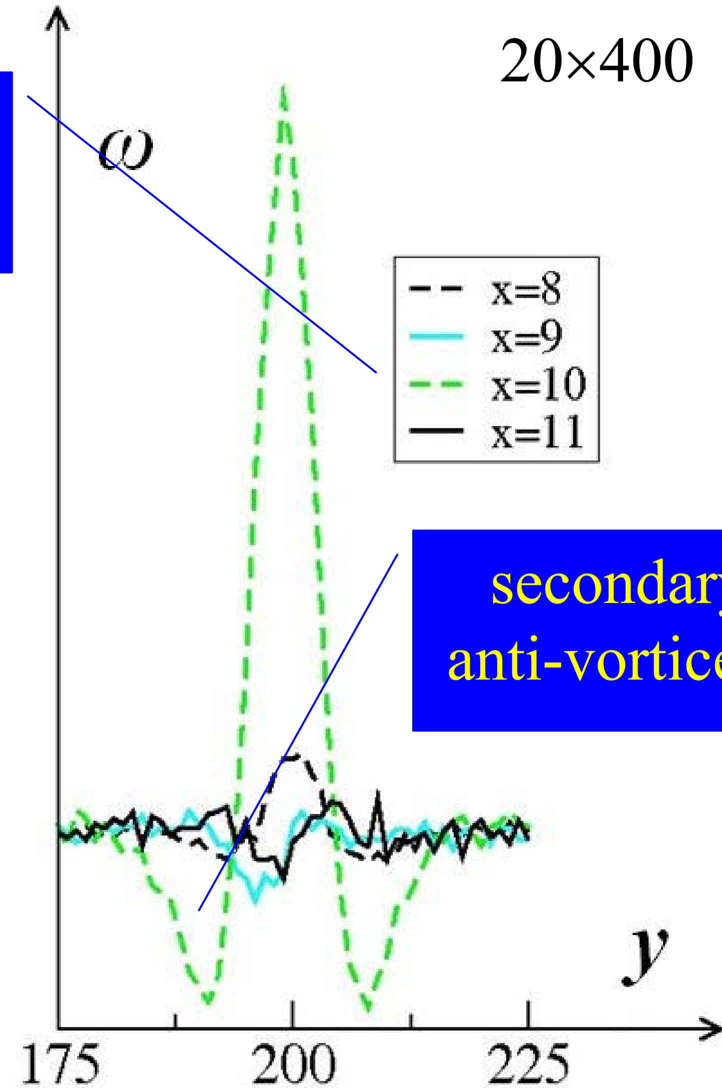
Simulations



Note localization!

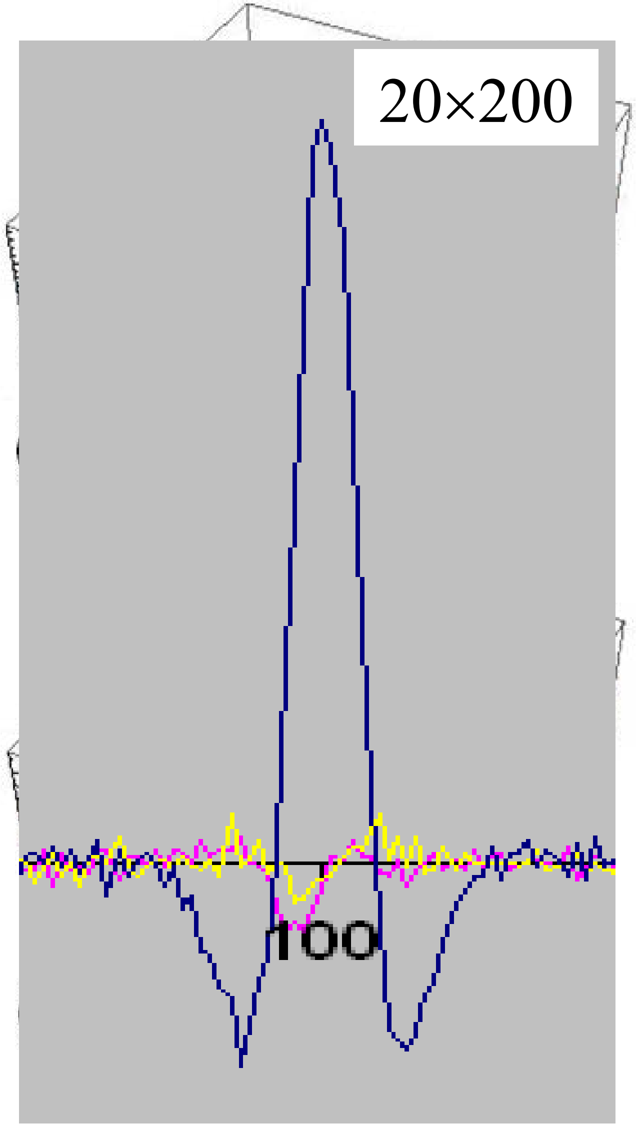
50×50

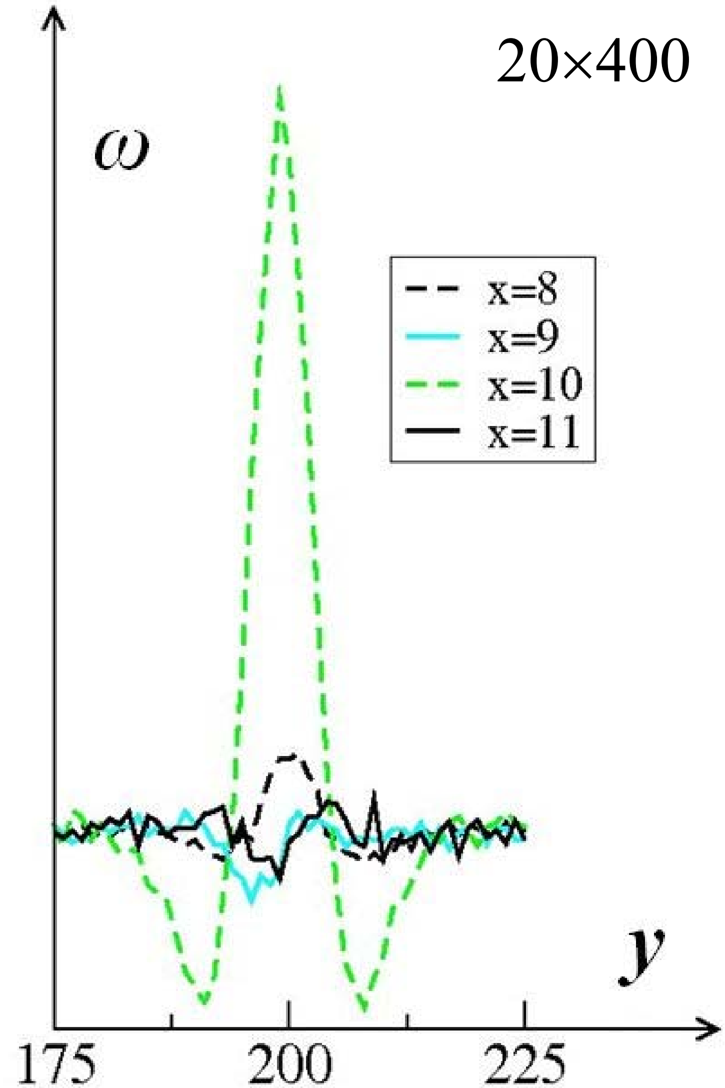
20×400



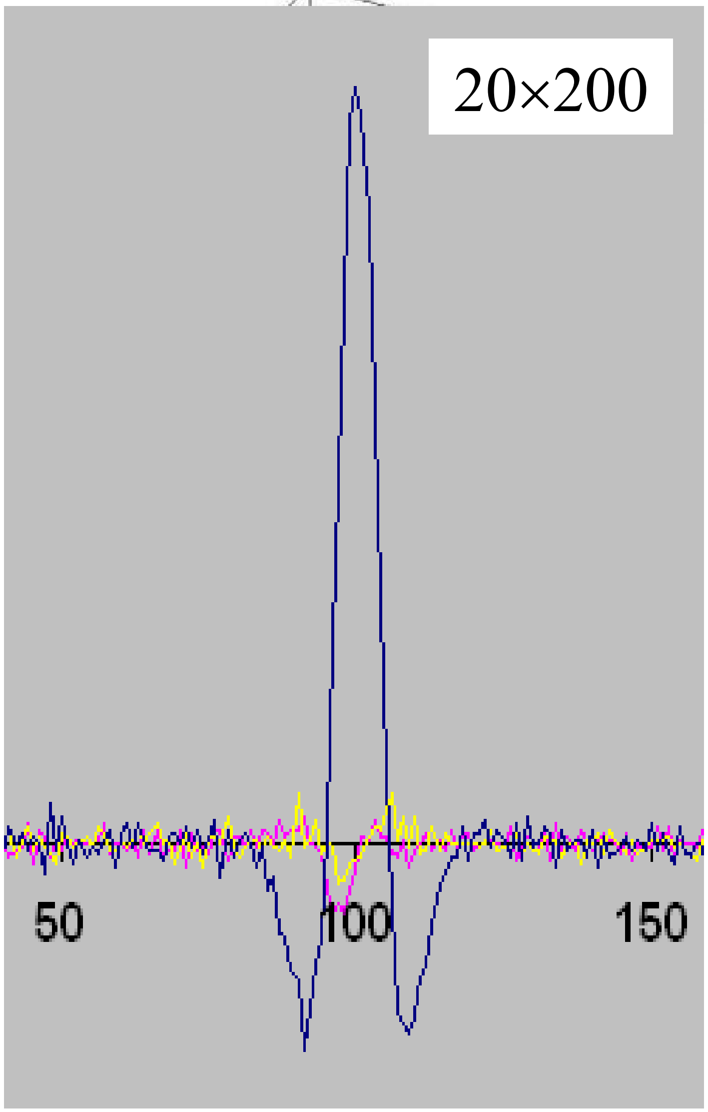
secondary, anti-vortices!!

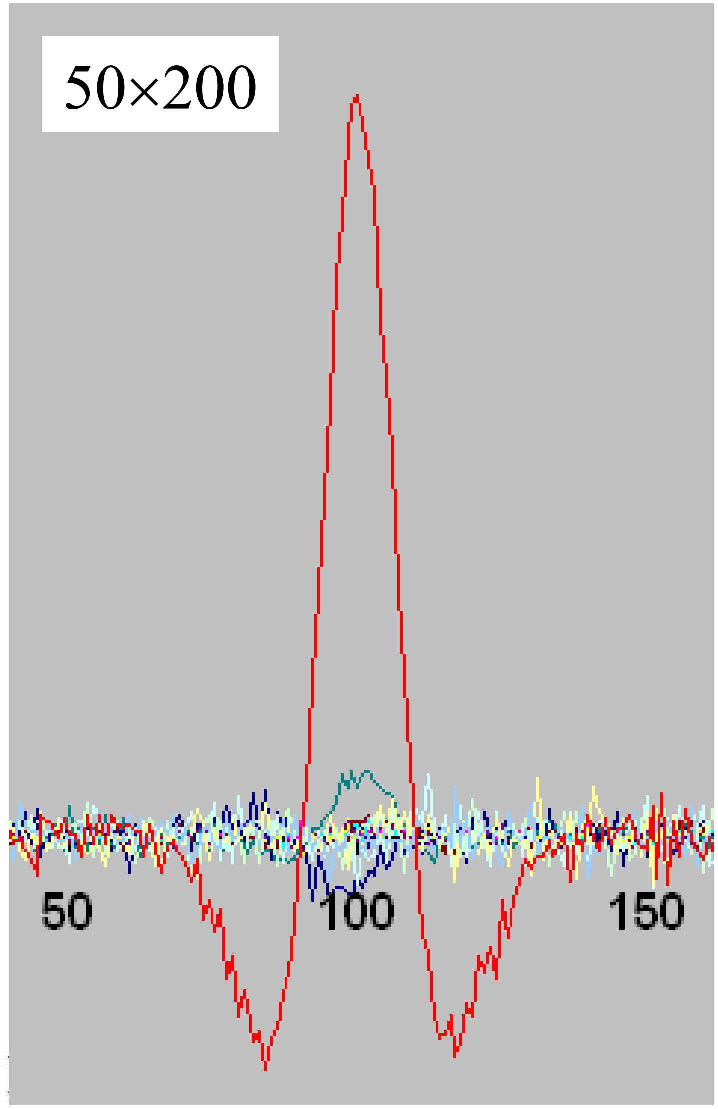
Simulations





Simulations





Currents and Curls

- $\boldsymbol{j}$ is "everywhere"; ω is localized!
- To probe the structure of ω, we studied a variety of L_x , L_y
- ...*e.g.*, 20×400; 20×200; 50×200…
- Most likely survives thermodynamic limit.

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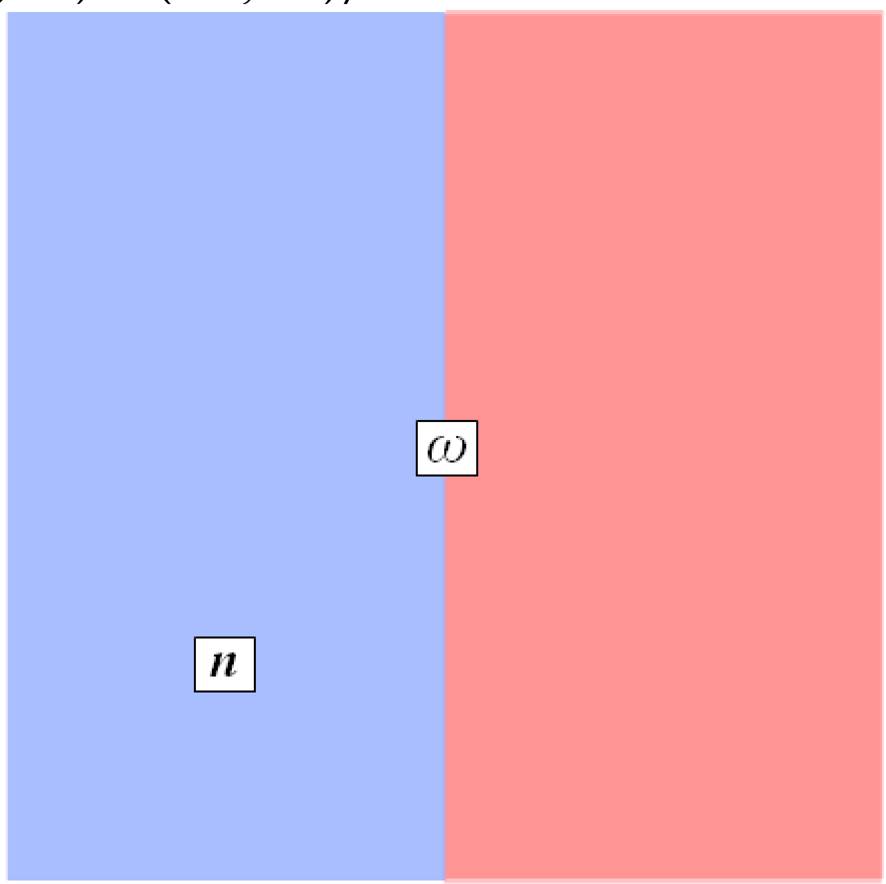
Is PinBC like gravity?

- A possible criticism is the PinBC…
- … breaks translational invariance;
- … does it effectively induce vortices?
- Restoring full PBC means, strictly, $\langle \omega \rangle = 0$ for finite systems (like $\langle m(\mathbf{x}) \rangle$ for ordinary lattice gas below T_O).
- Can still detect ω, by using *correlations* e.g., $\langle n(\mathbf{x})\ \omega(\mathbf{x}') \rangle$ (like $\langle ss \rangle$ for ordinary Ising magnets with PBC).
- "Long range order": let $|\mathbf{x} - \mathbf{x}'| \sim O(L)$.

$T' = T$ is the ordinary Ising lattice gas!

$\langle n(25,25)\ \omega(50,50) \rangle$



$L_x = L_y = 100$

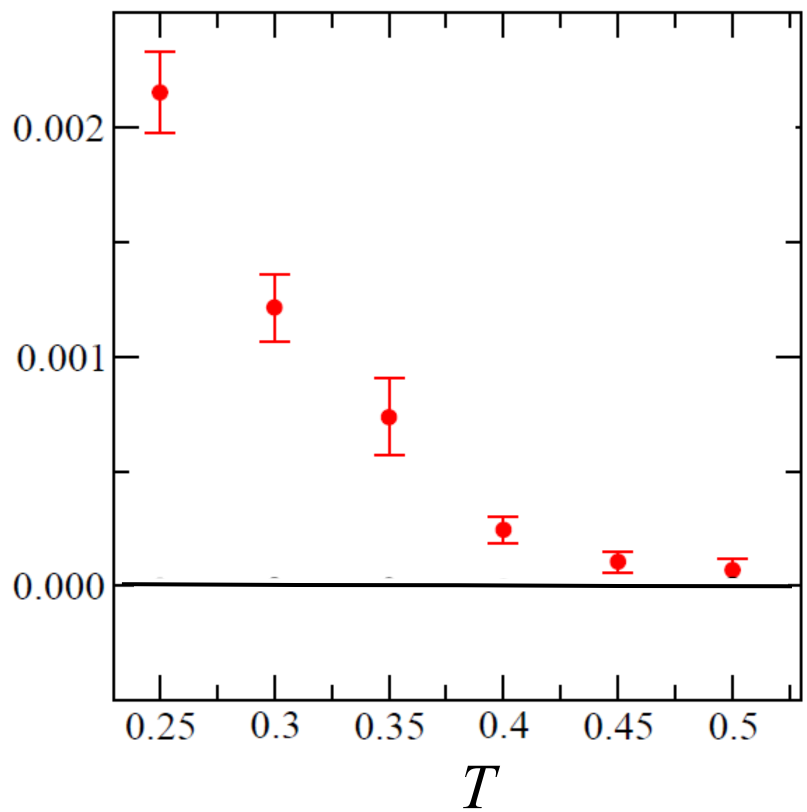
full PBC

$f = ½$

$\rho = ½$

$T' = T$ is the ordinary Ising lattice gas!

$\langle n(25,25)\ \omega(50,50)\rangle$



$L_x = L_y = 100$

full PBC

$f = ½$

$\rho = ½$

errors bars from
average over 24 runs

Irreversible Kolmogorov Loops

Another perspective of "non-equilibrium" physics

- Violation of detailed balance & *t* reversal
- No need of a Hamiltonian
- Simulations ⇔ Master equation

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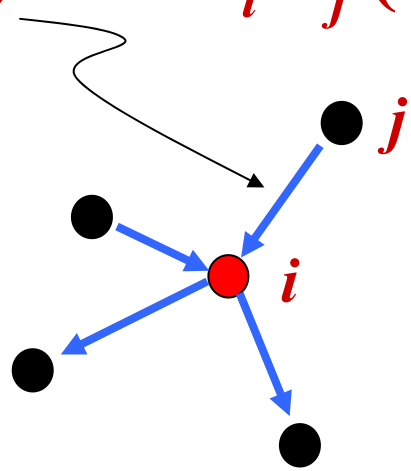
Notation and framework…

- Configurations: $C_i \quad i$
- Probability to find system: $P_i\,(t)$
- Master eqn: $\partial_t P_i\,(t) = \sum_{j \neq i} \left[w^j{}_i\, P_j\,(t) - w^i{}_j\, P_i\,(t) \right]$
- ***Net*** probability current… from j to i :

$$K^j{}_i\,(t) \;=\; w^j{}_i\, P_j\,(t) - w^i{}_j\, P_i\,(t)$$



Notation and framework…

- After long times, $P_i(t)$ settles to P^*_i , i.e. the stationary distribution: $\partial_t P^*_i = 0$
- … with t-independent prob. currents:

$$K^{*j}_i = w^j_i P^*_j - w^i_j P^*_i$$

- Rates respect detailed balance if

$$w^i_j P^{eq}_i = w^j_i P^{eq}_j$$

$$K^* \equiv 0 \Leftrightarrow \text{det. bal.}$$

Notation and framework…

- After long times, $P_i\,(t)$ settles to P^*_i , i.e. the stationary distribution: $\partial_t P^*_i = 0$
- … with *t*-independent prob. currents:

$$K^{*j}_{\ \ i} = w^j_{\ i} P^*_j - w^i_{\ j} P^*_i$$

- Rates violating detailed balance lead to ***NESS*** with non-zero K^*

- Detailed Balance was presented as

$$w^j{}_i / w^i{}_j = P^*{}_i / P^*{}_j$$

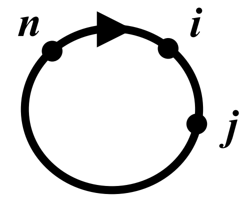
- . . . which give the impression that it "depends" on a known stationary distribution P^* !
- But, DB is an "intrinsic" property of the dynamics (Kolmogorov criterion 1936!):
  - consider closed loops in configuration space:

$$\mathscr{L} \equiv i \to j \to k \ldots \to n \to i$$

  - and the product of associated rates around the loop of the rates:

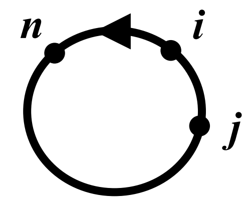
Theoretical considerations

$$\Pi[\mathscr{L}] \equiv w^i{}_j w^j{}_k \ldots w^n{}_i$$



– as well as the product of associated rates around the loop *in reverse*:

$$\Pi[\mathscr{L}_{rev}] \equiv w^i{}_n \ldots w^k{}_j w^j{}_i$$



- Dynamics has detailed balance ***iff***

$$\Pi[\mathscr{L}] = \Pi[\mathscr{L}_{rev}] \qquad \textit{for all loops}$$

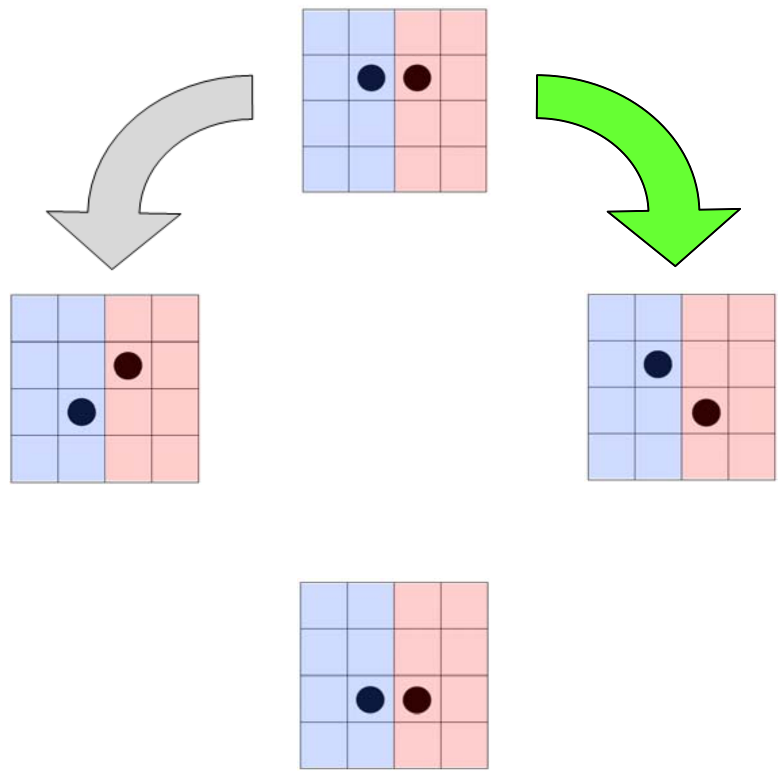
Irreversible Loops are key to ***NESS !***

Theoretical considerations

$$\Pi[\mathscr{L}_{rev}] = q\times 1\times q\times 1$$

$$\Pi[\mathscr{L}] = 1\times 1\times 1\times 1$$

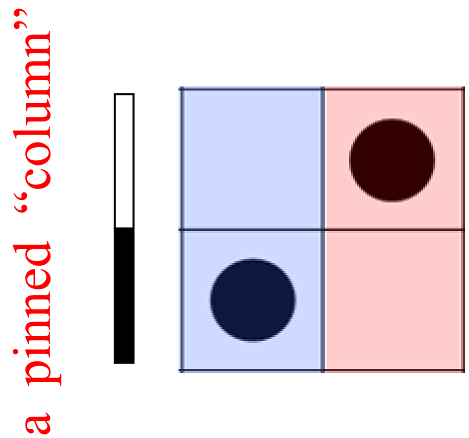
$$q \equiv exp\,[-J/k_B T]$$



Even the presence of a single *irreversible loop* is enough for d.b. violation and so, NESS

An "absolutely minimal" (exactly solvable) system

- Two particles in a 2×2, PinBC + FBC



An "absolutely minimal" (exactly solvable) system

- Two particles in a 2×2, PinBC + FBC
- Only 6 configurations; find $\boldsymbol{P}^*$ exactly
- Compute $\boldsymbol{K}^*$ and $\boldsymbol{j}$, ω (just ***one*** loop!)

…as a function of T

$$\omega = 2\frac{1-q^2}{7+5q^2}$$

$q \equiv exp\,[-J/\,k_B T\,]$

An "absolutely minimal"(exactly solvable) system

- Two particles in a 2×2, PinBC + FBC
- Too small to show phase transition

  … just a demonstration of $\omega \neq 0$
- $\langle n(\mathbf{x})\ \omega(\mathbf{x}')\rangle$ and PBC possible, but need at least 2×4.
- Up to 2×8 solvable numerically, showing similar results.

Mesoscopic approaches

field theory, hydrodynamics, Langevin eqns., etc.

…some preliminary observations/thoughts…

- Conservation law $\Rightarrow$ $\partial_t \rho = -\nabla \cdot \boldsymbol{j}$
- $\boldsymbol{j}$ has deterministic and noisy bits
- Both may have non zero *curl*…

  …but neither affects the evolution of ρ!
- $\boldsymbol{j}[\rho] \Rightarrow \omega[\rho]$ is a "slaved" field

…*unlike* in hydrodynamics, where

$\boldsymbol{v}$ (and so, ω) is an independent field.

Mesoscopic approaches

field theory, hydrodynamics, Langevin eqns., etc.

…some preliminary observations/thoughts…

- From "model B" and its relatives, we learn to write $\boldsymbol{j} = -\sigma\nabla\mu$, so that

$$\boldsymbol{j}[\rho] = -\sigma[\rho]\nabla(\delta\mathfrak{F}/\delta\rho) \quad \Rightarrow$$

$$\omega[\rho] = -\nabla\sigma \times \nabla(\delta\mathfrak{F}/\delta\rho)$$

- Assuming homogeneous mobility, $\sigma[\rho]$,

$$\nabla\sigma = -(\delta\sigma/\delta\rho)\nabla\rho$$

Mesoscopic ap

$$\omega[\rho] = -\nabla\sigma \times \nabla(\delta\mathfrak{F}/\delta\rho)$$

$$\nabla\sigma = -\,(\delta\sigma/\delta\rho)\,\nabla\rho$$

field theory, hydrodynamics,

…some preliminary observations/thoughts…

- Ordinarily, we also have

$$\nabla(\delta\mathfrak{F}/\delta\rho) = (\delta^2\mathfrak{F}/\delta\rho^2)\nabla\rho \quad \Rightarrow$$

$$\omega \;\propto\; \delta(x-x_{\mathrm{d}})$$

- Here, we may guess at $\mathfrak{F}[\mathbf{x},\rho]$ with explicit **x** coming from the defect line...
- so that, perhaps,

$$\nabla\big|_{\rho}(\delta\mathfrak{F}/\delta\rho) \propto \delta(x-x_{\mathrm{d}})$$

Mesoscopic approaches

field theory, hydrodynamics, Langevin eqns., etc.

…some preliminary observations/thoughts…

- … or perhaps this approach is deficient:
- ~~$\mathscr{F}[\mathbf{x},\rho]$, $\boldsymbol{j}[\rho]$, $\omega[\rho]$~~ and ρ is insufficient to capture some essentials of NESS, e.g.,
- persistent currents and loops ($\boldsymbol{j}$ *and* ω)
- HWDiehl: Perhaps the energy density (i.e., *n.n. correlations*) will play the crucial role?

What else ?

- Focus so far was non-zero $\boldsymbol{j}$ and ω …
  in a particular setting (2-D, f=1/2, $T < T_O$)
- Found discontinuous transitions…
  …as f is changed,
- Critical properties remain to be explored:
  anything "new" and relevant? or
  all new (i.e., NESS) properties hiding as corrections?
- Surprises even above criticality:

Periodic Ising chain (1-D)

- "Boring" equilibrium properties!

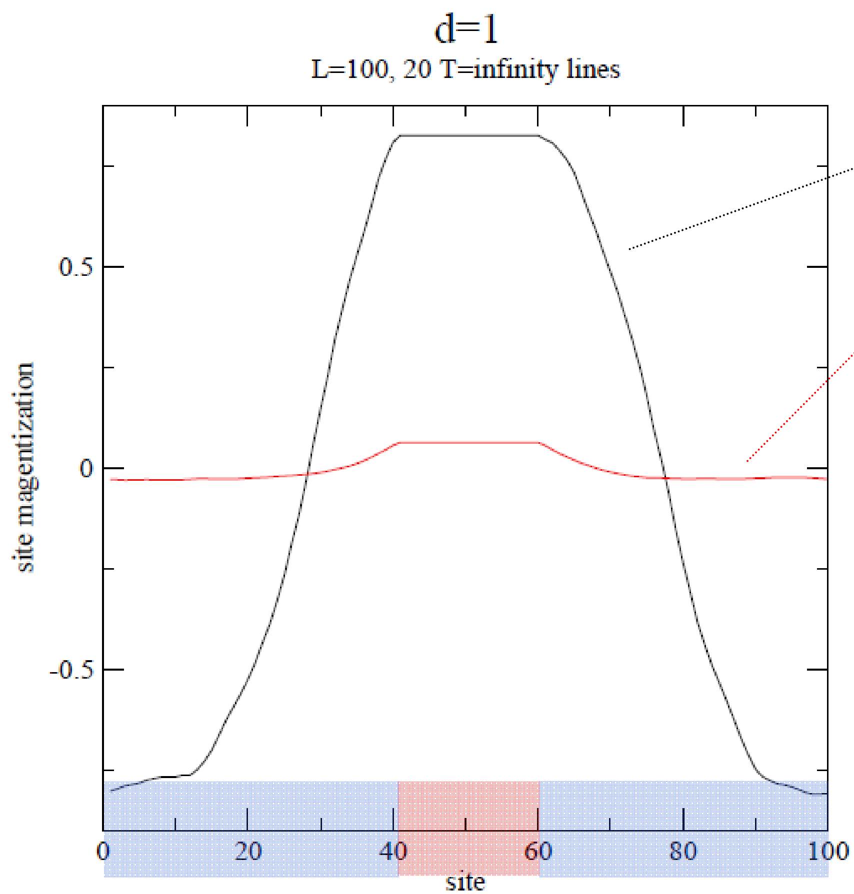
$$\langle s_j \rangle = 0 \; ; \; \langle n_j \rangle = \rho = 1/2$$

- Kawasaki update, with…

fraction f coupled to $T' = \infty$

(*preliminary* data next)

Periodic Ising chain (1-D)

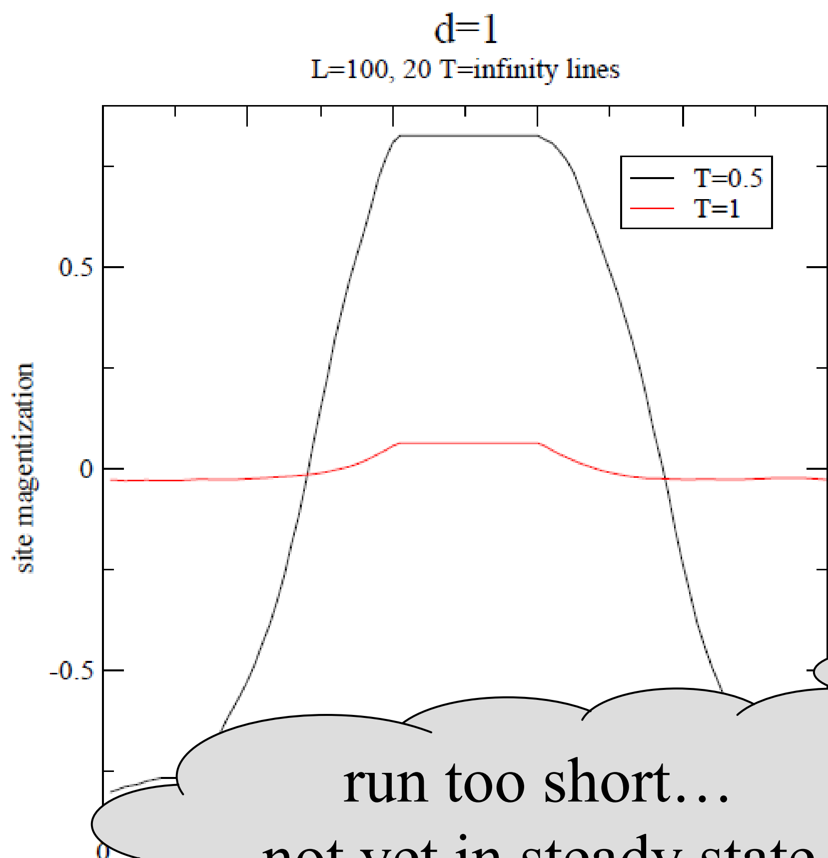


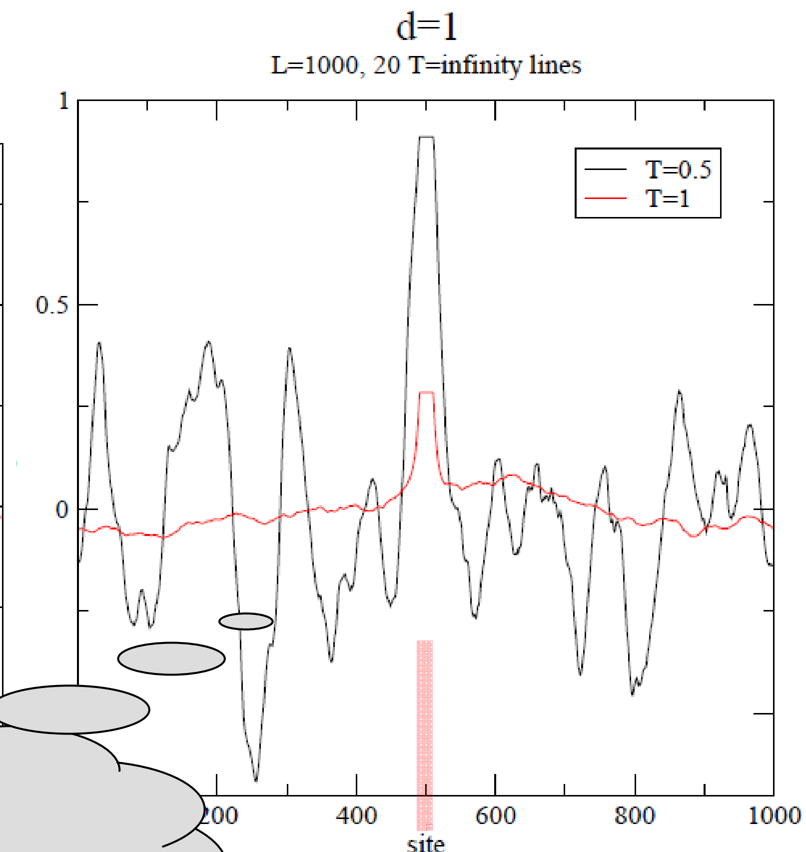
$T = 0.5$

$T = 1.0$

$$f = 20/100$$

Periodic Ising chain (1-D)



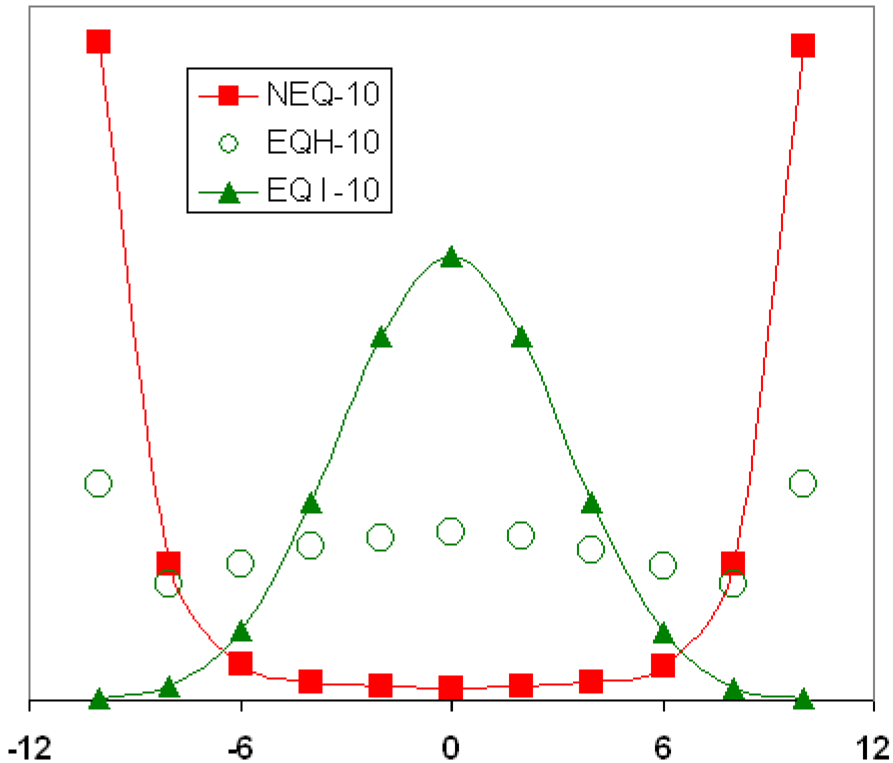


run too short…
not yet in steady state

f = 20

$f = 20/1000$

Periodic Ising chain (1-D)



$f = 10/50$

$T=1$ (spin J used)

one run of 10^9 MCS

time series with 10^5 total M's in window

compile histograms for both our model and two systems in equilibrium

EQH – equilibrium, homogeneous

EQ I – inhomogeneous; "two J model"

Conclusions

- Non-equilibrium systems, even very simple ones and in stationary states, challenge our intuition.
- Much to be done on this system
- Many others to be explored
- … and expect the ***unexpected*** !!

Come and join in the fun!