Non-equilibrium 2D Ising model with stationary uphill diffusion

Cristian Giardinà

UNIVERSITATIS STUDIORUM MUTINENSIS ET REGIENSIS 1175

UNIMORE
UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA

The results presented here have been obtained in collaboration with:

Matteo Colangeli (L'Aquila)

Claudio Giberti (Modena)

Cecilia Vernia (Modena)

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Martin Kroger (ETH)

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Outline

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2. Set up: model definition.
3. Hydrodynamics.
4. Numerical results.
5. Finite-size effects.
6. Perspectives.

1. Introduction

Boundary driven 2D Ising model

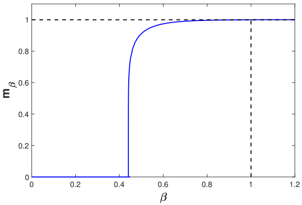
n.n. 2D Ising model: equilibrium

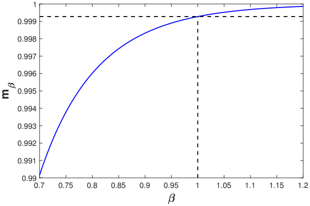
- model for ferromagnetism, exactly solvable (Onsager 1944)
- model for a fluid (lattice gas model)
- phase transition at inverse critical temperature

$$\beta_c = \frac{\ln(1+\sqrt{2})}{2} \approx 0.440686$$

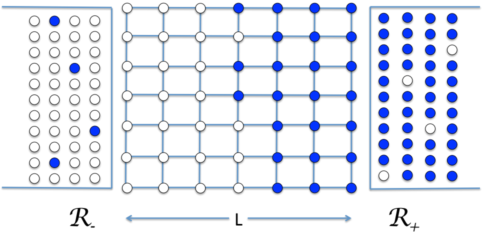
- spontaneous magnetization

$$m_\beta = \begin{cases} 0 & \text{if } \beta \leq \beta_c \\ \left[1 - \sinh^{-4}(2\beta)\right]^{1/8} & \text{if } \beta > \beta_c \end{cases}$$





Boundary driven 2D Ising model



Our setting:

- Kawasaki dynamics n.n. Ising 2D on $L \times L$ square
- Magnetic reservoirs $\mathcal{R}_{\pm}$ with magnetizations $m_{\pm}$ at the rigth/left boundary

Issues of this talk:

- structure of the non-equilibrium steady state as a function of the reservoirs magnetizations $m_{\pm}$
- Fick's law, sign of the current, magnetization profile, ...

2. Set up

Model definition

2D n.n. ferromagnetic Ising model

- Volume $\Lambda = [1, L]^2 \cap \mathbb{Z}^2$
- Spin variable: $\Lambda \ni i = (x, y) \longmapsto \sigma_i \in \{-1, 1\}$
- Hamiltonian

$$H_\Lambda(\sigma) = -\frac{1}{2} \sum_{\substack{i,j \in \Lambda \\ |i-j|=1}} \sigma_i \sigma_j + H_{b.c.}(\sigma)$$

  - vertical: periodic b.c.

$$\sigma_{(x,L+1)} = \sigma_{(x,1)}$$

  - horizontal: "$\frac{L}{4}$ b.c."

$$H_{b.c.}(\sigma) = -\frac{1}{2} \sum_{y=1}^{L} \sigma_{(1,y)} \sigma_{(1,y-\frac{L}{4})} - \frac{1}{2} \sum_{y=1}^{L} \sigma_{(L,y)} \sigma_{(L,y-\frac{L}{4})}$$

where $y - \frac{L}{4}$ stands for y minus the integer part of $\frac{L}{4}$ modulo L

Kawasaki dynamics + spin flips at the boundaries

Continuous time Markov process with rates:

- *bulk:* the spins on two n.n. sites i and j exchange values at rate

$$c(i,j;\sigma) = \mathbf{1}_{\sigma_i \neq \sigma_j} \cdot \begin{cases} 1 & \text{if } \Delta H(\sigma) = H(\sigma^{i,j}) - H(\sigma) \leq 0 \\ e^{-\beta \Delta H(\sigma)} & \text{otherwise} \end{cases}$$

- *reservoirs:* the spins at left/right boundary site i flip at rates

$$c_-(i;\sigma) = \frac{1 - \sigma_i m_-}{2} \quad \text{if } i = (1, y)$$

$$c_+(i;\sigma) = \frac{1 - \sigma_i m_+}{2} \quad \text{if } i = (L, y)$$

3. Hydrodynamics

Hydrodynamic limit: high temperature region

Conjecture 1 (uniqueness regime). Let $0 \leq \beta < \beta_c$.

Let $m(r,t), r \in [0,1], t \geq 0$ be the macroscopic magnetization profile.

$m(r,t)$ is the unique solution of:

$$\frac{\partial m}{\partial t} = \frac{\partial}{\partial r}\left(D(m)\frac{\partial m}{\partial r}\right)$$

$$m(0,t) = m_-, \quad m(1,t) = m_+$$

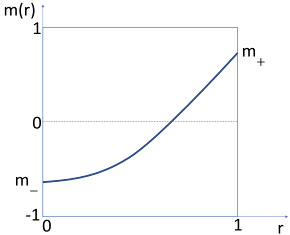
$$m(r,0) = m_0(r)$$

with $D(m) > 0$ given by the Green Kubo formula.

Remark: At $\beta = 0$, the process degenerates to stirring process and $D(m) = 1/2$.

Fick's law in the uniqueness regime

Stationary solution $m(r)$, $r \in (0,1)$



Current: $J = -D(m)\frac{dm}{dr} = \text{const.} < 0$ (downhill)

The statement should follow from:

- Varadhan, Yau: *Diffusive limit lattice gas with mixing conditions* (1997)
- Spohn, Yau: *Bulk Diffusivity of Lattice Gases Close to Criticality* (1995)
- Eyink, Lebowitz, Spohn: *Hydrodynamics of stationary non-equilibrium states for some stochastic lattice gas models* (1990)

Difficulties: non-gradient system, reservoirs, ...

Hydrodynamic limit: low temperature region

- The analysis is much more complex when $\beta > \beta_c$ because of phase-coexistence with regions (interfaces) where the magnetization profile is not slowly varying.

- If the system is in only one phase the hydrodynamic limit should still be described by a diffusion with D strictly positive. Thus if both m_+ and m_- are $\geq m_\beta$ (or both $\leq -m_\beta$) we expect that the Fick law is satisfied as when $\beta < \beta_c$.

Hydrodynamic limit: low temperature region

- What about hydrodynamics in the coexistence region (i.e. $\beta > \beta_c$, m_+ in the plus region, m_- in the minus region)?
- Spohn and Yau have proved that for $\beta > \beta_c$

$$D(m) > 0 \quad \text{if } |m| \geq m_\beta, \qquad D(m) = 0 \text{ otherwise}$$

- From now on, we assume $m_- = -m_+$

  We distinguish two regimes:
  - stable: $m_+ > m_\beta$
  - unstable: $m_+ < m_\beta$

Hydrodynamic limit, $m_+ > m_\beta$

Conjecture 2 (stable region): Let $\beta > \beta_c$ and $m_+ > m_\beta$.

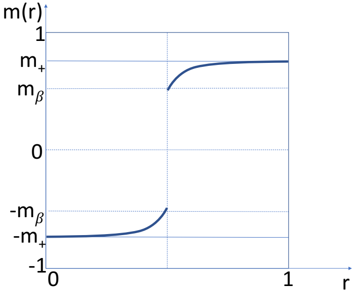
Let $m(r,t), r \in [0,1], t \geq 0$ be the macroscopic magnetization profile.

$(m(r,t), R_t)$ is the unique solution of the Free Boundary Problem

$$
\begin{aligned}
\frac{\partial m}{\partial t} &= \frac{\partial}{\partial r}\left(D(m)\frac{\partial m}{\partial r}\right) \qquad r \in [0,R_t) \cup (R_t,1] \\
m(0,t) &= -m_+, \quad m(R_t^-,t) = -m_\beta \\
m(R_t^+,t) &= m_\beta, \quad m(1,t) = m_+ \\
2m_\beta \dot{R}_t &= -D(m_\beta)\frac{\partial m}{\partial r}(R_t^+,t) + D(m_\beta)\frac{\partial m}{\partial r}(R_t^-,t) \\
m(r,0) &= m_0(r)
\end{aligned}
$$

Fick's law

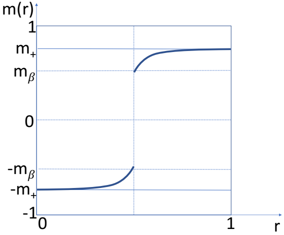
Stationary solution $(m(r), \frac{1}{2})$



$$J = -D(m)\frac{dm}{dr} = \text{const.} < 0 \quad \text{(downhill)}$$

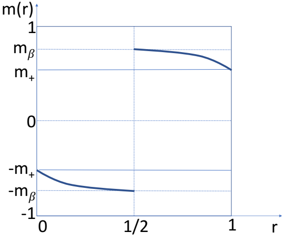
Stability of interface

$m_+ > m_\beta$



stable

$m_+ < m_\beta$



unstable (!)

Questions:

- What can we say when m_+ is in the spinodal region?
- What about Fick's law?
- Sign of the current?
- Optimal magnetization profiles?

4. Numerical simulations

Simulations

We implemented two algorithms:

- Kinetic Monte Carlo (continuos time)
- Metropolis Monte Carlo (discrete time)

Parameters:

- (Inverse) temperature $\beta = 1$ ($> \beta_c \approx 0.440686$)
- Size $L = 40$
- Initial conditions: independent Bernoulli, istanton-like, ± 1
- 10^{12} spin exchanges, 10^{10} steps (fluctuations 1%)

Observables

- *Current*

$$J = \lim_{T\to\infty} \frac{J_{x,y}(T)}{T} \qquad \forall\,(x,y)\in\Lambda$$

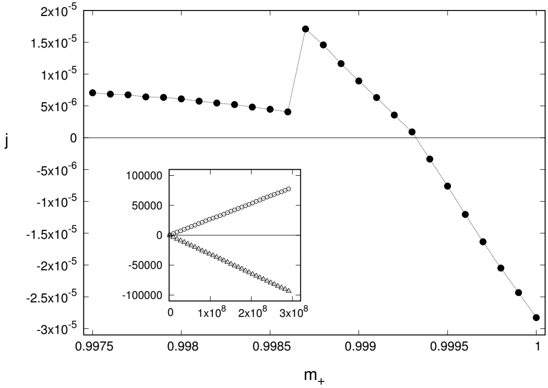
where $J_{x,y}(T)$ is the current up to time T between (x,y) and $(x+1,y)$, i.e.

$$\begin{aligned} J_{x,y}(T) &= \#\ \text{positive spins moving from left to right} \\ &- \#\ \text{positive spins moving from right to left} \end{aligned}$$

- *Magnetization profile*

$$m_x = \lim_{T\to\infty} \frac{1}{T}\int_0^T \left(\frac{1}{L}\sum_{y=1}^{L} \sigma_{(x,y)}(t)\right) dt \qquad\qquad x = 1,\ldots,L$$

Current



At $\beta = 1$ we found $m_{\text{crit}} \approx 0.9993$ such that

- $m_+ > m_{\text{crit}} \Longrightarrow J < 0$ downhill
- $m_+ < m_{\text{crit}} \Longrightarrow J > 0$ uphill

Remark: m_{crit} is very close to $m_{|_{\beta=1}} = 0.9992757$ (Onsager)

Movies

1. $m_+ = 0.9995 \ \ (> m_{\text{crit}} = 0.9993 \sim m_{|_{\beta=1}})$

Movies

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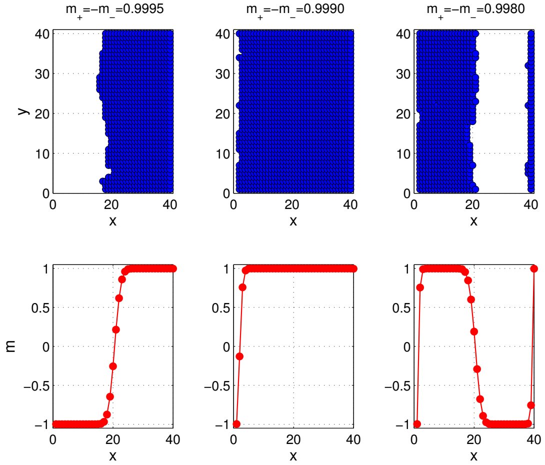
Movies

1. $m_+ = 0.9995 \ \ (> m_{\text{crit}} = 0.9993 \sim m_{|_{\beta=1}})$

2. $m_+ = 0.9990 \ \ (< m_{\text{crit}})$

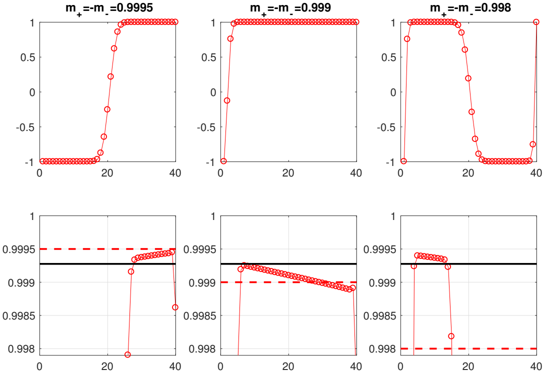
3. $m_+ = 0.9980 \ \ (< m_{\text{crit}})$

Magnetization profile



Stable   Metastable   Unstable

Zoom



Stable Metastable Unstable

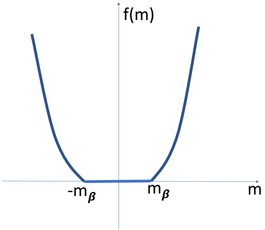
5. Finite-size effects

(I) metastable region

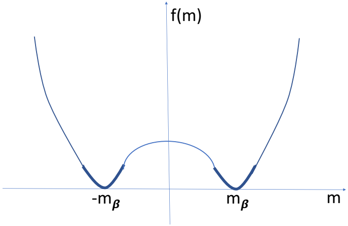
(II) critical value of m_+

(I) Metastable region

The central panel (with one bump) is due to “metastability”



$L = \infty$



$L < \infty$

For finite volumes, stable regions are larger:
phase separation occurs at $m = m^* < m_\beta$

Metastability: heuristics

Infinite volume Free Energy $f(m)$ with $f(m_\beta) = f(-m_\beta) = 0$.
Finite volume convex continuation for $m = m_\beta - \delta$ for small $\delta > 0$.

Compare:

1. homogeneous magnetization $m = m_\beta - \delta$
2. droplet of $-m_\beta$ in a sea of $+m_\beta$

$$(m_\beta - \delta)L^d = -m_\beta \gamma_d R^d + (L^d - \gamma_d R^d) m_\beta \qquad \gamma_d = \frac{\pi^{d/2}}{\Gamma(\frac{d}{2}+1)}$$

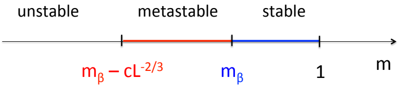
$$\frac{1}{2} f''(m_\beta)\delta^2 L^d = \tau_d R^{d-1} \qquad \tau_d = \text{surface tension}$$

Working out the algebra $\delta = c_d L^{-\frac{d}{d+1}}, \; R = c'_d L^{\frac{d}{d+1}}$

Metastability: Ising 2D

Consider the canonical Gibbs measure μ with magnetization m on the torus $[0, L]^2 \cap \mathbb{Z}^2$: (see for instance Biskup, Chayes, Kotecký, 2003)

- If $m \in (m_\beta - cL^{-2/3}, m_\beta)$, c small enough, then μ is supported by configurations with "small" contours (of size $\leq \log L$).
- If $m = m_\beta - cL^{-2/3}$ there is a droplet of size $L^{2/3}$.

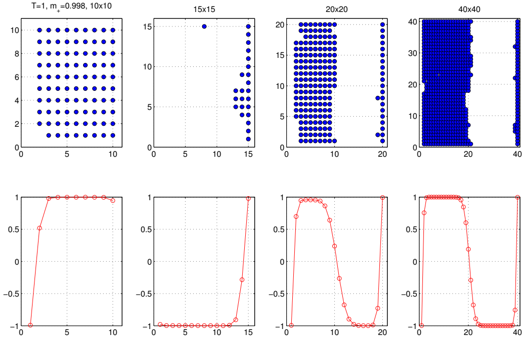


Thus:

- $(m_\beta - cL^{-2/3}, m_\beta)$ is the *plus metastable region*
- $(-m_\beta, -m_\beta + cL^{-2/3})$ is the *minus metastable region*

Metastability: simulations

Varying L, fixed $m_+ = 0.9995 \ \ (< m_{|\beta=1} = 0.99927)$



$L = 10$ $\quad L = 15$ $\quad L = 20$ $\quad L = 40$

(II) Critical value of m_+

- To determine the critical value m_{crit} of m_+, namely where the current changes sign, we have run *computer simulations of the conservative dynamics (without reservoirs) with empirical magnetization* $m = 0$.

- With this setting, the magnetization m_{eq} on the last column must coincides with the critical value m_{crit} of m_+ because:

  if $m_+ = m_{eq}$ *(and* $m_- = -m_{eq}$*) then the reservoirs are trying to impose a magnetization which is already there, the current in the presence of reservoirs is essentially the current without reservoirs (which is zero).*

- The value of m_{eq} is predicted by the theory of Wulff shape.

Wulff shape

- Consider the canonical Gibbs measure with Hamiltonian

$$H_\Lambda(\sigma) = -\frac{1}{2} \sum_{\substack{i,j \in \Lambda \\ |i-j|=1}} \sigma_i \sigma_j + H_{b.c.}(\sigma)$$

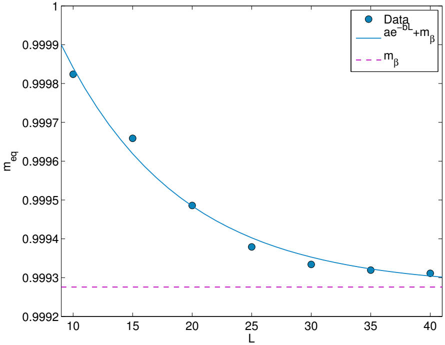
and magnetization $m = 0$. This is the Wulff problem, first studied by Dobrushin, Kotecký, Shlosman (1992).

- Typical configurations: *there is a vertical strip centered at $L/2$ of macroscopically infinitesimal thickness, to the right of the strip the magnetization is essentially m_β and to the left $-m_\beta$.*

- Without the additional hamiltonian $H_{b.c}$ the magnetization on the last column differs from m_β (or $-m_\beta$) and this is why we have added $H_{b.c}$ (Bodineau and Presutti (2003))

Finite volume effects

- If L is finite the magnetization of the last column is not exactly equal to m_β (or to $-m_\beta$). For $L \leq 40$ we found $m_{\text{crit}}(L) = m_{eq}(L)$
- Furthermore



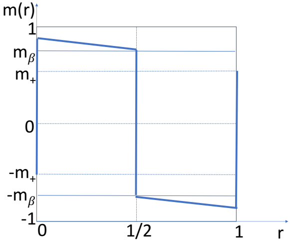
- Thus we claim $m_{\text{crit}} = m_\beta$ (in the infinite volume limit) and the current $J = 0$.

6. Perspectives

Hydrodynamic limit, $m_+ < m_\beta$

Conjecture 3 (unstable region): Let $\beta > \beta_c$ and $m_+ < m_\beta$.

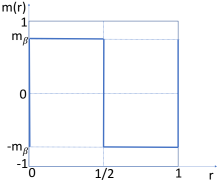
- $J > 0$ (uphill diffusion)
- The stationary magnetization profile has three discontinuities: two at the boundaries (bumps) and one in the middle.
- Fick's law is safisfied, except isolated points $\{0, \frac{1}{2}, 1\}$



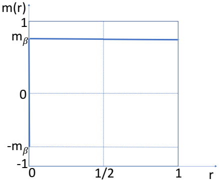
Hydrodynamic limit, $m_+ = m_\beta$

Conjecture 4 ("at criticality"): Let $\beta > \beta_c$.

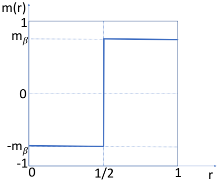
$$m_+(L) \nearrow m_\beta \text{ with } m_+(L) < m_\beta - cL^{-2/3}$$



$$m_+(L) \nearrow m_\beta \text{ with } m_+(L) > m_\beta - cL^{-2/3}$$



$$m_+(L) \searrow m_\beta$$



Some final comments

- stationary uphill diffusion in the boundary driven Ising 2D model
- Fick's law is satisfied
- role of reservoirs?
- experiments? (e.g. binary mixture)

THANK YOU FOR YOUR ATTENTION