Ficks law with phase transitions.

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INTRODUCTION

Main subject of the talk: *size of the interface fluctuations in $2d$ non equilibrium stationary states.*

It is well known since the work initiated by Gallavotti, 1972, that in the $2d$ Ising model at thermal equilibrium the interface fluctuates by the order of $\sqrt{N}$, N the size of the system.

We will see that in the presence of a stationary current produced by reservoirs at the boundaries the interface is much more rigid as it fluctuates only by the order $N^{1/4}$.

Talk based on a paper with Olla and Presutti and another in preparation with Merola and Olla.

The natural framework is the Ising model at low temperature with Kawasaki dynamics in the bulk and suitable Glauber processes at the boundaries which simulate interactions with thermal reservoirs.

This is a very difficult problem in the presence of phase transitions: it seems beyond the reach of the present techniques.

We will replace the Kawasaki dynamics in the bulk with the so called *stochastic phase field evolution* (which is still conservative).

For this model we have an explicit solution and the non equilibrium stationary measure is simply described by the Ising Gibbs measure in the presence of a linear slowly varying magnetic field.

The analysis of this measure indicates that the interface indeed fluctuates by the order $N^{1/4}$.

Plan of the talk

- Definition and properties of the stochastic phase field evolution with additional boundary processes.
- *Analysis of the interface in the Ising Gibbs measure with slowly varying external magnetic field*.
- *The SOS approximation and proof of the $N^{1/4}$ size of the fluctuations.*

The stochastic phase field evolution

This is a model introduced by Bertini, Buttà and Rüdiger, [1] as a microscopic version of the phase field equations much studied in the PDE's literature in connection with the Ginzburg-Landau functional.

The microscopic evolution is defined by:

- a spin flip, Glauber dynamics for the spin variable σ at a rate which depends on a space-time dependent field ϕ
- when the spin at x flips the field ϕ at x changes in such a way that the sum $\sigma_x + \phi_x$ is conserved.
- on top of that, the field ϕ evolves according to a linear Ginzburg - Landau diffusion.

[1] Rendiconti di Matematica, Vol. 19, 1999

$\sigma_x = \pm 1$, $\phi_x \in \mathbb{R}$, $x \in \Lambda_N$, $\Lambda_N \subset \mathbb{Z}^2 = N \times N$ square lattice centered at the origin.

We are going to define the bulk dynamics as a process reversible w.r.t. the Gibbs measure with Hamiltonian

$$H(\sigma, \phi) = H^{\text{ising}}(\sigma) + \frac{1}{2} \sum_{x \in \Lambda_N} \phi_x^2$$

H^{ising} is the usual Ising n.n. ferromagnetic Hamiltonian:

$$H^{\text{ising}}(\sigma) = - \sum_{\substack{x,y \in \Lambda_N \\ |x-y|=1}} \sigma_x \sigma_y$$

Generators in the bulk.

$$L_{\text{bulk}} = \sum_x L_x + \sum_x L_{x,x+e_i}$$

- L_x describes the spin flips Glauber dynamics (see next slide)
- $L_{x,x+e_i}$ acts only on the ϕ variables as a diffusion

$$L_{x,x+e_i} = -(\phi_x - \phi_{x+e_i})(\frac{\partial}{\partial \phi_x} - \frac{\partial}{\partial \phi_{x+e_i}}) + \frac{1}{\beta}(\frac{\partial}{\partial \phi_x} - \frac{\partial}{\partial \phi_{x+e_i}})^2$$

This describes an evolution for which the fields are randomly redistributed between two nearest-neighbour sites $(x, x + e_i)$ in such a way that the sum $\phi_x + \phi_{x+e_i}$ is conserved and there is a drift for them to become equal.

- Glauber dynamics for the spin variables: at rate

$$c_x(\sigma, \phi) = e^{-\frac{\beta}{2}[H((\sigma,\phi)^x)-H(\sigma,\phi)]}$$

$(\sigma, \phi)^x$ is the configuration obtained from (σ, ϕ) by

$$\sigma_x \to -\sigma_x$$

and

$$\phi_x \to \phi_x + 2\sigma_x$$

Thus the sum $\phi_x + \sigma_x$ is invariant .

By its definition the process in a torus is such that for any λ the Gibbs measure

$$d\nu_\lambda(\sigma, \phi) = \frac{1}{Z} e^{-\beta H^{\mathrm{ising}}(\sigma)} \prod_{x \in \Lambda_N} e^{-\frac{\beta}{2}\phi_x^2} \prod_{x \in \Lambda_N} e^{\beta\lambda(\sigma_x + \phi_x)} \, d\phi_x$$

is invariant (actually reversible).

The marginal of ν_λ on the spins is the usual Ising Gibbs measure with external magnetic field λ.

As we will see the same happens when the boundary processes are added: in such a case the external magnetic field is space dependent.

To impose “boundary conditions" we add Markov processes that act on the “upper" and "lower" boundaries in such a way to impose two different magnetic fields $\lambda_\pm$.

These processes involves only the ϕ variables and are Glauber dynamics reversible w.r.t. the Gibbs measure with Hamiltonian

$$\frac{1}{2}\sum_x \phi_x^2 - \lambda_\pm \sum_x \phi_x$$

Generators:

$$\sum_{x:x\cdot e_2=-N} L_{+,x} + \sum_{x:x\cdot e_2=N} L_{-,x}$$

$$L_{+,x} = -\Big(\phi_x - \lambda_+\Big)\frac{\partial}{\partial\phi_x} + \frac{1}{\beta}\Big(\frac{\partial}{\partial\phi_x}\Big)^2, \quad x : x \cdot e_2 = N$$

Analogously on the boundary $x \cdot e_2 = -N$

$$L_{-,x} = -\Big(\phi_x - \lambda_-\Big)\frac{\partial}{\partial\phi_x} + \frac{1}{\beta}\Big(\frac{\partial}{\partial\phi_x}\Big)^2, \quad x : x \cdot e_2 = -N$$

Here comes a miracle!

We can compute explicitly the invariant measure. [2]

Theorem *The invariant measure is*

$$d\mu_N = \frac{1}{Z} e^{-\beta H^{\text{ising}}(\sigma)} e^{\beta \sum_x \lambda_x(\sigma_x + \phi_x)} \prod_x e^{-\frac{\beta}{2}\phi_x^2} d\phi_x$$

with

$$\lambda_x = a\,\frac{x \cdot e_2}{2N} + b, \qquad a = \lambda_+ - \lambda_-, \quad b = \frac{\lambda_+ + \lambda_-}{2}$$

[2] DM, Olla, Presutti *A Note on Ficks Law with Phase Transitions* JSP, 2019

Remarks

- The proof is just computational.
- The marginal over the σ variables is the Ising Gibbs measure with external magnetic field λ_x.
- It is easy to see that for β large enough and $\lambda_+ > 0$, $\lambda_- = -\lambda_+$ in the upper half we see the plus phase and in the lower half the minus phase.
- This can be made sharp by letting $N \to \infty$ so that in macroscopic variables we see a flat interface at level 0 and the plus and minus phases in the upper and lower halves.
- We are however interested in the location of the interface at finite N.

In the sequel we fix β large and study the Gibbs measure in $[-N, N]^2 \cap \mathbb{Z}^2$ with zero boundary conditions.

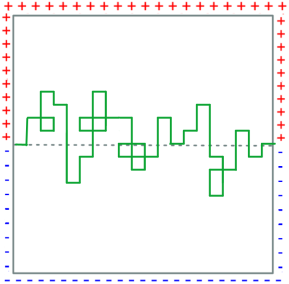
$$\nu_N(\sigma) = \frac{1}{Z} e^{-\beta H(\sigma)}$$

$$H(\sigma) = \sum_{\substack{x,y \in \Lambda_N \\ |x-y|=1}} \mathbf{1}_{\sigma_x \neq \sigma_y} - \sum_{x \in \Lambda_N} \frac{x \cdot e_2}{2N} \, \sigma_x$$

To underline the difficulties induced by the magnetic field, I start by recalling what happens when there is no magnetic field.

I thus consider boundary conditions that are + in the upper half and minus in the lower half of the square.

Then there is a contour which goes from the left end to the right one.



Gallavotti was the first one to study the structure of the interface and I will briefly recall his proof.

He describes the spin configurations in terms of contours: one of them γ being the interface while the others are disjoint connected and closed contours which do not intersect γ.

Thus the contours can be divided into those which are above and below γ.

The energy in the contours representation is simply the sum of the length of the contours, they however interact by exclusion.

Thus we can write the probability of an interface γ as

$$p_N(\gamma) = e^{-\beta|\gamma|} \frac{Z(M_\gamma^{\text{above}})Z(M_\gamma^{\text{below}})}{Z_N}$$

where M_γ^{above} and M_γ^{below} are respectively the regions above and below the interface γ and

$$Z(M_\gamma^{\text{above}}) = \sum_{\Gamma=(\gamma_1,..,\gamma_n)\subset M_\gamma^{\text{above}}} e^{-\beta \sum_i |\gamma_i|}$$

where Γ indicates a collection of disjoint contours.

Analogously for $Z(M_\gamma^{\text{below}})$.

The cluster expansion (valid for β large) allows to write

$$\log Z(M_\gamma^{\text{below}}) = \sum_{sp(I)\subset M_\gamma^{\text{below}}} \alpha(I)W(I)$$

$$\log Z(M_\gamma^{\text{above}}) = \sum_{sp(I)\subset M_\gamma^{\text{above}}} \alpha(I)W(I)$$

where

$$W(I) = \prod_{\gamma'} w(\gamma')^{I(\gamma')}, \qquad w(\gamma') = e^{-\beta|\gamma'|}$$

- $I(\gamma')$ are non negative integer valued functions on the space of all contours γ' in Λ_N. $I(\gamma')$ is the multiplicity of the contour γ'

- sp$(I) \subset A$ means that the support of I is made of $\gamma' \subset A$.

- $\alpha(I)$ are signed combinatorial coefficients with the property that $\alpha(I) \neq 0$ only if the support of I is connected, where γ' and γ'' are connected if $\gamma' \cap \gamma'' \neq \emptyset$.

The above series are convergent for β so large that the Kotecký-Preiss condition is satisfied.
Thus

$$Z(M_\gamma^{\text{below}})Z(M_\gamma^{\text{above}}) = \exp\Big\{ \sum_{sp(I)\cap\gamma=\emptyset} \alpha(I)W(I)\Big\}$$

$$\frac{Z(M_\gamma^{\text{below}})Z^+(M_\gamma^{\text{above}})}{Z_N} = \exp\{- \sum_{sp(I)\cap\gamma\neq\emptyset} \alpha(I)W(I)\}$$

The main point in the Gallavotti analysis is that the right hand side gives rise to an effective interaction between the jumps of the interface (called shapes by Gallavotti) which is treatable with the usual methods of Statistical Mechanics.

In the presence of the external magnetic field λ_x the partition function is not anymore represented in terms of contours.

However we may introduce “abstract contours" and write

$$Z(M_\gamma^{\text{above}}) = e^{\beta \sum_{x \in M_\gamma^{\text{above}}} \lambda_x} \sum_{\Gamma} \prod_{\gamma \in \Gamma} w^+(\gamma)$$

where Γ indicates a collection of disjoint contours.

$$Z(M_\gamma^{\text{below}}) = e^{-\beta \sum_{x \in M_\gamma^{\text{below}}} \lambda_x} \sum_{\Gamma} \prod_{\gamma \in \Gamma} w^-(\gamma)$$

The factors $e^{\pm\beta \sum_{x \in M_\gamma^{\text{above}}} \lambda_x}$ are maximal when the interface γ is flat and at level 0.

$w^\pm(\gamma)$ are ratios of partition functions but I will not give an explicit expression.

The combination of all that gives rise to an effective interaction similar to the one obtained by Gallavotti but with additional terms which depend on the location of the interface.

We conjecture that the above additional energy is responsible for localizing (when N is large) the interface in the strip $[-N^{1/4+\delta}, N^{1/4+\delta}]^2$, for any $\delta > 0$.

To understand the origin of the $N^{1/4}$ we neglect the statistical weights due to the partition functions (above and below the interface) and consider the simplest case where the interface is a graph.

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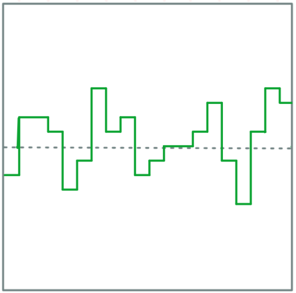
The SOS model

In the SOS model the interface γ is a graph of integer value functions s_x, $x \in \{-N, .., N\}$
By interpolation we think of it as a curve



The SOS Hamiltonian is

$$H(s) = \frac{1}{2N} \sum_{x=-N}^{N} s_x^2 + \sum_{x=-N+1}^{N} |s_x - s_{x-1}|$$

and the SOS Gibbs measure is

$$\nu(s) = e^{-H(s)} \Big[\sum_s e^{-H(s)} \Big]^{-1}$$

$s = (s_{-N}, s_{-N+1}, ..., s_N), \qquad s_x \in \mathbb{Z}$

This is related to our Ising Gibbs measure with space dependent magnetic field in the following way.

The spin configurations corresponding to the interface γ is made of spins equal to -1 below s_x and +1 above s_x (the interface is in the dual lattice).

The Ising energy of such configurations is $|\gamma|$, we normalise the energy by subtracting the energy of the flat interface so that the normalised energy is

$$\sum_{x=-N+1}^{N} |s_x - s_{x-1}| = |\gamma| - (2N + 1)$$

i.e. the sum of the lengths of the vertical segments.

The energy due to the external magnetic field is normalised by subtracting the energy of the configuration when all s_x are equal to 0. This is

$$2 \sum_{x=-N}^{N} \sum_{i=1}^{|s_x|} \frac{i}{2N} \approx \sum_{x=-N}^{N} \frac{s_x^2}{N}$$

Thus we get the SOS Hamiltonian

$$H(s) = \frac{1}{2N} \sum_{x=-N}^{N} s_x^2 + \sum_{x=-N+1}^{N} |s_x - s_{x-1}|$$

We rewrite the Gibbs measure $\nu(s) = \frac{1}{Z} e^{-\sum_x \frac{s_x^2}{2N}} e^{-|s_x - s_{x-1}|}$ as follows.

Call $\eta_x = s_x - s_{x-1}$ so that

$$s_x = s_{-N} + \sum_{y=-N+1}^{x} (s_y - s_{y-1}) = s_{-N} + \sum_{y=-N+1}^{x} \eta_y$$

Then $\{\eta_x\}_{x=-N,..,N}$ are i.i.d. with law $\pi(\eta) = \frac{1}{V} e^{-|\eta|}$,

The Gibbs measure is

$$\nu(s) = \frac{1}{Z} \prod_x \pi(\eta_x)\, e^{-\sum_{x=-N}^{N} \frac{s_x^2}{2N}}$$

Heuristics to justify $N^{1/4}$

Consider the random walk starting from 0 with value 0 for a time $\equiv$ length $N^{2\alpha}$

We want to determine for which values of α the contribution of the external magnetic field can be neglected.

The typical values of the random walk

$$s_x = \sum_{y=0}^{x} \eta_y, \qquad x \leq N^{2\alpha}$$

are of order N^{α}.

The energy of the magnetic field is then

$$\frac{N^{2\alpha}}{N} N^{2\alpha}$$

the first factor is the typical value of magnetic field the second factor is the length of the interval.

Thus if $\alpha = \frac{1}{4}$

If we take $\alpha = \frac{1}{4}$ and let $N \to \infty$, by the convergence of the random walk to a Brownian motion $B = \{B_s\}$

$$e^{-\frac{1}{2\sqrt{N}} \sum_{x=0}^{\sqrt{N}} \left(\frac{s_x}{N^{1/4}}\right)^2} d\pi(\eta) \to e^{-\frac{1}{2}\int_0^1 B_s^2 ds} dP(B)$$

Results in preparation:

- Typically $|s_x| \sim N^{1/4}$.
- The Gibbs measure can be described as a Markov process.
- On the spacial scale $\sqrt{N}$ the above Markov process is close to a stationary Ornstein-Uhlenbeck process.

$$
\begin{aligned}
\nu(s) &= \frac{1}{Z} \prod_{x} e^{-\frac{1}{2N}(s_x^2 + s_{x-1}^2)} \quad e^{-|s_x - s_{x-1}|} \\
&= \frac{1}{Z} T_N(s_{-N}, s_{-N+1})..T_N(s_{N-1}, s_N)
\end{aligned}
$$

where T_N (the transfer matrix) is the following operator

$$
T_N(s, \bar{s}) = e^{-\frac{1}{2N}(s^2 + \bar{s}^2)} \frac{e^{-|s - \bar{s}|}}{V}
$$

which is a symmetric, positive, bounded and compact operator in $L^2(\mathbb{Z})$.

By the Krein-Rutman theorem (a version of Perron-Frobenius) there is a maximal positive eigenvalue λ_N and a positive eigenvector $h_N(s) \in L^2$.
$\lambda_N > 0$ is not degenerate, its eigespace is one-dimensional.

$$\sum_{\bar{s}} T_N(s, \bar{s}) h_N(\bar{s}) = \lambda_N h_N(s), \qquad \sum_s h_N^2(s) = 1,$$

Then

$$P(s, s') = \frac{h_N(s')}{\lambda h_N(s)} T_N(s, s')$$

is a transition probability with invariant (actually reversible) measure given by $h_N^2(s)$.

As usual in Statistical Mechanics the properties of the Gibbs measure can be derived in terms of the Markov chain associated to P.

- h_N is symmetric, $h_N(s) = h_N(-s)$ and $\|h_N\|_\infty \leq 1$
- $$1 - \frac{c}{\sqrt{N}} \leq \lambda_N \leq 1$$
- $$h_N(s)\mathbf{1}_{|s| \geq cN^{1/4}} \leq C\frac{1}{N^{1/8}} e^{-c' \frac{|s|}{N^{1/4}}}$$
- The family of probability measures $\tilde{h}_N^2(r)dr$ on $\mathbb{R}$ is tight and any limit measure is absolutely continuous.

$$\tilde{h}_N^2(r) = N^{1/4} h_N^2([rN^{1/4}]), \qquad [] = \text{ integer part}$$

Iterate $n = \sqrt{N}$ times the equation $\sum_{\bar{s}} T_N(s,\bar{s}) h_N(\bar{s}) = \lambda_N h_N(s)$ and get

$$h_N(s) = \frac{1}{\lambda_N^n} e^{-\frac{1}{2N} s^2} \mathbb{E}_s(e^{-\frac{1}{2N} \sum_{x=1}^{n} s_x^2} h_N(s_n))$$

$\mathbb{E}_s$ is the expectation w.r.t. the random walk which starts from s. Any limit point $u(r)$ of $\tilde{h}_N(r)$ satisfies

$$u(r) = \frac{1}{\lambda} \mathbb{E}_r \left(e^{-\frac{1}{2} \int_0^1 B_s^2 ds} u(B_1) \right) \qquad (1)$$

where B_s is a Brownian motion with $B_0 = r$ furthermore $\lambda = \lim_{N \to \infty} \lambda_N^{\sqrt{N}}$ which exists.

The unique solution of (1) (up to a multiplicative constant) is $u(r) = \exp\{-r^2/2\}$ and $\lambda = e^{-\sigma/2}$.