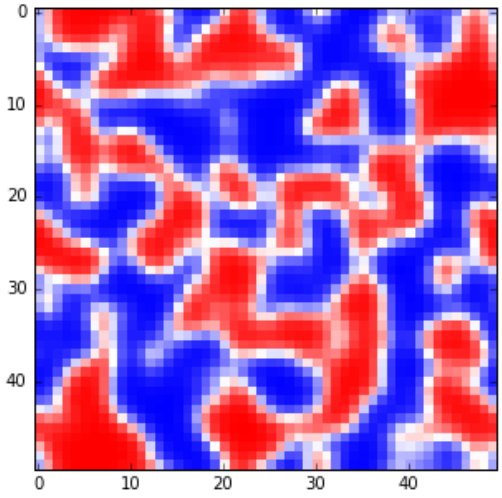
Internship report

Investigation of the time-dependent Ginzburg-Landau equation

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Paris, France
June 2017

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Introduction

The Laboratory of Theoretical and High Energy Physics (LPTHE) is a Joint Research Unit (UMR 7589) of the *University Pierre et Marie Curie* and the CNRS. It is affiliated with the CNRS Institute of Physics (INP). It comprises 19 CNRS researchers and 10 university professors.

The scientific activity at LPTHE is centered on the unifying principle of Quantum Field Theory, both in its most theoretical aspects and in its applications.

The following areas are represented at LPTHE:

- Mathematical Physics
- Strings, Branes and Fields
- Statistical and Condensed Matter Physics
- Particle Physics and Cosmology

More than a third of its members are also professors, which is a high ratio in the French theoretical physics community.

This internship was conducted under the supervision of **Leticia Cugliandolo**, who is a member of the Statistical and Condensed Matter Physics (MSMC) group of LPTHE.

The scientific activities of the MSMC group are varied. The Statistical Physics group covers such diverse areas as conformal field theory and studies of out of equilibrium phenomena. In Condensed Matter, the main interests are superconducting qubits, transport in hybrid systems, and electronic systems in low dimensions. [2]

1 Subject of the internship

Magnetism is a property dependent on the temperature of the magnet. If heated above a critical temperature T_c a ferromagnet becomes paramagnetic, for its internal structure becomes disordered. This structure is characterised by small domains, regions of similarly aligned spins inside the magnet. Thus, above T_c spins can no longer remain aligned due to large thermal fluctuations.

Consequently, if a paramagnet is suddenly cooled below its T_c or *quenched*, its spins will start to align. This can produce domains of differently oriented spins, for example a region of *up* spins within a larger area of *down* spins, as could be the case in the binary Ising model. Having this *up-down* interface is energetically unfavourable, and in time the smaller *up* domain will be consumed by the *down* domain. This domain growth or *coarsening* in an example of dynamics across 2nd order phase transitions.

This internship explored the evolution of domains and their properties via the 1D and 2D time-dependent Ginzburg-Landau (TDGL) equation for a field $\phi(\vec{x}, t)$. The field ϕ represents coarse-grained (spatially zoomed-out, in a sense) Ising spins.[1] The *a priori* inevident correspondence between the two models is achieved by introducing an internal double-well potential $V(\phi)$, to mirror the two discrete values of the Ising spins.

A continuum formulation is sometimes desired as it can provide insights that are not easy to obtain via the discrete description, for example by sometimes being more analytically tractable [10].

The TDGL equation is given by

$$\frac{\partial \phi}{\partial t} = \Delta\phi - V'(\phi), \tag{1}$$

A 1D field was investigated more extensively both numerically and analytically, as it is the simplest possible system, and the fastest to work with numerically.

The TDGL equation can be derived from Landau free energy functional by taking the variational derivative: $\frac{\partial \phi}{\partial t} = -\frac{\delta F}{\delta \phi}$ where F is defined [13] as

$$F[\phi(\vec{x}, t)] = \int d^d x \big[\frac{1}{2}(\nabla\phi)^2 + V(\phi)\big]. \tag{2}$$

In Eq. (2) the $(\nabla\phi)^2$ term represents the elastic energy – it *wants* to smooth out any fluctuations in the field, while the $V(\phi)$ term draws the field to one of its equilibrium values.

The work done concerned a particular double-well potential $V(\phi) = -\frac{u\phi^2}{2} + \frac{\lambda\phi^4}{4}$. A double-well potential was chosen so that its minima for the field ϕ would correspond to the two values the Ising spins can obtain, namely ± 1.

The effect of thermal fluctuations ξ was also taken into account, so the final and modified TDGL equation becomes

$$\frac{\partial \phi}{\partial t} = \Delta\phi - u\phi + \lambda\phi^3 + \xi. \tag{3}$$

The scaling hypothesis argues [1] that in domain growth processes following a quench to the ordered phase there exists a single growing length $R(t)$, away from the critical point where the correlation length ξ diverges, with which the observables of the system can be transformed into a scale invariant form – compressed into a *mastercurve*.

This length scale is time dependent and for a 1D TDGL equation has been shown [8] to be $R(t) \propto \log t$, while for the 2D case it is expected to be $R(t) \propto t^{\frac{1}{2}}$ [5].[2]

Kawasaki and Nagai [8] have determined the growing length for the one dimensional TDGL equation, as well as the form of the domain number function [7]. To obtain the domain numbers and compare with results of [8], the method outlined in [11] was used.

[1] The Ising model may seem rather simple, but that is deceptive, for, according to Mussardo [12], the model has also shown incredible ability to describe phase transitions and has a extraordinary theoretical richness.

[2] For the Ising model $R(t) \propto t^{\frac{1}{2}}$ for both $d = 1$ and $d = 2$.

This work follows the approach of [9] and assumes a steep potential $V(\phi)$; this translates to having a large barrier B between the double-well minima, as is explained in Sec. 2.1.3. This steepness results in both faster evolution of the domains, which is desired to minimize computational costs, and better pronounced domains [9] – the central objects of this paper.

The interaction between neighbouring domains in one dimension was derived analytically, following the steps explained by Privman in [13], and tested numerically.

The numerical tools needed for integrating of the TDGL equation and calculating various observables mentioned before, were developed from scratch by the author in Python, making use of the NumPy [3] library extensively.

1.1 Definitions

Throughout the paper the following definitions will be assumed and used:

- Domain – a region in space where the Ising spins are aligned in the same direction, and accordingly the coarse-grained field ϕ is at or near one of the minima of the double-well potential.
- Domain wall / kink – a region in space separating neighbouring domains of oppositely aligned Ising spins, and accordingly the coarse-grained field ϕ values of opposite minima of the double-well potential.
- Order parameter – a value characterising the order in a system. It is equal to zero for the unordered phase (high temperature limit) and nonzero below a phase transition into the ordered phase at some critical temperature T_c. A typical example is the total magnetization m of an Ising spin ensemble.
- Percolation – A grid is said to be *percolating* if there exists a continuous path of equally valued points from one side of it to the other side, either vertically or horizontally. In this paper, however, only points of equal signs, not values, were considered.

  An analogy can be made with electrical conduction – if the current can pass from one side of the material to the other, it is said to be conducting which corresponds to percolation.

2 Methods

This section provides an overview of the theorical and numerical methods used during the internship.

2.1 Theoretical methods

2.1.1 Coarse-graining

Sometimes a field theory is desired in place of a discrete theory. In such a case, a mapping from Ising spins to a field theory is done by a coarse-graining procedure over a given volume ΔV as follows:

$$\phi(\vec{x}, t) = \frac{1}{\Delta V} \sum_{i \in \Delta V} s_i(\vec{x}, t) \tag{4}$$

Thus, a discrete problem can be mapped to a quasi-continuous one, as the field $\phi(\vec{x}, t)$ can now take on non-integer values as well.

2.1.2 Time dependent Ginzburg - Landau (TDGL) equation

The TDGL equation is derived from the Landau free energy functional

$$F[\phi] = \int d^d x \big[\frac{1}{2}(\nabla\phi)^2 + V(\phi)\big]. \tag{5}$$

From this a field evolution equation with a non-conserved order parameter is found [13]

$$\frac{\partial\phi}{\partial t} = -\frac{\delta F}{\delta\phi} = \Delta\phi - V'(\phi) \tag{6}$$

For the particular double-well potential V the time-dependent Ginzburg-Landau equation is obtained for a field $\phi(\vec{r}, t)$ with thermal fluctuations ξ:

$$\frac{\partial\phi}{\partial t} = \Delta\phi - u\phi + \lambda\phi^3 + \xi, \tag{7}$$

where $u > 0$ and $\lambda > 0$ are constants characterising the potential acting of the field. This is the central equation of this internship.

2.1.3 Quench modelling

If a magnet is thermally quenched below its critical temperature, its spins will tend to align in some direction, thus creating a global magnetization and breaking the symmetry of the magnet.

A similar symmetry breaking behaviour can be obtained for a field ϕ by introducing an external double-welled potential $V(\phi)$. The field would be drawn to one of the potential wells and hence break the symmetry.

This paper explored the case of dimensions $d = 1$ and $d = 2$, with a double-well potential $V(\phi)$ in the form of

$$V(\phi) = -\frac{u\phi^2}{2} + \frac{\lambda\phi^4}{4} \tag{8}$$

with $u, \lambda > 0$ and minima at $\phi_0 = \pm\sqrt{\frac{u}{\lambda}}$. The height of the potential barrier between the two wells is denoted $B = u/4 \cdot (u/\lambda) = u/4$, since throughout the simulations this ratio was kept constant at 1 so as to preserve the field equilibrium values ϕ_0 at ± 1. Thus, the depth of the barrier is proportional to u.

2.1.4 Correlation function

It is interesting to look at the correlations between spins. Nearby spins tend to be correlated, meaning that they are likely pointing in the same direction [12].

There are many ways to probe correlations mathematically. This work used the two-point equal-time correlation function

$$C(\vec{r}) = \langle \phi_i \phi_{i\pm r} \rangle, \tag{9}$$

where r is the distance between the points and the brackets represent an ensemble average.

The correlation length ξ gives the characteristic length of these correlated regions and can be defined mathematically via the correlation function

$$C(\vec{r}) \approx e^{-|\vec{r}|/\xi}. \tag{10}$$

2.1.5 Domain numbers

An interesting observable to consider is the domain number at a given time t, defined as:

$$n(l,t) = \frac{\#\text{ of domains of size } l}{\text{length of the system}}. \tag{11}$$

In $d = 1$ Kawasaki and Nagai found [7] that this is an exponential distribution with a cut-off for low sizes. This cut-off size is expected to grow as more and more domains flip and thus disappear, increasing the average domain (and correlation) length.

In $d = 2$ the domain number distribution function is found [6] to be

$$n(A,t) \simeq 2c/(A + \lambda t)^2, \tag{12}$$

where A gives the area of the domain and c and λ are constants.

2.1.6 Exponential decay

From equation (6) the the way in which stationary domain wall approaches the saturation values $\pm\phi_0$ can be deduced [13], by setting $\frac{\partial\phi}{\partial t} = 0$ and expanding the potential in powers of $\epsilon = \pm 1 \mp \phi$, since the field saturates at a value of ± 1.

For the $\epsilon = 1 - \phi$ case one obtains

$$\phi'' = -\frac{d^2\epsilon}{dx^2} = V'(1-\epsilon) = V'(1) - V''(1)\epsilon + o(\epsilon^2). \tag{13}$$

Noting that $V'(1) = 0$ the solution of the differential equation gives

$$\phi \propto 1 - e^{-[V''(1)]^{\frac{1}{2}}x}. \tag{14}$$

The exact solution of the 1D TDGL equation and thus the form of the kink is given by Tagami in [14] and takes the form of

$$\phi(x) = \sqrt{\frac{u}{\lambda}} \tanh\left(\sqrt{u/2}\; x\right). \tag{15}$$

2.1.7 Percolation

The 2D field grids were tested for percolation. In this context a percolating lattice would correspond to a divergent correlation length ξ since periodic boundary conditions are used for all fields/lattices. Such divergence would indicate a macroscopic domain and thus magnetization for a system of Ising spins.

Since the fields were initialized with randomly distributed values, a grouping into positive and negative values was made, so that there remained only two *species* of points which were then tested for these continuous or percolating paths.

2.2 Numerical methods

2.2.1 Integration of TDGL equation

The field $\phi(\vec{x}, t = 0)$ was initialized randomly with each field value drawn from a Gaussian distribution $\mathcal{N}(0, 1)$. As explained, the evolution of the field ϕ is given by the TDGL equation:

$$\frac{\partial \phi}{\partial t} = \Delta\phi - u\phi + \lambda\phi^3 + \xi, \tag{16}$$

which in the discretized version for explicit $\phi(x_n, t_{i+1})$ becomes:

$$\frac{\phi(x_n, t_{i+1}) - \phi(x_n, t_i)}{\Delta t} = \phi''(x_n, t_i) - u\phi(x_n, t_i) + \lambda\phi^3(x_n, t_i) + \xi. \tag{17}$$

Periodic boundary conditions were used throughout all the calculations: $\phi(\vec{x}, t) = \phi(\vec{x} + \vec{L}, t)$, where L is the length of the lattice used. These lengths ranged from 10 to $40'000$ for various calculations.

The calculation of the second derivative depends on the space dimension, as ilustrated in Table (1).

1D	$a^2\phi''(x_n) = \phi(x_{n+1}) + \phi(x_{n-1}) - 2\phi(x_n)$
2D	$a^2\phi''(x_n) = \phi(x_{n+1}, y_n) + \phi(x_{n-1}, y_n) + \phi(x_n, y_{n+1}) + \phi(x_n, y_{n-1}) - 4\phi(x_n)$

Table 1: Calculations of second derivatives for a given time t_i that is omitted for brevity. Here a is the spatial step size of the grid.

In this paper *one iteration* or *step* is considered as the evolution field values from $\phi(x, t_i)$ to $\phi(x, t_{i+1})$ for $\forall x$. The values of the field after an iteration were updated all at once, after being calculated successively for each point separately and saved in a temporary array.

The temperature fluctuation term ξ was assumed zero for $T = 0$, otherwise it was also drawn from a gaussian distribution $\mathcal{N}(0, \alpha T^2)$, where α is some proportionality constant, because for white noise thermal fluctuations

$$\langle \xi(t)\xi(t') \rangle \ = 2k_b T\delta(t - t') \quad \Rightarrow \quad \sigma_\xi \propto \sqrt{T}, \tag{18}$$

where σ_ξ is the standard deviation of these fluctuations and the $\langle \xi(t)\xi(t') \rangle$ signifies the ensemble averaged correlation of thermal noise. As can be seen, the white noise is delta correlated.

For equation (17) to yield convergent results, $2\Delta t \leq a^2$ has to hold [4]. This condition was validated numerically.

Many calculations were performed on the Linux based cluster of the *LPTHE*, accessible via an SSH connection.

2.2.2 Percolation algorithms

In order to check for percolation it is necessary to find domains in a lattice. This was implemented recursively using a depth-first-search (DFS).

To determine whether a particular cluster spans the whole lattice the concept of distance to the root site was used, as illustrated below.

```
percolating = False
for site in sites:
    if site not visited:
        root = site
        roots.add(root) # the array containing the root sites
        findDomain(root)

findDomain(root): # finds the sites belonging to the domain containing the root
    findAllSites(root)
    for foundSite in sameDomainSites:
        distance[foundSite] = findDistanceToRoot(foundSite)
        if distance[foundSite] - distance[neighborsOfFoundSite] not 1:
        percolating = True
```

The rationale is that if two neighbouring sites of the same domain have distances to the root site that differ by more than a lattice step, the algorithm has to have found them by going in different directions from the root site, and thus, the cluster has to span the whole lattice.

3 Results

3.1 1D fields

The integration of the TDGL equation permits one to observe the evolution of the field ϕ, as illustrated with a domain disappearance of a 1D field in Fig. 1.

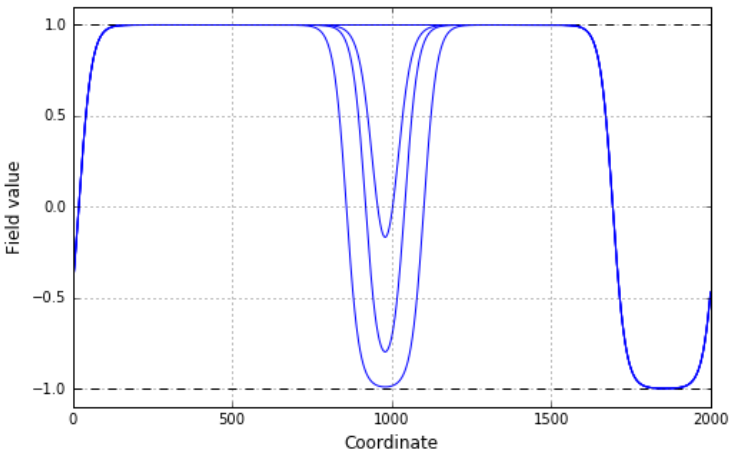
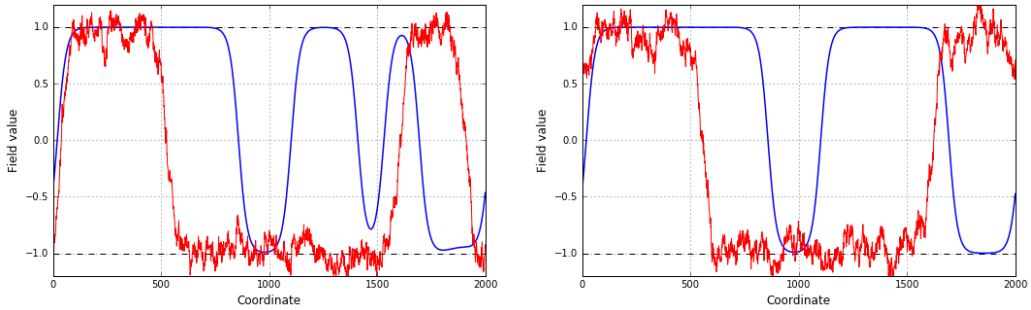


Figure 1: The progressive disappearance of a domain at coordinate 1000. Different curves represent the field configuration at different times $t = 10, 401, 402, 403$ steps.

This domain flipping illustrates that the order parameter is not conserved by the TDGL equation, as the macroscopic magnetization of the corresponding Ising spin ensemble would change in such an event. Thus, the TDGL equation can also be considered dissipative, as after this domain flip there remain less domain walls and hence *elastic* energy in the system.

3.1.1 Temperature effects

The effect of temperature (thermal fluctuations ξ) is illustrated in Fig. 2. Both fields were initialized with identical values.



(a) 1 iteration after initialization.

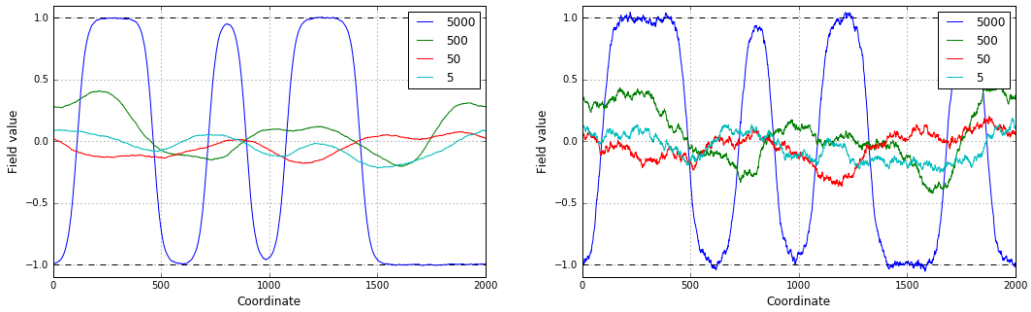
(b) 3 iterations after initialization.

Figure 2: Field evolution for different temperatures. Here the blue curve corresponds to $T = 0$, the red to $T = 0.2B$.

Temperature can completely change the distribution of domains in a field (and correspondingly, a magnet), for example in Fig. 2b the domains in the region from 1200 to 1500 are opposite.

3.1.2 Effects of potential steepness

As mentioned earlier this paper followed the approach of [9] and used a steep potential or large u and λ values. Figure 3 illustrates the effect of the parameters for equally initialized fields at some time t, that is equal for all the fields.



(a) $T = 0.01B$ (b) $T = 0.1B$

Figure 3: The effects of potential steepness for different temperatures. The legend shows values of $u(= \lambda)$. E stands for the height of the potential barrier between the two minimum wells.

It can be observed that the field evolves faster in a steeper potential. That is desirable due to computational costs.

Lack of knowledge of this fact caused a problem in the beginning of the internship, as a gradual potential was used and thus no domain formation was observed even for long times. That led to rigorous code inspection, but no faults in the code were found, it was all a matter of the potential steepness.

3.1.3 Exponential saturation

The exponential description of the field profile of Sec. 2.1.6 was validated numerically as can be seen in Fig. (4).

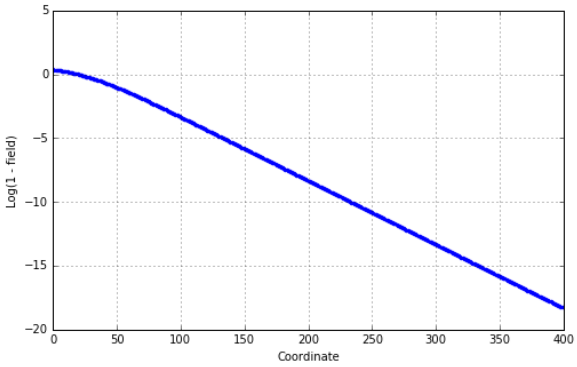
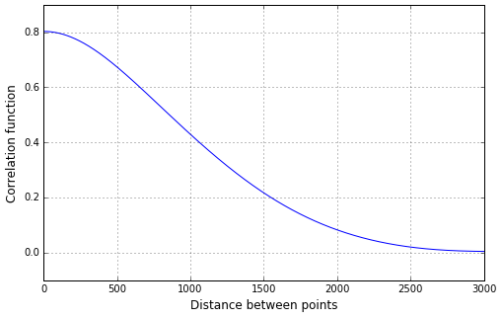


Figure 4: Log of the left side of the field profile of Fig. 1.

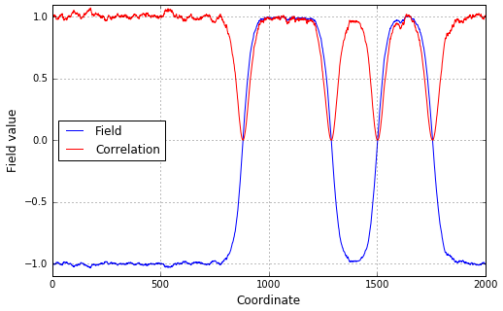
Fig. 4 demonstrates that the curve becomes linear almost instantly, suggesting that the approximation in Sec. 2.1.6 holds not only for values of ϕ very close to ± 1, which is expected according to the hyperbolic tangent relationship shown in [14].

3.1.4 Correlations

The author was unable to find correlation functions for the 1D TDGL equation in the scientific literature, so it was not possible to compare the obtained results with already established ones. An example of the calculated correlation function is provided in Fig. 5a. The curve was obtained as the average of 20 samples.



(a) An example of a correlation function for a 16'000 point field.



(b) Field profile overlayed with self-correlation function $C(r = 0)$.

Figure 5: Correlation functions.

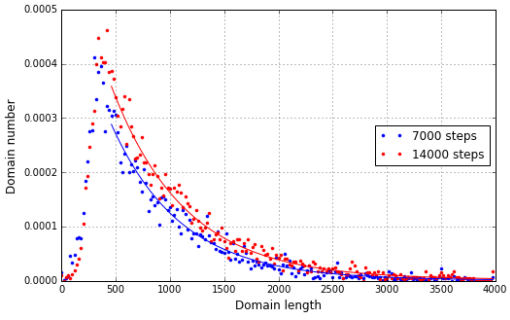
It is important to note that the correlation function is not equal to 1 at vanishing distance, as is usually the case. This is explained by Fig. 5b where the culprit is immediately visible. The correlation function drops rapidly on domain walls, thus bringing down the average value. This discrepancy could be accounted for by normalizing the correlation function.

3.1.5 Domain numbers & Scaling hypothesis

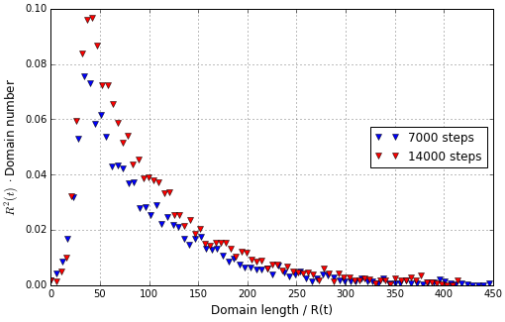
The determination of domain numbers was computationally the most expensive, so it was done completely on the cluster.

To test the prediction of the exponential distribution and the cut-off length of [7] and the logarithmic scaling function prediction of [8], domain numbers were obtained for different times. In retrospect, if the times used had been more distant we would have observed more pronounced differences between the two data series.

Nonetheless, Fig. 6a clearly demonstrates the existence of a cut-off length, below the domain number drops abruptly. The cut-off length is proportional to the correlation length ξ and so is expected to growth in logarithmically with time. The tail of the exponential distribution of the domain numbers is equally clear, hence the predictions of [8] are validated.



(a) Domain numbers for different times.



(b) Scaled domain numbers.

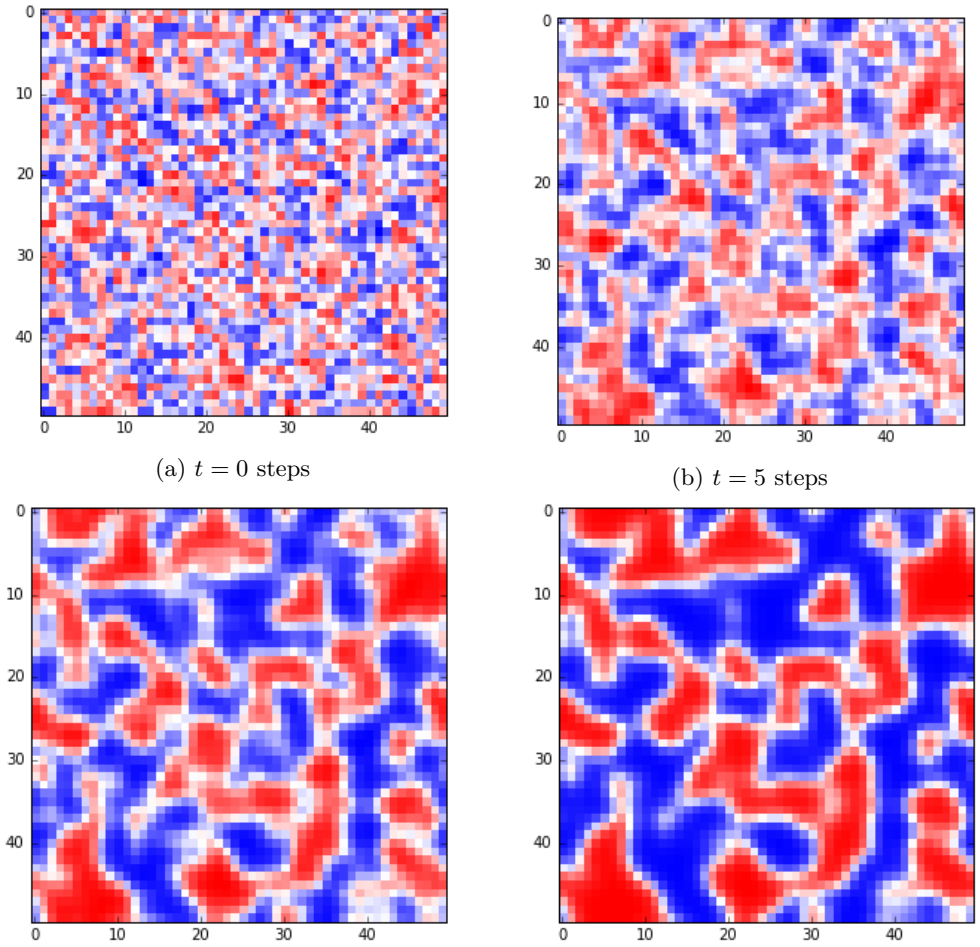
Figure 6: Domain numbers

The validity of the logarithmic scaling function is less obvious in Fig. 6b, but the data seems to be *compressed* into a single *mastercurve*. More different times should be tested to make more conclusive statements.

3.2 2D fields

An example of a 2D field just after initialization can be seen in Fig. 7a and its evolution in Fig. 7.

The disappearance of islands/domains can be seen in multiple regions of the lattice. In the Ising spin model this behaviour would correspond to the flipping of spins.



(a) $t = 0$ steps

(b) $t = 5$ steps

(c) $t = 10$ steps

(d) $t = 15$ steps

Figure 7: The evolution of a 2D field on a 50x50 grid, here $\Delta t = 0.000005$. The intensity of each color corresponds to larger absolute values. Blue represents negative values, red – positive and zero is given by the white color.

The calculations for 2D fields were actually a lot faster due to the small number of grid points, 2500 in the figures below, as opposed to many many thousand in 1D fields.

Flat domain walls are expected to be stable at $T = 0$, because for flat walls the $\Delta\phi$ term of the TDGL equation vanishes – there is no *elastic* curvature and thus the field remains stationary.

If calculated for long enough, just as in the 1D case, the field eventually relaxes to one of its equilibrium values, signifying a broken symmetry and correspondingly a macroscopic magnetization in the Ising spin model sense.

Unfortunately, when it was time to investigate the 2D fields at least as thoroughly as 1D fields by calculating the domain numbers, correlation functions and other observables, it was already June, so no deeper analysis was performed.

3.2.1 Percolation

Following the method outlined in Sec. 2.1.7, Fig. 8 was obtained. It is observed, that the fields tend to become percolating rather fast.

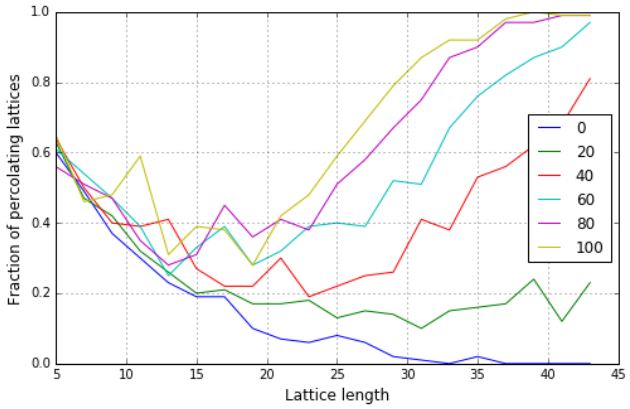


Figure 8: Emergence of percolation during time evolution. The legend gives the number of calculated time steps, here $\Delta t = 0.000005$.

4 Conclusion

First of all, I would like to express a deep gratitude to Leticia Cugliandolo, my supervisor. She accepted me as her intern and was always distinctively supportive and helpful. Having her as my supervisor made this internship a really pleasant experience.

During the 2 months I spent at the *LPTHE*, I learned a lot and grew as a possible future researcher as well. This internship gave me a glimpse of statistical field theory (SFT), scientific computing and the world of research in general.

While I acquired some foundations of SFT, many computational physics concepts and tricks to ensure optimal performance of code, and even ran my code for the first time ever on a cluster via an SSH connection, I feel that the most valuable experience I draw from these last 2 months is the exposure to the ways of a researcher.

Until the beginning of the internship I had always been pretty sure about doing a PhD, but now I am as doubtful as ever. The everyday life of a researcher, at least to the extent that I experienced it, is a lot harder than I expected, mostly due to the lack of certainty.

It is very easy to get lost and spend time on unsolvable problems or dead-ends. It was hard to search the papers and not know, whether I'm not finding a paper because of my humble searching skills or because such a paper has not been published. This experience made me appreciate the role of supervisors in scientific endeavours even more.

In addition, I took some time to get adjusted to the very flexible daily schedule. It was not simple at the beginning, as I was used to the tight lecture planning. Now I have optimized my temporal organization so that I can arrive and stay late at the lab.

On the other hand, I have never been as certain about my fondness of theoretical physics as I am now, not least because of the good support of mine, the book of Mussardo [12], showed me the ubiquity of theoretical physics. In particular, Mussardo explains how the Potts model, a generalization of the Ising model, can be mapped to the Four Color Theorem of pure mathematics. I found that extraordinarily satisfying and am anxious to learn more about SFT and its links to QFT.

I really like the very concept of doing an internship as part of the program. It makes the program more diverse and exposes students to learning various aspects of not only scientific knowledge and the everyday life of scientists.

I enjoyed my stage and feel it was a great learning experience in many ways.

Aigars Langins

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