Universal finite-size scaling function of non-conserved q-states Potts model

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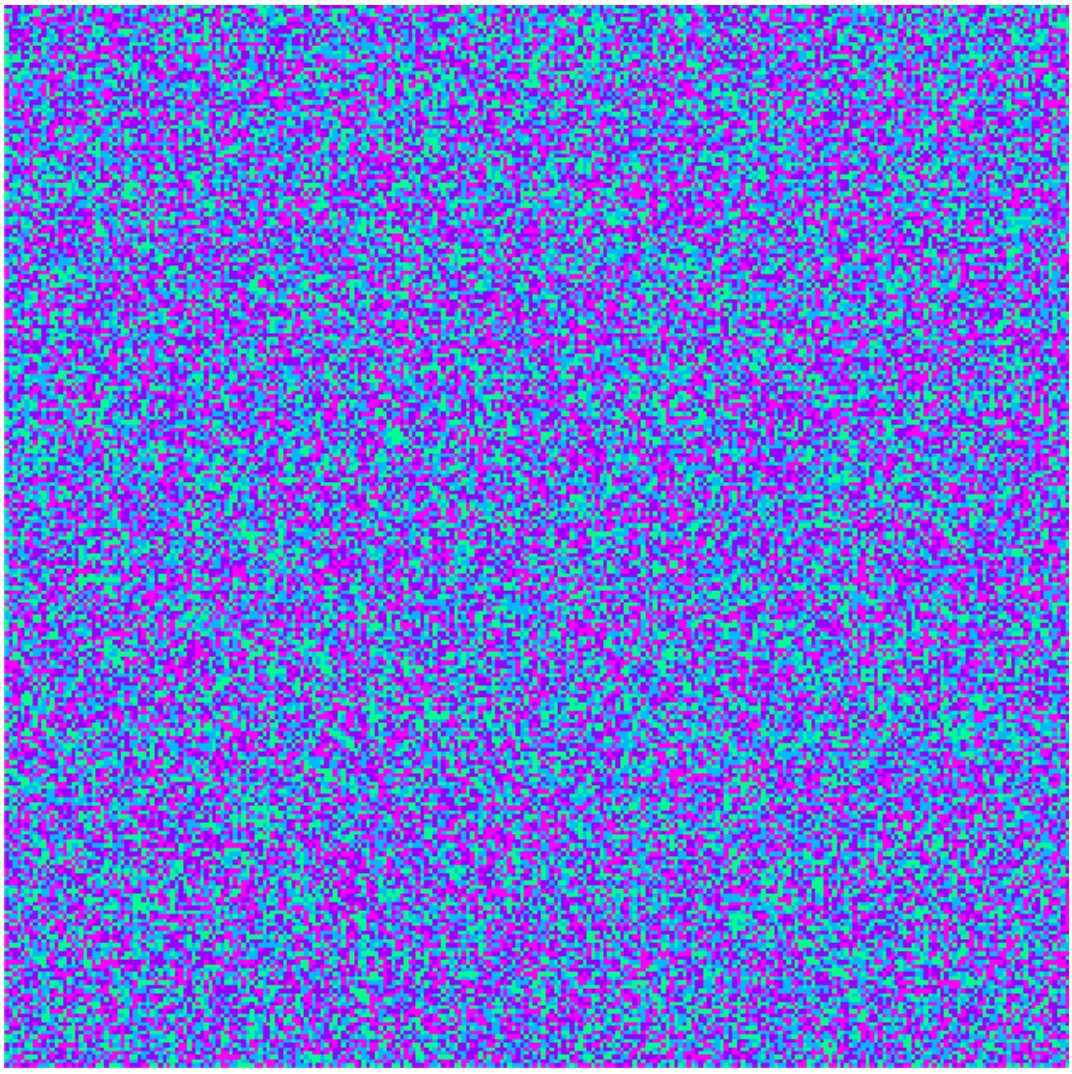

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Abstract

From Monte Carlo simulation of the non-conserved q-states Potts model, an investigation of the domain growth that occurs after a quench from the homogeneous phase to a temperature below the critical point, is presented. The general concept of this simulation technique is introduced, as well as a derivation of the physical laws governing the domain coarsening process, namely the Allen-Kahn-equation. In order to demonstrate how observables which are determined by such physical laws are calculated from the state of the simulated system, a general presentation of the Potts model and correlation functions is given. With respect thereto, the finite-size scaling technique is introduced. The thesis aims to use this technique to find a finite-size scaling function, describing the domain coarsening process, which is universal with respect to the q parameter of the Potts model.

Contents

1 Introduction

Consider a system that consists of different components, for example two liquids that compose a mixture or two kinds of elementary spin (e.g. up and down) that form a magnet. At high temperatures, such systems are typically in a homogeneous phase. Each elementary unit is only weakly correlated to its neighborhood and the whole structure looks random. But when the system is quenched to a temperature below the critical threshold, an ordered phase will occur: The two liquids of a mixture separate and the spins of a magnet align either up or down. In the first case, the overall amount of each liquid remains constant. Such a system is regarded to have a conserved order parameter, when the concentration of one liquid is adopted as the order parameter. In the second case, all elementary spins will finally be aligned in the same direction, but either up or down, so the order parameter is not conserved. If one adopts the overall magnetization as the order parameter of the system, i.e. $M = \text{Number}_{\text{spinUP}} - \text{Number}_{\text{spinDOWN}}$ and $N = \text{Number}_{\text{spinUP}} + \text{Number}_{\text{spinDOWN}}$ as the number of all spins, it is roughly zero in the homogeneous phase where $\text{Number}_{\text{spinUP}} \approx \text{Number}_{\text{spinDOWN}}$ and either $M = +N$ or $M = -N$ in the ordered phase, when the spins are either all up or all down.

But the transformation of the system from the homogeneous phase into the ordered phase does not happen instantaneously. Domains of one component each are formed and grow with time until the ordered phase is established. This domain coarsening is typically considered to be a scaling phenomenon, i.e. at each time t the structure looks roughly the same up to a scaling factor. The scaling hypothesis will be made precise in an section 3.4. But first of all, the dynamics of the domain coarsening process are reviewed and a growth law for the domain size evolution is derived, since this is crucial for the further investigation of the scaling behavior.

1.1 Growth law for the domain coarsening

The following derivation of the growth law adopts the approach provided by A. J. Bray in his article "Theory of phase-ordering kinetics" (1994).

To investigate the time evolution of a system, one is interested in the Landau free energy functional. With an order parameter field $\phi(x, t)$ that describes the state of

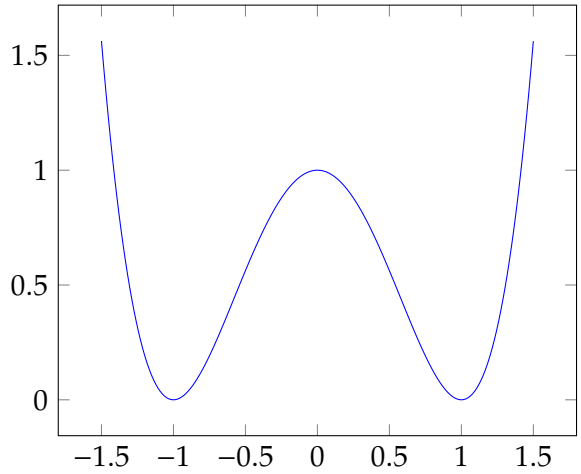


Figure 1.1: Double well structure of the potential $V(\phi)$

the system and a potential $V(\phi)$, the functional takes the following form:

$$F[\phi] = \int \mathrm{d}^d x \frac{1}{2}((\nabla\phi)^2 + V(\phi)) \tag{1.1}$$

For a non conserved order parameter field, the system evolves under the terms of a reaction diffusion equation:

$$\frac{\partial\phi}{\partial t} = -\frac{\partial F}{\partial\phi} = \nabla^2\phi - V'(\phi) \tag{1.2}$$

For an understanding of the domain coarsening dynamics, one has to examine the movement of the domain walls. Since the order parameter field remains constant there over time, the wall profile is the solution of the equation $\partial_t\phi = 0$. If one considers only the movement of one wall and adopts coordinates g normal to this wall, equation 1.2 yields:

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}g^2} = V'(\phi) \tag{1.3}$$

At large distances from the wall, the order parameter has the boundary conditions $\phi(\pm\infty) = \pm 1$. It is also valid to set $\phi(0) = 0$, i.e. to set the center of the wall at $g = 0$. With these boundary conditions, an integration of (1.3) provides the following equation:

$$\left(\frac{\mathrm{d}\phi}{\mathrm{d}g}\right)^2 = 2V'(\phi) \tag{1.4}$$

To establish a dynamical formula that captures the movement of the wall, it is helpful to consider the movement to be driven by a surface tension. Such a property can be

derived via an integration of 1.1 over the normal coordinates, which provides the energy per unit area of wall, i.e. the surface tension or surface energy:

$$\sigma = \int_{-\infty}^{\infty} \mathrm{d}g \left(\frac{\mathrm{d}\phi}{\mathrm{d}g}\right)^2 = \int_{-1}^{1} \mathrm{d}\phi \sqrt{2V(\phi)} \tag{1.5}$$

This equation can be linearized at $\phi = \pm 1$ i.e. at $g = \pm\infty$, which gives an exponential formula:

$$\phi \sim \exp(-[V(\pm 1)]^{\frac{1}{2}}|g|) \quad \text{for} \quad g \to \pm\infty \tag{1.6}$$

So the order parameter field ϕ decays exponentially fast away from the walls which means that the system's energy resides there. This implies that the curvature of the walls, i.e. the imbalances of the free energy, is the driving force for the dynamics of the system. If one considers a spherical domain with radius R which is decreased by $\mathrm{d}R$, the work $4\pi F R^2 \mathrm{d}R$ has to be brought about. At the same time, the surface energy σ decreases by $8\pi\sigma R \mathrm{d}R$. Because of energy conservation both terms can be set equal, which implies that a force F drives the movement of the domain wall:

$$F = \frac{2\sigma}{R} \tag{1.7}$$

If one considers a friction of η during the movement, this driving force leads directly to an equation of motion:

$$\eta \frac{\mathrm{d}R}{\mathrm{d}t} = -\frac{2\sigma}{R} \tag{1.8}$$

Since it is not clear a priori why domains should have a spherical shape, it is necessary to consider generally curved surfaces as well. The results for this case were first derived by S. M. Allen and W. J. Cahn in their article "A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening" (1979). Since close to a domain wall, the nabla operator can be rephrased as $\nabla\phi = (\partial\phi/\partial g)_t \hat{g}$ with $\hat{g}$ normal to the wall, the l.h.s. of equation 1.2 reads as $(\partial^2\phi/\partial^2 g)_t + (\partial\phi/\partial g)_t \nabla\hat{g} - V'(\phi)$. For the r.h.s. one finds $(\partial\phi/\partial t)_g = -(\partial\phi/\partial g)_t (\partial g/\partial t)_\phi$, so equation 1.2 takes the following form:

$$-\left(\frac{\partial\phi}{\partial g}\right)_t \left(\frac{\partial g}{\partial t}\right)_\phi = \left(\frac{\partial\phi}{\partial g}\right)_t \nabla\hat{g} + \left(\frac{\partial^2\phi}{\partial^2 g}\right)_t - V'(\phi) \tag{1.9}$$

The last two terms cancel because the wall profile ist considered to be controlled by equation 1.3. Dividing by $(\partial\phi/\partial g)_t$ and setting $v = (\partial g/\partial t)_\phi$ yields the Allen-Kahn equation:

$$v = -\nabla\hat{g} = -K \tag{1.10}$$

The Allen-Kahn equation is consistent with the result for a surface tension driven growth of spherical domains in equation 1.8 because $K = 2/R$ and $\sigma = \eta$. Insomuch as the movement of the walls is proportional to the growth of the domain size $L(t)$

and since the curvature can be rephrased as $K \sim 1/L$, the Allen-Kahn equation reads as $\mathrm{d}L/\mathrm{d}t = -1/L$, which has the following solution:

$$L(t) \sim t^{\frac{1}{2}} \tag{1.11}$$

To put in a nutshell: In systems with a non-conserved order parameter, where distinct phases with different potential energy occur, domains should grow after a phase-transition with an exponent 1/2. The question is now, how a system with such clearly defined properties could be simulated and observed.

1.2 Monte Carlo simulation

For the description of classical systems, there exist traditionally two very different mathematical aproaches: The first one consists of differential equations, which imply a determistic view of the world. For fixed boundary conditions, the complete trajectory of a particle can be calculated. But already for a system of three particles with attractive forces, the descriptive differential equation is not analytically solvable. And the most objects of our natural enviroment contain even more particles: A liter water consists of roughly 3.3×10^{25} water molecules. However, many properties of macroscopic objects do not rely on their exact microscopic configuration. Therefore one uses a stochastic approach, namely statistical mechanics, to describe these objects.

For the dynamical evolution of a statistical system, a mixture of both approaches is often helpful, so that the system evolves in a "flow of both deterministic and stochastic processes" (Metropolis and Ulam 1949). The most common method is the monte carlo simulation, which was first suggested by E. Fermi and further developed by S. Ulam, J. v. Neumann and N. Metropolis in the context of neutron diffusion as a part of the U.S. nuclear weapons project. The codename "Monte Carlo" was used since the project was strictly confidential and refers to gambling due to the randomness exploited by the method (Metropolis et al. 1987).

The main goal of the monte carlo method is to estimate expectation values $\langle O \rangle$ of an given esemble (Janke 2013, p. 96):

$$\langle O \rangle = \sum_{\text{states } \omega} O(\omega) \exp -\beta \mathcal{H}(\omega)/\mathcal{Z} \tag{1.12}$$

This sum can not be computed because the number of possible microstates ω of the system is far too high. One solution approach would be a stochastic sampling of the state space: The huge sum of equation 1.12 is restricted to a randomly chosen set of microstates. But usually, the area of the state space that yields a small $\mathcal{H}(\omega)$ and therefore significally contributes to the $O(\omega) \exp -\beta \mathcal{H}(\omega)$ sum, is very small. A random sampeling of the state space would probably miss this region and could not

be used for a good estimation of the full sum (Janke 2013, p. 97). The idea is to set up a Markov-chain that lets the system evolve into a region of the state space that has a higher probabilty to occur and a lower energy. The sum over the whole state space can then be estimated with a sum over a Markov chain:

$$\langle O \rangle = \sum_{\text{states } \omega} O(\omega) \exp -\beta \mathcal{H}(\omega)/\mathcal{Z} \quad \approx \quad \bar{O} = \frac{1}{N} \sum_{k=1}^{N} O(\omega^{(k)}) \tag{1.13}$$

Here, $\omega^{(k)}$ is the kth microstate of the Markov chain. Since microstates occur with probabilty $\mathcal{P}^{\text{eq}}(\omega_i) = \exp -\beta \mathcal{H}/\mathcal{Z}$ in thermal equilibrium, the transition probability W_{ij} of microstate ω_i transforming into microstate ω_j must obey the *detailed balance condition* (Hastings 1970, p. 99):

$$W_{ij} \mathcal{P}^{\text{eq}}(\omega_i) = W_{ji} \mathcal{P}^{\text{eq}}(\omega_j) \tag{1.14}$$

The most common way to set up a Makrov-chain is the standard Metropolis algorithm, which follows two steps: First, a transition of microstate ω_i to microstate ω_j is randomly proposed. This occurs with the *selection probability* f_{ij} which is symmetric ($f_{ij} = f_{ji}$). This transition is accepted with the *acceptance probability* w_{ij}:

$$w_{ij} = \begin{cases} 1 & E_j < E_i \\ \exp -\beta(E_j - E_i) & E_j > E_i \end{cases} \tag{1.15}$$

The transition probability of the Markov chain is therefore:

$$W_{ij} = \begin{cases} f_{ij} w_{ij} & i \neq j \\ f_{ii} - \sum_{j \neq i} f_{ij}(1 - w_{ij}) & i = j \end{cases} \tag{1.16}$$

From this it follows immediately that W_{ij} is actually an appropriate probability distribution, i.e. that it fullfills $W_{ij} \geq 0 \, \forall \, i, j$ and $\sum_j W_{ij} = 1 \, \forall \, i$. Moreover, it does fullfill the detailed balance condition in equation 1.14.

The quest is now to find physical models, which mimic natural objects and their phenomena very well, but can be simulated at the same time with a Markov chain.

1.3 Potts model

The Potts model was formulated by R. B. Potts in his dissertation (Potts 1952) and is a generalization of the Ising model (Ising 1925). While in the Ising model each site σ_i of an n-dimensional lattice is in a state $\sigma_i = +1$ or $\sigma_i = -1$, in the q states Potts model each lattice point can adopt a state $\sigma_i = 0, 1, \ldots q - 1$. The Ising states are meant to represent spins which are alligned parallel or antiparallel to a particular direction. The generalized version of this are spins pointing in one of q different directions. But

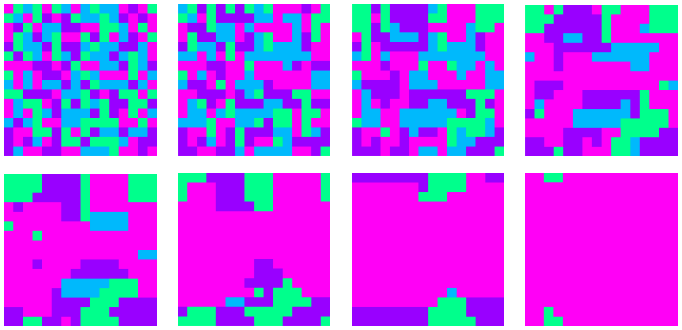


Figure 1.2: Lattice with 16×16 sites at different MC steps

the Hamiltonian for a system that involves the angle between neighboring spins is much more complicated and Potts was not able to determine the critical points for values of $q > 4$. Therefore he suggested a simpler Hamiltonian similar to the Ising model. Without any external field and for next neighbor interaction it takes the following form:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j} \tag{1.17}$$

The $\langle ij \rangle$ term indicates summation over all neighboring states and $\delta_{\sigma_i \sigma_j}$ is the Kronecker delta. The original form of the Hamiltonian which involves a $\cos \theta$ term for the angle between neighboring spins is nowadays known as the Clock model.

For $J > 0$ the Hamiltonian (1.17) takes minimal values if all lattice sites are in the same state, so this is called the *ferromagnetic Potts model*, whereas the $J < 0$ case is called the *antiferromagnetic Potts model*. Since for dimension 2, the model is equivalent to the ice-rule vertex model, the critical temperature can be deduced (Wu 1982, p. 254):

$$T_c = \frac{J}{k_\mathrm{B} \ln (1 + \sqrt{q})} \tag{1.18}$$

The phase transitions that occur at this temperature are of second order for $q \leq 4$ and of first order for $q > 4$. In dimensions higher than 2, first order phase transitions appear at lower q-values and for dimensions $d \geq 6$ even continuous transitions take place (Wu 1982, p. 238).

1.4 Implementation

The aim of this thesis is to investigate the domain growth in a two-dimensional Potts lattice after a quench from the homogeneous phase to a temperature $T < T_\mathrm{C}$. The initial configuration is therefore completely random as one can see in figure 1.2, which represents the behavior of the system at $T \to \infty$. Starting with the initial configuration, local updates according to the algorithm in equation 1.15 with a $T < T_\mathrm{C}$ are

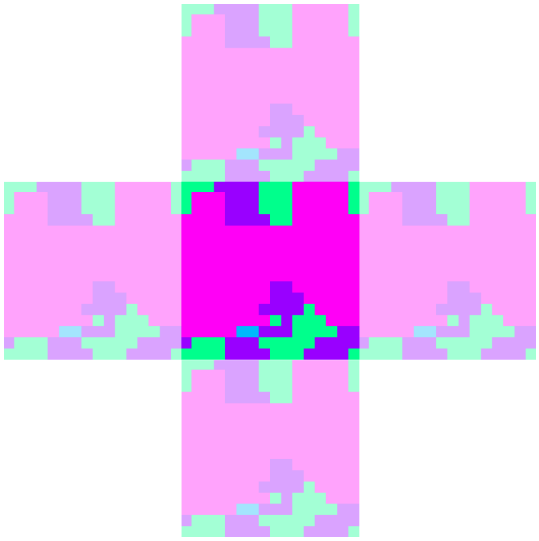


Figure 1.3: Visualization of the periodic boundary conditions

performed. This corresponds to an immediate quench from the homogeneous phase to a temperature below the critical point. For a quadratic lattice with $N = L \times L$ sites, N such local updates at randomly chosen lattice sites form a Monte Carlo step (MC step). Since the acceptance probability is $w_{ij} = 1$ for $\omega_i = \omega_j$ because of $E_j = E_i$, such trivial "non-updates" are avoided by proposing only $\sigma_{i,j}^{\text{new}} \neq \sigma_{i,j}^{\text{old}}$. If the site (i, j) is for example in the state $\sigma_{i,j}^{\text{old}} = 2$ in a $q = 4$ Potts lattice, an update is randomly chosen among $\sigma_{i,j}^{\text{new}} = 0$, $\sigma_{i,j}^{\text{new}} = 1$ and $\sigma_{i,j}^{\text{new}} = 3$. It is either rejected or accepted with a probability according to equation 1.15 and N such propositions are sequentially conducted in one MC step.

1.5 Boundary conditions

The Hamiltonian (1.17) is defined to sum only over neighboring lattice sites. For a quadratic two-dimensional lattice, this means that every lattice point (i, j) has the four neighbors $(i, j+1)$, $(i+1, j)$, $(i, j-1)$ and $(i-1, j)$. A local update at this lattice point thus affects only four terms in the Hamiltonian:

$$\begin{aligned} \Delta E = (&\delta_{\sigma_{i,j}^{\text{new}} \sigma_{i,j+1}} + \delta_{\sigma_{i,j}^{\text{new}} \sigma_{i,j-1}} + \delta_{\sigma_{i,j}^{\text{new}} \sigma_{i+1,j}} + \delta_{\sigma_{i,j}^{\text{new}} \sigma_{i-1,j}}) \\ -(&\delta_{\sigma_{i,j}^{\text{old}} \sigma_{i,j+1}} + \delta_{\sigma_{i,j}^{\text{old}} \sigma_{i,j-1}} + \delta_{\sigma_{i,j}^{\text{old}} \sigma_{i+1,j}} + \delta_{\sigma_{i,j}^{\text{old}} \sigma_{i-1,j}}) \end{aligned} \tag{1.19}$$

In order for all states of the lattice to evolve under the same conditions, a proper treatment of the outer edges and corners is necessary, which have only three or two neighbors, respectively. In most cases, periodic boundary conditions are applied: As one can see in figure 1.3, lattice points on the left edge ($i = 0$) are assigned

to points on the right adge $i = L$ as their neighbors and vice versa. Equivalently, lattice points on the upper edge $(j = 0)$ are assigned to points on the lower adge $(j = L)$ as their neighbors and vice versa. This adjustment is called *periodic boundary conditions*, whereby the system evolves as if it were part of an infinitely large lattice. Nevertheless, the finite lattice size can interfere in the domain growth. A discussion of such *finite size effects* will therefore follow the analysis of the presented data.

2 Observables

In order to compare the behavior of the model with physical laws, it is necessary to evaluate the observables in a considerate and transparent way. For phase ordering dynamics, one is particularly interested in morphology describing functions, such as the correlation function, which is examined in the following section. The correlation function can be used to calculate a measure for the domain sizes, a method which will be discussed along with a more direct way of calculating the domain size.

2.1 Correlation function

A correlation function is generally a measure of the order of a system. Contingent of the spatial or temporal distance between two variables, the function indicates the statistical correlation between them. Correlation is to be understood as the degree of which a pair of variables is linearly related. In the Ising model for example, the correlation between two Ising spins Φ_i and Φ_j is determined by $\Phi_i\Phi_j$, which is 1 for two equal, i.e. strongly correlated spins and -1 for two different, i.e. weakly correlated spins. In order to determine a spatial correlation function $C(r)$, the average correlation of all spins with the distance r is computed. This is also called the equal-time correlation function:

$$C^{\text{Ising}}(r) = \langle \Phi_i \Phi_j \rangle - \langle \Phi_i \rangle \langle \Phi_j \rangle \tag{2.1}$$

Since the aim of this thesis is to examine the development of the domain structure over time, it is necessary to work out the spatial correlation function at different MC

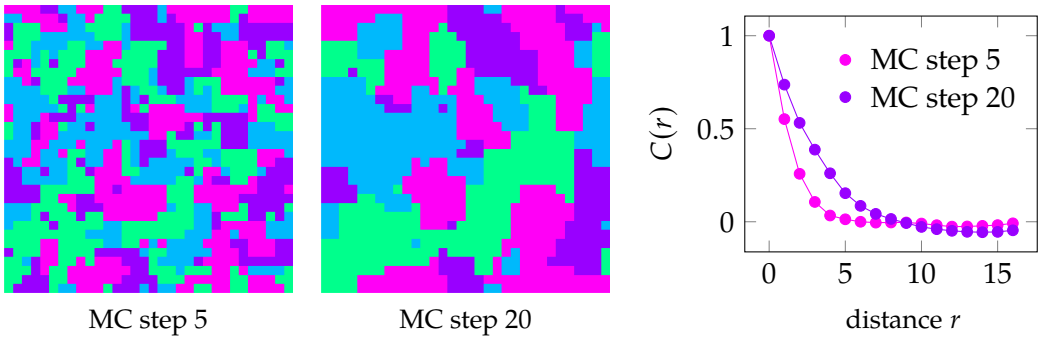
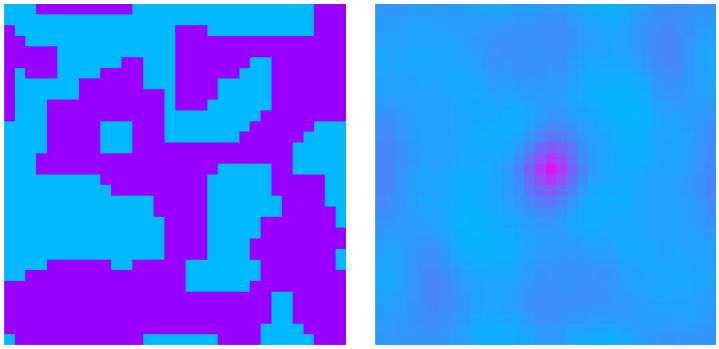


Figure 2.1: Correlation functions of two Potts lattice configurations



Ising lattice arranged FFT data

Figure 2.2: Ising lattice and real part of twofold FFT

steps. One can view the correlation functions of two $q = 4$ potts configurations in figure 2.1, where the second lattice is in a more ordered state and the correlation between lattice sites thus decays slower. The correlation function in a Potts lattice is defined very similarly to the Ising model:

$$C(r) = \frac{1}{q} \sum_{n=1}^{q} \left[\langle \Phi_i^n \Phi_j^n \rangle - \langle \Phi_i^n \rangle \langle \Phi_j^n \rangle \right] \tag{2.2}$$

Here, for each of the q states, all Potts variables are transformed into Ising spins with $\Phi_i^n = 2\delta_{\sigma_i n} - 1$ and the sum of the q Ising correlation functions is divided by q.

Computation via FFT

A direct calculation of the correlation function is in most cases not practicable, since the correlation of each lattice site with all sites at distance r is to be determined. The number of operations for a lattice with N points is therefore N^2, which is why it is called an $O(N^2)$ process. With an algorithm called *fast Fourier transform* (*FFT*), the number of operations can be reduced to $O(N \log_2 N)$ (Flannery et al. 1992, p.504). The FFT algorithm is a sophisticated way of computing the Fourier transform of discrete data sets with a length that is a power of two, which is also why all Potts lattices analyzed in this thesis have sizes $128, 256, 512$ and 1024. The difference between $O(N^2)$ and $O(N \log_2 N)$ processes is immense: For a 1024×1024 lattice with roughly 10×10^6 points this means 2 weeks of CPU time with the direct method an only 30 seconds with the FFT method on a microsecond cycle time computer (Flannery et al. 1992, p.504). One can see the twofold FFT plot of a 32×32 Ising lattice in figure 2.2. Since a Fourier transform already arranges the variables of a field due to spatial correlation, it is sufficient to sum over lattice sites at distance r from the center in order to determine the correlation function.

2.2 Domain length

The computation of the average size of the domains is not trivial, since they come in various shapes and arrangements. However, it is not necessary to identify all clusters and their radii respectively. A quantity which is proportional to the actual domain sizes is completely sufficient, because one is interested in the exponents of growth laws and not the actual amplitudes. The two algorithms used in this thesis are the following:

Direct method

First the Potts lattice is converted into q Ising lattices, following the same transformation rule as in 2.2. Then one determines the number of domain walls in each row, i.e. points that have a right neighbor with a different spin, and in each column, i.e. points that have a lower neighbor with a different spin. The Lattice size divided by the number of domain walls gives a measure for the average domain size.

Via the correlation function

The domains are strongly correlated areas of the lattice, since they consist of identical states. Their walls mark a limit of the correlation of the containing sites to their neighbors and the decay of the correlation function is therefore a good measure for the average domain size. One can choose for example the zero-crossing, i.e. the r for which $C(r) = 0$, as an indicator, but any other threshold is equally justified. In fact, for this thesis $C(r) = 0.5$ was elected, because zero-crossings may not occur at late times. But even the 0.5 crossing is not sufficient to examine the saturation process, since the correlation function becomes $C(r) = 1$ for completely ordered systems. For this kind of analysis, one therefore uses the direct method, but in order to study the scaling hypothesis or growth laws, an application of both methods makes the implications more trustworthy.

3 Methods

In the following sections, the computational methods used throughout this thesis are examined using the example of the time evolution of a 128×128 lattice with 100 different initial configurations. The two earlier proposed methods of domain length calculation are contrasted and the time evolution is checked for a power law behavior in section 3.2. In the subsequent section a frequently arising problem, metastable final states, is demonstrated and the proper treatment is discussed. Section 3.3 deals with the question, whether noise canceling procedures interfere with the correct calculation of domain lengths. Finally, the finite-size scaling technique is introduced in section 3.4.

3.1 Domain length computation

In order to determine which of the methods for domain length calculation discussed in section 2.2 is to be preferred, one has to compare the data they produce. In figure 3.1 the method which uses the 0.5-crossing of the correlation function is contrasted with the direct estimation. A noise-canceling over 4 neighbors was performed at the beginning of both computing processes. The graphs depict a domain expansion behavior that is very well correlated to the growth law in equation 1.11. The slower growth of the directly computed data at early times might be due to the noise canceling routine presented in section 3.3. This procedure effectively reduces the size of small domains and the direct method might cope with this problem in a different way than the correlation function, since it expects equally distributed domains over the whole lattice.

The plot of the averaged correlation-measured evolution ends at MC step 3162, because at the next point of evaluation, some lattices were already in the final one-state equilibrium for which the correlation function diverges. Nevertheless, not all initial configurations reach the final equilibrium this early. The lattice evolution which is illustrated in figure 3.2 terminates shortly after MC step 10000 but exhibits a strange behavior: The domain length seems to decrease at late times, which is clearly an artifact, as the corresponding lattice plots reveal. In this particular case, the annihilation of the turquoise colored phase and vertical growth of the purple colored phase gives rise to a faster decaying correlation function and thus to a 0.5-crossing at shorter distance. Due to the quadratic shape of the lattice, phases at late times very often exhibit rectangular shapes that extend either horizontally or vertically

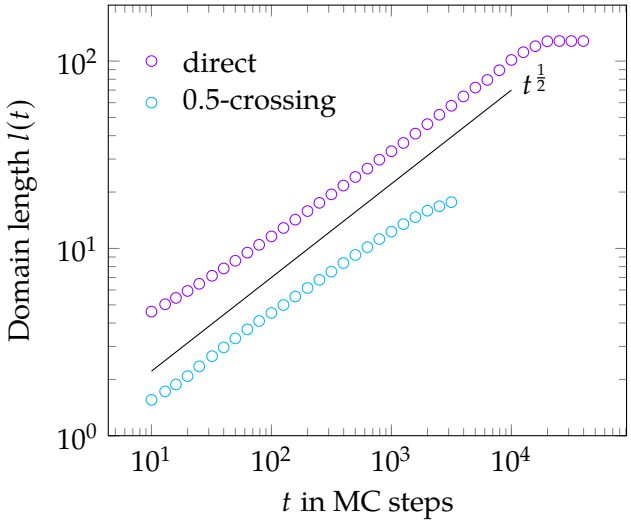


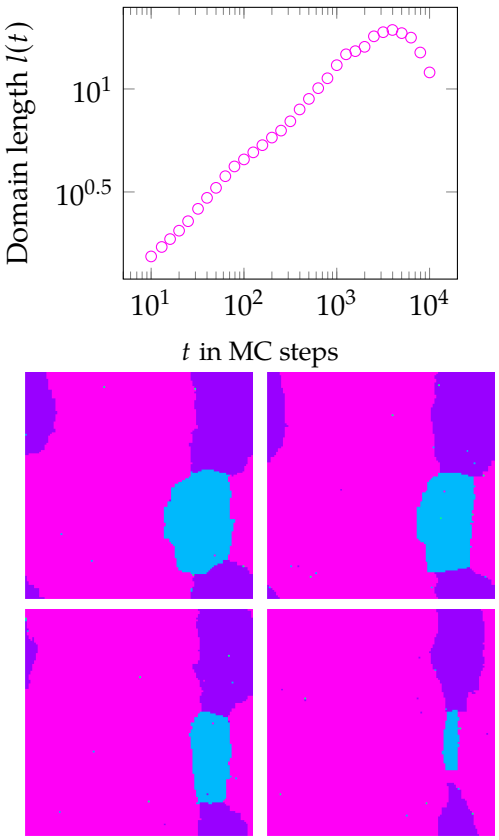
Figure 3.1: Domain length evolution in 128×128 Potts lattice with $q = 4$, averaged over 100 initial configurations. Comparison of directly computed data and 0.5-crossings of the correlation function. Noise-canceling was performed in both cases.

over the entire width before they vanish or even persist, as discussed in section 3.2. Since the correlation function is defined in a rotationally symmetric way, it is not a good indicator of the domain size for such oddly shaped phases. The descent of some correlation-based evolution data sets at late times thus causes the soft bending of the averaged evolution plot in figure 3.1.

It follows from this analysis that a direct computation of the domain sizes should be preferred. Both methods clearly reveal a time evolution according to the growth law derived in section 1.1 at early times, but the directly computed data set shows such behavior more consistently before saturation begins, whereas the correlation-based evolution deviates early and is not able to capture the passage into one-phase equilibrium.

3.2 Local minima

Since lattice configurations with only one phase correspond, according to the Potts Hamiltonian in equation 1.17, to the lowest internal energy, one would at first glance expect from all growth processes to terminate in such a state. But the Metropolis algorithm minimizes not internal energy but the free energy which can have local minima separated from the global minimum by high potential barriers. Thus lattices sometimes get stuck in such pseudo-equilibrii, a problem which is very common in



Lattice at MC steps 5012, 6310, 7943 and 10000

Figure 3.2: Domain length evolution of one particular 128×128 lattice with $q = 4$, computed via the 0.5-crossing of the correlation function. The configurations which correspond to the last four data points were plotted on the right.

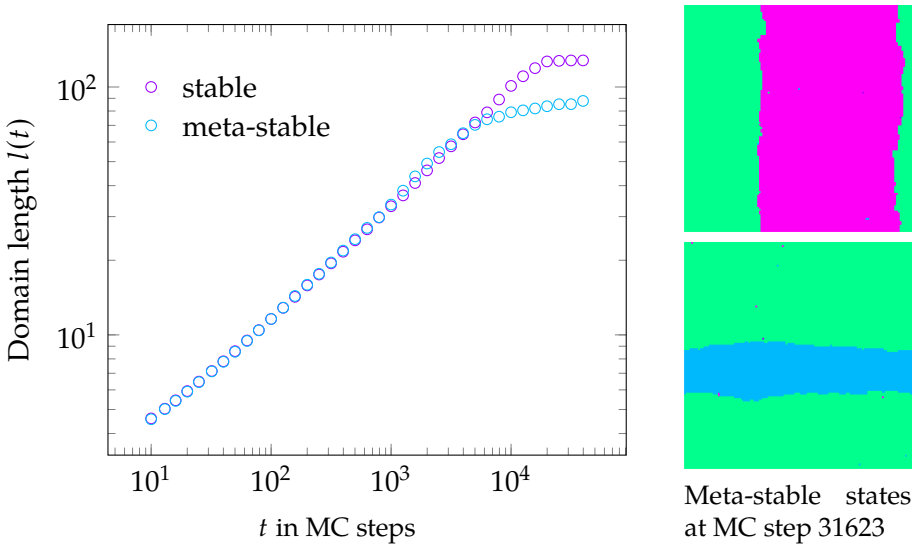


Figure 3.3: The purple data points correspond to lattices which do not achieve the final one-phase equilibrium but get stuck in a meta-stable state, which was observed in 21 of the 100 evolution processes. Two of such meta-stable final configurations are plotted on the right hand. The purple data points correspond to the remaining 79 growth instances, which terminated in one-phase equilibrium. Both data sets were averaged over the corresponding number of 21 and 79 instances respectively.

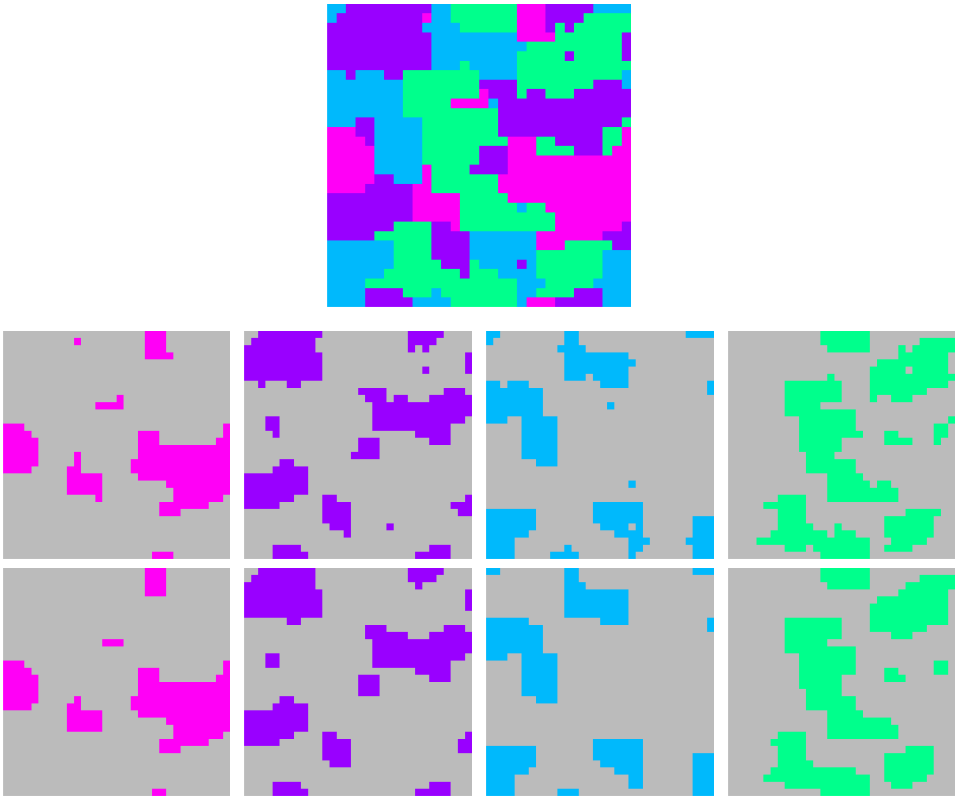


Figure 3.4: Transformation of a 32×32 Potts lattice into four Ising lattices and subsequent noise canceling

Monte Carlo simulation. Since eventually a finite-size scaling with respect to the system size is desired, such multi-phase final states will in most instances be removed from the data sets.

3.3 Noise canceling

The randomness of the update algorithm has the effect that singular lattice points in a domain of one specific phase can suddenly adopt a different phase since the probability of this event to happen is low but not zero. Such defects disappear as fast as they appeared but nevertheless interfere with the domain length computation. A noise canceling routine is therefore applied before the measurement is performed, which does of course not influence the lattice itself but just acts on snapshots of it. The noise canceling routine is carried out for all of the q Ising lattices, which are generated during the process of domain length computation, because it is more well-defined for this model: Each spin at lattice point (i, j) is replaced with the spin that occurs most often in the four nearest neighbor sites $(i+1, j)$, $(i-1, j)$, $(i, j+1)$,

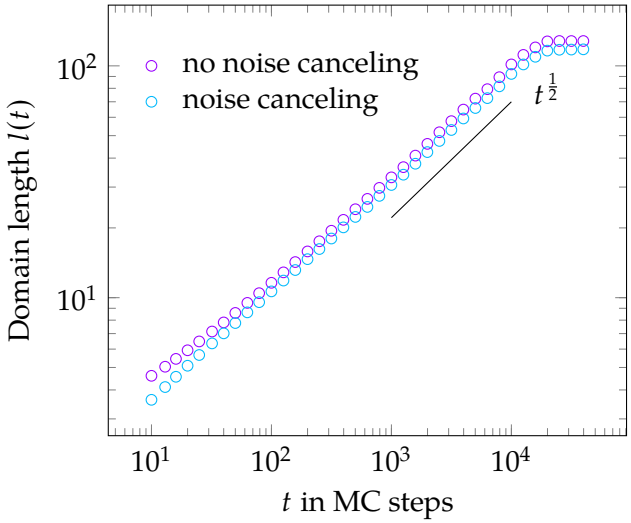


Figure 3.5: Domain length evolution in 128×128 lattice with $q = 4$, computed with the direct method after a noise canceling routine (purple) and without noise canceling (blue) respectively. Averaged over 100 initial configurations.

$(i, j-1)$ and (i, j) itself. At these five sites, either spin +1 or spin −1 is the most common since 5 is an odd number, whereas in the $q = 5$ model, all five sites could be occupied by a different state and the nearest neighbor rule could not be applied. One can see an example of the noise canceling routine in figure 3.4. Apparently, it affects the domain expansion only at early times, when it might effectively reduce the domain size. Since lattice point defects affect the domain length computation in the equilibrium, the graph in figure 3.5 saturates at a slightly lower length.

3.4 Finite size scaling analysis

Thermodynamic quantities of a system that slowly passes the critical temperature while remaining in equilibrium can be characterized during the transition period via critical exponents. For any quantity X one can write:

$$X = X_0 |T - T_C|^{-x} \tag{3.1}$$

T_c is the critical temperature, X_0 the amplitude and x the critical exponent. For example, the equilibrium correlation length ξ exhibits the following critical behavior with an exponent v:

$$\xi = \xi_0 |T - T_C|^{-v} \tag{3.2}$$

The equilibrium correlation length is a measure for the distance at which microscopic variables are correlated, in such a way that the correlation function can be

approximated with $C(r) \sim \exp(-r/\xi)$. Equation 3.1 and 3.2 can be combined to express the critical behavior of any quantity X in terms of the correlation length:

$$X = \tilde{X}_0 \xi^{\frac{x}{v}} \tag{3.3}$$

Here, $\tilde{X}_0 = X_0 \xi_0^{-x/v}$ is just an adjusted growth amplitude. However, in computer simulation physics, the correlation length of microscopic variables in a system is limited by the finite system size L, which is in this case the size of a quadratic lattice. In fact, for $\xi \to L$, the critical behavior of the thermodynamic variables can be in terms of the system size (Landau and Binder 2014, S.80):

$$X = \tilde{X}_0 L^{\frac{x}{v}} \tag{3.4}$$

In order to deal with this limiting behavior, one introduces a scaling variable $y = L/\xi$ and a scaling function $Y(y)$ which connects the lattice size dependence and the correlation length dependence of thermodynamic quantities:

$$X = L^{\frac{x}{v}} Y(y) \tag{3.5}$$

This scaling function has to obey $Y(y) = \tilde{X}_0$ for $y \to 0$ and $Y(y) \sim y^{-x}$ for $y \ll 1$ in order to obey the two behaviors in equation 3.3 and equation 3.4.

These considerations are, however, not sufficient to describe the domain coarsening process, since it expresses the non-equilibrium dynamics of a phase transition. At this point, a theory of great importance comes into play: The *scaling hypothesis*, which claims that during the coarsening process, there exists a characteristic length scale $l_c(t)$ such that the domain structure is, in a statistical sense, independent of time when all lengths are scaled by $l_c(t)$ (Bray 1994, S.6). For the spatial correlation function for example, which describes the morphology of the system and therefore also the domain structure, one can find a master function:

$$C(r,t) = f\left(\frac{r}{l_c(t)}\right) \tag{3.6}$$

While the scaling function of equation 3.5 allows one to describe the behavior of thermodynamic quantities in the equilibrium case in a temperature-independent way, with the analogies $\xi_c \equiv l(t)$ and $1/t \equiv |T - T_C|$ one can also find a scaling function, which describes the dynamics of the characteristic length in a time-independent way:

$$l_c(t) = l_{\max} Y(y) \tag{3.7}$$

In Potts lattices, the characteristic length is equal to the average domain size $l(t)$, which evolves according to the power law of equation 1.11. One should therefore use a scaling variable $y = l_{\max}^{1/\alpha}/t$ so that the scaling function has the two limiting behaviors $Y(y) = 1$ for $y \to 0$ and $Y(y) \sim y^{-\alpha}$ for $y \ll 1$. For non-conserved dynamics, α is equal to $\frac{1}{2}$, as demonstrated in section 1.1.

3.5 Universal finite size scaling function

In statistical physics, *universality* is the observation, that a lot of systems behave very similar at criticality. Theoretical models with different dynamics can, if their dimension and symmetries are equal, belong to the same *universality class*, which means their thermodynamic or dynamic quantities exhibit equal critical exponents at phase transitions. The Potts models with different q values are certainly instances of the same universality class and one can therefore aim to find a *universal scaling function* in a finite size scaling analysis.

4 Results

In the subsequent sections, the data obtained in various simulation processes is presented, all referring to the domain length evolution in Potts lattices with different q values, quench temperatures T and lattice sizes L. The domain length is computed via the direct method discussed in section 3.1, since the correlation function was considered to be not very faithful in order to measure this observable. Noise reduction was performed before each computation of the domain size and multi-phase final states were in most instances filtered out, which is also indicated in the caption of each data plot.

4.1 Different lattice sizes for $q = 4$

In figure 4.1 the domain length evolution in $q = 4$ Potts lattices with four different sizes is plotted, all at quench temperature $T = 0.5T_C$. One can see that the data of smaller system sizes follows the one for larger lattices until saturation occurs, which suggests that interference of finite size effects with the domain growth happens only at very late times. At early times, the evolution is slower than the growth law, which probably has its origins in the noise canceling routine, as discussed in section 3.3. After the Potts lattice is transformed into q different Ising lattices, the noise reduction may drastically contract some of the domains, relative to their yet small size.

The finite-size scaling analysis exhibits a collapse of data, as shown in figure 4.2, with the exception of large y values. These correspond to early times, where the scaling law is apparently not fulfilled. The $y^{-1/2}$ behavior begins at $y = 1.295$, which implies a finite-size unaffected scaling and power law growth of the domains until $l(t) \approx 0.9L$.

In figure 4.3, one can see a collapse of the averaged correlation functions in a 64×64 Potts lattice with $q = 4$, achieved by a scaling with the domain size. This implies, as proposed in section 3.4, that the domain size is a characteristic length scale of the system, which fulfills the scaling hypothesis.

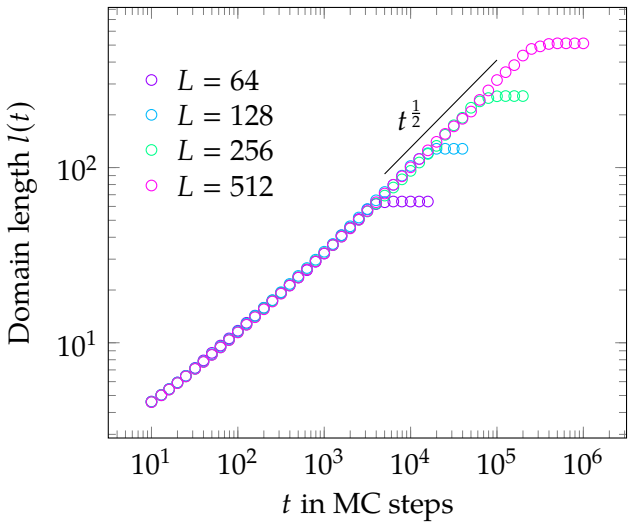


Figure 4.1: Domain length evolution for $q = 4$ Potts lattice with four different lattice sizes, all at quench temperature $T = 0.5T_C$. Data is averaged over 100 initial configurations, whereby evolutions without one-phase final equilibrium were filtered out.

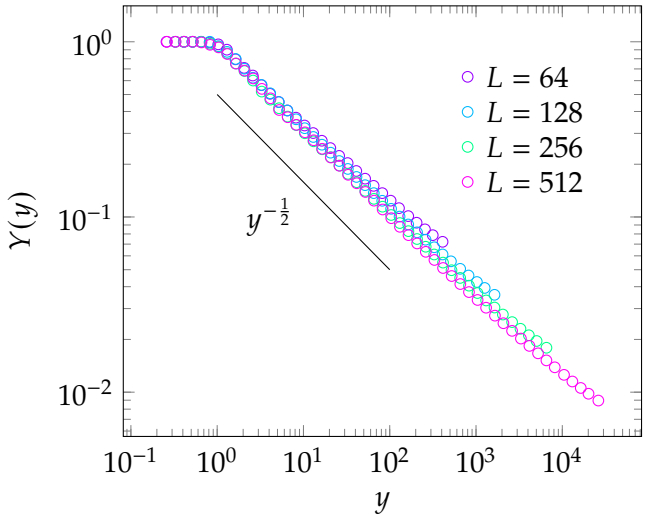


Figure 4.2: Scaling functions for $q = 4$ Potts lattices with four different lattice sizes, all at quench temperature $T = 0.5T_C$ (Scaling of the data sets of figure 4.1).

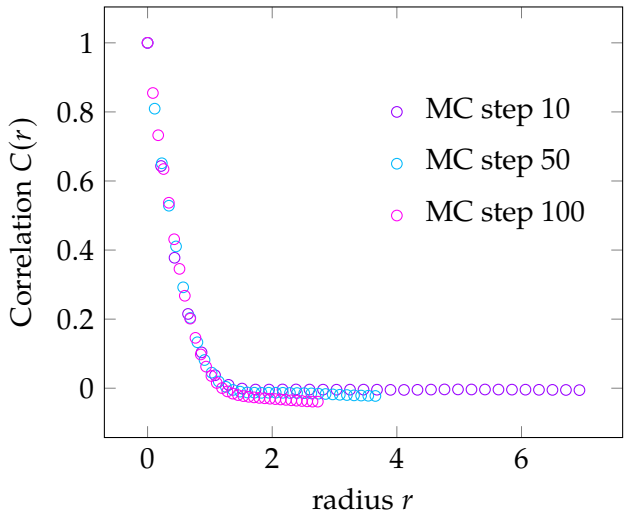


Figure 4.3: Scaling of the correlation functions of $q = 4$ Potts 64×64 lattice with domain length $l(t)$.

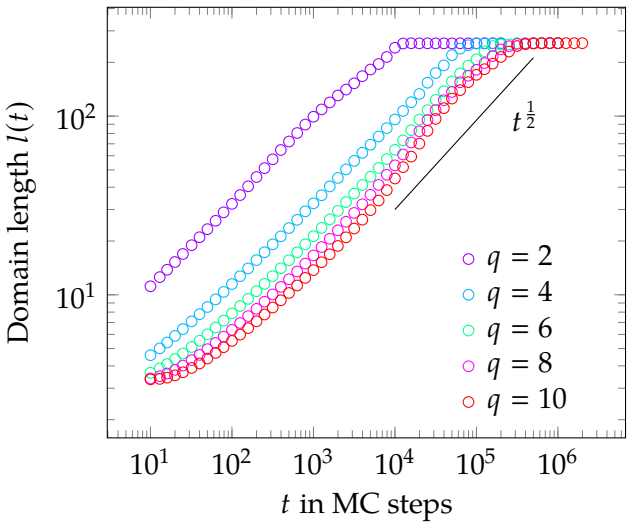


Figure 4.4: Domain length evolution in 256×256 Potts lattices with $q = 2, 4, 6, 8, 10$, all at quench temperature $T = 0.5T_C$. Data is averaged over 100 initial configurations, whereby evolutions without one-phase final equilibrium were filtered out.

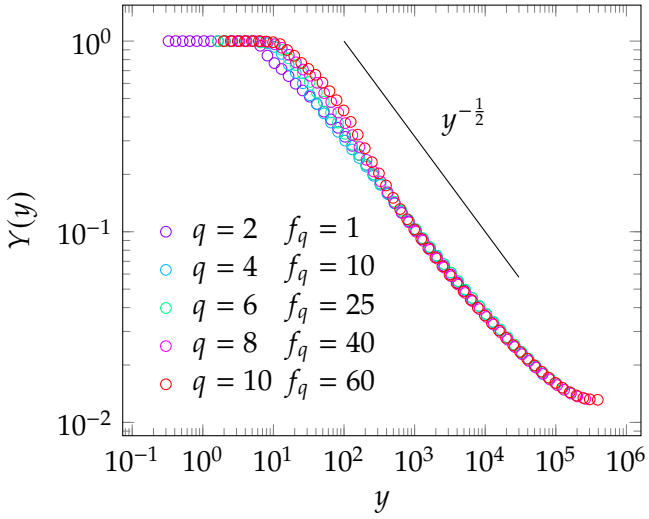


Figure 4.5: Scaling functions in 256×256 Potts lattices with $q = 2, 4, 6, 8, 10$, all at quench temperature $T = 0.5T_C$ (Scaling of the data sets of figure 4.4).

4.2 Different q values

Next, the focus lies on the domain growth in lattices with different q values. In figure 4.4 one can see the evolution of domain sizes in a 256×256 lattice for $q = 2, 4, 6, 8, 10$ settings. Already at MC step 10, very different average domain sizes can be detected, whereby the size expands with the inverse of the q value. Nevertheless, a growth exponent of $\frac{1}{2}$ accurately describes the evolution at some times in all instances. For the $q = 10$ lattice, a rather early onset of finite size effects could be an explanation for the unexpected behavior, but this seems physically not very intuitive. The diffusion reaction equation 1.2 might not be suited to deal with large q values, but this question is beyond the scope of this thesis.

The plots apparently exhibits power law growth for all q values at least in some periods, but with different growth amplitudes. One can take care of this fact in the finite size scaling analysis by implementation of a metric factor f_q into the scaling variable:

$$y_q = f_q \frac{l_{\max}^{\frac{1}{\alpha}}}{t} \tag{4.1}$$

With such a modification, one can empirically determine the metric factors by an optimum collapse exercise, where α is fixed to $\frac{1}{2}$. The result is depicted in figure 4.5 along with the corresponding metric factors, which already give an idea about their dependence on q. The scaling confirms that the growth behavior, regardless of the value of q, in finite systems, can be described by a universal scaling function $Y(y)$.

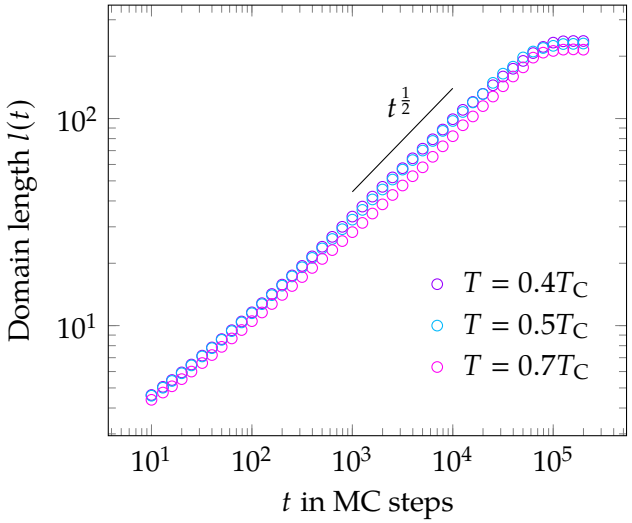


Figure 4.6: Domain length evolution for 256×256 Potts lattice with $q = 4$ at quench temperatures $T = 0.4T_C, 0.5T_C, 0.7T_C$. Data is averaged over 100 initial configurations, whereby multi-phase final states were not filtered out.

4.3 Different quench temperatures

Domain coarsening was also investigated for different quench temperatures. As it is apparent from the data in figure 4.6, where lattices of size 256×256 in $q = 4$ configuration were quenched to temperatures $T = 0.4T_C, 0.5T_C, 0.7T_C$, the growth behaviors again only differ by an amplitude, while the growth exponent is not affected at all. This could be explained by a higher diffusivity in equation 1.2 at higher temperatures.

4.4 Conclusion

The aim of this thesis was to find a universal scaling function for the domain coarsening process in Potts lattices with different q values. In order to compute the domain lengths, the direct method was discovered to be more appropriate than the method based on correlation functions. However, multi-phase final states turned out to be a recurring problem, affecting roughly 20 % of all initial configurations in $q = 4$ lattices and even more for larger q values. Such evolutions had to be sorted out, since they are considered to be unphysical and disturb the finite-size scaling analysis. It could be inferred that meta-stable final states reveal a fundamental problem of lattice-based simulations of natural objects.

Taking care of all these considerations, the domain coarsening process was found to be accurately described by a power law with exponent $\frac{1}{2}$ following from the Allen-

Kahn-equation. The scaling of correlation functions at different MC steps suggest, that the domain size is a characteristic length scale of the system according to the scaling hypothesis. Moreover, a finite size scaling analysis was able to provide a universal scaling function for different q values, suggesting that equal dynamics determine the coarsening process in all Potts models. Additionally, this seems to hold true for all temperatures below the critical point.

Since the finite-size scaling analysis demonstrated to be very well applicable for domain growth, it might be insightful to explore related systems, such as the clock model. There, the Hamiltonian is more similar to physical spin systems, which would also shed light on the question, whether meta-stable final states can be avoided in lattice simulations.

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