2D non-conserved Ising Model: Scaling Form of the Structure Factor and Numerical Evidence for the Dynamic Scaling Exponent

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Abstract: We present numerical evidence for the domain size scaling relation $L \propto t^{1/z}$ in the scaling regime of Spinodal Decomposition of quenched Model A systems (2D Ising model) using Model Monte Carlo simulations and time-dependent Ginzburg-Landau theory. We show that the scaling form of the structure factor leads to found scaling relations and determine the universal dynamic scaling exponent z. We find a value of $1/z = 0.416 \pm 0.032$ and $1/z = 0.327 \pm 0.004$ for the Monte Carlo and TDGL models respectively. We also study how $1/z$ behaves in a convergence study of increasing system system size. All codes are available on a public GitHub repository under: `https://github.com/MACIEK1JAREMA/Spinodal_Decomps`

I. INTRODUCTION

The Ising model describes a variety of systems whilst foregoing some of the underlying physics. Since its introduction to explain ferromagnetism [1], it has been applied in many areas of scientific research - from describing the structure of multi-metal alloys [2] to modelling how languages change over time [3]. Although a simple model it nonetheless exhibits interesting properties. This paper will focus on the spinodal decomposition of a 2D Ising model and examine the scaling dynamics universal to 2D systems through the dynamic scaling exponent z.

Spinodal decomposition occurs when a system above its critical temperature T_c is "quenched" to $T < T_c$. That is, the temperature instantly drops below T_c. The phase transition that would take place if T_c were approached slowly from $T > T_c$ does not take place instantaneously. Instead, under quenching, the system slowly relaxes into an equilibrium state, which is seen by formation and propagation of ordered domains. These domains possess a characteristic length scale, which is directly related to system's correlation length ξ, characterised by the dynamic critical exponent z by its relation to the time τ since quenching [4]:

$$\tau = \xi^z \tag{1}$$

It has previously been shown that $z = 2$ for infinite systems, which has been extensively tested numerically [5–8] and experimentally [9]. A simple argument can be made to find the theoretical value of z. The velocity of the domain walls v is proportional to their curvature by the Allen-Cahn equation [2, 10, 11] which is inversely proportional to average domain sizes L. If the system only exhibits a single length scale then $v = dL/dt$ and we can solve:

$$\frac{dL}{dt} = \frac{1}{L} \tag{2}$$

to give

$$L \propto t^{\frac{1}{2}} \tag{3}$$

which compares with equation 1 showing $z = 2$.

This relation can be confirmed by tracking average domain sizes over time using a structure factor $S(\boldsymbol{k}, t)$ (power spectrum of the system distribution, characterising fluctuation sizes [12]).

It has also been proposed that such behaviours stem from a universal scaling form of the system's structure factor [12].

We test both of these results in 2D Ising systems using Monte Carlo (MC) simulations and time dependant Ginzburg-Landau (TDGL) models.

II. THEORY

A. Time-Dependent Ginzburg-Landau Theory

Through coarse-graining methods, we can take averages over regions of a given spin system to acquire some space $\boldsymbol{x}$ and time t dependent scalar order parameter $\phi(\boldsymbol{x}, t)$ which describes the system's behaviour. For spin systems, ϕ can be interpreted as the mean magnetisation over a region. The free energy of the 2D system can be written as the functional over 2D space [2]:

$$F[\phi] = \int \left(\frac{1}{2} |\nabla \phi|^2 + V(\phi) \right) d\boldsymbol{x} \tag{4}$$

with some potential V.
Under time-evolution, the system minimises the free energy F [13]. This means we can equate the ϕ-derivative of equation 4 to the time derivative of ϕ, which yields the time-dependent Ginzburg-Landau equation:

$$\frac{\partial \phi}{\partial t} = \nabla^2 \phi - \frac{\partial V}{\partial \phi} \tag{5}$$

The typical Ginzburg-Landau form of potential is the symmetric $V = \frac{1}{2}\phi^2 + \frac{1}{4}\phi^4$ [13] corresponding to systems at $T = 0$, guaranteeing quenching by $T < T_c$. Substituting this into equation 5 yields the following non-linear differential equation that can be used to investigate spinodal decomposition:

$$\frac{\partial \phi}{\partial t} = \nabla^2 \phi + \phi(1 - \phi^2) \tag{6}$$

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B. Metropolis Monte Carlo

The Metropolis Monte Carlo algorithm [14] uses the assumption of detailed balance [15] to construct a matrix of probabilities for single spin-flip transitions from configuration i to j as:

$$p_{ji} = \begin{cases} 1, & \Delta E_{ji} < 0 \\ e^{-\frac{\Delta E_{ji}}{T}}, & \Delta E_{ji} > 0 \end{cases} \tag{7}$$

where T is the system temperature, $k_B = 1$ and ΔE_{ji} is the difference in energy between configuration j and i. The flip transitions can then be implemented by randomly selecting a spin of the lattice, and flipping it at corresponding probability or leaving it unchanged. Completing as many of these attempts as spins present in the system is defined as 1 Monte Carlo Step (MCS).

C. Structure Factor and Dynamic Scaling

The structure factor characterises the size of fluctuations (domains) in the system as a power spectrum of spatial frequency k. It is found by the square-modulus of the Fourier transform [13] of the order parameter $\phi(\boldsymbol{x}, t)$ (in TDGL) or the spin configuration $s(\boldsymbol{x}, t)$ (in MC):

$$S_{\mathrm{TDGL}}(\boldsymbol{k}, t) = |\mathscr{F}(\phi(\boldsymbol{x}, t))|^2 \tag{8}$$

$$S_{\mathrm{MC}}(\boldsymbol{k}, t) = |\mathscr{F}(s(\boldsymbol{x}, t))|^2 \tag{9}$$

with spins at lattice sites from vector $\boldsymbol{x} = (i, j)$.

Time evolution of average domain size $L(t)$ can be quantified by $S(|\boldsymbol{k}|, t)$-weighted mean of $|\boldsymbol{k}|$, calculated through:

$$\langle |\boldsymbol{k}(t)| \rangle = \frac{2\pi}{L(t)} = \frac{\sum S(|\boldsymbol{k}|, t)|\boldsymbol{k}|^2 \mathrm{d}k}{\sum S(|\boldsymbol{k}|, t)|\boldsymbol{k}| \mathrm{d}k} \tag{10}$$

where $S(|\boldsymbol{k}|, t)$ comes from circular averaging $S(\boldsymbol{k}, t)$, done by finding its mean over an annulus of radius $|\boldsymbol{k}|$ and width $\mathrm{d}k$. This gives rise to the extra k factor in the numerator and denominator.

In the scaling regime, the system shows fractal behaviour, where small fluctuations at one time, when re-scaled, resemble large fluctuations of late time behaviour. This can be imposed by proposing that the Structure factor follows a particular scaling form [12]:

$$S(|\boldsymbol{k}|, t) = a(t) f(k t^{\alpha}) \tag{11}$$

By enforcing the condition that the structure factor is normalised for all values of t, the form of the function $a(t)$ can be derived by making the substitution $y = kt^{\alpha}$.

$$t^{-2\alpha}\, a(t) \int_0^{\infty} y f(y) dy = 1 \tag{12}$$

where the integral is definite and hence independent of t, thus the only way this can be true for all t is if $a(t) = t^{2\alpha}$. We can show that the system will follow a growth-law for the single characteristic length-scale of the system's ordered domains by using equations 10 and 11 with found $a(t)$:

$$\frac{2\pi}{L(t)} = \frac{\int_0^{\infty} t^{2\alpha} f(kt^{\alpha}) k^2 dk}{\int_0^{\infty} t^{2\alpha} f(kt^{\alpha}) k dk} \tag{13}$$

and using the same substitution as in equation 12, we can then find the relation for $L(t)$

$$\frac{2\pi}{L(t)} = t^{\alpha} \int_0^{\infty} f(y) y^2 dy \tag{14}$$

$$L(t) \propto t^{\alpha} \tag{15}$$

which compared to equation 1, gives the scaling exponent by noticing $\alpha = 1/z$ in the scaling regime when $\xi = L$.

III. NUMERICAL METHODS

A. Monte Carlo Method

The system was initialised into a random (high T) configuration of spins on a 2D lattice (`numpy` array of -1 and +1 entries) of size $N \times N$ using coupling $J = 1$. It was then simulated at temperature $T = 0.1T_c$ to achieve quenching and observe spinodal decomposition.

The evolution was done numerically by Metropolis Monte Carlo as described in section II B. Calculating ΔE was optimised by setting up `numpy.roll` matrices of neighbours with imposed periodic boundary conditions (PBCs). We ensured N to be even for a periodic rather than anti-periodic boundary condition and used predominantly powers of 2 for efficient fast Fourier Transforms. The flipping process was optimised [16] by comparing the exponential factor $r = e^{-\frac{\Delta E_{ji}}{T}}$ to a random number $z : 0 \leq z \leq 1$ and flipping when $r > z$. This works as $\Delta E < 0$ leads to $r > 1$ and thus always $r > z$, while at $\Delta E > 0$, the probability of flipping ($r > z$) is proportional to r as in equation 7. The code was written to be `numba` [17] compatible allowing us to run large system sizes in our limited time frame.

Structure factors were found from Fourier transforms as in equation 8. In the interest of time only a small number of time steps were saved from evolution and used for statistics. The system properties depend on the initial configuration, thus it was necessary to average the structure factor over many initial conditions (stated with each result, limited by computational power). Found Structure factors at each time step were also normalised to $t = 0$ via $S(|\boldsymbol{k}|, t)/S(|\boldsymbol{k}|, 0)$ to mitigate initial condition effects despite them not affecting the time dependence. We then calculated the weighted-k average from equation 10, and used it to find the corresponding length scale L for each saved time step. A final log-log plot of L against t provided the scaling exponent $1/z$. With this result we re-scaled the structure factor plots as described in section II C to show universality of the scaling form. Finally, we quantify the effects of finite sizes by checking for convergence of this value with varying N, finding errors on each value of $1/z$ from the spread over different initial conditions as this error far exceeds the error in the L vs t gradient.

B. TDGL Method

We follow the same set up as the above described Monte Carlo, but using a 2D `numpy` array of values continuously ranging from -1 (totally spin-down region) to +1 (totally spin-up region) to save configurations of the order parameter.

To simulate quenching, the initialised random state (high T) was evolved using equation 6 corresponding to $T < T_c$ by $T = 0$.

Numerical solving of TDGL was done by first discretizing the Laplacian term on a grid of sites i, j and spacing $\Delta x = 1$ giving:

$$\nabla^2\phi \approx \frac{\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1} - 4\phi_{i,j}}{(\Delta x)^2} \quad (16)$$

then evolved it with the extra potential using `SciPy`'s `odeint` module. The proceeding analysis followed the methods stated above for Monte Carlo section III A.

IV. RESULTS

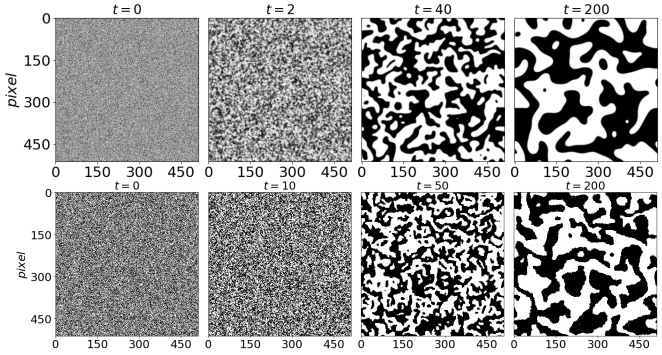

FIG. 1: Evolution of a random 512x512 system until t=200 showing spinodal decomposition. Top from TDGL, bottom from MC. Times are not comparable by nature as neither `odeint` t steps nor MCS relate to physical time, but results look qualitatively similar for chosen time steps. White denotes down spins up spins are black.

Figure 1 qualitatively shows dynamic scaling hypothesis during spinodal decomposition as final snapshots of each model look self-similar to smaller regions of the previous snapshot.

We then produce structure factors (shown on column 1 of figure 3) and calculate corresponding L for all saved time steps.

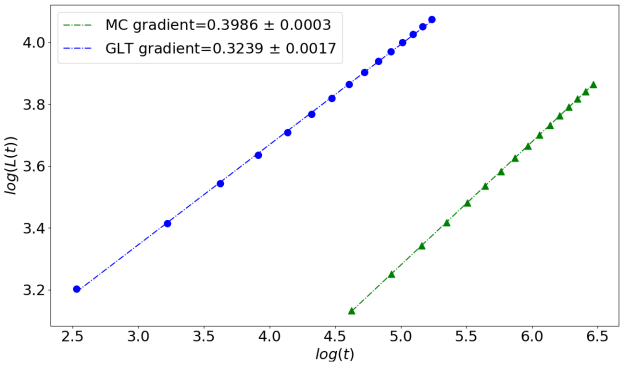

FIG. 2: Log-log plot of average domain size L against time step t indicating power-law behaviour. The gradient provides the power, $1/z$, for dynamic scaling exponent z. Dotted lines are found by linear regression using `scipy`. MC was averaged over 60 initial conditions while TDGL used 20 due to computational limitations. Both ran for $N = 1024$ and saved 16 time steps.

As expected, the logarithmic plot of L against t on figure 2 is a straight-line, showing a power law behaviour as per equation 3. The horizontal shift comes from the discrepancy in the definition of "time" between the two models, and is also expected to account for vertical deviations, which otherwise would match (as seen in figure1) to indicate similar average domain sizes. These indicate the following results:

$$\frac{1}{z_{\mathrm{MC}}} = 0.3986 \pm 0.0003 \quad (17)$$

$$\frac{1}{z_{\mathrm{TDGL}}} = 0.3239 \pm 0.0017 \quad (18)$$

where quoted errors come only from spread in the data on $log(L)$ vs $log(t)$. Larger errors enter when considering the spread of data-points over results from different initial conditions, which we report below.

Theoretically for non-conserved order parameters we expect a value of $z = 2$ giving $1/z = 0.5$ [18], although it is commonly acknowledged that numerically found values are $1/z \approx 0.45$ due to finite size effects [2, 19].

We then show universality of the structure factor in figure 3 following equation 11 with found $a(t)$.

Finally, figure 4 shows a study of finite size effects, resulting in growth of $1/z$ with increasing N. Although it is not possible to conclude convergence to $1/z = 0.5$ by extrapolation, primarily due to limited number of points from computational cost of the calculations, finite size effects can be seen to play a significant role in affecting our results.

The errors are now much larger as they include effects of initial conditions.

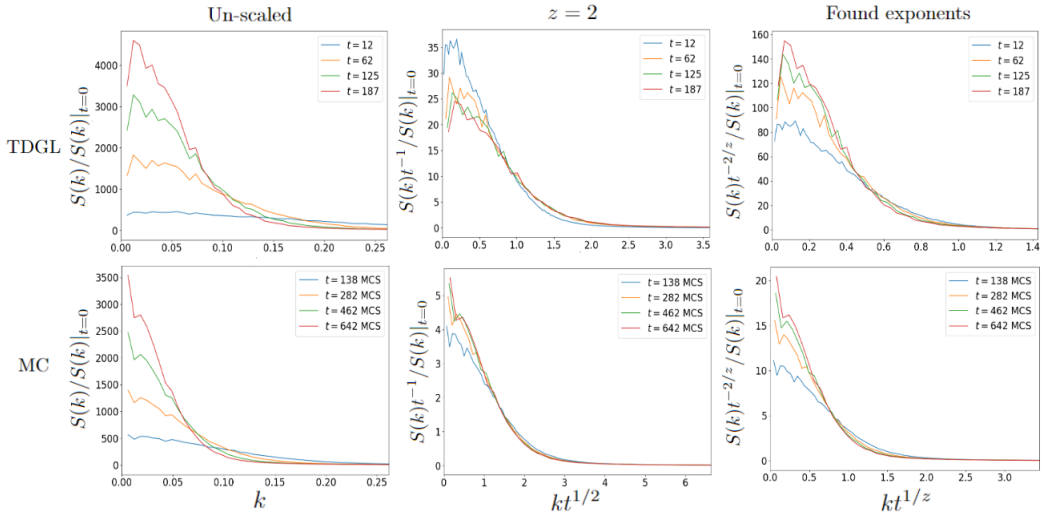

FIG. 3: Structure factors from both TDGL (top) and MC (bottom) as originally calculated (column 1), re-scaled using equations derived in section II C for known $z = 2$ (column 2) and our results quoted in equation 17 (column 3). Same parameters as those for figure 2.

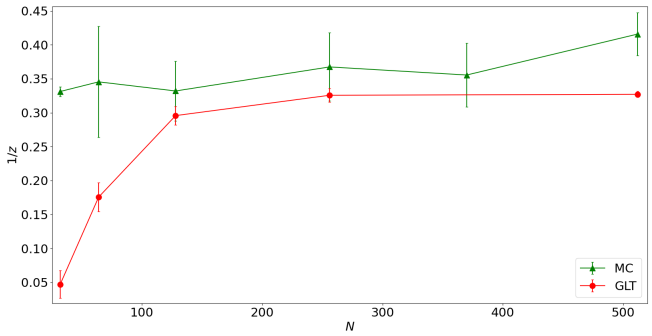

FIG. 4: Changes of the end result with system size to investigate finite size effects. Errors are found by the standard error on the mean over different initial conditions as these were orders of magnitude larger than errors from the gradient on $\log(L)$ vs $\log(t)$. Same parameters as before stated.

From these, we conclude our final results of:

$$\frac{1}{z_{\mathrm{MC}}} = 0.416 \pm 0.032 \tag{19}$$

$$\frac{1}{z_{\mathrm{TDGL}}} = 0.327 \pm 0.004 \tag{20}$$

V. DISCUSSION

We produce high quality simulations of 2D Ising systems using both models which show qualitatively correct behaviour. Quantitative checks were carried out by tracking excess energy of the system stored in domain walls and showing its expected scaling as $\Delta E \propto \frac{1}{L} \propto t^{-1/2}$ (available on our GitHub)[20]. Their structure factors show expected increase in frequency of low k (large L) over time as system equilibriates.

Extracting L at different time steps was carried out nominally. However, the corresponding errors were vastly underestimated by only using spread in the line after averaging over different initial conditions. Instead, we should have used the spread of extracted $1/z$ for each repeat, as was done for figure 4. Once these were included, from figure 4 we can see the far better agreement with the expected $1/z = 0.45$ [2, 19] of stated final results in equation 19, with more reasonably sized errors. Importantly, our values grow with system size, showing that found discrepancies are effects of finite size systems. For optimum results, we may require larger system sizes being simulated with more repeats. Optimally, matching previous works [19] using $N = 1024$ we need 160 repetitions, and more for smaller systems. The universality of the structure factors is a stricter constraint and hence is expected to be more difficult to achieve. It is also hard to quantify, but our curves qualitatively show reasonable collapse, especially using the limiting exponent of $1/z = 0.5$ (column 2 of figure 3).

Monte Carlo methods show better agreement with results in literature, due to similarity in methods. The value of TDGL is too low, but agrees with ones numerically found by other collaborations [21] (from its theoretical simplifications). The errors are also more reasonable as compared to TDGL results due to its deterministic evolution as compared to random MC. The two methods also differ by TDGL quenching to $T = 0$ by its potential and MC using $T = 0.1T_c$.

VI. CONCLUSION

We observe spinodal decomposition in 2D spin systems and find a value for the dynamic scaling exponent z close to and approaching the theoretical value with increasing system size. Some literature reports values closer to $1/z = 0.5$ [22, 23], although many obtain values similar to our own [21], despite variations in methods.

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