



Licentiate Thesis

# Examining Hausdorff dimension and Scaling behaviour in Worm algorithm

Simon Rydell

Theoretical Particle Physics, Department of Theoretical Physics,  
School of Engineering Sciences  
Royal Institute of Technology, SE-106 91 Stockholm, Sweden

Stockholm, Sweden 2018

Typeset in L<sup>A</sup>T<sub>E</sub>X

Akademisk avhandling för avläggande av teknologie licentiatexamen (TeknL) inom ämnesområdet teoretisk fysik.

Scientific thesis for the degree of Licentiate of Engineering (Lic Eng) in the subject area of Theoretical physics.

TRITA-FYS-2010:05

ISSN

ISRN KTH/FYS/--10:05--SE

© Simon Rydell, May 2018

Printed in Sweden by Universitetsservice US AB, Stockholm May 2018

## Abstract

2.3 The Metropolis Monte Carlo method The principle of importance sampling in statistical physics as suggested by Metropolis et al. [83] is as follows. In Fig. 2.1 we generated numbers  $x$  and from a uniform distribution. In the evaluation of something like (2.1), we could instead imagine generating the configurations  $\mu \equiv \{\theta_i\}_{i=1}^N$  not uniformly, but in such a way that the number of hits and misses are roughly equal. The estimated expectation value after  $M$  generated configurations  $\mu_n$  can be written

$$\langle O \rangle = \frac{\sum_{n=1}^M O_{\mu_n} e^{\beta H \mu_n}}{\sum_{n=1}^M e^{\beta H \mu_n}} \quad (1)$$

for states  $\mu_n$  generated with uniform probability. If we instead were to draw configurations with probabilities according to their Boltzmann weights, the estimator is simply an unweighted arithmetic average

$$\langle O \rangle \approx \sum_{n=1}^M O_{\mu_n} \quad (2)$$

for states  $\mu_n$  generated with probability  $e^{-\beta \mu_n}$

The remaining question is then how one generates configurations with probability according to their Boltzmann weights. In practice, the importance sampling discussed above is obtained with a Markov chain through the Metropolis method [83]. Metropolis Monte Carlo works by proposing a new configuration  $j$  from an old configuration  $i$  with a proposal distribution  $g(i \rightarrow j)$ , which is accepted with a specified probability  $A(i \rightarrow j) = \min(1, e^{-\beta \Delta E})$  where  $\Delta E = E_j - E_i$ . Consider the time evolution of the probability of being in state  $i$ ,

$$\frac{dp_i}{dt} = \sum_j [p_j P(j \rightarrow i) - p_i P(i \rightarrow j)] \quad (3)$$

where  $P(i \rightarrow j)$  is the probability of transitioning from  $i$  to  $j$ . The first and second terms on the right-hand side correspond to the rate of transitioning into and out of the state  $i$  respectively. In equilibrium the time derivative is zero and (2.5) is fulfilled if (but not only if)

$$p_j P(j \rightarrow i) = p_i P(i \rightarrow j) \quad (4)$$

The condition of (2.6) is called detailed balance and is a sufficient but not necessary condition for Metropolis Monte Carlo given that states are generated ergodically, see [84, 88]. Ergodicity means that each state is reachable from every other state in a finite time, however a non-ergodic calculation may still yield useful information within an ergodic class [84]. In a simulation, the probability of transitioning from  $i$  to  $j$  is the product of the proposal and acceptance probabilities, that

is  $P(i \rightarrow j) = g(i \rightarrow j)A(i \rightarrow j)$  which after insertion into the balance equation (2.6) gives

$$\frac{p_i}{p_j} \frac{g(j \rightarrow i) \min(1, e^{-\beta(E_i - E_j)})}{g(i \rightarrow j) \min(1, e^{-\beta(E_j - E_i)})} = \frac{e^{-\beta E_i}}{e^{-\beta E_j}} \quad (5)$$

assuming that the proposal distribution is symmetric. The Metropolis Monte Carlo method thus generates a chain of configurations where each configuration appears with a probability proportional to its Boltzmann weight. The estimation of thermal averages can thus be done via arithmetic averaging of the form (2.4) by starting with some initial configuration  $\mu_0$  and generating a chain  $\mu_1, \dots, \mu_M$  via the Metropolis scheme.

### 2.5 Phase transitions: definition and classification

The thermodynamical bulk free-energy density  $f = \beta^{-1} \ln(Z)/V$  depends on the coupling parameters of the Hamiltonian, and thermodynamic functions are calculated via differentiation of the free energy. Such thermo-dynamic functions may exhibit discontinuities at certain sets of coupling parameters, for which the free energy is not analytic. Such sets can be taken as definitions of phase boundaries which separate phases (i.e. regions of analyticity). The crossing of a phase boundary is then understood as a phase transition. It should be noted that the definition in terms of analytic free-energy is not completely general, considering the BKT-transition. For further details of mathematical aspects of phase transitions, we refer to [94] and for a more physical discussion to [95].

By the Ehrenfest classification [96] phase transitions are classified by the order of the derivative of the free energy which has a discontinuity at the critical point. If a first order derivative (e.g. entropy, internal energy) is discontinuous, then the phase transition is of first order. If a second order derivative (e.g. heat capacity) is discontinuous, the phase transition is of second order, and so on.

The Ehrenfest classification is however discouraged [95, 98], for example there may be divergences rather than discontinuities in thermodynamic functions (as for the 2D Ising model without external field, where the heat capacity diverges logarithmically at  $T_c$ ). The modern classification of phase transitions is binary where a phase transition is either ‘first-order’ (there is a latent heat for a temperature-driven transition) or ‘continuous’ (no latent heat) [98, 95].

5. Partition function A problem of statistical mechanics is to calculate the partition function, that is calculating the trace of  $e^{-\beta H}$ , a task most straightforwardly written as

$$Z = \sum \langle \alpha_n | e^{-\beta H} | \alpha_n \rangle \quad (6)$$

$$= \sum e^{-\beta E_i} \quad (7)$$

where the  $|\alpha_n\rangle$  is a complete orthonormal set and  $E_i$  the energy eigenvalues of  $H$ . In this form, it is necessary to determine the eigenvalues  $E_i$  of the Hamiltonian operator, and then carry out the sum over all corresponding weights  $e^{-\beta E_i}$ , as

Feynman put it [132] a ‘hopelessly difficult’ calculation. Instead we reformulate the problem in terms of imaginary time path integrals [132, 69, 133].

Imaginary-time path integral reformulation of the partition function First, we outline the reformulation of (5.5) in terms of path integrals, with the Bose-Hubbard model (5.2) in mind. Following the derivation in [69], first denote the statistical operator It then follows that

$$\rho(\beta) = e^{-\beta H} \quad (8)$$

$$\partial \rho = -H \rho \quad (9)$$

## 0.1 Derivation for Ising 2D Worm

The Ising model energy

$$E = -J \sum_{\langle ij \rangle} S_i S_j \quad (10)$$

Let  $K = \beta J$  where  $\beta = 1/k_B T$ .

$$\beta E = -K \sum_{\langle ij \rangle} S_i S_j \quad (11)$$

The partition function  $Z$ .

$$Z = \sum_{\text{all states}} e^{-\beta E} = \sum_{\text{all states}} e^{K \sum_{\langle ij \rangle} S_i S_j} = \sum_{\text{all states}} \prod_{\langle ij \rangle} e^{K S_i S_j} \quad (12)$$

Since  $S_i S_j = \pm 1$  in the Ising model, Euler identities can be used to expand the exponential in (12).

$$\begin{aligned} e^{K S_i S_j} &= \frac{e^K + e^{-K}}{2} + S_i S_j \frac{e^K - e^{-K}}{2} \\ &= \cosh(K) + S_i S_j \sinh(K) \\ &= \{T = \tanh(K)\} \\ &= (1 + T S_i S_j) \cosh(K) \end{aligned}$$

For  $N$  spins there are  $2N$  bonds, therefore the partition function is

$$\begin{aligned}
Z &= \sum_{\text{all states}} \Pi_{\langle ij \rangle} (1 + T S_i S_j) \cosh(K) \\
&= \cosh^{2N}(K) \cdot 2^N \left( 2^{-N} \sum_{\text{all states}} \Pi_{\langle ij \rangle} (1 + T S_i S_j) \right) \\
&= \cosh^{2N}(K) \cdot 2^N Z'
\end{aligned}$$

And

$$\begin{aligned}
Z' &= 2^{-N} \sum_{\text{all states}} \Pi_{\langle ij \rangle} (1 + T S_i S_j) \\
&= 2^{-N} \sum_{S_1=\pm 1} \sum_{S_2=\pm 1} \dots \sum_{S_N=\pm 1} \left( 1 + T \sum_{l=1} S_l S_{l+1} + T^2 \sum_{l=2} (S_l S_l)(S_{l-1} S_{l+1}) + \dots \right)
\end{aligned}$$

Where the sums  $\sum_{l=L}$  should be interpreted as the sum over all sets where the link length is  $L$ . Link length is the coupling between  $S$ -terms as

$$\begin{aligned}
(S_1 S_2) &- \text{Open with length 1} \\
(S_1 S_2)(S_2 S_3) &- \text{Open with length 2} \\
(S_1 S_2)(S_2 S_3)(S_3 S_4)(S_4 S_1) &- \text{Closed with length 4}
\end{aligned}$$

Since  $\sum_{S_i=\pm 1} S_i = 0$ , only terms with an even number of  $S_i$  are contributing to  $Z'$ . We will call these terms closed, indicating that they represent a closed loop if we were to draw the link lengths between the sites. The sum over all contributing terms gives a factor of  $2^N$ , canceling the  $2^{-N}$ .

We can now rewrite  $Z'$  in terms of loop lengths.

$$Z' = \sum_L g(L) T^L \quad (13)$$

Where  $g(L)$  is the number of loops with length  $L$ . Finally we can write the expression for the partition function.

$$Z = 2^N \cosh^{2N}(K) \sum_L g(L) T^L \quad (14)$$

### 0.1.1 Energy calculation

$$E = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{J}{Z} \frac{\partial Z}{\partial K} \quad (15)$$

Therefore

$$\begin{aligned}
\frac{\partial Z}{\partial K} &= 2^N 2N \cosh^{2N-1}(K) \cdot \frac{\partial \cosh(K)}{\partial K} Z' + 2^N \cosh^{2N}(K) \cdot \frac{\partial Z'}{\partial K} \\
&= 2^N \cosh^{2N}(K) \left( 2N \tanh(K) Z' + \frac{\partial Z'}{\partial K} \right) \\
&= 2^N \cosh^{2N}(K) \tanh(K) \left( 2N Z' + \frac{1}{\tanh(K)} \frac{\partial Z'}{\partial K} \right)
\end{aligned}$$

Examine  $\tanh^{-1}(K) \frac{\partial Z'}{\partial K}$ .

$$\begin{aligned}
\tanh^{-1}(K) \frac{\partial Z'}{\partial K} &= \tanh^{-1}(K) \frac{\tanh(K)}{\partial K} \sum_L g(L) L \tanh^{L-1}(K) \\
&= \frac{1}{\tanh^2(K) \cosh^2(K)} \sum_L g(L) L \tanh^L(K) \\
&= \frac{Z'}{\sinh^2(K)} \frac{\sum_L g(L) L \tanh^L(K)}{\sum_L g(L) \tanh^L(K)} \\
&= \frac{Z'}{\sinh^2(K)} \langle L \rangle
\end{aligned}$$

And finally

$$E = -J \tanh(K) \left( 2N + \frac{\langle L \rangle}{\sinh^2(K)} \right) \quad (16)$$

where

$$\langle L \rangle = \frac{\sum_L g(L) L \tanh^L(K)}{\sum_L g(L) \tanh^L(K)} \quad (17)$$

### 0.1.2 Heat capacity

$$C = \frac{\partial E}{\partial T} = -\beta^2 \frac{\partial E}{\partial \beta} = -K \beta \frac{\partial E}{\partial K} \quad (18)$$

Let  $A = 2N + \frac{1}{\sinh^2(K)} \langle L \rangle$ . Then

$$\frac{E}{J} = -\tanh(K) A \quad (19)$$

and

$$\frac{1}{J} \frac{\partial E}{\partial K} = -\frac{\partial \tanh(K)}{\partial K} A - \tanh(K) \frac{\partial A}{\partial K} \quad (20)$$

where

$$\begin{aligned}
\frac{\partial A}{\partial K} &= \langle L \rangle \frac{\partial \sinh^{-2}}{\partial K} + \tanh^{-1}(K) \sinh^{-2}(K) (\langle L^2 \rangle - \langle L \rangle^2) \frac{\partial \tanh(K)}{\partial K} \\
&= \frac{1}{\sinh^2(K) \tanh(K)} \left( -2\langle L \rangle + \frac{\langle L^2 \rangle - \langle L \rangle^2}{\cosh^2(K)} \right)
\end{aligned}$$

and finally

$$C = \frac{K^2}{\sinh^2(K)} \left( \frac{\langle L^2 \rangle - \langle L \rangle^2}{\cosh^2(K)} - E \tanh(K) - 2\langle L \rangle \right) \quad (21)$$



# Preface



# Contents

Abstract . . . . .	iii
0.1 Derivation for Ising 2D Worm . . . . .	v
0.1.1 Energy calculation . . . . .	vi
0.1.2 Heat capacity . . . . .	vii
<b>Preface</b>	<b>ix</b>
<b>Contents</b>	<b>xi</b>
<b>I Introduction and background material</b>	<b>1</b>
<b>1 Introduction</b>	<b>3</b>
<b>2 Background</b>	<b>5</b>
<b>3 Method</b>	<b>7</b>
3.1 Worm Algorithm . . . . .	7
3.2 Graph Labeling . . . . .	7
3.2.1 Hoshen Kopelman . . . . .	7
3.3 Fractals . . . . .	8
3.4 Box dimension . . . . .	8
3.5 Graph Dividing Algorithm . . . . .	8
<b>4 Graph Division and Hausdorff Dimension</b>	<b>11</b>
<b>5 Connection between Hausdorff Dimension and Scaling Behaviour</b>	<b>13</b>
5.1 Error Estimation . . . . .	13
5.1.1 Bootstrap . . . . .	13
<b>6 Results</b>	<b>15</b>
<b>7 Summary and conclusions</b>	<b>17</b>
7.1 Pseudo Code for Box Division Algorithm . . . . .	17

<b>8 Appendix</b>	<b>19</b>
<b>Bibliography</b>	<b>19</b>

## Part I

# Introduction and background material



# Chapter 1

## Introduction





## Chapter 2

# Background



# Chapter 3

## Method

### 3.1 Worm Algorithm

### 3.2 Graph Labeling

#### 3.2.1 Hoshen Kopelman

To find the clusters a modified version of the Hoshen Kopelman algorithm was used. A raster scan is used to label disjoint sets into groups with some canonical label[12]. It is a variant on the union-find algorithm and is most easily described through the associated functions. Intuitively, applying the find function on a site  $i$  returns the canonical, often implemented as the smallest, label in the cluster that  $i$  belongs to. Union uses find to ensure that two sites  $i$  and  $j$  are connected by setting the canonical label of  $i$  to that of  $j$  (or vice versa).

An example implementation would be to have a 2D graph without periodic boundary conditions of zeros and ones, where a site is occupied if it has a one associated with it, and unoccupied otherwise. A disjoint set here is a number of occupied sites neighbouring each other with unoccupied sites surrounding them. For simplicity one can start in the lower left corner, moving right and up, while search for neighbours left and down, ensuring that if a neighbouring site is occupied, it has been labeled before.

Start by setting each site to a unique label, putting all sites in individual clusters. Go through the lattice until an occupied site  $i$  is found. Search the neighbours below and to the left. If none of these neighbours are occupied, label  $i$  have a unique label and move to the next site. If  $i$  has one occupied neighbour it must have been labeled before, so  $i$  inherits the neighbours label. Finally if both neighbours are occupied, site  $i$  must be connecting a cluster and a union is performed on the neighbours to join their labels. A final pass through the lattice using the find function ensures that all sites have their canonical label.

In this paper an occupied site corresponds to a site with connections to the neighbouring sites (in the 2D example above, each site could have four such connections). In the original paper by Hoshen and Kopelman the labels for the sites who did not originally carry the canonical label, were set to a negative integer, symbolizing that they were aliases. A positive value was used at the canonical label, showing the number of sites in that cluster. This was not used in this project since the number of links in a cluster is not necessarily equal to the number of sites.

### 3.3 Fractals

Everyone agrees that the dimension of a point is zero, and that of a smooth line is one, but what about a set of points? A definition could be to say that the dimension is the minimum number of coordinates needed to describe every point in the set. Effectively, a point would describe itself, and a curve could be parametrized to the distance of some point on the same curve.

The situation is more complex when examining fractals. Take for example the Koch curve, it starts out as a line segment of length  $L_0$ , and successively adds a ‘bump’, making the total length  $L_1 = 4/3 \cdot L_0$ . Continuing this trend gives for the  $n$ th iteration a line length of  $L_n = (4/3)^n \cdot L_0$ , and so for the final fractal the length is infinite. Now any two point on the curve has a distance of infinity between them, so parametrization is impossible, but the area is still finite, so the dimension should be somewhere between one and two.

A useful concept here is the similarity dimension, defined by the scaling of each iteration. If  $m$  is the number of similar elements after an iteration and  $r$  is the scaling factor, the dimension is defined as  $m = r^d$ , or equivalently

$$d = \frac{\ln m}{\ln r} \quad (3.1)$$

So for the Koch curve, each segment is divided into fourths with each having one third the length from the previous iteration, giving it a dimension of  $\ln 4 / \ln 3 \approx 1.26$ .

### 3.4 Box dimension

### 3.5 Graph Dividing Algorithm

In order to calculate the box dimension the lattice needs to be divided into boxes of decreasing size. A step by step instruction of a graph dividing algorithm is provided below, and an implementation in pseudocode is available in the Appendix at Section 7.1.

For brevity some abbreviations are introduced.

$d =$ dimension	$l_i =$ side length of the current box
$l_0 =$ side length of the smallest box allowed	$e_j^i =$ vector of length $l_i/2$ in the $j$ 'th direction
$\text{perm}(v) =$ All permutations of $v$	$s_i =$ starting site of the current box

1. If  $l_i \geq l_0$ , go to 2, else stop.
2. Save all sites in the current box, starting for  $s_i$  going  $l_i$  in  $d$  directions.
3. Find all starting points for new boxes.

- (i) Form the matrix  $E^i = (e_0^i, e_1^i, \dots, e_d^i)^T$
- (ii) For all vectors  $v_k$  in  $\text{perm}(0, 0, \dots, 0)$ ,  $\text{perm}(1, 0, \dots, 0)$ ,  
 $\dots$ ,  $\text{perm}(1, 1, \dots, 1)$ , create the new start  $s_k^i$  as

$$s_k^i = v_k E^i$$

4. For each start  $s_k^i$ :
  - (i)  $s_i = s_k^i$ ,  $l_i = l_i/2$
  - (ii) Go to 1.



## Chapter 4

# Graph Division and Hausdorff Dimension





## Chapter 5

# Connection between Hausdorff Dimension and Scaling Behaviour

### 5.1 Error Estimation

In this thesis a number of error estimation techniques were used to know how much data was needed for each measurement. In this section the techniques will be described intuitively.

#### 5.1.1 Bootstrap

Bootstrap is a resampling method to examine a probability distribution. In this thesis it was used to estimate the error propagation of parameters in curve fitting.

Given a set  $\mathbf{x}$  of  $N$  measurements from an unknown distribution  $\hat{\phi}$ , some statistical calculation of interest can be done as  $\theta = s(\mathbf{x})$ . A resampling  $\mathbf{x}_0$  of  $\mathbf{x}$  comprised of  $N$  random measurements from  $\mathbf{x}$  (where one measurement can be included several times), can then be used to calculate  $\theta_0^* = s(\mathbf{x}_0)$ . Repeating this  $N_B$  times gives an estimate  $\theta^* = (\theta_0^*, \theta_1^*, \dots, \theta_{N_B}^*)$  of the distribution  $\hat{\theta}$ . Assuming  $N_B$  is large then, by the central limit theorem,  $\hat{\theta}$  is a normal distribution with some standard deviation  $\sigma_\theta$  that can be used as an error estimation for  $\theta$ .



## Chapter 6

# Results



## Chapter 7

# Summary and conclusions

### 7.1 Pseudo Code for Box Division Algorithm



## Chapter 8

## Appendix





# Bibliography

- [1] S. H. Strogatz, *Nonlinear Dynamics and Chaos With Applications to Physics, Chemistry, and Engineering*, 2 ed. (Westview Press Inc, Boulder, Colorado, 2014).
- [2] Y. Holovatch, *Order, Disorder and Criticality* (WORLD SCIENTIFIC, 2004).
- [3] J. Hove, S. Mo and A. Sudbø, *Hausdorff Dimension of Critical Fluctuations in Abelian Gauge Theories*, Physical Review Letters **85**, 2368 (2000).
- [4] D. Schleicher, *Hausdorff Dimension, Its Properties, and Its Surprises*, The American Mathematical Monthly **114**, 509 (2007).
- [5] N. Prokofev and B. Svistunov, *Comment on Hausdorff Dimension of Critical Fluctuations in Abelian Gauge Theories*”, Physical Review Letters **96** (2006).
- [6] O. Melchert, C. Norrenbrock and A. Hartmann, *Negative-weight Percolation: Review of Existing Literature and Scaling Behavior of the Path Weight in 2d*, Physics Procedia **57**, 58 (2014).
- [7] A. Raboutou *et al.*, *Fractal vortices in disordered superconductors*, Physica A: Statistical Mechanics and its Applications **207**, 271 (1994).
- [8] X. Dong *et al.*, *Phase transitions in 3D gravity and fractal dimension*, Journal of High Energy Physics **2018** (2018).
- [9] M. Wallin *et al.*, *Superconductor-insulator transition in two-dimensional dirty boson systems*, Physical Review B **49**, 12115 (1994).
- [10] N. Prokofev and B. Svistunov, *Worm Algorithms for Classical Statistical Models*, Physical Review Letters **87** (2001).
- [11] W. Janke and A. M. J. Schakel, *Fractal structure of spin clusters and domain walls in the two-dimensional Ising model*, Physical Review E **71** (2005).
- [12] J. Hoshen and R. Kopelman, *Percolation and cluster distribution. I. Cluster multiple labeling technique and critical concentration algorithm*, Physical Review B **14**, 3438 (1976).