

# KZM on Si(1, 0, 0) Surface

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## **Summary**

Abstract

English:

Abstract

Deutsch



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# 1 Introduction

## 1.1 Motivation

In the area of semiconductor technology, silicon has become the cornerstone material driving the innovations that power our modern world. Its versatility, reliability, and abundance have solidified its position as the basic building block of the semiconductor industry, making Silicon responsible for large parts of the recent human revolution. Its semiconducting properties facilitate the creation of wafers and integrated circuits, which are the centerpieces of computers, smartphones and virtually any recent electrical device.

The most important part of integrated circuits are transistors as they function as switches which make up binary numbers and logic gates that every processor uses to do math. The speed at which processors do math is majorly influenced by the number of transistors available and therefore the pursuit of further miniaturization is crucial in performance enhancement. Up to date transistors approach wire diameters of  $\approx 5$  nm (reference?) and therefore approach atomic scales as the diameter of a silicon atom and the lattice constant are around 0.2 nm or 0.55 nm respectively. At these scales surface effects play an ever increasing role in influencing the behavior and conductivity of the wires. Manufacturers actually really have difficulties controlling the current flow through the channels of the transistors, so a better understanding of the behavior of the surface is critical to ensure progress in classical computing.

A specific important silicon surface is the Si(001) surface of monocrystalline silicon which in transistors forms an interface with the oxide layer that is constructed around the silicon wires to isolate them from their environment. The Si(001) surface is also the surface wafers are cut along. The orientation of the cut is important since many of a crystal's structural and electronic properties are highly anisotropic. Each direction offers distinct paths for transport (Sources on Wikipedia for Wafers).

The Si(001) surface undergoes/ shows an order-disorder phase transition between two surface reconstructions. While static properties like possible reconstructions, their energies and electronic structures are thoroughly investigated, the dynamic properties are not yet well understood. A rich dynamic phenomenon to consider is the Kibble-Zurek mechanism which

describes the unavoidable non adiabatic evolution of systems as they cross a phase boundary during a quench. The quench time is directly related to the scaling of the number of domains with different order. The number of those domain boundaries again influences the electronic properties of the surface.

## 1.2 Thesis structure

This thesis aims to contribute to the understanding of the dynamic behavior of Si(001) during a quench. The already existing discrete Ising like description of the surface is therefore extended to an continuous XY-like model and adapted to the silicon surface. Well established molecular dynamics methods are used in combination with state of the art parallel programming and gpu acceleration techniques to overcome the many numerical obstacles that are inherent to the nature of phase transitions. The used langevin type stochastic differential equations are motivated from a quantum point of view. Renormalization group techniques are employed to set a theoretical baseline for the investigation of the phase transition.

chapter 2 firmly concludes the current viewpoint on and knowledge of the Si(001) surface and its order-disorder phase transition. chapter 3 explores the renormalization group description of phase transitions to create a theoretical understanding of the following. It introduces the concept of universality and the methods of finite size scaling which are used to investigate and interpret the simulation results. Chapter 4 explains the used numerics and motivates our description form a quantum point of view. Also the XY model used to describe the Si(001) surface is introduced and investigated. The results of various investigations like the quenches, but also static measurements are written in Chapter 5. In chapter 6 the main points of the thesis are summarized and an outlook for possible further investigations are given. The appendix contains calculations to various parts of the work as well as benchmarks for the simulation.

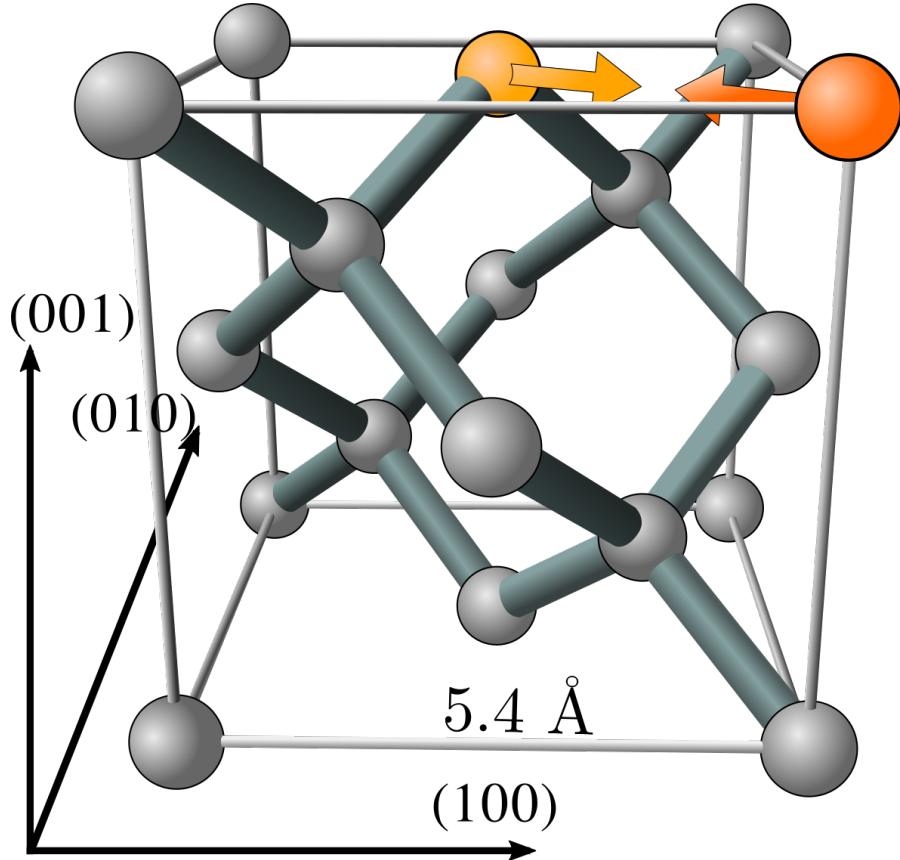
The simulation is written in **C++** using **CUDA** and **Thrust**. The evaluation and plotting is done in **python**. The whole source code can be obtained at [github.com](https://github.com).

The surface is semiconducting [18, 51, 17]

## 2 The Si(0,0,1) Surface

### 2.1 Surface Reconstruction

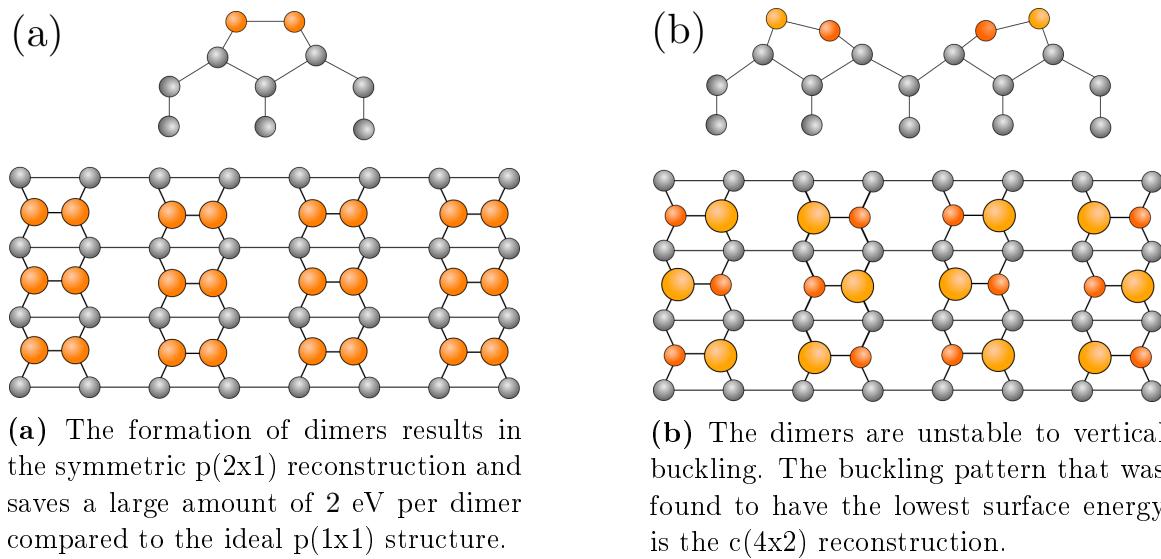
Below a temperature of  $T = 1687$  K silicon crystallizes in a diamond cubic crystal structure Figure 2.1 with a lattice constant of  $a = 5.431$  Å [50]. When cutting this crystal structure along the (001) plane, the resulting system exhibits a surface reconstruction. Surface atoms are left with two dangling bonds. One of those dangling bonds can be invested into forming a dimer with the neighboring Si atom in (110) direction [11], which leads to a large reduction of surface energy of 2 eV per dimer [45].



**Figure 2.1:** The crystalline structure of Si in its solid state is shown. The orange colored atoms form a dimer when cutting the diamond structure along the (001) plane. The arrows on the left are normal to their corresponding planes. (TODO cite origin from wikipedia, mark your alterations)

The resulting dimers can further reduce their energy by vertical buckling. The dimers tilt to

an angle of about  $\approx 18^\circ$ , which lowers the surface energy by another 0.2 eV per dimer. The buckling comes with a charge transfer of  $\approx 0.1e$  [7, 30] and the resulting coulomb interaction leads to an alternating buckling of the dimers like shown in Figure 2.2b. The surface reconstruction with the lowest energy was through theoretical [45] and experimental [7] methods found to be the c(4x2) reconstruction as it minimizes the electrostatic interaction energy as well as the surface stress. The alternative buckling in both directions suggests an antiferromagnetic interaction along and across the dimer rows, but the interaction across the row is actually ferromagnetic. However the diagonal interactions overpower the perpendicular interactions so that the interaction across dimer rows can be modeled to be antiferromagnetic in both directions.



**Figure 2.2:** The structure of the silicon surface after forming dimer (a) and after buckling (b) is shown.

## 2.2 Phase Transition of the Si(0,0,1) Surface

The Si(001) surface exhibits an order-disorder phase transition from the disordered p(2x1) (Figure 2.2a) phase to the ordered c(4x2) reconstruction at a critical temperature of about  $T_c \approx 200$  K [48]. This continuous phase transition will be of central importance in the following discussion. We say that the p(2x1) structure is disordered since the surface only appears during experiments to be in this phase due to thermal fluctuations and flipping of the dimers.

The Silicon surface is strongly anisotropic which leads to long streaks of order along ( $\parallel$ ) the dimer rows and short domains of order across ( $\perp$ ) the dimer rows. In [6] it was found that the ratio of correlation lengths is  $\frac{\xi_{\parallel}}{\xi_{\perp}} \approx 5.2$ . The lattice spacing along the dimer rows is  $a_{\parallel} = 3.84$  Å, while across it is  $a_{\perp} = 2a_{\parallel} = 7.68$  Å (see Figure 2.1).

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To understand the phase transition of the Si(001) surface we need to have a general understanding of phase transitions.



# 3 Phase Transitions

Under phase transitions in the most classical sense one understands the transition from an unordered state to an ordered state when changing an external parameter, mostly the temperature  $T$ , through a certain critical value, for example  $T_c$ . Phenomenologically one could say that the driving force behind the phase transition is the minimization of the free energy  $F = U - TS$ , with internal energy  $U$  and entropy  $S$ . Below the critical temperature, the internal energy  $U$  is minimized which usually comes with some kind of ordering that depends on the microscopic hamiltonian.

## Mathematical definition:

In the **thermodynamic limit** (system volume  $V \rightarrow \infty$  or number of sites  $N \rightarrow \infty$ ), we can give a mathematical definition of a phase transition. Consider our system to be dependent on a set of coupling constants  $[K]$ , which for example can be temperature  $T$ , pressure  $p$  or interaction strength  $J$ . We define the free energy per site as

$$f[K] = \lim_{N \rightarrow \infty} \frac{F[K]}{N} \quad (3.1)$$

If the thermodynamic limit  $\lim_{N \rightarrow \infty}$  exists, we can give a precise definition of a phase boundary. The  $d$  coupling constants  $[K]$  span the so called phase diagram. The free energy density  $f[K]$  is analytic almost everywhere in this  $d$ -dimensional phase space, except from the possibility of non-analyticities at certain points, lines, planes, etc. up to dimensionality  $d-1$ . The connected areas of analyticity are called **phases** and non-analyticities with dimension  $d-1$  are called **phase boundaries** or **critical manifolds**. Since  $f[K]$  has to be continuous everywhere, the phase boundaries come in two classes:

1. at least one of the first derivatives  $\frac{\partial f}{\partial K_i}$  is discontinuous across the phase transition. This case belongs to the **first-order phase transition**.
2. all derivatives  $\frac{\partial f}{\partial K_i}$  are continuous. This transition is called the **continuous phase transition**.

The free energy density gives reasonable, when the correlation length  $\xi$ , which is basically the spatial extent of fluctuations in the system, is much smaller than the system size  $L$ , so  $\xi \ll L$ . The phase transition of the silicon surface belongs to the continuous phase transitions.

Phase transitions exhibit rich phenomena like the divergence of the correlation length  $\xi$  at the critical point. The reason for the universality of this behavior across different systems will be outlined in the next section with the help of renormalization group theory.

### 3.1 Renormalization Group Considerations

The renormalization group (RG) theory is a general framework to study phase transitions and particle physics. It uses scale invariance arguments, meaning the self-similarity properties of systems at different length scales, to systematically investigate properties of the system. In the following basic considerations as well as important results shall be presented.

Imagine an infinite two dimensional lattice with Ising-like spins on each site. Just as Kadanoff [24] we consider a square of length  $l$  in lattice spacing units  $a = 1$  and map their combined  $l^2$  spins to a single value  $\pm l^2$ . Afterwards we renormalize their combined block spin to be either  $+1$  or  $-1$ . The new blocks of spins define a new Ising-like system, but on a different length scale with a new lattice spacing  $la$  like shown in . The proposal is now that there exists a new set of coupling parameters  $[K^l]$  so that the total free energy stays the same. In terms of the free energy density we can write

$$f[K] = l^{-2} f[K^l], \quad (3.2)$$

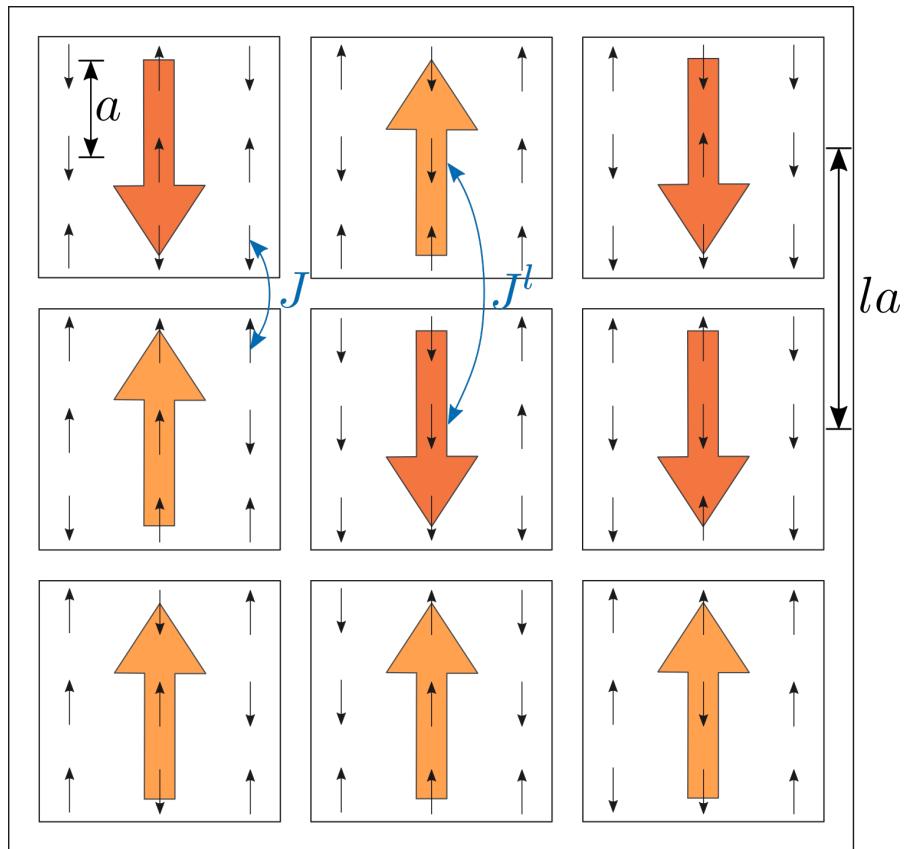
since the free energy density after the transformation has to be larger as we measure in a larger length scale. The same considerations can be made for the correlation length:

$$\xi[K] = l \xi[K^l]. \quad (3.3)$$

Suppose we know how the coupling constants change under an RG transformation  $R_l$ :

$$[K^l] = R_l[K]. \quad (3.4)$$

This is the starting point for us to comprehend why phase transitions exhibit singular behavior. The idea is that even though the partition function is a sum of exponentials which are analytic in  $[K]$ , the singularities can arise after an infinite number of RG iterations. As we begin to apply RG transformations, our system traces out a trajectory in coupling constant space ( $[K^{(1)}] \rightarrow [K^{(2)}] \rightarrow [K^{(3)}] \rightarrow \dots$ ). This trajectory could in principle, for example, go in circles, but in practice, we almost always find that the system is attracted to fixed points. The behavior of a system near a fixed point is the origin of scaling and lets us extract important information, like the shape of the phase diagram.



**Figure 3.1: PLACEHOLDER.** In Kadanoffs block spin picture, one combines a number  $l^2$  of spins to a new spin. The composite spin takes on the value of the majority of spins. The block spin is the standard example for a renormalization group transformation. Under the RG transformation, the relevant length scales change from  $a$  to  $la$ .

A fixed point of the RG map satisfies

$$[K^{(*)}] = R_l[K^{(*)}] . \quad (3.5)$$

At this point the correlation length transforms according to

$$\xi[K^{(*)}] = \xi[K^{(*)}]/l , \quad (3.6)$$

meaning that the correlation length either has to be 0 or  $\infty$ . The same is true for the free energy density. In proximity of a fixed point we may? write down the initial coupling constants as

$$K_i = K_i^{(*)} + \delta K_i \quad \text{and} \quad K_i^l = R_l(K_i^{(*)} + \delta K_i) = K_i^{(*)} + \delta K_i^l . \quad (3.7)$$

A RG Transformation of those coupling constants is dependent on all coupling constants  $K_i^l = K_i^l[K] = K_i^l(K_1^{(*)} + \delta K_1, K_2^{(*)} + \delta K_2, \dots)$ . We taylor expand  $K_i^l$  around the fixed point  $[K^{(*)}]$  to obtain the linearized RG Transformation:

$$K_i^l = K_i^{(*)} + \sum_j \frac{\partial K_i^l}{\partial K_j} \Big|_{K_j=K_j^{(*)}} \delta K_j + O((\delta K_j)^2) = K_i^{(*)} + \delta K_i^l + O((\delta K_j)^2) . \quad (3.8)$$

We write down the partial derivatives as a matrix

$$M_{ij}^l = \frac{\partial K_i^l}{\partial K_j} \Big|_{K_j=K_j^{(*)}} \quad (3.9)$$

and construct an eigenvalue problem:

$$M^l k^{(\sigma)} = \lambda_l^{(\sigma)} k^{(\sigma)} , \quad (3.10)$$

where  $\sigma$  labels the eigenvalues. Because two consecutive RG Transformations by  $l_1$  and  $l_2$  have to yield the same result as one with  $l_1 l_2$ , we know that

$$M^{l_1} M^{l_2} = M^{l_1 l_2} , \quad \text{implying that} \quad \lambda_{l_1}^{(\sigma)} \lambda_{l_2}^{(\sigma)} = \lambda_{l_1 l_2}^{(\sigma)} . \quad (3.11)$$

implying that

$$\lambda_{l_1}^{(\sigma)} \lambda_{l_2}^{(\sigma)} = \lambda_{l_1 l_2}^{(\sigma)} . \quad (3.12)$$

Setting  $l_2 = 1$  yields  $\lambda_{l_1}^{(\sigma)} \lambda_1^{(\sigma)} = \lambda_{l_1}^{(\sigma)}$  which lets conclude that  $\lambda_1^{(\sigma)} = 1$ . Differentiating Equa-

tion 3.12 with respect to  $l_2$  yields

$$\begin{aligned} \frac{d}{dl_2} \left( \lambda_{l_1}^{(\sigma)} \lambda_{l_2}^{(\sigma)} \right) &= \frac{d}{dl_2} \lambda_{l_1 l_2}^{(\sigma)} \\ \lambda_{l_1}^{(\sigma)} \left( \frac{d}{dl_2} \lambda_{l_2}^{(\sigma)} \right) + \left( \frac{d}{dl_2} \lambda_{l_1}^{(\sigma)} \right) \lambda_{l_2}^{(\sigma)} &= l \frac{d}{d(l_1 l_2)} \lambda_{l_1 l_2}^{(\sigma)} \\ \left( \frac{d}{dl_2} \lambda_{l_2}^{(\sigma)} \right) \lambda_{l_1}^{(\sigma)} &= l \frac{d}{d(l_1 l_2)} \lambda_{l_1 l_2}^{(\sigma)} . \end{aligned} \quad (3.13)$$

Setting now  $l_2 = 1$  gives the differential equation

$$\frac{d}{dl_2} \lambda_{l_2}^{(\sigma)} \Big|_{l_2=1} \lambda_{l_1}^{(\sigma)} \equiv y_\sigma \lambda_{l_1}^{(\sigma)} = l \frac{d}{dl_1} \lambda_{l_1}^{(\sigma)} \Rightarrow \frac{d}{dl_1} \lambda_{l_1}^{(\sigma)} = \frac{y_\sigma}{l} \lambda_{l_1}^{(\sigma)} . \quad (3.14)$$

A solution to Equation 3.14 is

$$\lambda_l^{(\sigma)} = l^{y_\sigma} \quad (3.15)$$

with  $y_\sigma$  as defined above, being independent of  $l$ . This is an important result on the way to show the origin of scaling. Since the  $k^{(\sigma)}$  are vectors in the coupling constant space, we deduce from Equation 3.10 that some differences in coupling constants  $\delta K$  grow or shrink when applying RG transformations, depending on the  $\lambda_l^\sigma$ . There are three cases:

1. **Relevant** directions and eigenvalues:  $|\lambda_l^{(\sigma)}| > 1$ , meaning that  $y_\sigma > 0$  and  $\delta K$  in direction of  $k^{(\sigma)}$  grow.
2. **Irrelevant** directions and eigenvalues:  $|\lambda_l^{(\sigma)}| < 1$ , meaning that  $y_\sigma < 0$  and  $\delta K$  in direction of  $k^{(\sigma)}$  shrink.
3. **Marginal** directions and eigenvalues:  $|\lambda_l^{(\sigma)}| = 1$ , meaning that  $y_\sigma = 0$  and  $\delta K$  in direction of  $k^{(\sigma)}$  do not change.

After many RG transformations, only the relevant eigenvalues will be important, as the influence of the others will negligible in comparison. If we differ from the fixed point in a relevant direction, the differences to the fixed point will become larger and the RG transformation flow will flow out of the fixed point. Deviations in irrelevant direction will flow into the fixed point again.

Consider a system with only one coupling constant, in this case the temperature, and choose  $T$  in the vicinity of a fixed point  $T^{(*)}$ . Apply a RG transformation to  $T$  so that  $T^l = R_l(T)$  and then consider the difference

$$T^l - T^{(*)} = R_l(T) - T^{(*)} . \quad (3.16)$$

Using Equation 3.8 we can rewrite

$$R_l(T) = T^{(*)} + \delta T^l = T^{(*)} + \frac{\partial T^l}{\partial T} \Big|_{T=T^{(*)}} \delta T = T^{(*)} + \lambda_l \delta T \quad (3.17)$$

since  $M^l$  has only one component and  $\delta T$  is therefore automatically in eigenvector direction. Equation 3.16 then becomes in terms of the reduced temperature  $\varepsilon = \frac{T-T^{(*)}}{T^{(*)}}$

$$\varepsilon^{(l)} = \lambda_l \varepsilon \stackrel{\text{Equation 3.15}}{=} \varepsilon l^{y_\varepsilon}. \quad (3.18)$$

After  $n$  RG iterations one obtains

$$\varepsilon^{(nl)} = (l^{y_\varepsilon})^n \varepsilon. \quad (3.19)$$

Now consider again how the correlation length transforms after  $n$  RG transformations:

$$\xi(\varepsilon) = l^n \xi(\varepsilon^{nl}) = l^n \xi(l^{ny_\varepsilon} \varepsilon) \quad (3.20)$$

Substituting  $\tau = l^{ny_\varepsilon} \varepsilon$  into Equation 3.20 yields

$$\xi(\varepsilon) = \tau^{1/y_\varepsilon} \varepsilon^{-1/y_\varepsilon} \xi(\tau) \quad (3.21)$$

This is the origin of scaling and universality!

## 3.2 Universality and static scaling

The last section traced the origin of universality and scaling in phase transitions. This section will deal with the term universality and its implications in more detail.

Scaling laws like Equation 3.21 can be derived for many different quantities of a system. In the context of phase transitions, **static scaling** means the power law dependence of a system quantity **in equilibrium**, like the correlation length  $\xi$ , on a coupling parameter, like the temperature  $T$ . The exponent of this power law is called the **critical exponent**. Important scaling laws include the scaling of (in the notation of [42])

- the specific heat  $C_H$ :  $T_c C_H \approx A^\pm |\varepsilon|^{-\alpha}$ ,
- the order parameter  $\Psi$  or  $M$ :  $|M| \approx B |\varepsilon|^{-\beta}$ ,
- the susceptibility  $\chi$ :  $\chi \approx C^\pm |\varepsilon|^{-\gamma}$ ,
- and the correlation length  $\xi$ :  $\xi \approx f^\pm |\varepsilon|^{-\nu}$ .

The prefactors of the power laws are called the **critical amplitudes** and  $\nu, \alpha, \dots$  are the mentioned critical exponents. The superscript  $\pm$  denotes whether the phase transition is approached from below ( $-$ ) or above ( $+$ ) the critical temperature  $T_c$ . The critical exponents are the same on both sides of the transition, but the amplitudes vary.

These scaling laws are only valid in the thermodynamic limit for  $\varepsilon \rightarrow 0$ , so infinitely close to the critical point. Otherwise they exhibit **corrections to scaling** that result out irrelevant and marginal eigenvalues of the RG transformations as well as **finite size** corrections.

Systems that share the same set of critical exponents belong to the same **universality class**. In the last section we motivated that this might be a result of symmetry considerations and indeed, it is found that which universality class a system belongs to usually only depends on

- the **symmetry group** of the system hamiltonian,
- the **dimensionality** of the problem,
- and whether the **interaction** between the components is **short-ranged**.

In contrast to the critical exponents, the critical amplitudes are not universal, but their ratios, for example  $f^+/f^-$ , are.

The concept of universality is very useful to investigate real systems at the critical point. As a result of scale invariance and self similarity, the microscopic dynamics of a system become irrelevant at  $\varepsilon = 0$  and its behavior can then be approximated by a simplified, hopefully exactly solvable model.

The extraction of critical exponents is notoriously difficult for various reasons, one being the inaccessibility of the thermodynamic limit  $\lim_{N \rightarrow \infty}$ , another **critical slowing down** (see section 3.4). The following section will explain the mentioned finite size corrections to static scaling and illustrate how one can make use of them to analyze critical exponents.

### 3.3 Finite size scaling and critical exponent extraction

Recall how the free energy density Equation 3.2 transforms and that it depends on the system size  $L = lL^{(l)}$ :

$$f([K], L^{-1}) = l^{-2} f\left([K^{(l)}], L^{(l)-1}\right) = l^{-2} f\left([K^{(l)}], lL^{-1}\right) . \quad (3.22)$$

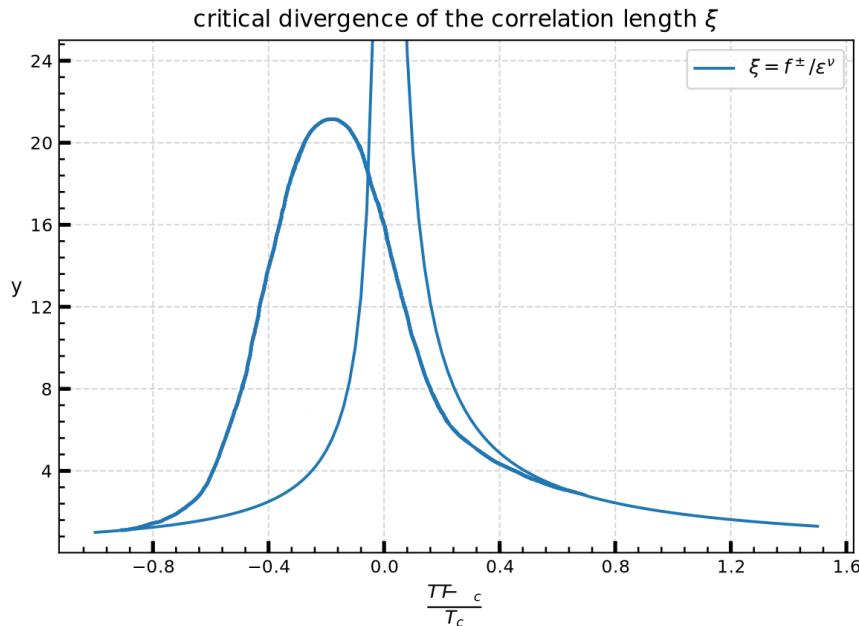
Let  $K_1 = \varepsilon$  be the reduced temperature. Close to the critical point we can use Equation 3.18 to write Equation 3.22 in terms of eigenvalues:

$$f(\varepsilon, K_2, \dots, L^{-1}) = l^{-2} f(\varepsilon l^{y_\varepsilon}, K_2 l^{y_2}, \dots, l L^{-1}) . \quad (3.23)$$

The system size behaves like a relevant eigenvalue with a value of

$$\lambda_L = 1 \quad \text{implying that} \quad y_L = 1 . \quad (3.24)$$

This means that the system size has to be tuned to criticality to let the phase transition occur, which is in accord with our interpretation that phase transitions only occur in the thermodynamic limit, i.e. if  $L^{-1} = 0$ . As a result real, finite systems deviate from the behavior that the scaling laws dictate. For example, the actual correlation length cannot outgrow the system size  $\xi \leq L$  and so the divergence of  $\xi$  is rounded at the phase transition. Additionally the peak is shifted to a lower critical temperature Figure 3.2, so the phase transition appears to happen at a different point.



**Figure 3.2:** PLACEHOLDER. In the thermodynamic limit, the correlation length  $\xi$  diverges at the critical point according to a power law. For finite systems, the singularity of  $\xi$  appears rounded and the peak position is shifted to a lower temperature.

TODO:

Consider again the correlation length and Equation 3.20:

$$\xi(\varepsilon, L^{-1}) = l \xi(\varepsilon l^{y_\varepsilon}, l L^{-1}) = \varepsilon^{-\nu} F_\xi(L^{-1} \varepsilon^{-\nu}) \quad (3.25)$$

with  $F_\xi$  as in Equation 3.21. Introducing a new scaling function  $F' = (L\varepsilon^\nu)^{-1}F_\xi$  yields

$$\xi(\varepsilon, L^{-1}) = \varepsilon^{-\nu}(L\varepsilon^\nu)F'(L\varepsilon^\nu) = LF'(L\varepsilon^\nu) . \quad (3.26)$$

In the limit  $L \rightarrow \infty$  and close to  $\varepsilon = 0$ ,  $\xi$  has to scale like  $\xi(\varepsilon, 0) \propto \varepsilon^{-\nu}$ . Taylor expansion around  $\varepsilon = 0$  somehow yields

$$\frac{L}{\xi(\varepsilon, L^{-1})} = A + B\varepsilon L^{1/\nu} + O(\varepsilon^2) \quad (3.27)$$

TODO end

This equation is an important result since it can be used to calculate two important quantities. Firstly, curves of  $L/\xi(\varepsilon, L^{-1})$  for different  $L$  intersect at the critical point  $\varepsilon = 0$ , so by determining this intersection one can extract the critical temperature  $T_c$ , which is usually not known a priori. Secondly by computing the gradient

$$\frac{\partial}{\partial \varepsilon} \left( \frac{L}{\xi(\varepsilon, L^{-1})} \right) = BL^{1/\nu} \quad (3.28)$$

for various  $L$ , one can determine the critical exponent  $\nu$ . This method is easier than, for example, trying to fit to the original scaling law Equation 3.21 because of the reasons mentioned at the end of section 3.2.

### 3.3.1 Binder Cumulant

A popular quantity to apply Equation 3.27 is the Binder cumulant  $U_L$ , introduced by K. Binder in [4]. It is defined as

$$U_L = \frac{\langle M_L^4 \rangle}{\langle M_L^2 \rangle^2} , \quad (3.29)$$

$M_L$  being the order parameter of a system of size  $L$ .  $\langle \cdot \rangle$  denotes the ensemble average, meaning the average over different realizations of the same system. Its finite size scaling is given in analogue to Equation 3.27 by

$$U_L = U_L^* + U\varepsilon L^{1/\nu} (1 + WL^{-\omega} + \dots) , \quad (3.30)$$

including the corrections resulting out of the largest irrelevant eigenvalue  $1/|y_1| = \omega$ . In practice, to extract the critical exponent  $\nu$ , one fits to

$$\ln \left( \frac{\partial U_L}{\partial \varepsilon} \right) \approx \ln (UL^{1/\nu}) = \ln(U) + \frac{1}{\nu} \ln(L) . \quad (3.31)$$

$U_L$  has a value of  $U_L = 1$  far below the phase transition, approaches  $U_L = 3$  above the phase transition and exhibits the intersection in between at  $U_L = U_L^*$ . It is generally easy to compute and extract out of the system.

### 3.3.2 The correlation length ratio $\frac{\xi}{L}$

TODO

## 3.4 Dynamic Scaling and the Kibble-Zurek mechanism

### 3.4.1 The relaxation time $\tau$ and the critical exponent $z$

With the Binder cumulant we saw a way to extract the static scaling exponent  $\nu$ . Aside static scaling, phase transitions show another phenomenon, called **dynamic scaling**. The topic of dynamic critical phenomena deals with how long the fluctuations in the system on the largest lengthscale take to equilibrate. This time is called the the **relaxation time** and it is found to scale like

$$\tau = \tau_\xi \xi(\varepsilon)^z , \quad (3.32)$$

with the new **dynamic critical exponent**  $z$ . (TODO RG explanation for this scaling?).

Plugging in the known scaling of  $\xi(\varepsilon)$  from section 3.2 yields

$$\tau = \tau_\xi \xi(\varepsilon)^z = \tau_\xi (f^\pm |\varepsilon|^{-\nu})^z := \tau_\varepsilon |\varepsilon|^{-\nu z} . \quad (3.33)$$

As the correlation length diverges, so does the relaxation time. This makes intuitively sense, since infinite correlation length implies that infinitely far apart components of the system had "time to talk", and for that to happen, it would take an infinite amount of time. This is what is meant with the in section 3.2 mentioned critical slowing down. As a system approaches  $\varepsilon \rightarrow 0$ , it takes longer and longer to equilibrate. It then becomes computationally a challenge to let large systems equilibrate. But since static scaling laws involve only quantities in equilibrium and are only valid in the thermodynamic limit for  $\varepsilon \rightarrow 0$ , large, critical systems have to be considered. This dilemma was partially solved by the finite size techniques of section 3.3.

### 3.4.2 Quenches and the freezeout of domains

The **Kibble-Zurek mechanism** (KZM) [53, 54] shall be a central point of the upcoming investigations and will be explained in the following.

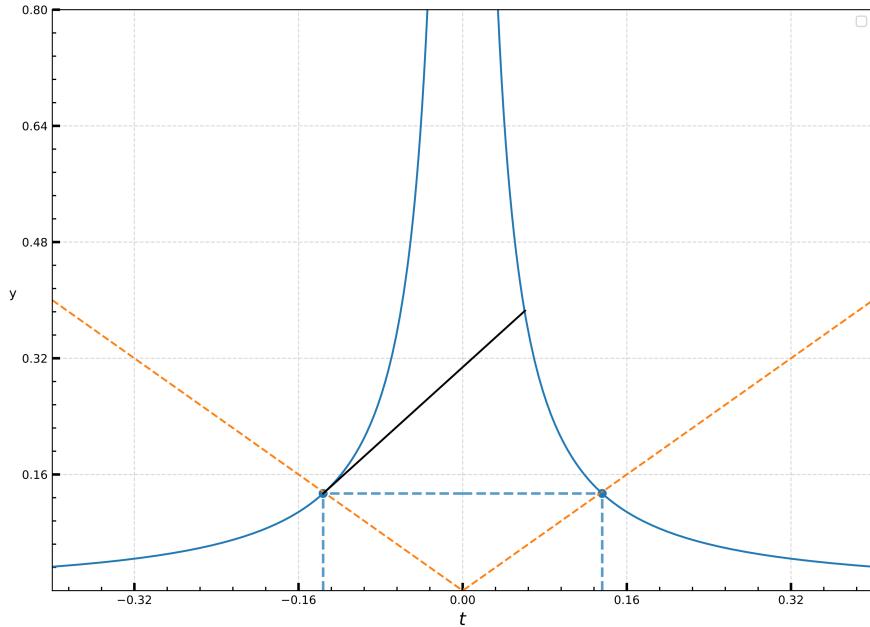
Consider a linear quench, meaning the cooling down of a system linear in time  $t(?)$ . We characterize the speed of cooling by the **quench timescale**  $\tau_Q$ :

$$\varepsilon(t) = \frac{t}{\tau_Q} . \quad (3.34)$$

For slow quenches sufficiently far away from the critical point, the system will evolve adiabatically, meaning that system quantities like  $\xi$  assume their equilibrium values. As we get closer to the phase transition, the change in  $\xi$  becomes faster and faster since it's time derivative  $\frac{\partial}{\partial t}\xi(\varepsilon(t))$  diverges. At the latest when  $\frac{\partial}{\partial t}\xi(\varepsilon(t))$  outgrows the speed of sound the system cannot keep up with the change in the equilibrium correlation length and therefore diverges from its equilibrium behavior Figure 3.3. The timepoint  $\hat{t}$  of divergence from the equilibrium behavior is called the **freezeout** since the current state of the system effectively becomes frozen in comparison with the equilibrium values. One Assumption of the KZM is that this freezeout roughly happens when the current relaxation time  $\tau$  equals the time that is left until the critical point is crossed:

$$\tau(\hat{t}) = \hat{t} . \quad (3.35)$$

Another is that the system quantities after the quench will have only reached approximately



**Figure 3.3:** PLACEHOLDER. The freezeout of the current state of the system happens roughly at  $\tau(\hat{t}) = \hat{t}$ . After that, the system continues to evolve in its maximum speed until the critical point is crossed and the actual values intersect with the equilibrium values.

their equilibrium value at  $\hat{t}$ . Combining

$$\hat{t} = \varepsilon(\hat{t})\tau_Q \quad \text{and} \quad \hat{t} = \tau(\hat{t}) = \tau(\varepsilon(\hat{t})) = \tau_\varepsilon |\varepsilon(\hat{t})|^{-\nu z} \quad (3.36)$$

yields the reduced temperature at  $\hat{t}$ :

$$|\varepsilon(\hat{t})| = \left( \frac{\tau_\varepsilon}{\tau_Q} \right)^{\frac{1}{1+\nu z}} . \quad (3.37)$$

For  $\xi$  this means:

$$\xi \approx \hat{\xi} := \xi(\varepsilon(\hat{t})) = \xi_0 / |\varepsilon(\hat{t})|^\nu = \xi_0 \left| \frac{\tau_Q}{\tau_\varepsilon} \right|^{\frac{\nu}{1+\nu z}}, \quad (3.38)$$

so the frozen value of the correlation length scales with the quench timescale like  $\hat{\xi} \propto \tau_Q^{\frac{\nu}{1+\nu z}}$ . The freezeout of the correlation length implies domains of order  $\propto \hat{\xi}^2$ . The domains of order are separated by **domain walls**, which represent a defect in the order of the surface. Such defects may have influences on different properties of the surface, including conductivity, an important value for the semi conductor industry. Knowledge of how the defect density on the surface behaves might help to prepare ideal silicon surfaces.

# 4 Simulating Dynamics

While most numerical studies of phase transitions rely on monte carlo techniques, this work, inspired by Laguna and Zurek [29], focuses on the use of **stochastic differential equations**. Their mathematical basics and a derivation of a Langevin equation for our case will be outlined in the following.

## 4.1 Stochastic differential equations and the Langevin equation

Put simply, stochastic differential equations are the stochastic generalizations of common differential equations like

$$y(t + dt) = y(t) + A(y(t), t)dt . \quad (4.1)$$

Equation 4.1 describes a **continuous, memoryless, deterministic** process. For every time-point  $t + dt$  one can predict the value  $y(t + dt)$  knowing the values  $y(t)$ ,  $dt$  and  $t$ . SDEs describe continuous, memoryless **stochastic** processes, also called continuous **markov processes**, meaning for every timepoint we can assign definite probabilities to all possible  $y(t+dt)$ . These properties impose relatively strict limitations on a generalization of Equation 4.1. It turns out, that the generalization must be of the form [15].

$$y(t + dt) = y(t) + A(y(t), t)dt + D^{1/2} (y(t), t) n(t)(dt)^{1/2} . \quad (4.2)$$

$n(t)$  is a sample value of a normal distribution around zero with standard deviation one  $\mathcal{N}(0, 1)$ . Equation 4.2 is called the standard form **Langevin equation** and it represents an update formula for the continuous markov process. To obtain the widely used **differential or white noise** form of the Langevin equation, we define the **Gaussian white noise process**  $\Gamma(t)$  by

$$\Gamma(t) := \lim_{dt \rightarrow 0} \mathcal{N}(0, 1/dt) \equiv \frac{n(t)}{(dt)^{1/2}}, \quad (4.3)$$

rearrange Equation 4.2

$$\frac{y(t+dt) - y(t)}{dt} = A(y(t), t) + D^{1/2}(y(t), t) \frac{n(t)}{(dt)^{1/2}} \quad (4.4)$$

and take the limit  $dt \rightarrow 0$ , leading to

$$\frac{d}{dt}y(t) = A(y(t), t) + D^{1/2}(y(t), t)\Gamma(t) . \quad (4.5)$$

$A(y(t), t)$  is called the **drift** and  $D(y(t), t)$  is called the **diffusion** function. Important properties of the white noise process  $\Gamma(t)$  are

$$\langle \Gamma(t) \rangle = 0 \quad \text{and} \quad \langle \Gamma(t)\Gamma(t+t') \rangle = \delta(t') . \quad (4.6)$$

### 4.1.1 Ornstein-Uhlenbeck process and Brownian motion

The Ornstein-Uhlenbeck process is central to the mathematical description of Brownian motion, which will be used to model the movement of the silicon dimers. The Ornstein-Uhlenbeck process is a continuous Markov process with drift and diffusion functions of the form

$$A(y(t), t) = -\frac{1}{\tau}y(t) \quad \text{and} \quad D(y(t), t) = c . \quad (4.7)$$

The constants  $\tau$  and  $c$  are the **relaxation time** and the **diffusion constant**. Plugging the drift and diffusion functions into Equation 4.2 yields

$$y(t+dt) = y(t) - \frac{1}{\tau}y(t)dt + c^{1/2}n(t)(dt)^{1/2} . \quad (4.8)$$

$y(t)$  is normally distributed, since  $y(dt)$  is normally distributed as the sum of a constant depending on  $y(0)$  and the normal variable  $n(dt)$ .  $y(2dt)$  is normally distributed being the linear combination of two statistically independent normal variables  $y(dt)$  and  $n(2dt)$ . Continuation shows the normal distribution of  $y(t)$ . The differential equations for the first and second moment of  $y$  are

$$\langle y(t+dt) \rangle = \langle y(t) \rangle - \frac{1}{\tau} \langle y(t) \rangle dt \quad \text{and} \quad (4.9)$$

$$\langle y^2(t+dt) \rangle = \langle y^2(t) \rangle - \frac{2}{\tau} \langle y^2(t) \rangle dt + cdt \quad (4.10)$$

Solving these equations with the initial condition  $y(0) = y_0$  yields the mean

$$\langle y(t) \rangle = y_0 e^{-t/\tau} \quad (4.11)$$

and the variance

$$\langle y^2(t) \rangle - \langle y(t) \rangle^2 = \frac{c\tau}{2} (1 - e^{-2t/\tau}) . \quad (4.12)$$

of  $y(t)$ . This determines the distribution of  $y(t)$  to be

$$y(t) = \mathcal{N}\left(y_0 e^{-t/\tau}, \frac{c\tau}{2} (1 - e^{-2t/\tau})\right) \xrightarrow{t \rightarrow \infty} \mathcal{N}\left(0, \frac{c\tau}{2}\right) . \quad (4.13)$$

Consider now a particle that is coupled to a reservoir of temperature  $T$  resulting in a dissipative drag force  $-\frac{\eta}{m}p(t)$  proportional to a dampening constant  $\eta$  as well as a fluctuating force  $F(t)$ . By Newton's second law, its equation of motion is given by

$$\frac{d}{dt}p(t) = -\frac{\eta}{m}p(t) + F(t) , \quad (4.14)$$

which we identify with the Langevin equation for the Ornstein-Uhlenbeck process Equation 4.8

$$\frac{d}{dt}p(t) = -\frac{1}{\tau}p(t) + c^{1/2}\Gamma(t). \quad (4.15)$$

From classical statistical thermodynamics we know that the velocity of the particle will eventually be distributed in a Maxwell-Boltzmann fashion:

$$p(t \rightarrow \infty) = \mathcal{N}(0, mk_B T) . \quad (4.16)$$

Comparing Equation 4.13 and Equation 4.16 shows that

$$\frac{c\tau}{2} = mk_B T \quad \text{or equivalently} \quad c = 2k_B T \eta , \quad (4.17)$$

implying that the dampening constant or respectively the relaxation time and the diffusion constant are not independent. For a particle in a potential  $V(x)$  one eventually obtains the equations of motions

$$\frac{d}{dt}x(t) = \frac{1}{m}p(t) \quad \text{and} \quad (4.18)$$

$$\frac{d}{dt}p(t) = -\frac{\eta}{m}p(t) - \frac{\partial V(x)}{\partial x} + \sqrt{2k_B T \eta} \Gamma(t) . \quad (4.19)$$

Methods of solution of the Langevin equation will be presented in section 4.3. But first we will talk about the applicability of the Langevin equation for the silicon surface.

## 4.2 Caldeira-Leggett Master equation

### 4.2.1 Motivation of the master equation

The silicon surface is a complex system subject to quantum mechanical interactions in between the surface atoms, as well as the silicon bulk and it is therefore anything but clear that we can use a classical Langevin equations to approximate its behavior.

A quantum mechanical microscopic theory is needed to live up to the silicon surface. Systems that are coupled to an environment are subject of the theory of open quantum systems, which will be used to derive a set of coupled Langevin equations.

Consider the **Caldeira-Leggett model** [9] for a quantum mechanical particle of mass  $m$ , moving in a potential  $V(\hat{x})$ . We can write down it's **free Hamiltonian**  $\hat{H}_S$  as

$$\hat{H}_S = \frac{1}{2m} \hat{p}^2 + V(\hat{x}) , \quad (4.20)$$

with the position and momentum operators  $\hat{x}$  and  $\hat{p}$ . The bath, which is the silicon bulk, is modeled as a set of harmonic oscillators with frequencies  $\omega_n$ . The bath hamiltonian can be written in terms of the bosonic annihilation and creation operators  $\hat{b}_n^\dagger$  and  $\hat{b}_n$ , or in terms of the canonically conjugated position  $\hat{x}_n$  and momentum  $\hat{p}_n$  operators of the  $n$ -th oscillator:

$$\hat{H}_B = \sum_n \hbar \omega_n \left( \hat{b}_n^\dagger \hat{b}_n + \frac{1}{2} \right) = \sum_n \left( \frac{1}{2m_n} \hat{p}_n^2 + \frac{1}{2} m_n \omega_n^2 \hat{x}_n^2 \right) \quad (4.21)$$

We assume that the coordinate  $\hat{x}$  of the Brownian particle is linearly coupled to the coordinates  $\hat{x}_n$  of the bath oscillators, yielding for the interaction Hamiltonian  $\hat{H}_I$

$$\hat{H}_I = -\hat{x} \otimes \sum_n \kappa_n \hat{x}_n = -\hat{x} \otimes \sum_n \kappa_n \sqrt{\frac{\hbar}{2m_n \omega_n}} (\hat{b}_n + \hat{b}_n^\dagger) = -\hat{x} \otimes \hat{B} , \quad (4.22)$$

with the coupling constants  $\kappa_n$ . To ensure positivity of the combined Hamiltonian  $\hat{H}_{SB}$ , a **counter-term**

$$\hat{H}_c = \sum_n \frac{\kappa_n^2}{2m_n \omega_n^2} \hat{x}^2 \quad (4.23)$$

is added. The counter term is in the following absorbed into the system hamiltonian. The hamiltonian of the combined system, or the universe, is given by

$$\hat{H}_{SB} = \hat{H}_S + \hat{H}_B + \hat{H}_I . \quad (4.24)$$

Since it is neither possible, nor required to solve the dynamics of the whole hamiltonian, we will be looking for a probabilistic description of the surface. In the quantum mechanical terms this means we will derive an equation for the system density matrix  $\hat{\rho}_S$ . Starting point is the von Neumann equation for  $\hat{\rho}_{SB} := e^{i(\hat{H}_S + \hat{H}_B)t} \hat{\rho}_{SB} e^{-i(\hat{H}_S + \hat{H}_B)t}$  in **interaction picture** with respect to  $\hat{H}_S + \hat{H}_B$ :

$$\frac{\partial}{\partial t} \hat{\rho}_{SB}(t) = -i \left[ \hat{\mathbf{H}}_I(t), \hat{\rho}_{SB}(t) \right]. \quad (4.25)$$

To derive an equation for  $\hat{\rho}_S$  the reservoir degrees of freedom are traced out:

$$\begin{aligned} \frac{\partial}{\partial t} \hat{\rho}_S(t) &= \text{tr}_B \left\{ \frac{\partial}{\partial t} \hat{\rho}_{SB}(t) \right\} = -i \text{tr}_B \left\{ \left[ \hat{\mathbf{H}}_I(t), \hat{\rho}_{SB}(t) \right] \right\} \\ &= -i \text{tr}_B \left\{ \left[ \hat{\mathbf{H}}_I(t), \hat{\rho}_{SB}(0) \right] \right\} - \int_0^t dt' \text{tr}_B \left\{ \left[ \hat{\mathbf{H}}_I(t), \left[ \hat{\mathbf{H}}_I(t'), \hat{\rho}_{SB}(t') \right] \right] \right\} \\ &= - \int_0^t dt' \text{tr}_B \left\{ \left[ \hat{\mathbf{H}}_I(t), \left[ \hat{\mathbf{H}}_I(t'), \hat{\rho}_S(t') \otimes \bar{\rho}_B \right] \right] \right\} \end{aligned} \quad (4.26)$$

The second line in Equation 4.26 is obtained by integrating Equation 4.25 and solving for  $\hat{\rho}_{SB}(0)$ . Under the **Born approximation**, which assumes that the reservoir density matrix is stationary and we can decompose  $\hat{\rho}_{SB}(t) = \hat{\rho}_S(t) \otimes \bar{\rho}_B$ , the trace  $\text{tr}_B \left\{ \left[ \hat{\mathbf{H}}_I(t), \hat{\rho}_{SB}(0) \right] \right\} = 0$  vanishes, yielding the third line of Equation 4.26. Afterwards we apply the **markov approximation** [31] by first replacing  $\hat{\rho}_S(t') \rightarrow \hat{\rho}_S(t)$ , then substituting  $\tau = t - t'$ , as well as sending the upper limit of the integral to infinity. This is permissible as the integrand disappears sufficiently fast. We obtain the **Redfield-II** master equation

$$\frac{\partial}{\partial t} \hat{\rho}_S(t) = - \int_0^\infty d\tau \text{tr}_B \left\{ \left[ \hat{\mathbf{H}}_I(t), \left[ \hat{\mathbf{H}}_I(t - \tau), \hat{\rho}_S(t) \otimes \bar{\rho}_B \right] \right] \right\}. \quad (4.27)$$

Transforming Equation 4.27 back to the Schrödinger picture gives

$$\frac{\partial}{\partial t} \hat{\rho}_S(t) = -i \left[ \hat{H}_S, \rho_S(t) \right] - \int_0^\infty d\tau \text{tr}_B \left\{ \left[ \hat{H}_I, \left[ \hat{\mathbf{H}}_I(-\tau), \hat{\rho}_S(t) \otimes \bar{\rho}_B \right] \right] \right\}. \quad (4.28)$$

The integral in the second term of Equation 4.28 can be rearranged (section A.1) to

$$\int_0^\infty d\tau \left( \frac{i}{2} D(\tau) [\hat{x}, \{\hat{\mathbf{x}}(-\tau) \cdot \hat{\rho}_S(t)\}] - \frac{1}{2} D_1(\tau) [\hat{x}, [\hat{\mathbf{x}}(-\tau), \hat{\rho}_S(t)]] \right), \quad (4.29)$$

with the noise kernel  $D(\tau)$  and dissipation kernel  $D_1(\tau)$  defined as in section A.1. In the markov approximation we already mentioned that the integrand decays sufficiently fast. This is because the noise and dissipation kernels disappear on the timescale of the relaxation  $\tau_B$  of the reservoir. When doing the markov approximation we assume that this timescale is much shorter than the relaxation time of the system  $\tau_S$ . We now make use of this again by

approximating  $\hat{\mathbf{x}}(-\tau)$  in the integrand by its free dynamics

$$\hat{\mathbf{x}}(-\tau) = \hat{\mathbf{x}} - \hat{p}\tau . \quad (4.30)$$

Plugging this approximation into Equation 4.29 enables to evaluate the integrals (see section A.1). This eventually results in the **Caldeira-Leggett master equation**

$$\frac{d}{dt} \rho_S(t) = \underbrace{-i [\hat{H}_S, \rho_S(t)]}_{\text{free dynamics}} - \underbrace{i\gamma [\hat{x}, \{\hat{p}, \rho_S(t)\}]}_{\text{dissipative term}} - \underbrace{2\eta m k_B T [\hat{x}, [\hat{x}, \rho_S(t)]]}_{\text{thermal fluctuations}} . \quad (4.31)$$

$\gamma$  is a damping constant that enters the calculation through a parametrization of the spectral density function. The first term in the Caldeira-Leggett master equation describes the free dynamics of the system and resembles the form of the **von Neumann** equation. The second term is the dissipative part proportional to the damping constant  $\eta$ , which enters the calculation through the parameterization of the spectral density function ???. The thermal fluctuations of the reservoir are captured in the third term proportional to the temperature  $T$  determined by the state of the reservoir  $\bar{\rho}_B$ , which follows the **Bose-Einstein distribution**.

### 4.2.2 Equations of motion

From Equation 4.31 one can derive equations of motion for arbitrary observables via

$$\frac{d}{dt} \langle \hat{A} \rangle = \text{tr} \left\{ \hat{A} \frac{d}{dt} \hat{\rho}_S(t) \right\} . \quad (4.32)$$

The results of Equation 4.32 for  $\hat{x}$ ,  $\hat{p}$  and  $\hat{p}^2$  compared to the equations of brownian motion of subsection 4.1.1

$$\begin{aligned} \frac{d}{dt} \langle \hat{x} \rangle &= \frac{1}{m} \langle \hat{p} \rangle , & \frac{d}{dt} \langle x(t) \rangle &= \frac{1}{m} p(t) , \\ \frac{d}{dt} \langle \hat{p} \rangle &= - \left\langle \frac{\partial V(\hat{x})}{\partial \hat{x}} \right\rangle - \eta \langle \hat{p} \rangle , & \frac{d}{dt} \langle p(t) \rangle &= - \left\langle \frac{\partial V(x)}{\partial x} \right\rangle - \eta \langle p(t) \rangle , \\ \frac{d}{dt} \langle \hat{p}^2 \rangle &= - \left\langle \hat{p} \frac{\partial V(\hat{x})}{\partial \hat{x}} + \frac{\partial V(\hat{x})}{\partial \hat{x}} \hat{p} \right\rangle & \frac{d}{dt} \langle p^2(t) \rangle &= - \left\langle 2p(t) \frac{\partial V(x)}{\partial x} \right\rangle \\ &\quad - 2\eta \langle \hat{p}^2 \rangle + 2\eta k_B T , & &\quad - 2\eta \langle p^2(t) \rangle + 2\eta k_B T . \end{aligned}$$

The two equation sets show the same structure. Especially interesting is the last term in the equations for the second moment of the impuls, which is the diffusion constant in the case of Brownian motion, match. It is therefore possible to derive the diffusion constant from microscopic considerations. We conclude that the equations of motion Equation 4.18 and Equation 4.19 are the classical correspondence to the preceding equations for  $\langle \hat{x} \rangle$  and  $\langle \hat{p} \rangle$  and move on to use them to describe the silicon surface. Since the silicon dimers interact,

the potential  $V(x) = V(x, x_i)$  is a function of the coordinates of the other dimers, leading to a **coupling** between the differential equations. Additionally,  $V(x, x_i)$  is **nonlinear** in  $x$ , eventually yielding a coupled set of nonlinear stochastic differential equations of the kind of Equation 4.19. An analytic solution is impossible and therefore we turn to numerical solutions in the next section.

### 4.3 Numerical methods and molecular dynamics

The update form Equation 4.2 of the Langevin equation are very useful for their numerical solution. A simple method of solution is the straight implementation of Equation 4.2, which is called the **Euler-Maruyama method** [25]. In practice one solves a system of first order stochastic differential equations

$$x_i(t + dt) = x_i(t) + \frac{1}{m} p_i(t) dt , \quad (4.33)$$

$$p_i(t + dt) = p_i(t) - \frac{\eta}{m} p_i(t) dt - \frac{\partial V(x_i(t), \{x\})}{\partial x_i} dt + \sqrt{2k_B T \eta} n_i(t) \sqrt{dt} . \quad (4.34)$$

The Euler-Maruyama method is straightforward to implement and computationally inexpensive, but shows discretization artefacts even for small stepsizes  $dt$ . Since usually the integration of the equations of motion takes much less time than the evaluation of  $V(x_i, \{x\})$  [13], many efforts have been made to improve the weak convergence (see [25]) of integration schemes.

The topic of simulating microscopical systems by numerically solving Newton's equations of motion is called **Molecular dynamics**. Molecular dynamics is widely used in biophysics, chemical physics but also material sciences. Larini et al [32] compare some of the integration schemes that have been developed over the time. They show that the popular Brunger-Brooks-Karplus [8] scheme (BBK method) is robust method with a number of general advantages. It is given by [21]:

half a kick

$$p_i(t + \frac{1}{2}dt) = (1 - \frac{1}{2}\eta dt) p_i(t) - \frac{1}{2}dt \frac{\partial V(x_i(t), \{x\})}{\partial x_i} + \frac{1}{2}\sqrt{2\eta k_B T} n_i(t) \sqrt{dt} ,$$

drift

$$x_i(t + dt) = x_i(t) + p_i(t + \frac{1}{2}dt) dt , \quad (4.35)$$

half a kick

$$p_i(t) = \left(1 + \frac{dt}{2}\eta\right)^{-1} \left( p_i(t + \frac{dt}{2}) - \frac{1}{2}dt \frac{\partial V(x_i(t+dt), \{x\})}{\partial x_i} + \frac{1}{2}\sqrt{2\eta k_B T} n_i(t + dt) \sqrt{dt} \right) .$$

Compared to higher order schemes like the fourth-order Hamiltonian Runge-Kutta scheme, that require multiple potential evaluations, the BBK method is faster with limited loss of

accuracy. The BBK integration step is slightly slower than the Euler-Maruyama one but it makes up through its much greater stability regarding larger stepsizes, ultimately resulting in much faster simulation speeds. The stability of the schemes is compared in appendix ??.

We now know why and how we can describe the silicon surface with langevin equations. The following section will deal with the modeling of the several times mentioned potential.

## 4.4 The Model

### 4.4.1 The Ising model

The Ising model is well known and has been used several times ([6, 43, 19, 47]) to study the Si(001) surface. Brand et al. [7] even found that the phase transitions shows Ising-like critical exponents. Their results may be relevant for the following investigations and therefore the Ising model will be shortly discussed below.

The 2D Ising model describes spins  $\sigma_{i,j} = \pm 1$  on a lattice. We consider the anisotropic case on a rectangle without external field. Its nearest neighbor Hamiltonian is given by

$$H = - \sum_{i,j} (J_{\parallel} \sigma_{i,j} \sigma_{i,j+1} + J_{\perp} \sigma_{i,j} \sigma_{i+1,j}) , \quad (4.36)$$

with  $J_{\delta}$  being the effective nearest neighbor coupling strengths. The 2D anisotropic Ising model is analytically solvable [41] and exhibits a continuous phase transition at

$$\sinh \left( \frac{2|J_{\parallel}|}{k_B T} \right) \sinh \left( \frac{2|J_{\perp}|}{k_B T} \right) = 1. \quad (4.37)$$

The equilibrium correlation lengths for  $T > T_c$  can be determined from the coupling constants [36] by

$$\frac{\xi_{\delta}(T)}{a_{\delta}} = \left( \ln \left[ \coth \left( \frac{|J_{\delta}|}{k_B T} \right) \right] - \frac{2|J_{\delta}|}{k_B T} \right)^{-1} , \quad (4.38)$$

with  $a_{\delta}$  being the lattice spacing in  $\delta$  direction and  $\bar{\delta}$  marking the direction perpendicular to  $\delta$ .

The ansatz is to map the equilibrium positions of the silicon dimers Figure 2.2b to the ising spin values  $\sigma_{i,j} = \pm 1$ . Then, by measuring the correlation lengths  $\xi_{\delta}$ , the effective coupling constants  $J_{\delta}$  can be determined by the usage of Equation 4.38. Afterwards, one is left with a simple theoretical model of the Si(001) system, that is hopefully helpful in understanding and predicting the behavior of the surface.

The Ising model gives name to its universality class. It is characterized by a continuous phase transition with a scalar order parameter and  $\mathbb{Z}_2$ -Symmetry. An overview of the relevant critical exponents is given in Table 4.1. Since the Ising model has only discrete states, it is not suitable

$\nu$	$z$	$\frac{\nu}{1+\nu z}$
1	$2.1667 \pm 0.0005$	$0.3158 \pm ?$

**Table 4.1:** The static critical exponents of the Ising universality class can be calculated analytically [10]. The value for  $z$  is the estimate of Nightingale et al. [39], who used MC techniques.

for a modeling with differential equations.

#### 4.4.2 The classical XY-Model

The classical XY-model and the Ising model can be viewed as two special cases of the Potts model [44] which generalizes the Ising model to allow  $q$ , instead of two, uniformly on a circle distributed states. The XY-model is obtained in the limit  $q \rightarrow \infty$  and therefore includes a continuity of values on the unit circle. It is thus suitable to be described by langevin equations and still related to the Ising model.

The XY hamiltonian with nearest neighbor interactions is given by

$$\begin{aligned} H &= - \sum_{i,j} (J_{\parallel} \vec{s}_{i,j} \cdot \vec{s}_{i,j+1} + J_{\perp} \vec{s}_{i,j} \cdot \vec{s}_{i+1,j}) \\ &= - \sum_{i,j} (J_{\parallel} \cos(\vartheta_{i,j} - \vartheta_{i,j+1}) + J_{\perp} \cos(\vartheta_{i,j} - \vartheta_{i+1,j})) , \end{aligned} \quad (4.39)$$

with the unit-length vectors

$$\vec{s}_{i,j} = \begin{pmatrix} \cos \vartheta_{i,j} \\ \sin \vartheta_{i,j} \end{pmatrix} \quad (4.40)$$

characterizing the state of the lattice site. Although the exact solution of the 2D XY model is intractable, Mattis [35] used a transfer matrix approach to approximate an analogue to Equation 4.37:

$$\frac{2k_B T_c}{J_{\parallel}} \ln \left( \frac{2k_B T_c}{J_{\perp}} \right) = 1 \quad \text{with} \quad J_{\parallel} \geq J_{\perp} . \quad (4.41)$$

A relation between the coupling constants and the correlation lengths is not available at the moment. TODO maybe you can derive one! That would be sick... but you cant even recalcu-

late the 1D XY calculation...

The 2D XY model does not exhibit a phase transition in the conventional sense, as the **Mermin-Wagner theorem** [37] prohibits the breaking of its continuous  $O(2)$  symmetry through short-range interactions. Instead, the system shows a **Kosterlitz-Thouless transition** [26, 3] characterized by an exponential divergence of the correlation length. The bare 2D XY model is part of no universality class as the universal power laws are not applicable.

We can add a  $p$ -fold symmetry breaking field of strength  $h$  to the XY hamiltonian

$$H = - \sum_{i,j} (J_{\parallel} \cos(\vartheta_{i,j} - \vartheta_{i,j+1}) + J_{\perp} \cos(\vartheta_{i,j} - \vartheta_{i+1,j})) + h \sum_{i,j} \cos(p\vartheta_{i,j}), \quad (4.42)$$

explicitly breaking the  $O(2)$ -symmetry. Those fields may very well be experimentally realized by crystalline anisotropies. The Migdal lattice recursion scheme [38] implies that for  $T \rightarrow 0$ , the field  $h$  is a relevant variable in the sense of section 3.1. The perturbations caused by  $h$  will grow as  $T$  shrinks, eventually forcing the system into a state of broken symmetry in which one of the directions  $\vartheta = 2\pi n/p, n \in [0, p-1]$  is preferred. Hence any  $h$  will lead to deviations in critical behavior from the classical XY-Model. José and Kadanoff [23] found that the symmetry broken XY model exhibits a continuous phase transition with critical exponents characteristic of a  $p$ -state Potts model, leading to Ising like critical behavior in the case of  $p = 2$ . This makes the 2D XY model with twofold symmetry breaking field ideal to explore the dynamics of the Si(001)-surface.

#### 4.4.3 Adaptation to the Si(001) surface

In the following some customization steps will be shown to adapt the XY model in a way to optimally resemble the experimentally observed properties of the silicon surface.

Since the silicon dimers do not have a distinguished direction in contrary to the spin vectors of the XY model, we define the right dimer to point along the arrow Figure 4.1. Additionally, a flip of the pointer by  $\pm\pi$  results in the same state, effectively cutting the state space in half. Measuring from the (001) axis (Figure 2.1), the angles will be restricted to  $\vartheta \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ . This

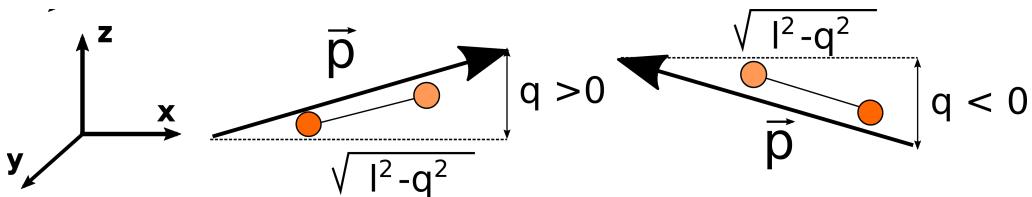


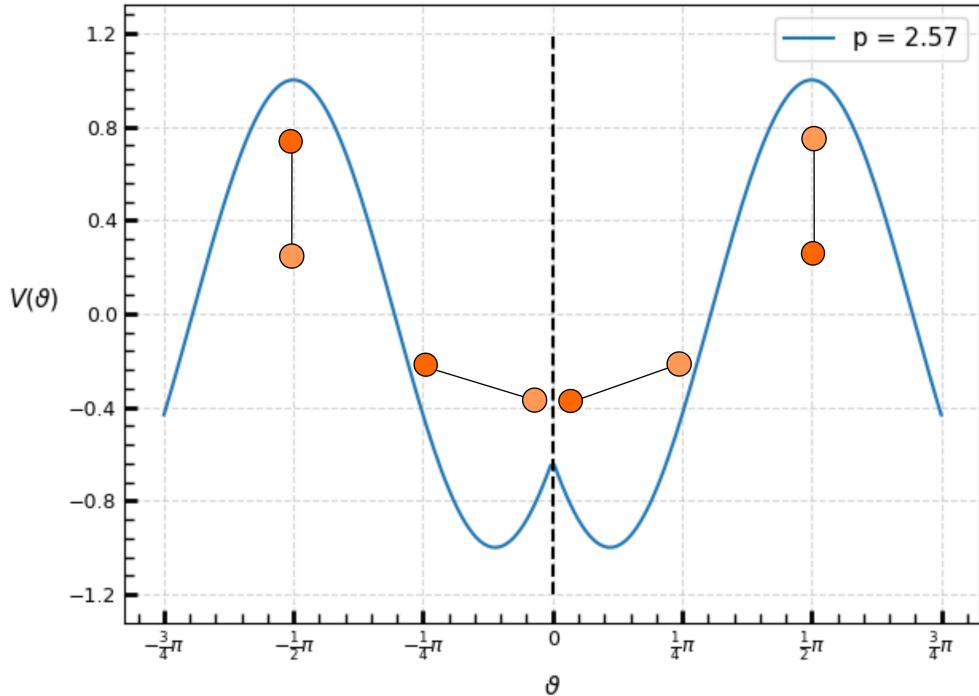
Figure 4.1: PLACEHOLDER

is achieved by adding a factor  $m = 2$  into the  $J_\delta \cos(m\Delta\vartheta_{i,j})$  terms. As stated in chapter 2, the dimers are buckled by  $18^\circ$  corresponding to an angle  $\vartheta^\pm = \pm 72^\circ \approx \pm \frac{2}{5}\pi$ . The equilibrium positions of Equation 4.42 are determined by the symmetry breaking field and the parameter  $p$  since the interaction is  $O(2)$ -symmetric. The minima satisfy

$$\cos(p\vartheta^\pm) = -1 , \quad \text{implying that} \quad p \approx 2.57 , \quad (4.43)$$

to ensure to reproduce the experimental equilibrium positions. The resulting potential of the symmetry breaking field is shown in Figure 4.2.

A suitable order parameter for this model is



**Figure 4.2:** The external field in combination with the restriction of  $\vartheta$  leads to the shown potential. The angle is measured from the (110) axis for illustration purposes. The Dynamics of the dimers for sufficiently low temperatures will take place around  $\vartheta = 0$ , the bucklings of  $\vartheta = \pm \frac{1}{2}\pi$  will almost never be reached.

$$M_L = \frac{1}{L^2} \sum_{i,j} m(\vartheta_{i,j}) \quad \text{with} \quad m(\vartheta) = \sin\left(\frac{p}{2}\vartheta\right) , \quad (4.44)$$

as the  $m(\vartheta)$  have maxima at  $\vartheta^+$  and minima at  $\vartheta^-$  satisfying  $m(\vartheta^+) = -m(\vartheta^-)$ .

Since in the XY-model the natural conjugated coordinate is the angle  $\vartheta$  and therefore the equations of motions Equation 4.18 have to be adapted to rotary motion. The velocity is replaced by the angle velocity  $\alpha$  in this case.

Equation 4.42 yields the force

$$\begin{aligned} \frac{\partial V(\{\vartheta\})}{\partial \vartheta_{i,j}} = & J_{\parallel} m \left( \sin(\vartheta_{i,j} - \vartheta_{i+1,j}) + \sin(\vartheta_{i,j} - \vartheta_{i-1,j}) \right) \\ & + J_{\parallel} m \left( \sin(\vartheta_{i,j} - \vartheta_{i,j+1}) + \sin(\vartheta_{i,j} - \vartheta_{i,j-1}) \right) \\ & + hp \sin(p\vartheta_i) . \end{aligned} \quad (4.45)$$

Eventually, the langevin equations to integrate become

$$\frac{d}{dt} \vartheta_{i,j}(t) = \omega_{i,j}(t) , \quad (4.46)$$

$$\frac{d}{dt} \omega_{i,j}(t) = -\frac{\eta}{I} \omega_{i,j}(t) - \frac{1}{I} \frac{\partial V(\{\vartheta\})}{\partial \vartheta_{i,j}} + \sqrt{\frac{2k_B T \eta}{I^2}} \Gamma(t) , \quad (4.47)$$

with  $\frac{\partial V(\{\vartheta\})}{\partial \vartheta_{i,j}}$  given in Equation 4.45. The implementation of the solution of this coupled set of stochastic differential equations will be the subject of the next section.

$$\ddot{\vartheta}_{i,j} = -\frac{\eta}{I} \dot{\vartheta}_{i,j} - \frac{1}{I} V'_{i,j} + \sqrt{\frac{2k_B T \eta}{I^2}} \Gamma_{i,j} \quad (4.48)$$

# 5 Implementation and Results

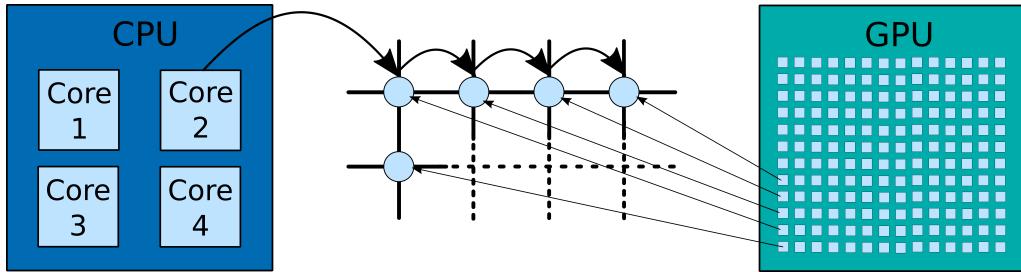
To reduce finite size corrections it is beneficial to consider as large systems as possible. Combined with the critical slowing down described in section 3.4 the problem at hand inherently generates an arbitrarily large computational cost. On top comes the stochastic nature of the system, requiring to run many simulations to extract ensemble averages, as well as the need to avoid discretization errors and ensure convergence when implying Equation 4.35 by choosing a small  $dt$ . This makes an efficient and fast implementation a crucial part of our investigations.

## 5.1 GPU programming

Besides the difficulties just described, there is an advantage that can be made use of. The langevin equations for the different lattice sites may be coupled through the potential Equation 4.45, but the integration step for  $t + dt$  only depends of the  $\vartheta_{i,j}(t)$  of the previous step, meaning that the integrations can be performed simultaneously. This allows for heavy parallelization, making the problem predestined for a GPU implementation.

The main difference between a conventional single core implementation on a central processing unit (CPU) and one on a graphical processing unit (GPU) is the number of processing cores involved. While CPUs only have few ( $\sim 10$ ) powerful processing cores, GPUs are made up of more than  $\sim 10^4$  cores. The CPU solves problems in a sequential matter, doing calculation after calculation making it suitable for usecases where the next step directly depends on the one before. In contrast, the GPU is able to perform many independent calculations real time simultaneously on its different cores. In situations where this is applicable, GPU implementations yield a significant speedup of up to a factor of  $10^3$ . A concept of the different solution approaches is shown in Figure 5.1.

For performance reasons the implementation took place (?) in C++ using **Thrust** [49] as high level interface for Nvidia's parallel computing platform **Cuda** [40]. The source code can be found at <https://github.com/andiw99/Master-Arbeit>. The architecture is inspired by Ahnert et al.'s work [1].



**Figure 5.1:** A CPU using single core processing would integrate the langevin equation for lattice site  $i$  and move on to site  $i + 1$ . The use of multi core processing would allow the CPU to integrate 4 sites simultaneously. In contrast, using GPU programming enables to evaluate the langevin equation at about  $10^4 - 10^5$  sites at the same time.

## 5.2 Benchmarks

Since an analytic solution of our model is intractable, proper benchmarks are vital to ensure the correctness of our simulation. Furthermore the stepsize used in Equation 4.35 has to be analyzed to ensure convergence as well as a balance between the discretization error and efficiency.

The Benchmarks that were conducted are

- the statistics of independent harmonic oscillators with thermal coupling,
- the equilibrium distribution of particles in a cosine potential,
- the equilibrium distribution of a system composed of two particles in a cosine potential with cosine interaction

The equation that describes the time evolution of probability densities of brownian motion is the **Fokker-Planck equation**. When talking about the probability density  $p(x, v, t)$  in terms of particle velocity  $v$  and position  $x$  it is often referred to as the **Klein-Kramers-** or **Smoluchowski** equation and written as

$$\frac{\partial}{\partial t} p(x, v, t) = \left( -\frac{\partial}{\partial x} v + \frac{\partial}{\partial v} \left( \eta v - \frac{1}{m} \frac{\partial}{\partial x} V(x) \right) + \frac{\eta k_B T}{m} \frac{\partial}{\partial v^2} \right) p(x, v, t). \quad (5.1)$$

The Fokker-Planck equation and the langevin equations (Equation 4.18 and Equation 4.19) are virtually identical and can be converted into each other. Ensemble averages over paths of langevin equations result in the probability distribution satisfying Equation 5.1. The steady state distribution of the Fokker-Planck equation is the canonical distribution

$$p(x, v) \propto e^{\beta \left( \frac{1}{2} mv^2 + V(x) \right)}, \quad (5.2)$$

allowing for an easy way to verify long term behavior.

### 5.2.1 Thermal harmonic oscillators

For a quadratic potential

$$V(x) = \frac{1}{2}\omega^2x^2, \quad (5.3)$$

the Fokker-Planck equation is analytically solvable [46]. This makes it ideal to confirm correct dynamics of the simulation. The analytic solution for the second moment of  $x(t)$  reads

$$\langle x^2 \rangle(t) = \frac{\eta k_B T}{m(\lambda_+ - \lambda_-)^2} \left[ \frac{\lambda_+ + \lambda_-}{\lambda_+ \lambda_-} + \frac{4}{\lambda_+ + \lambda_-} (e^{-(\lambda_+ + \lambda_-)t} - 1) - \frac{1}{\lambda_+} e^{-2\lambda_+ t} - \frac{1}{\lambda_-} e^{-2\lambda_- t} \right], \quad (5.4)$$

with

$$\lambda_{\pm} = \frac{1}{2} \left( \eta \pm \sqrt{\eta^2 - 4\omega^2} \right) \quad (5.5)$$

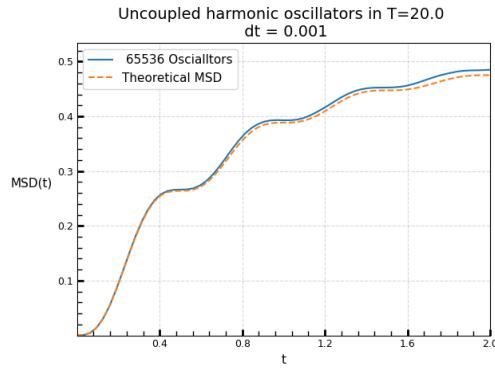
In Figure 5.2 we compare  $\langle x^2 \rangle(t)$  calculated from  $\approx 65000$  path, simulated by either the Euler-Maruyama- or the BBK method, with the theoretical result. The BBK algorithm with  $dt = 0.05$  and the Euler-Maruyama method with  $dt = 0.001$  yield similar small deviations from the theoretical curve, suggesting that the BBK method can be used up to much larger stepsizes. Besides, the validity of both methods for thermal harmonic oscillators is given for both methods for small enough stepsizes.

### 5.2.2 Particles in a cosine potential

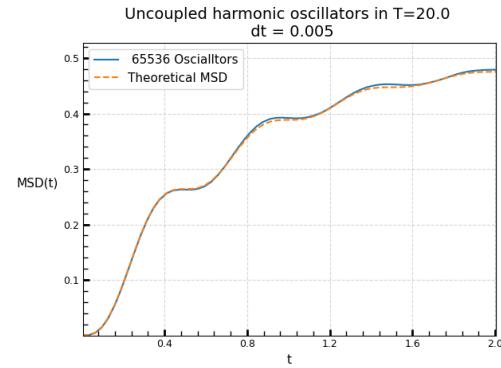
Another valuable Benchmark is the edge case of weakly interacting particles with  $J = 0$ . We will confirm that probability distribution calculated from ??? particle paths will approach the theoretical equilibrium distribution given by inserting Equation 4.42 for  $J_{\delta} = 0$  into Equation 5.2.

In Figure 5.3 we show the calculated integrated probability density  $p(x) = \int p(x, v)dv$  is plotted. The BBK method shows virtually no discretization errors up to a stepsize of  $dt = 0.05$ . For the Euler-Maruyama method large discretization errors show up for stepsizes one magnitude smaller.

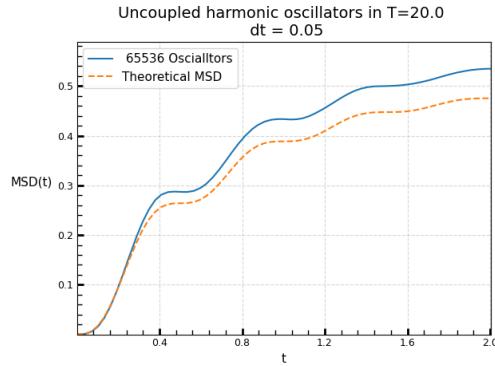
Again, for sufficiently small stepsizes the long term behavior of our simulation is verified.



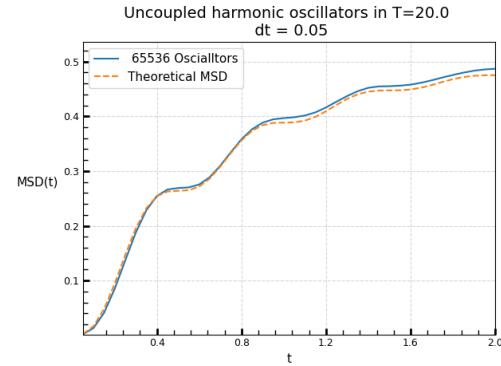
(a) The Euler-Maruyama method with a stepsize of  $dt = 0.001$  results in small but noticeable deviations.



(b) The BBK method with a stepsize of  $dt = 0.005$  reproduces the theoretical curve very well.

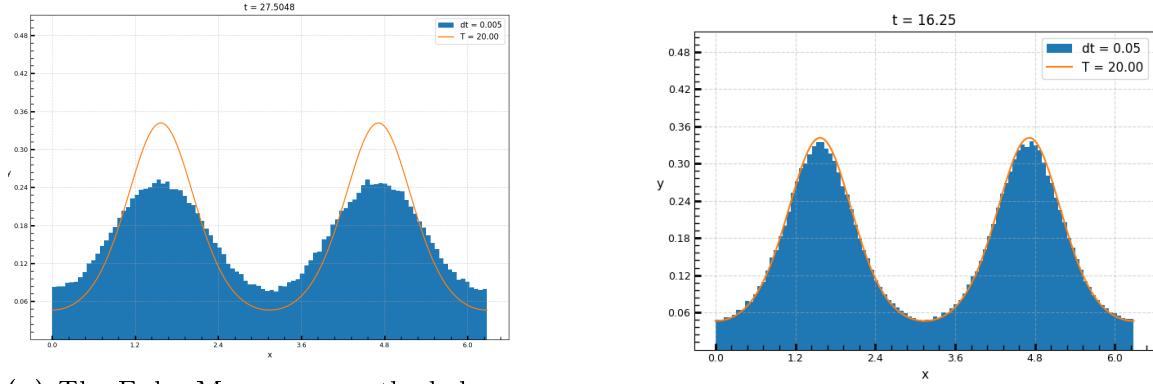


(c) The Euler-Maruyama method with a stepsize of  $dt = 0.05$  results in large deviations.



(d) The BBK method with a stepsize of  $dt = 0.05$  results in small but noticeable deviations.

**Figure 5.2:** The calculated  $\langle x^2 \rangle(t)$  of thermal harmonic oscillators are compared for the Euler-Maruyama- and the BBK method with different stepsizes



(a) The Euler-Maruyama method shows significant discretization errors regarding  $p(x)$  even for a comparatively small step-size of  $dt = 0.005$ .

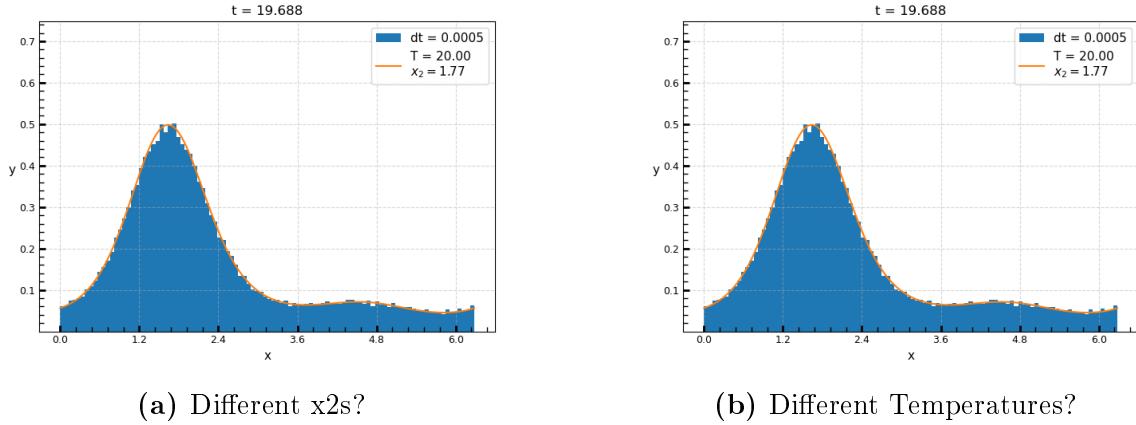
(b) The BBK method shows almost no deviation from the theoretical  $p(x)$  even for a stepsize of  $dt = 0.05$ .

**Figure 5.3:** The integrated probability distributions  $p(x)$  calculated from ??? particle paths are compared to the theoretical equilibrium distribution for the Euler-Maruyama method and the BBK Algorithm. It was made sure that the systems were completely relaxed, meaning that the effects of the starting position vanished and the shape of the probability distribution did not change anymore.

### 5.2.3 Two interacting particles in a cosine potential

The third benchmark has the purpose of verifying the correct behavior of the interaction. Since the equilibrium distribution becomes a high dimensional function  $p(\{x_i\}, \{v_i\})$ , a suitable representation is possible in the case of system consisting of two particles. The object of examination is again the equilibrium probability distribution of the Fokker-Planck equation.

In Figure 5.4 we now show cuts of the integrated probability density  $p(x_1, x_2) = \int p(x_1, x_2, v_1, v_2) dv_2 dv_1$  with a constant  $x_2$ . It is verified that simple interacting systems are driven to their equilibrium by the method of langevin integrations. The statistical- and discretization errors vanish for many samples and small stepsizes.



**Figure 5.4:** Cuts of the integrated probability distributions  $p(x_1, x_2)$  with a constant  $x_2$  calculated from ??? particle paths are compared to the theoretical equilibrium distribution. It was made sure that the systems were completely relaxed, meaning that the effects of the starting position vanished and the shape of the probability distribution did not change anymore.

## 5.3 Results

In the following the results of the explained simulation will be presented. We will start with the examination of the critical exponents of our model.

The parameters will be measured in units of  $J_\perp = 1$  and the initially used ratio  $J_\parallel/J_\perp = 31.1$  is the one from Brand et. al [6]. The external field  $h = 5$  is chosen small compared to  $J_\parallel$  to ensure approximate validity of Equation 4.41. The strength of  $h$  should not influence the kind of phase transition we observe as long as it is finite, but may influence  $T_c$ . Both coupling strengths are negative to reproduce the c(4x2) symmetry. To conclude, as long as not otherwise stated, the in the following used model parameters of Equation 4.42 are

$$J_\perp = -1, \quad J_\parallel = -31.1 \quad \text{and} \quad h = 5. \quad (5.6)$$

The dampening is set to  $\eta = 1.5$ . Our method of correlation length extraction section A.2 works best if  $\xi_\delta \ll L_\delta$ . Since the Si(001) surface exhibits a large correlation length anisotropy  $\frac{\langle \xi_\parallel/a_\parallel \rangle}{\langle \xi_\delta/a_\delta \rangle} \approx 10$ , it is useful to ensure that the system sizes share a similar ratio. This way we can analyze larger correlation lengths without increasing the computational cost. The following systems have a ratio of  $\frac{L_\parallel}{L_\perp} = 8$  if not stated otherwise. The used stepsize is  $dt = 0.01$

### 5.3.1 static scaling

Since the phase transition of the Si(001) surface seems to belong to the Ising universality class [7], our simulation should reproduce this. The XY model with a  $p$ -fold symmetry breaking external field belongs to the Ising universality class for  $p = 2$  [23], but the question remains if

this is still true for our adaptation (subsection 4.4.3) with a rational number  $p \approx 2.57$ .

Therefore, the finite size techniques and the Binder cumulant described in section 3.3 and subsection 3.3.1 are employed to extract the critical exponent. The magnetization is calculated using Equation 4.44. We initialize totally ordered systems as suggested in [5], that is all dimers are alternatively buckled. We run multiple small independent systems simultaneously on a single GPU to achieve optimal parallelization. We run long simulations to ensure the thermalization of the systems. During the run, we document the Binder cumulant  $U_L(t)$  to be able to afterwards determine a timepoint  $t_{equil}$  after which we judge the cumulant to be equilibrated. The cumulant is subject to statistical fluctuations, so to obtain useful averages it can be made use of the ergodic hypotheses. Instead of running many simulations and averaging the latest value of  $U_L$ , we simulate systems for long times  $t_{long}$  and calculate the ensemble average as the time average

$$\overline{U}_L = \frac{1}{(t_{long} - t_{equil})} \int_{t_{equil}}^{t_{long}} U_L(t) dt . \quad (5.7)$$

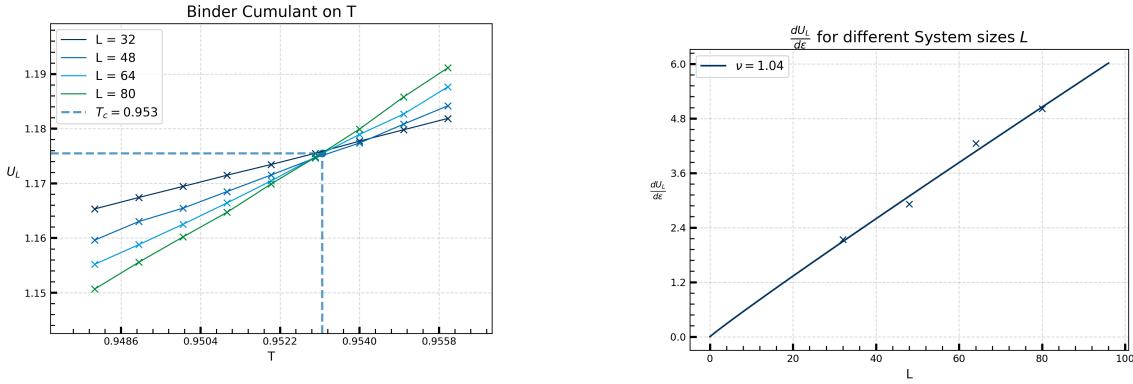
In Figure 5.5 the results for ??? systems simulated until  $t_{long} = ???$  are shown for temperatures very close to  $T_c$ . The critical point was approached by estimating the critical temperature with Equation 4.41 yielding  $T_c^{est} \approx 0.618$ , examining the general area for the phase transition and then iteratively closing in. The more precise  $T_c$  shall be determined, the closer the temperatures have to lie at  $T_c$ . The closer two temperatures lie, the easier it is for statistical fluctuations to smear their relative position and therefore the more averages you need. The same is true for the calculation of the critical exponent  $\nu$ . The derivative  $\frac{\partial U_L}{\partial \varepsilon}$  is calculated through a simple central difference. Afterwards the function Equation 3.31 is fitted to  $\frac{\partial U_L}{\partial \varepsilon}(L)$ . The result  $\nu = 1.04$  is in good agreement with the theoretical critical exponent of the Ising model  $\nu = 1$ . The matching of the static critical exponent verifies our numerics as well as the assumption that our modification of the XY model still belongs to its expected universality class.

### 5.3.2 dynamic scaling

The dynamic universality classes are subgroups of the static universality classes and our model could very well be in a different dynamic universality class than the 2D Ising model. In the following multiple methods will be employed to extract the dynamic critical exponent  $z$ .

#### The Kibble-Zurek mechanism

The first method will be the extraction through Equation 3.38 and the Kibble-Zurek mechanism. Since we already gained knowledge of  $\nu$  we can fit the exponent  $\nu/(1 + \nu z)$  to quenched correlation lengths deduce  $z$ .



(a) The Binder cumulants intersect at  $T_c = 0.953$ . The intersection is determined by the minimum squared error between the cumulants.

(b) The derivatives  $\frac{\partial U_L}{\partial \varepsilon}$  scale like  $\propto L^\nu$ . The fitting results in  $\nu = 1.04$  which is in good accordance with the Ising model.

**Figure 5.5:** The results for  $\bar{U}_L$  of ??? averaged systems of different sizes simulated for a time of  $t_{long} = ???$  are shown. The estimated equilibration time is  $t_{equil} = ???$ .

The used quench protocol, i.e the manner in which the system is cooled down, will be a simple isotropic, linear quench like Equation 3.34. The starting temperature  $\varepsilon(t_{start})$  is chosen to be sufficiently far away to observe adiabatic system evolution before crossing the freezeout point  $\varepsilon(t_{start}) < \varepsilon(\hat{t})$ . The end temperature  $\varepsilon(t_{end})$  is chosen in symmetric distance from the transition point  $|\varepsilon(t_{start})| = |\varepsilon(t_{end})|$ .

In Figure 5.6 the results for the quench of our system are shown. A fit of the frozen correlation lengths  $\hat{\xi}$  to Equation 3.38 is performed in ?? and ?. Only the datapoints in the phase space where the Kibble-Zurek mechanism should be valid are used. It was made sure that  $\hat{\xi}_\delta \ll L_\delta$  so that section A.2 is still applicable. The extracted KZM exponent of  $\nu/(1+\nu z)$  is unusually large and suggests that  $z < 2$ .

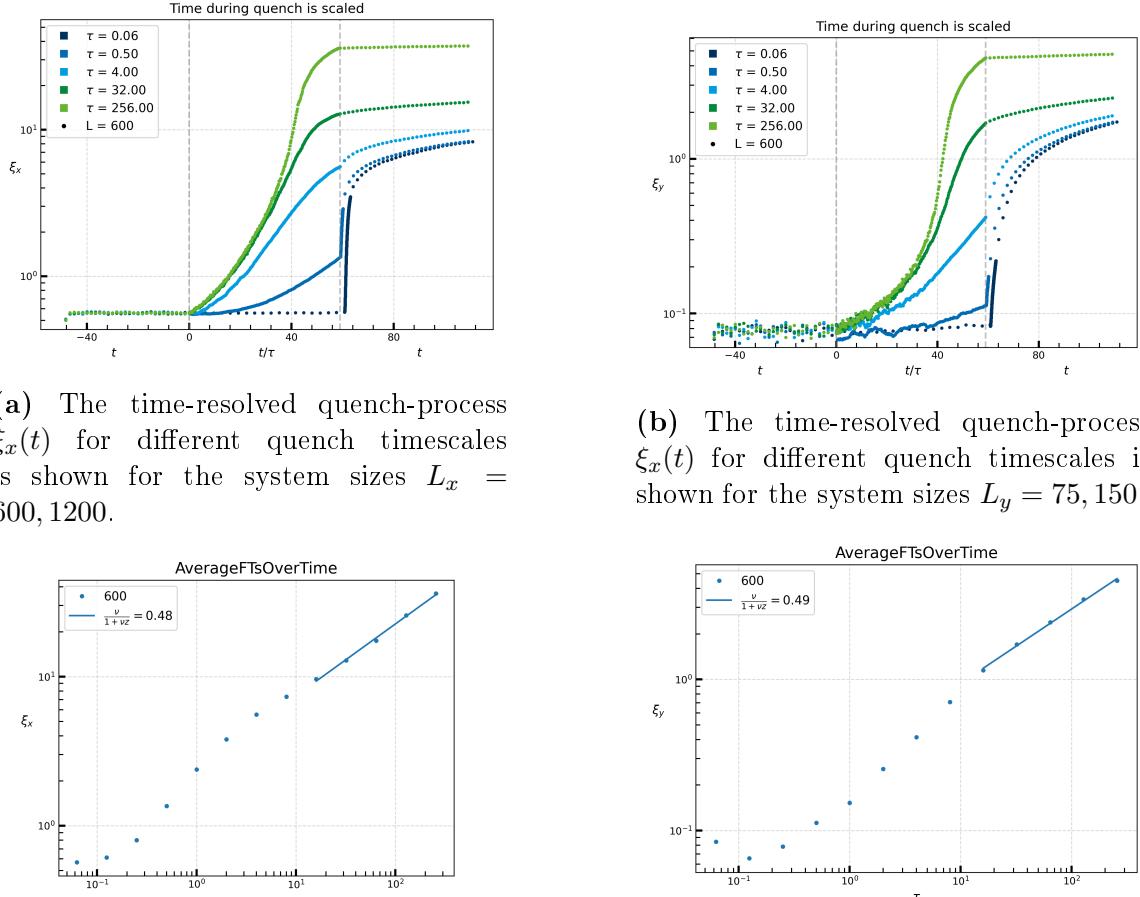
A KZM independent  $z$  extraction method is needed to verify the correct critical exponent.

### Relaxation of the Binder cumulant

A simple way to examine the dynamic critical exponent is to consider the relaxation of the Binder cumulant including finite size scaling. This method was introduced by Li et. al [33] and will be used in the following to extract the dynamic critical exponent.

The basis is the time-resolved finite size scaling of the  $(n)$ -th moment of the magnetization

$$M^{(n)}(t, \varepsilon, L) = b^{-n\beta/\nu} M^{(n)}(b^{-z}t, b^{1/\nu}\tau, b^{-1}L) , \quad (5.8)$$



(a) The time-resolved quench-process  $\xi_x(t)$  for different quench timescales is shown for the system sizes  $L_x = 600, 1200$ .

(b) The time-resolved quench-process  $\xi_x(t)$  for different quench timescales is shown for the system sizes  $L_y = 75, 150$ .

(c) The frozen correlation length  $\hat{\xi}_x(\tau)$  depending on the quench timescale is investigated. A fit of the data to Equation 3.38 is calculated and drawn in the appropriate area.

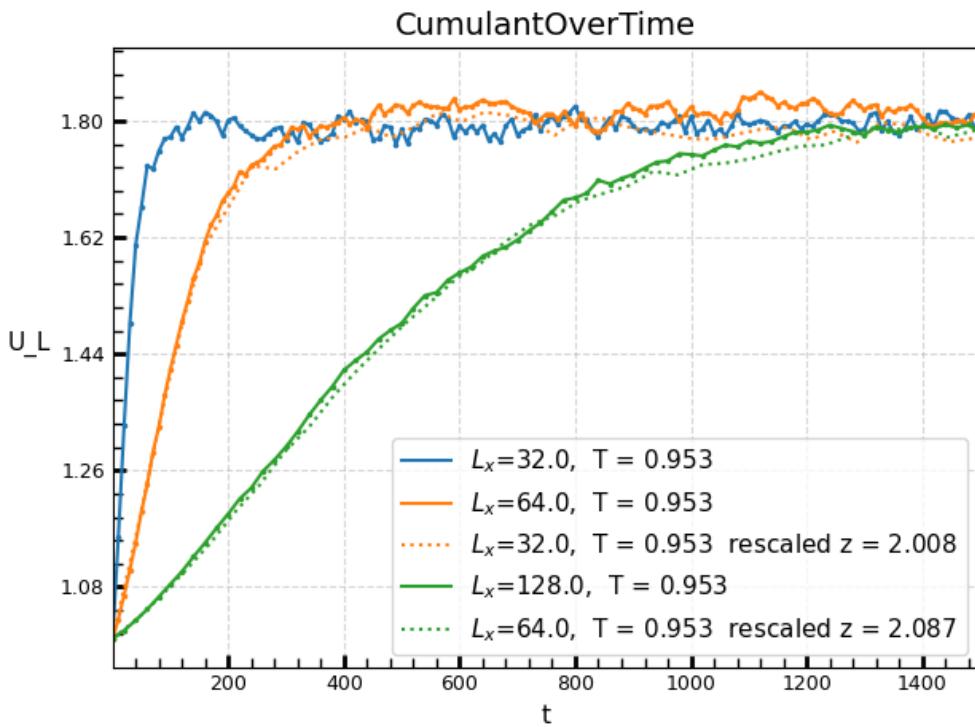
(d) The frozen correlation length  $\hat{\xi}_y(\tau)$  depending on the quench timescale is investigated. A fit of the data to Equation 3.38 is calculated and drawn in the appropriate area.

**Figure 5.6:** The results of the quenches are investigated using the Kibble Zurek mechanism. The Kibble-Zurek mechanism is valid where the system is at the start of the quench able to adiabatically follow the process. When the quench is so fast that the system cannot follow the quench even at the start, the frozen correlation length is the equilibrium correlation length of the starting temperature and no scaling is observed.

with  $b = \frac{L}{L'}$  being the spatial rescaling factor. Janssen et. al [22] determined that the initial correlation length must be very short for Equation 5.8 to be valid. Therefore the investigated systems will be prepared in a high temperature, low order state. Following the definition of the Binder cumulant Equation 3.29, one can relate the Binder cumulant of systems of different sizes at the critical point  $\varepsilon = 0$  by

$$U(t, 0, L_1) = U(b^{-z}t, 0, L_2), \quad \text{with} \quad b = \frac{L_1}{L_2} \quad (5.9)$$

The exponent  $z$  is easily obtained by searching a time rescaling factor  $b^{-z}$  such that the recorded curves for  $U_{L_1}$  and  $U_{L_2}$  collapse. Since the sample systems are prepared in a high temperature state where  $U_L = 3$ , we expect a relaxation from this value to the equilibrium  $U_L^*$  which is, at  $\varepsilon = 0$ , the same for every system size. The results for the rescalings  $32 \rightarrow 64$  and



**Figure 5.7:** The best rescaling of  $U_{L_1} \rightarrow U_{L_2}$  is selected by minimizing the squared error between the interpolated curves. The result of the rescaling from  $64 \rightarrow 128$  yields a dynamic critical exponent of  $z = 2.08$ , close to the best known value for the Ising universality class (see Table 4.1).

$64 \rightarrow 128$  calculated from ??? sample paths are shown in Figure 5.7. The rescaling  $64 \rightarrow 128$  is to be trusted more than the  $32 \rightarrow 64$  since it minimizes the finite size corrections to the scaling law Equation 5.8. Its result  $z = 2.08$  is very close to the best available dynamical critical exponent of the Ising model  $z_{Ising} = 2.14$ . With this the calculated KZM exponent of  $\nu/(1 + z\nu) = 0.33$  stands in harsh contradiction to the exponent obtained directly from the quench  $\nu/(1 + z\nu) = 0.45$ . Since it is from symmetry considerations very plausible that our

model for silicon would show the Ising dynamical exponent, we would expect that the deviation stems from the Kibble-Zurek scaling. Since the system sizes used in the quenches is already very large, strong finite size corrections to the Kibble-Zurek scaling can be ruled out as cause of the deviation. The same is true for the discretization error of our stepsize since the same quenches have been recalculated with a smaller stepsize. Since the correctness of our simulation has otherwise been verified, the most sensible explanation for the large Kibble-Zurek scaling exponent is that the cause has to be a systematic difference in the expected Kibble-Zurek mechanics (???). An idea could be the existence of subleading scalings like reported in [28] caused by other scaling fields than the temperature. In our case such a scaling field could be the strength of the external potential  $h$ .

In the following we will investigate the effect of the strength of  $h$  on the dynamical critical exponent as well as the Kibble-Zurek exponent.

### 5.3.3 The correlation length amplitudes $\xi_\delta^+$

The static scaling law of the correlation length  $\xi_\delta$  above the critical temperature ( $\varepsilon > 0$ ) given by Equation 3.21 can be rewritten as

$$\xi_\delta(\varepsilon) = \xi_\delta^+ \varepsilon^{-\nu}, \quad (5.10)$$

with the so called correlation length amplitude  $\xi_\delta^+$ . The + sign denotes the amplitude above the critical temperature. The correlation lengths in the Ising model are directly related to the temperature and the coupling constants  $J_\delta$ . Their relation above the critical temperature is given by Equation 4.38. An expansion of Equation 4.38 around the critical temperature  $T_c$  leads to a simple relation between the coupling constants and the correlation length amplitudes,

$$\sinh\left(\frac{2|J_\delta|}{k_B T_c}\right) = \frac{\xi_\delta^+ / a_\delta}{\xi_\delta^- / a_\delta}. \quad (5.11)$$

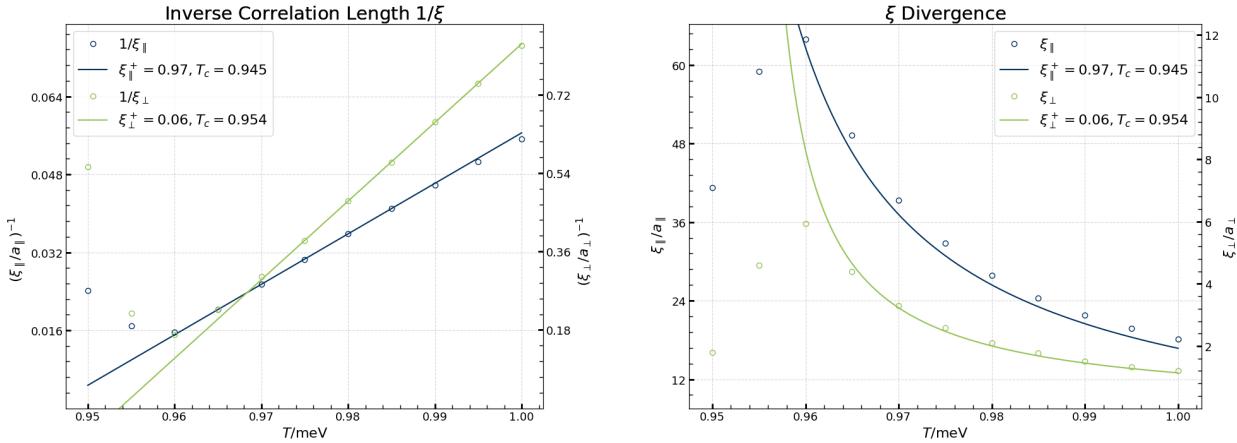
This relation is exceptionally useful, as it can be used to determine the coupling energies  $J_\delta$  from the measured correlation lengths and critical temperatures as is done in [6], [7]. The value that is obtained here for the amplitude ratio in units of the lattice constants is  $(\xi_\parallel^+ / a_\parallel) / (\xi_\perp^+ / a_\perp) = 10.3$ .

A relation like Equation 5.11 for the XY model with a symmetry breaking field is not known at the moment and efforts to derive one were unsuccessful. So a direct relation of the correlation length ratio to the model couplings  $J_\delta, h$  and even  $p$  is not possible. But since the symmetry broken XY model and the Ising model have shown to behave quite similar in the previous

investigations, it is reasonable to examine the correlation length amplitude ratio for the Ising coupling constant ratio  $J_{\parallel}/J_{\perp} = 31.1$ .

The amplitude ratio is investigated by preparing the system in a random state and letting it relax at a fixed temperature  $T \gtrsim T_c$ . To judge whether the system is relaxed and at the same time obtain a precise value for the equilibrium correlation length,  $\xi$  is monitored on the run in the spirit of Equation 5.7. Every  $n_s = 100$  steps,  $\xi_{\delta}$  is calculated and saved. After reaching a minimum step threshold, every  $n_{\sigma} = 5n_s$  steps also the mean  $\bar{\xi}_{\delta}$  as well as its error  $\sigma_{\bar{\xi}_{\delta}}$  is calculated. The correlation of  $\xi(t)$  and  $\xi(t + n_s dt)$  has to be taken into consideration if  $n_s dt < \tau$  (see section A.3). When calculating mean and error, a fraction  $p_{\tau} = 1/2$  of correlation lengths is ignored in order to account for the equilibration of the system. After falling below a maximum relative error of  $\sigma_{max}/\bar{\xi}_{\delta} = 0.01$  for both directions, the run is terminated. The used system size is chosen as large as numerically feasible to minimize finite size effects around the critical temperature  $T_c$ .

The results for the equilibrium  $\xi_{\delta}$  for a system of size  $L_x = ?$  are shown in Figure 5.8. To



**Figure 5.8:** (a) The inverse correlation length  $\xi^{-1}$  of a system of size  $L_x = ?$  equilibrium is measured and shown for temperatures  $T \gtrsim T_c$ . The line is a linear fit with the parameters  $\xi_{\delta}^+$  and  $T_c$ . (b) The divergence of  $\xi$  is measured around  $T \gtrsim T_c$ . The line is calculated by Equation 5.10, using the parameters obtained by the fit of (a).

extract the correlation length amplitude  $\xi_{\delta}^+$ , the scaling of  $\xi_{\delta}^{-1}$  was considered, which is given by

$$\xi_{\delta}^{-1}(T) = \frac{1}{\xi_{\delta}^+} \left( \frac{T - T_c}{T_c} \right) = -\frac{1}{\xi_{\delta}^+} + (T_c \xi_{\delta}^+)^{-1} T , \quad (5.12)$$

if the result  $\nu = 1$  is used. Therefore  $\xi$  behaves linearly in  $T$  around the critical point. Which datapoints shall be included is decided by selecting the best linear regression in the parameters of  $\xi_{\delta}^+$  and  $T_c$  of at least 4 consecutive datapoints that agree with the previously determined critical temperature  $T_c^{UL}$ . The quality of the fit is determined by the  $r^2$ -value of the regression.

A minimum  $r^2$ -value of  $r_{min}^2 = 0.98$  is required to accept a successful fit. (TODO) maybe just choose the regression that has a minimum  $r^2$  value and is as close to  $T_c$  as possible?) Close to  $T_c$  finite size effects become visible. To illustrate this,  $\xi$  is recalculated at the questionable datapoints for a system of size  $L'_x = 2L_x$ . At this point I am not sure why the correlation length becomes smaller already at temperatures slightly larger than  $T_c$ , the RG theory actually predicts that the maximum of  $\xi$  should be shifted to a lower temperature?. The correlation length ratio of  $\xi_{\parallel}^+/\xi_{\perp}^- = ?$  is smaller than expected for the Ising model. Reasons for this could be influences of the symmetry breaking field and structural difference in the relationship of the coupling constants and the correlation lengths. The influence of the symmetry breaking field on the amplitude ratio will be investigated in the following.

### 5.3.4 quantitative

Since the dimer interaction is a kind of dipole interaction [43], our XY-model interaction might not reproduce quantitative results of the real system. In the following some quantitative considerations will be done anyway.

Since the numbers used in a simulation are all dimensionless, one has to think about what those numbers represent in physical quantities. Since the mass  $m$ , or for rotational motion equivalently the moment of inertia  $I$ , is not implemented into the simulation, it is easiest to measure all quantities in multiples of  $I$ . Natural units will be used in the following. The moment of inertia is approximated as two point masses  $m_{Si} \approx 28u = 26$  GeV with a distance of  $2r \approx 2 \text{ \AA} \approx 10 \text{ keV}^{-1}$ , yielding

$$I \approx 2m_{Si}r^2 \approx 2(26 \text{ GeV}) (5 \text{ keV}^{-1})^2 = 1300 \text{ meV}^{-1}. \quad (5.13)$$

The dimensionless angular velocity  $\Omega$  in units of  $I$  is

$$\Omega(t) = I\omega(t). \quad (5.14)$$

The dimensionless version of Equation 4.47 becomes

$$\begin{aligned} \Omega_{i,j}(t + dt) &= \Omega(t) - \eta\Omega_{i,j}(t)\frac{dt}{I} - I\frac{\partial V(\{\vartheta\})}{\partial\vartheta_{i,j}}\frac{dt}{I} + \sqrt{\frac{2T\eta}{I^2}}n(t)I\sqrt{dt} \\ &= \Omega(t) - \eta\Omega_{i,j}(t)d\sigma - \frac{\partial v(\{\vartheta\})}{\partial\vartheta_{i,j}}d\sigma + \sqrt{2\kappa\eta}n(t)\sqrt{d\sigma}, \end{aligned} \quad (5.15)$$

with the dimensionless quantities

$$\sigma = t/I, \quad (5.16)$$

$$v(\vartheta) = IV(\vartheta), \quad \text{and} \quad (5.17)$$

$$\kappa = IT. \quad (5.18)$$

The second line of Equation 5.15 is what is implemented in the simulation. To get the physical values, the equation has to be divided by the moment of inertia  $I$ . The position coordinate  $\vartheta$  of the dimer however does not have to be converted since the dimensionless form of Equation 4.46

$$\begin{aligned} \vartheta(t + dt) &= \vartheta(t) + \Omega(t)d\sigma = \vartheta(t) + I\omega(t)\frac{dt}{I} \\ &= \vartheta(t) + \omega(t)dt \end{aligned} \quad (5.19)$$

equals the dimensionful form.

The used dimensionless stepsize of  $d\sigma = 0.01$  corresponds to a physical stepsize of

$$dt = Id\sigma = 1300 \text{ meV}^{-1} \cdot 0.01 \approx 0.01 \text{ ns}, \quad (5.20)$$

which is very reasonable since this stepsize is of the order of magnitude of the fast hight temperature flipping of the dimers (source? BrandCritical). The dimensionless critical temperature has a value of

$$\kappa_c = 1300 \text{ meV}^{-1} \cdot 16.43 \text{ meV} \approx 22100, \quad (5.21)$$

using the experimental critical temperature  $T_c = 16.43 \text{ meV}$  of Brand et. al [6]. Assuming a ratio of  $J_{\parallel}/J_{\perp} = 31$ , Equation 4.41 can be used to together with  $T_c$  to estimate the values of  $J_{\delta}$ . We get

$$J_{\perp} = 2.66 \text{ meV} \quad \text{and} \quad J_{\parallel} = 82.46 \text{ meV}, \quad (5.22)$$

corresponding to the dimensionless values  $j_{\delta} = IJ_{\delta}$  of

$$j_{\perp} = 3580 \quad \text{and} \quad j_{\parallel} = 110980. \quad (5.23)$$

The question now is how to choose  $h$  in order not to change the phase transition again. Therefore a perturbation based version of Equation 4.41 including  $h$  would be very useful. And the dampening is also crucial to the timescales on which the system evolves. There is probably no way of estimating this? Or there might be one but that is surely not possible in

2 months...

For the addition of  $h$ : you know the form of the phase diagram of the XY model, and I think you even know the kind of function it describes. What you probably don't know are the prefactors, etc. You can fit them but they probably are dependent on  $J$ ? It is not dependent on  $\eta$  at least.

The equilibrium position of the dimers is determined by the strength of repulsion  $J_{\parallel}$  and  $J_{\perp}$ , the amplitude of the symmetry breaking field  $h$  and the position of its minima determined by the parameter  $p$ . In the case of ferromagnetic interaction, the equilibrium position is solely determined by  $p = \frac{18}{7}$  which yields the experimental equilibrium position of  $\vartheta^* = \frac{7}{18}\pi = 70^\circ$  (measuring from the z-Axis). We can also infer that  $p > 2$  as  $p = 2$  means that the equilibrium position of the symmetry breaking field is at  $\vartheta = \pi/2$ , corresponding to a horizontal dimer. Since we see from DFT calculations that even the buckling itself without any constraint on the configuration decreases the energy, this is not realistic. The two constraints conclude to  $p \in [2, 2.57]$  Consider now a specific lattice site of a system in total equilibrium, meaning that the site's buckling angle is  $\vartheta = \vartheta^*$  and the buckling angle of all its neighbors is  $\vartheta_{NN} = -\vartheta^*$ . The condition that  $\frac{\partial H(\vartheta)}{\partial \vartheta} \Big|_{\vartheta=\vartheta^*} = 0$  gives

$$-4 \sin(4\vartheta^*) \left( \frac{J_{\parallel} + J_{\perp}}{h} \right) = p \sin(\vartheta^* p) . \quad (5.24)$$

This is a transcendental equation that determines the parameter  $p$  in dependence of the coupling constants,  $h$  and the desired equilibrium position. For the experimental  $\vartheta^*$ ,  $\sin(4\vartheta^*) \approx -1$ , leading to the simpler form

$$4 \frac{J_{\parallel} + J_{\perp}}{h} = p \sin\left(\frac{7\pi}{18}p\right) . \quad (5.25)$$

The right hand side of this equation is monotonically decreasing on the interval  $[2, 2.57]$ , so a solution is only possible if

$$\frac{J_{\parallel} + J_{\perp}}{h} \leq \frac{1}{4} \cdot 2 \cdot \sin\left(\frac{14}{18}\pi\right) \approx \frac{1}{3} \quad (5.26)$$

### Fitting the model parameters to DFT calculations

Numerous investigations calculated configuration energies of the Si(001) [14, 45] surface by density functional theory (DFT) methods and fitted the Ising model parameters accordingly [43, 20, 19, 52]. We can trace their path and use their configuration energies to get a feeling of the dimension of our coupling parameters.

The model in use has 4 parameters that influence the configuration energy, being the interaction

couplings  $J_{\parallel}, J_{\perp}$ , the strength  $h$  and the position, characterized by  $p$ , of the symmetry breaking field. Another unknown is the binding energy of the lowest configuration  $E_0$ , in our case being the absolute energy of the  $c(4 \times 2)$  configuration. Since  $p$  is inside a  $\cos(p\theta)$ , the fitting of the model parameters will result in a 5-dimensional non linear system of equations, which could be a bit tedious to solve. An approximation that is probably still fairly accurate would be to determine  $p$  solely from the equilibration angle of the asymmetric  $p(2 \times 1)_a$  configuration. Since in this configuration all dimers have the same buckling angle by definition, the dimer interaction cannot influence the equilibrium angle, since there is i.e. no repulsion involved that could shift the minimum of the symmetry breaking field. The caveat is that we have to assume that the surface configuration does not or only slightly change the strength and shape of the symmetry breaking field, which is in the real world system generated by the silicon bulk. If that's the case, the angle that is observed in the  $p(2 \times 1)_a$  configuration directly determines  $p$  since

$$\cos(\vartheta_{p(2 \times 1)_a} p) \approx -1 \quad \Rightarrow \quad p = \pi/\vartheta_{p(2 \times 1)_a}. \quad (5.27)$$

Pillay et. al [43] found a buckling angle of  $\approx 17.2^\circ$  resulting in  $\vartheta_{p(2 \times 1)_a} = 72.8^\circ$  and  $p = 2.473$ . With this simplification we obtain a linear system of equations

$$c(4 \times 2) : \quad \cos(4\vartheta^{(1)}) \quad J_{\parallel} + \cos(4\vartheta^{(1)}) \quad J_{\perp} + \cos(\vartheta^{(1)} p) h = E_0 \quad (5.28)$$

$$p(2 \times 2) : \quad \cos(4\vartheta^{(2)}) \quad J_{\parallel} + \quad J_{\perp} + \cos(\vartheta^{(2)} p) h = E_0 + E_{p(2 \times 2)} \quad (5.29)$$

$$p(2 \times 1)_a : \quad \quad \quad J_{\parallel} + \quad J_{\perp} + \cos(\vartheta^{(3)} p) h = E_0 + E_{p(2 \times 1)} \quad (5.30)$$

$$p(4 \times 1) : \quad \quad \quad J_{\parallel} + \cos(4\vartheta^{(4)}) \quad J_{\perp} + \cos(\vartheta^{(4)} p) h = E_0 + E_{p(4 \times 1)} \quad (5.31)$$

I am not sure whether the NN interaction describes the  $(4 \times 1)$  (or some other configurations) correctly. I think that  $J_{\perp}$  is effectively antiferromagnetic is only valid in the  $c(4 \times 2)$  configuration. I think the equations for  $p(2 \times 1)_a$  and  $p(4 \times 1)$  are just wrong and have to include diagonal interactions. This would add another parameter to my calculation and I would need another configuration energy. Including NNN interactions, so the diagonal interaction  $J_x$  we get for the system of equations from above: WAIT this is wrong right? The  $J_x$  should not have the cosine prefactor in the first line since the diagonal neighbors have the same buckling

angle

$$\cos(4\vartheta^{(1)})J_{||} + \cos(4\vartheta^{(1)})J_{\perp} - 2\cos(4\vartheta^{(1)})J_{\times} + \cos(\vartheta^{(1)}p)h = E_0 \quad (5.32)$$

$$\cos(4\vartheta^{(2)})J_{||} + J_{\perp} - 2J_{\times} + \cos(\vartheta^{(2)}p)h = E_0 + E^{(2)} \quad (5.33)$$

$$J_{||} + J_{\perp} + 2J_{\times} + \cos(\vartheta^{(3)}p)h = E_0 + E^{(3)} \quad (5.34)$$

$$J_{||} + \cos(4\vartheta^{(4)})J_{\perp} + 2\cos(4\vartheta^{(4)})J_{\times} + \cos(\vartheta^{(4)}p)h = E_0 + E^{(4)} \quad (5.35)$$

$$J_{||} + J_{\perp} + 2J_{\times} + \cos\left(\frac{\pi}{2}p\right)h = E_0 + E^{(5)} \quad (5.36)$$

$$\cos(4\vartheta^{(1)})J_{||} + \cos(4\vartheta^{(1)})J_{\perp} + 2J_{\times} + \cos(\vartheta^{(1)}p)h = E_0 \quad (5.37)$$

$$\cos(4\vartheta^{(2)})J_{||} + J_{\perp} + 2\cos(4\vartheta^{(2)})J_{\times} + \cos(\vartheta^{(2)}p)h = E_0 + E^{(2)} \quad (5.38)$$

$$J_{||} + J_{\perp} + 2J_{\times} + \cos(\vartheta^{(3)}p)h = E_0 + E^{(3)} \quad (5.39)$$

$$J_{||} + \cos(4\vartheta^{(4)})J_{\perp} + 2\cos(4\vartheta^{(4)})J_{\times} + \cos(\vartheta^{(4)}p)h = E_0 + E^{(4)} \quad (5.40)$$

$$J_{||} + J_{\perp} + 2J_{\times} + \cos\left(\frac{\pi}{2}p\right)h = E_0 + E^{(5)} \quad (5.41)$$

where we added another equation for the  $p(2 \times 1)_s$  configuration where its angle is defined to be  $\vartheta^{(5)} = \pi/2$ . We need that one as we have to determine another coupling constant now. We could use the values from Inoue et al. as they have those 5 configurations that we want to use, but I am not sure whether those values are accurate and we don't really know the angles, we only know the  $\Delta z$  displacement but not the bond length. We can eliminate  $E_0$  from the equations by subtracting the  $c(4 \times 2)$  configuration energy to obtain:

$$(\cos(4\vartheta^{(2)} - \cos(4\vartheta^{(1)}))J_{||} + (1 - \cos(4\vartheta^{(1)}))J_{\perp} - 2(1 - \cos(4\vartheta^{(1)})) \quad (5.42)$$

$$(1 - \cos(4\vartheta^{(1)}))J_{||} + (1 - \cos(4\vartheta^{(1)}))J_{\perp} + 2(1 + \cos(4\vartheta^{(1)})) \quad (5.43)$$

$$J_{||} + \cos(4\vartheta^{(4)})J_{\perp} + 2\cos(4\vartheta^{(4)})J_{\times} + \cos(\vartheta^{(4)}p)h \quad (5.44)$$

$$J_{||} + J_{\perp} + 2J_{\times} + \cos\left(\frac{\pi}{2}p\right)h \quad (5.45)$$

Approximating that  $\varphi^{(i)} = 19^\circ$  so  $\vartheta^{(i)} = \vartheta = 81^\circ = 1.42$  the prior equation system simplifies

to

$$0 \quad J_{\parallel} + (1 - \cos(4\vartheta))J_{\perp} + 2(\cos(4\vartheta) - 1)J_{\times} + 0h = E_{p(2 \times 2)} \quad (5.46)$$

$$(1 - \cos(4\vartheta))J_{\parallel} + 0J_{\perp} + 2(\cos(4\vartheta) - 1)J_{\times} + 0h = E_{p(4 \times 1)} \quad (5.47)$$

$$(1 - \cos(4\vartheta))J_{\parallel} + (1 - \cos(4\vartheta))J_{\perp} + 0J_{\times} + 0h = E_{p(2 \times 1)} \quad (5.48)$$

Fitting yields

$$J_{\parallel} = 115.6 \text{ meV} \Rightarrow j_{\parallel} = 150000 \quad (5.49)$$

$$J_{\perp} = -17.3 \text{ meV} \quad (5.50)$$

$$J_{\times} = -9.5 \text{ meV} \quad (5.51)$$

$$J_{\perp}^{eff} = J_{\perp} - 2J_{\times} = 1.8 \text{ meV} \Rightarrow j_{\perp} = 2340 \quad (5.52)$$

Dabrowski and Scheffler [12] describe the movement of the dimer to be in a double well potential with a barrier height of  $E_B = 100$  meV. The same argumentation can be applied to [20] leading to  $E_B = 170$  meV. In our model the potential barrier can be specified as

$$h \left(1 + \cos\left(p \frac{\pi}{2}\right)\right) = E_B . \quad (5.53)$$

Together with Equation 5.24 we have two more equations at hand to determine the location of the minimum  $p$  and strength  $h$  of the symmetry breaking field. Fitting with the  $E_B$  value of Inoue et. al yields

$$h = 1324 \text{ meV} \Rightarrow h_{num} = 1722500 \quad (5.54)$$

$$p = 2.33 \quad (5.55)$$

The numerical values are very large, this would mean that we would have to decrease the stepsize to ensure numerical stability, but then the quenches and stuff would take a really short time in real time? Is this a problem? The equilibration and stuff should not take longer right because everything should be scale invariant. If we calculate the critical temperature that the bare XY model would have with the current values we would get

$$T_c = \quad (5.56)$$

### 5.3.5 other

## 5.4 Discussion

# **6 Summary and Lookout**

## **6.1 Summary**

## **6.2 Lookout**



# A Appendix

## A.1 Caldeira-Leggett calculation

Starting point for this calculation is Equation 4.28. Consider the trace in the second term in Equation 4.28:

$$\text{tr}_B \left\{ \left[ \hat{H}_I, \left[ \hat{\mathbf{H}}_I(-\tau), \hat{\rho}_S(t) \otimes \bar{\rho}_B \right] \right] \right\} = \text{tr}_B \left\{ \left[ \hat{x} \otimes \hat{B}, \left[ \hat{\mathbf{x}}(-\tau) \otimes \hat{\mathbf{B}}(-\tau), \hat{\rho}_S(t) \otimes \bar{\rho}_B \right] \right] \right\}. \quad (\text{A.1})$$

Multiplying out the commutator yields

$$(\text{A.1}) = \text{tr}_B \left\{ +\hat{x}\hat{\mathbf{x}}(-\tau)\hat{\rho}_S(t) \otimes \hat{B}\hat{\mathbf{B}}(-\tau)\bar{\rho}_B - \hat{x}\hat{\rho}_S(t)\hat{\mathbf{x}}(-\tau) \otimes \hat{B}\bar{\rho}_B\hat{\mathbf{B}}(-\tau) \right. \\ \left. - \hat{\mathbf{x}}(-\tau)\hat{\rho}_S(t)\hat{x} \otimes \hat{\mathbf{B}}(-\tau)\bar{\rho}_B\hat{B} + \hat{\rho}_S(t)\hat{x}\hat{\mathbf{x}}(-\tau) \otimes \bar{\rho}_B\hat{\mathbf{B}}(-\tau)\hat{B} \right\}. \quad (\text{A.2})$$

The factors belonging to the Hilbert space of the system can be pulled out of the trace. Additionally we use the cyclic property of the trace as well as the expectation value representation  $\langle \hat{A} \rangle = \text{tr}(\hat{A}\rho)$  to obtain

$$(\text{A.2}) = \left( \hat{x}\hat{\mathbf{x}}(-\tau)\hat{\rho}_S(t) - \hat{\mathbf{x}}(-\tau)\hat{\rho}_S(t)\hat{x} \right) \langle \hat{B}\hat{\mathbf{B}}(-\tau) \rangle \\ + \left( \hat{\rho}_S(t)\hat{\mathbf{x}}(-\tau)\hat{x} - \hat{x}\hat{\rho}_S(t)\hat{\mathbf{x}}(-\tau) \right) \langle \hat{\mathbf{B}}(-\tau)\hat{B} \rangle. \quad (\text{A.3})$$

We can rewrite  $\langle \hat{B}\hat{\mathbf{B}}(-\tau) \rangle = \frac{1}{2}\langle [\hat{B}, \hat{\mathbf{B}}(-\tau)] \rangle + \langle \{\hat{B}, \hat{\mathbf{B}}(-\tau)\} \rangle$  and likewise  $\langle \hat{\mathbf{B}}(-\tau)\hat{B} \rangle$  which yields

$$(\text{A.3}) = \frac{1}{2} \left\langle \left[ \hat{B}, \hat{\mathbf{B}}(-\tau) \right] \right\rangle \left( +\hat{x}\hat{\mathbf{x}}(-\tau)\hat{\rho}_S(t) + \hat{x}\hat{\rho}_S(t)\hat{\mathbf{x}}(-\tau) - \hat{\mathbf{x}}(-\tau)\hat{\rho}_S(t)\hat{x} \right. \\ \left. - \hat{\rho}_S(t)\hat{\mathbf{x}}(-\tau)\hat{x} \right) \\ \frac{1}{2} \left\langle \left\{ \hat{B}, \hat{\mathbf{B}}(-\tau) \right\} \right\rangle \left( \hat{x}\hat{\mathbf{x}}(-\tau)\hat{\rho}_S(t) - \hat{x}\hat{\rho}_S(t)\hat{\mathbf{x}}(-\tau) - \hat{\mathbf{x}}(-\tau)\hat{\rho}_S(t)\hat{x} \right. \\ \left. + \hat{\rho}_S(t)\hat{\mathbf{x}}(-\tau)\hat{x} \right). \quad (\text{A.4})$$

The position operator terms can be combined to

$$[\hat{x}, \{\hat{\mathbf{x}}(-\tau), \hat{\rho}_S(t)\}] = \hat{x}\hat{\mathbf{x}}(-\tau)\hat{\rho}_S(t) + \hat{x}\hat{\rho}_S(t)\hat{\mathbf{x}}(-\tau) - \hat{\mathbf{x}}(-\tau)\hat{\rho}_S(t)\hat{x} - \hat{\rho}_S(t)\hat{\mathbf{x}}(-\tau)\hat{x} \quad (\text{A.5})$$

$$[\hat{x}, [\hat{\mathbf{x}}(-\tau), \hat{\rho}_S(t)]] = \hat{x}\hat{\mathbf{x}}(-\tau)\hat{\rho}_S(t) - \hat{x}\hat{\rho}_S(t)\hat{\mathbf{x}}(-\tau) - \hat{\mathbf{x}}(-\tau)\hat{\rho}_S(t)\hat{x} + \hat{\rho}_S(t)\hat{\mathbf{x}}(-\tau)\hat{x} . \quad (\text{A.6})$$

Plugging Equation A.5 into Equation A.4 yields for the trace of Equation A.2:

$$\begin{aligned} \text{tr}_B \left\{ \left[ \hat{H}_I, \left[ \hat{\mathbf{H}}_I(-\tau), \hat{\rho}_S(t) \otimes \bar{\rho}_B \right] \right] \right\} &= \frac{1}{2} \left\langle \left[ \hat{B}, \hat{\mathbf{B}}(-\tau) \right] \right\rangle [\hat{x}, \{\hat{\mathbf{x}}(-\tau), \hat{\rho}_S(t)\}] \\ &\quad \frac{1}{2} \left\langle \left\{ \hat{B}, \hat{\mathbf{B}}(-\tau) \right\} \right\rangle [\hat{x}, [\hat{\mathbf{x}}(-\tau), \hat{\rho}_S(t)]] \end{aligned} \quad (\text{A.7})$$

We will now try to find expressions for  $\langle [\hat{B}, \hat{\mathbf{B}}(-\tau)] \rangle$  and  $\langle \{\hat{B}, \hat{\mathbf{B}}(-\tau)\} \rangle$ . The interaction picture operator  $\hat{\mathbf{B}}(-\tau)$  can be calculated by it's definition

$$\begin{aligned} \hat{\mathbf{B}}(-\tau) &= e^{i\hat{H}_B(-\tau)} \hat{B} e^{-i\hat{H}_B(-\tau)} = e^{i\hat{H}_B(-\tau)} \sum_n \kappa_n \sqrt{\frac{\hbar}{2m_n\omega_n}} \left( \hat{b}_n + \hat{b}_n^\dagger \right) e^{-i\hat{H}_B(-\tau)} \\ &= \sum_n \kappa_n \sqrt{\frac{\hbar}{2m_n\omega_n}} \left( \hat{\mathbf{b}}_n(-\tau) + \hat{\mathbf{b}}_n^\dagger(-\tau) \right) . \end{aligned} \quad (\text{A.8})$$

For the transformation of the bosonic creation and annihilation operators one can derive a differential equation

$$\begin{aligned} \frac{d}{dt} \hat{\mathbf{b}}_n^{(\dagger)}(-\tau) &= \frac{d}{dt} \left( e^{-i\hat{H}_B\tau} \hat{b}_n^{(\dagger)} e^{i\hat{H}_B\tau} \right) = -i e^{-i\hat{H}_B\tau} \left[ \hat{H}_B, \hat{b}_n^{(\dagger)} \right] e^{i\hat{H}_B\tau} \\ &= (-i) e^{-i\hat{H}_B\tau} \hat{b}_n^{(\dagger)} e^{i\hat{H}_B\tau} = (-i)\omega_n \hat{\mathbf{b}}_n^{(\dagger)}, \end{aligned} \quad (\text{A.9})$$

and solve it under the initial condition  $\hat{\mathbf{b}}_n^{(\dagger)}(0) = \hat{b}_n^{(\dagger)}$ . The solution to Equation A.9 is

$$\hat{\mathbf{b}}_n^{(\dagger)}(-\tau) = \hat{b}_n^{(\dagger)} e^{(-i)\omega_n\tau}, \quad (\text{A.10})$$

leading to

$$\hat{\mathbf{B}}(-\tau) = \sum_n \kappa_n \sqrt{\frac{\hbar}{2m_n\omega_n}} \left( \hat{b}_n e^{i\omega_n\tau} + \hat{b}_n^\dagger e^{-i\omega_n\tau} \right) . \quad (\text{A.11})$$

Now we can calculate the commutator  $[\hat{B}, \hat{\mathbf{B}}(-\tau)]$ :

$$\begin{aligned}
[\hat{B}, \hat{\mathbf{B}}(-\tau)] &= \sum_{n,k} \frac{\kappa_n \kappa_k}{2\sqrt{\omega_n \omega_k}} \left[ \hat{b}_n^\dagger + \hat{b}_n, \hat{b}_k e^{i\omega_k \tau} + \hat{b}_k^\dagger e^{-i\omega_k \tau} \right] \\
&= \sum_{n,k} \frac{\kappa_n \kappa_k}{2\sqrt{\omega_n \omega_k}} \left\{ [\hat{b}_n^\dagger, \hat{b}_k] e^{i\omega_k \tau} + [\hat{b}_n, \hat{b}_k^\dagger] e^{-i\omega_k \tau} \right\} \\
&= \sum_{n,k} \frac{\kappa_n \kappa_k}{2\sqrt{\omega_n \omega_k}} \left\{ \delta_{nk} e^{-i\omega_k \tau} - \delta_{nk} e^{i\omega_k \tau} \right\} \\
&= \sum_n \frac{\kappa_n^2}{2\omega_n^2} \left\{ e^{-i\omega_k \tau} - e^{i\omega_k \tau} \right\} \\
&= -2i \sum_n \frac{\kappa_n^2}{2\omega_n^2} \sin \omega_n \tau
\end{aligned} \tag{A.12}$$

Since this is a constant  $\langle [\hat{B}, \hat{\mathbf{B}}(-\tau)] \rangle = [\hat{B}, \hat{\mathbf{B}}(-\tau)]$ . By introducing the reservoir spectral density

$$J(\omega) = \sum_n = \frac{\kappa_n^2}{2\omega_n} \delta(\omega - \omega_n) , \tag{A.13}$$

Equation A.12 may be written as an integral

$$\langle [\hat{B}, \hat{\mathbf{B}}(-\tau)] \rangle = -2i \int_0^\infty d\omega J(\omega) \sin \omega \tau . \tag{A.14}$$

Under Born approximation, the reservoir is in thermal equilibrium so that the density matrix can be written as

$$\bar{\rho}_B = \frac{e^{-\beta H_B}}{\text{tr}(e^{-\beta H_B})} = \frac{1}{Z} e^{-\beta H_B} . \tag{A.15}$$

## A.2 Correlation Length calculation

The two-point equal time correlation function of the XY model in 2D is defined as

$$C(x, y) = \langle \vec{s}_{0,0} \vec{s}_{x,y} \rangle . \tag{A.16}$$

The brackets  $\langle \cdot \rangle$  denote the ensemble average

$$\langle \vec{s}_{0,0} \vec{s}_{x,y} \rangle = \frac{1}{Z} \int \prod_i d\vartheta_i \vec{s}_{0,0} \vec{s}_{x,y} e^{-\beta H(\{\vartheta\})} \tag{A.17}$$

I don't know where you have this definition from but i guess you can calculate it like this in the case of discrete states. But in XY model we don't have discrete states?

For the 2D anisotropic Ising Model, we can write down the Correlation Function in the limit for large distances as

$$C(x, y) \sim \frac{f_{\gtrless}(\theta)}{r^{\vartheta_{\gtrless}}} e^{-r/\xi_{\gtrless}(\theta)} \quad \text{with} \quad r = \sqrt{x^2 + y^2}. \quad (\text{A.18})$$

With known Functions  $f_{\gtrless}(\theta)$  and  $\xi_{\gtrless}(\theta)$  depending on the angle of the correlation vector and the Temperature  $T \gtrless T_c$ . We also know from mean field theory that (No, we also know from KT and stuff that the correlation function decays exponentially above the critical temperature [27, 16])

$$C(x, y) \sim e^{-r(x,y)/\xi(x,y)}. \quad (\text{A.19})$$

We hope that the correlation function of the XY model has a similar form and proceed.

This is the definition of the correlation length  $\xi$ . The correlation length is a measure for the lengthscale over which perturbations of a system relax in space.

We are mainly interested in the correlation lengths in the directions along and across the dimer row and therefore define the correlation functions in those directions as

$$C_{\perp}(x) = \langle \vec{s}_{0,0} \vec{s}_{x,0} \rangle \sim e^{-x/\xi_{\perp}} \quad \text{and} \quad C_{\parallel}(y) = \langle \vec{s}_{0,0} \vec{s}_{0,y} \rangle \sim e^{-y/\xi_{\parallel}}. \quad (\text{A.20})$$

Consider the fourier transforms of  $C_{\delta}(r)$

$$S_{\delta}(k) = \sum_{r=0}^{N_{\delta}-1} C_{\delta}(r) e^{-2\pi i \frac{kr}{N_{\delta}}}, \quad (\text{A.21})$$

with  $N_{\delta}$  being the number of lattice sites in the direction of  $\delta$ . Set now without loss of generality  $\delta = \perp$  to obtain

$$\begin{aligned} S_{\perp}(k) &= \sum_{x=0}^{N_{\perp}-1} C_{\perp}(x) e^{-2\pi i \frac{kx}{N_{\perp}}} = \sum_{x=0}^{N_{\perp}-1} \langle \vec{s}_{0,0} \vec{s}_{x,0} \rangle e^{-2\pi i \frac{kx}{N_{\perp}}} = \sum_{x=0}^{N_{\perp}-1} \langle s_{0,0}^0 s_{x,0}^0 \rangle e^{-2\pi i \frac{kx}{N_{\perp}}} \\ &\quad + \sum_{x=0}^{N_{\perp}-1} \langle s_{0,0}^1 s_{x,0}^1 \rangle e^{-2\pi i \frac{kx}{N_{\perp}}}. \end{aligned} \quad (\text{A.22})$$

The ensemble average can be computed by a sum over an infinite lattice

$$\langle s_{0,0}^{\kappa} s_{x,0}^{\kappa} \rangle = \lim_{N_{\perp} \rightarrow \infty} \lim_{N_{\parallel} \rightarrow \infty} \frac{1}{N_{\perp} N_{\parallel}} \sum_{i=0}^{N_{\perp}} \sum_{j=0}^{N_{\parallel}} s_{i,j}^{\kappa} s_{i+x,j}^{\kappa}. \quad (\text{A.23})$$

An approximation is possible by using a finite lattice with large dimensions  $N_{\delta}$ . Inserting Equation A.23 into Equation A.22 and replacing the sum  $\sum_x$  with a sum over  $q = i + x$  yields

$$S_{\perp}(k) = \frac{1}{N_{\perp}N_{\parallel}} \sum_{\kappa,q,i,j} s_{i,j}^{\kappa} s_{q,j}^{\kappa} e^{-2\pi i \frac{k(q-i)}{N_{\perp}}} = \frac{1}{N_{\perp}N_{\parallel}} \sum_{\kappa,q,i,j} \left( \sum_{p=0}^{N_{\parallel}} \delta_{p,j} \right) s_{i,j}^{\kappa} s_{q,p}^{\kappa} e^{-2\pi i \frac{k(q-i)}{N_{\perp}}}. \quad (\text{A.24})$$

In the second step we have inserted a productive one in the form of a sum over a Kronecker delta. The Kronecker delta can be written as a sum over complex exponentials

$$\delta_{p,j} = \frac{1}{N_{\parallel}} \sum_{l=1}^{N_{\parallel}} e^{2\pi i \frac{l(j-p)}{N_{\parallel}}}. \quad (\text{A.25})$$

Inserting this representation into Equation A.24 gives

$$\begin{aligned} S_{\perp}(k) &= \frac{1}{N_{\perp}N_{\parallel}^2} \sum_l \sum_{\kappa} \sum_{q,p,i,j} s_{i,j}^{\kappa} s_{q,p}^{\kappa} e^{-2\pi i \frac{k(q-i)}{N_{\perp}}} e^{2\pi i \frac{l(p-j)}{N_{\parallel}}} \\ &= \frac{1}{N_{\perp}N_{\parallel}^2} \sum_l \sum_{\kappa} \left( \sum_{i,j} s_{i,j}^{\kappa} e^{2\pi i \left( \frac{ki}{N_{\perp}} + \frac{lj}{N_{\parallel}} \right)} \right) \left( \sum_{q,p} s_{q,p}^{\kappa} e^{-2\pi i \left( \frac{kq}{N_{\perp}} + \frac{lp}{N_{\parallel}} \right)} \right). \end{aligned} \quad (\text{A.26})$$

The expressions in the parentheses are the fourier transforms  $\tilde{s}_{k,l}^{\kappa}$ , or respectively the conjugated fourier transform, of the  $s_{i,j}^{\kappa}$  lattice:

$$\begin{aligned} S_{\perp}(k) &= \frac{1}{N_{\perp}N_{\parallel}^2} \sum_l \sum_{\kappa} \left( \tilde{s}_{k,l}^{\kappa} \right)^* \tilde{s}_{k,l}^{\kappa} \\ &= \frac{1}{N_{\perp}N_{\parallel}^2} \left( \sum_l |\tilde{s}_{k,l}^0|^2 + \sum_l |\tilde{s}_{k,l}^1|^2 \right). \end{aligned} \quad (\text{A.27})$$

This way we can calculate  $S_{\perp}(k)$  by calculating the 2D fourier transforms of the lattices  $s_{i,j}^0 = \cos \vartheta_{i,j}$  and  $s_{i,j}^1 = \sin \vartheta_{i,j}$ . The analogue result is valid for  $S_{\parallel}(k)$ .

To eventually extract the correlation length, we consider again Equation A.24 and insert the asymptotic behavior of  $C_{\delta}$  Equation A.20 to obtain

$$S_{\delta}(k) \sim \sum_r^{N_{\delta}-1} e^{-|r|/\xi_{\delta}} e^{-2\pi i \frac{kr}{N_{\delta}}} = \frac{2\xi_{\delta}}{1 + 4\pi^2 \xi_{\delta}^2 k^2}, \quad (\text{A.28})$$

showing that  $S_{\delta}(k)$  behaves like a lorentzian function around  $k = 0$ . Calculating  $S_{\delta}(k)$  by means of Equation A.27 and fitting to the lorentzian Equation A.28 yields  $\xi_{\delta}$  as fitting parameter.

### A.3 Error calculation on moving averages

[34] (appendix C) An average  $\bar{f}$  that is calculated by the means of Equation 5.7 has a non trivial relationship with it's variance  $\sigma_{\bar{f}}$ . The reason for this is that  $f(t)$  and  $f(t + mdt)$  might be, and most probably are, correlated. This means that observables at different times are not independent of each other and therefore have to be treated accordingly.

As a reminder, the average  $\bar{f}$  is calculated as

$$\bar{f} = f_T = \frac{1}{T} \int_0^T ds f(s) , \quad (\text{A.29})$$

with  $T$  being the total time of the simulation or the the time interval we want to average over. To estimate the error on  $f_T$  we consider the variance of the average  $f_T$  ([13] appendix D, [2] (p. 438 ff))

$$\begin{aligned} \sigma_{\bar{f}}^2 &= \langle f_T^2 \rangle - \langle f_T \rangle^2 \\ &\approx \frac{1}{T} \int_{-\infty}^{\infty} dt C_f(t), \end{aligned} \quad (\text{A.30})$$

with  $C_f(t)$  being the autocorrelation or time correlation function

$$C_f(t) = \langle f(s)f(s+t) \rangle - \langle f(s) \rangle^2 . \quad (\text{A.31})$$

The step performed in Equation A.30 is valid in the limit of  $T \gg \tau_C$ , that the sampling time  $T$  is much larger than the characteristic decay time of the autocorrelation function  $\tau_C$ .  $\tau_C$  is defined as

$$\tau_C = \frac{1}{2} \int_{-\infty}^{\infty} dt C_f(t)/C_f(0) . \quad (\text{A.32})$$

So that we can express  $\sigma_{\bar{f}}^2$  in terms of  $\tau_C$

$$\sigma_{\bar{f}}^2 = \frac{2\tau_C}{T} C_f(0) . \quad (\text{A.33})$$

Looking at Equation A.31, we can see that  $C_f(0)$  reduces to the variance of  $f$

$$C_f(0) = \sigma_f^2 . \quad (\text{A.34})$$

Rewriting  $T = n_s \tau_s$  with  $n_s$  being the number of measured samples and  $\tau_s$  being the time

between the samples, the variance of the mean  $\bar{f}$  can be expressed as

$$\sigma_{\bar{f}}^2 = \frac{2\tau_C}{\tau_s} \frac{\sigma_f^2}{n_s}, \quad (\text{A.35})$$

revealing that the variance of  $\bar{f}$  is by a factor of  $\frac{2\tau_c}{\tau_s}$  larger than the naive approach of uncorrelated measurements would yield. Since it is practically not possible to integrate Equation A.31 from  $-\infty$  to  $\infty$ , we approximate  $\tau_c$  by

$$\tau_C \approx \frac{1}{2} \int_{-T/2}^{T/2} dt C_f(t)/C_f(0). \quad (\text{A.36})$$



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## **Erklärung**

Hiermit erkläre ich, dass ich diese Arbeit im Rahmen der Betreuung am Institut für ??? Physik ohne unzulässige Hilfe Dritter verfasst und alle Quellen als solche gekennzeichnet habe.

Vorname Nachname  
Dresden, Monat 2019