Non-equilibrium phase transitions
An Introduction

Lecture I

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\mode<presentation>{{
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\usepackage[english]{babel}
\usepackage[latin1]{inputenc}
\usepackage{helvet}
\usepackage[T1]{fontenc}
\usepackage{graphicx}
\usepackage{multimedia}
\title{Non-equilibrium phase transitions}
\subtitle{An Introduction}
\author{Haye Hinrichsen}
\institute{University of W"rzburg, Germany}
Outline

1. Introduction
   - Stochastic Many-Particle Systems
   - Equilibrium Statistical Mechanics
   - Equilibrium and Nonequilibrium Dynamics

2. Directed Percolation
   - From Isotropic to Directed Percolation
   - The DP Phase Transition
   - DP Lattice Models
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Classical Statistical Physics

- At a given instance of time the system is in a certain configuration $c$.
- All possible configurations $c$ form a set of configurations $\mathcal{C}$.
- Transitions $c \rightarrow c'$ from one configuration to a different one occur spontaneously at a certain rate $w_{c\rightarrow c'}$. 
Transition rates

Configurations $c$

Transition rates $w_{c \rightarrow c'}$

$c1$

$c4$

$c3$

$c2$
...trivial, but often a source of mistakes...

- Rates are **probabilities per unit time**.
- Rates carry the same dimension as $1/t$.
- The numerical value of a rate can be larger than 1.
- In a computer simulation rates have to be multiplied by a time interval $\Delta t$ to get a probability.

```plaintext
if (w*dt < random(0,1)) ...
```
1. Choose an initial configuration and set $t = 0$.

2. Compute total outgoing rate $W_c = \sum_{c' \in C} w_{c \rightarrow c'}$.

3. Select new configuration $c'$ with probability $w_{c \rightarrow c'} / W_c$.

4. Increase $t$ by $1 / W_c^*$.

5. Monitor quantities of interest and continue while $t < t_{max}$.

* Approximation, good if $t \gg 1 / W_c$
Approximation:

Poisson statistics (like radioactive decay) → regular intervals

Spontaneous events:

Regular time increments:
The individual trajectory of a classical stochastic system is unpredictable.

**Probability Distribution**

\[ P_t(c) \] is the probability to find the system at time \( t \) in the configuration \( c \).

\[
\sum_{c \in C} P_t(c) = 1
\]

The evolution of \( P_t(c) \) is predictable.
The **master equation** is a linear deterministic evolution equation that describes the flow of probability:

\[
\frac{\partial}{\partial t} P_t(c) = \sum_{c'} w_{c' \rightarrow c} P_t(c') - \sum_{c'} w_{c \rightarrow c'} P_t(c) .
\]

In the continuum also called **Fokker-Planck equation**. *(do not mix up with Langevin equations, see below.)*
List all the probabilities in a vector:

$$|P_t\rangle = \begin{pmatrix} P_t(c_1) \\ P_t(c_2) \\ P_t(c_3) \\ \vdots \end{pmatrix} \in [0, 1]^{\otimes |\mathcal{C}|}$$

Write Master equation in a compact form:

$$\partial_t |P_t\rangle = -\mathcal{L} |P_t\rangle$$

$\mathcal{L}$ is called **Liouville operator**.
The Lioville operator $\mathcal{L}$ is defined by the matrix elements

$$\langle c' | \mathcal{L} | c \rangle = -w_{c \rightarrow c'} + \delta_{c, c'} \sum_{c''} w_{c \rightarrow c''}.$$  

Formal solution:

$$|P_t\rangle = e^{-\mathcal{L}t} |P_0\rangle,$$

where $|P_0\rangle$ is the initial probability distribution at $t = 0$

...looks like quantum mechanics...
Compact Notation – Conservation of Probability

Probability conservation

\[ \sum_{c \in C} P_t(c) = 1 \]

can be expressed as

\[ \langle 1 | P_t \rangle = 1 , \]

where

\[ \langle 1 | := \sum_{c \in C} \langle c | = (1, 1, 1, 1, \ldots, 1) \]

\[ \Rightarrow \langle 1 | \mathcal{L} = 0 \]
Compact Notation – Structure of $\mathcal{L}$

The matrix of the time evolution operator in configuration basis

- has positive entries on the diagonal,
- has negative non-diagonal entries,
- and **the sum over columns vanishes**.

Example: $\mathcal{L} = \begin{pmatrix} 2 & -3 & -5 \\ -1 & 5 & -1 \\ -1 & -2 & 6 \end{pmatrix}$

Such matrices are called **intensity matrices**.
Solving the Master Equation by Diagonalization

The master equation can be solved by **diagonalization** of $\mathcal{L}$:

1. Solve eigenvalue problem:

   $$\mathcal{L}|\phi_i\rangle = \lambda_i |\phi_i\rangle$$

2. Express initial state $|P_0\rangle$ in terms of eigenvectors:

   $$|P_0\rangle = \sum_i a_i |\phi_i\rangle$$

3. Write down the solution:

   $$|P_t\rangle = e^{-\mathcal{L}t}|P_0\rangle = \sum_i a_i e^{-\lambda_i t} |\phi_i\rangle$$

   *solution = sum over exponentially decaying eigenmodes*
The time evolution operator

- is non-Hermitean, meaning that left and right eigenvectors to the same eigenvalue may have different representations.
- Because of \( \langle 1 | \mathcal{L} = 0 \) there is at least one eigenvalue \( \lambda_0 = 0 \), representing the stationary state.
- All eigenvalues have a non-negative real part.
- Eigenvalues may occur in complex-conjugate pairs.

complex? damped oscillations?
Complex Eigenvalues of $\mathcal{L}$ – Chemical Oscillations

Belusov-Zhabotinsky-Reaction

\[
\begin{align*}
\text{BrO}_3^- + \text{Br}^- &\rightarrow \text{HBrO}_2 + \text{HOBr} \\
\text{HBrO}_2 + \text{Br}^- &\rightarrow 2\text{HOBr} \\
\text{BrO}_3^- + \text{HBrO}_2 &\rightarrow 2\text{HBrO}_2 + 2\text{Ce}^{4+} \\
2\text{HBrO}_2 &\rightarrow \text{BrO}_3^- + \text{HOBr} \\
\text{Br}^- + \text{Ce}^{4+} &\rightarrow 1/2\text{Br}^- 
\end{align*}
\]

http://online.redwoods.cc.ca.us/instruct/darnold/deproj/
Chemical oscillations occur in activator-inhibitor reactions:
Complex Conjugate Eigenvalues - Chemical Oscillations

Even spatio-temporal oscillations can be observed...
Complex Conjugate Eigenvalues - Chemical Oscillations

...and may be simulated by partial differential equations:
Classical Stochastic Dynamics compared to Quantum Mechanics

<table>
<thead>
<tr>
<th>Quantum Mechanics</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\int \psi^*(x)\psi(x)dx = 1$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Classical Stochastic Dynamics</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sum_c P_t(c) = 1$</td>
</tr>
</tbody>
</table>

...look similar, but differ significantly.
Relaxation times

- The relaxation time of an eigenmode $|\phi_i\rangle$ is $(\text{Re} \lambda_i)^{-1}$

- Systems with finite configuration space relax to their stationary state exponentially within finite time determined by the eigenvalue with the smallest real part.

- Conversely: Systems exhibiting infinite relaxation times or power laws must have an infinite configuration space.
Relaxation times

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- Conversely: Systems exhibiting infinite relaxation times or power laws must have an infinite configuration space.
Spectrum of the Time Evolution Operator

Relaxation times

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System in Equilibrium with a Heat Bath
In equilibrium Nature maximizes the entropy $S$ of the entire system.

The total entropy is extensive: $S = S_1 + S_2$

The total energy is conserved: $E = E_1 + E_2$

$$\Rightarrow \frac{\partial S_1}{\partial E_1} = - \frac{\partial S_1}{\partial E_1} = \frac{\partial S_2}{\partial E_2}$$

$\Rightarrow$ The quantity $\frac{1}{T} := \frac{\partial S}{\partial E}$ is the same in both subsystems.

**Temperature** $\Leftrightarrow$ equilibrium & energy conservation.
Compute the probability to find system 1 in a certain configuration $c$.

\[ P(c) \propto \# \text{ of possible configurations of the bath}. \]

\[
\begin{align*}
P(c) & \propto \exp \left( \frac{1}{k_B} S_2(E_2) \right) = \exp \left( \frac{1}{k_B} S_2(E - E_1) \right) \\
& \approx \exp \left( \frac{1}{k_B} \left( S_2(E) - \frac{\partial S_2(E)}{\partial E} E_1 + \ldots \right) \right) \\
& \propto \exp \left( - \frac{E_1}{k_B T} \right).
\end{align*}
\]
Equilibrium Statistical Mechanics

- In **equilibrium** statistical mechanics there is no notion of *time*.

- Equilibrium models are defined by an energy functional $c \rightarrow E(c)$.

- In equilibrium statistical mechanics we get the probability distribution for free!

---

- **Nonequilibrium** models are defined by a set of transition rates.

- In nonequilibrium statistical mechanics the probability distribution is obtained by solving the master equation.
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There are two types of stochastic dynamical processes:

1. **Equilibrium dynamics:**
   Dynamical processes which relax towards a stationary state described by an equilibrium ensemble.

2. **Nonequilibrium dynamics:**
   All other processes.
Equilibrium and Nonequilibrium Dynamics

All systems with stochastic dynamics
Equilibrium and Nonequilibrium Dynamics

Equilibrium dynamics

Non-equilibrium dynamics
Equilibrium and Nonequilibrium Dynamics

- Ising
- Potts
- Non-equilibrium dynamics
Example:
The following dynamical processes

1. Ising Heat bath dynamics
2. Glauber-Ising model
3. Ising Metropolis dynamics
4. Ising Kawasaki dynamics*
5. Swendsen-Wang cluster algorithm
6. Wolf cluster algorithm
7. ...

relax towards a stationary state which is precisely the equilibrium ensemble of the Ising model.

Proof needed!
A system is said to obey **Detailed Balance** if the probability currents between pairs of configurations compensate each other:

\[ P_{eq}(c) w_{c \rightarrow c'} = P_{eq}(c') w_{c' \rightarrow c} . \]
Detailed Balance implies Stationarity ...

...but not vice versa:

\[ P(A) = P(B) = P(C) = \frac{1}{3} \]
Broken detailed balance in the stationary state implies that the stationary state of the system is **not** in equilibrium.

In particular, irreversible one-way flow...

...is always out of equilibrium.
Physical Conditions for Nonequilibrium

Non-stationary situations:
- quasi-equilibrium
- non-equilibrium
Physical Conditions for Nonequilibrium

Flow of energy through the system:
Physical Conditions for Nonequilibrium

Flow of particles through the system:
Continuous phase transitions at equilibrium:

- can be categorized into **universality classes**.
- are particularly well understood in two dimensions, where *conformal invariance* leads to a classification scheme.

**Nonequilibrium phase transitions**?
Phase transitions into absorbing states

An **absorbing state** is a configuration from where the system cannot escape:

![Mousetrap and mouse](borrowed from stud.fh-wedel.de)

Systems with *reachable* absorbing states are out of equilibrium.

Standard example: **Directed Percolation** (DP).
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From Isotropic to Directed Percolation
From Isotropic to Directed Percolation

isotropic percolation

directed percolation
Directed Percolation in a Random Diode Network
The preferred direction can be interpreted as time $t$. 

<table>
<thead>
<tr>
<th>$t$</th>
<th>$N(t)$</th>
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<tbody>
<tr>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
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<tr>
<td>5</td>
<td>2</td>
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<tr>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td>7</td>
<td>3</td>
</tr>
</tbody>
</table>
DP is easy to simulate

```c
#include "xwindows.h"

void GerichtetePerkolation (int N, double p, int T) 
{
    int i,j,r,t,s[N];
    for (i=1; i<=N; ++i) s[i]=1;
    for (t=0; t<T; ++t)
    {
        for (i=1; i<=N; ++i) if (s[i]) Plot(i,t);
        for (r=1; r<N; ++r)
        {
            i=rndint(N); j=(i+1)%N;
            if (s[i] or s[j])
            {
                if (rnd()<p) s[i]=s[j]=1;
                else s[i]=s[j]=0;
            }
        }
    }
}

void main (void)
{
    const double p=0.81;
    const int N=500, T=500;
    InitGeneral(); OpenWindow(N,T);
    GerichtetePerkolation (N,p,T);
}
DP is easy to simulate
DP as a Reaction-Diffusion Process

(a) death process \( A \rightarrow 0 \)
(b-c) diffusion
(d) offspring production \( A \rightarrow 2A \)
(e) coagulation \( 2A \rightarrow A \)
DP as a Simple Model for Epidemic Spreading

Infection:

Recovery:
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DP exhibits a Phase Transition

...starting with a fully active lattice:

\[ p < p_c \]  \[ p = p_c \]  \[ p > p_c \]
DP exhibits a Phase Transition

...starting with a single active site:

\[ \text{position } i \]

\[ p < p_c \] \[ p = p_c \] \[ p > p_c \]
Let us measure $\langle N(t) \rangle$ for various $q$.
#include <fstream.h>
using namespace std;
const int T=1000;    // number of updates
const int R=10000;   // number of independent runs
const double p=0.6447;  // percolation probability

double rnd(void) { return (double)rand()/0x7FFFFFFF; }

int main (void)
{
  int s[T][T],N[t],i,t,r;
  for (t=0; t<T; t++) N[t]=0;   // clear cumulative particle number
  for (r=0; r<R; r++) {   // loop over R runs
    s[0][0]=1;         // place initial seed
    for (t=0; t<T-1; t++) {     // temporal loop
      for (i=0; i<=t+1; ++i) s[t+1][i]=0;   // clear new config
      for (i=0; i<=t; ++i) if (s[t][i]==1) {   // loop over active sites
        N[t]++;               // count active sites
        if (rnd()<p) s[t+1][i]=1;       // random activation left
        if (rnd()<p) s[t+1][i+1]=1;     // random activation right
      }
    }
    ofstream os ("N.dat");         // write average N(t) to file
    for (t=0; t<T-1; t++) os << t << ' ' << (double)N[t]/R << endl;
}
Directed Percolation

This is the Output (via xmgrace):

\[
\begin{align*}
\langle N(t) \rangle & \quad p=0.7 \\
p & = 0.65 \\
p & = 0.6447 \text{ (critical)} \\
p & = 0.64 \\
p & = 0.6
\end{align*}
\]
Result for $\langle N(t) \rangle$:

- For $q < q_c$ $\langle N(t) \rangle$ crosses over to an **exponential** decay.
- For $q > q_c$ $\langle N(t) \rangle$ tends to a **linear** increase.
- At $q = q_c$ $\langle N(t) \rangle$ increases **algebraically** as $t^\theta$ with an exponent $\theta \approx 0.302$. 
**WARNING**: NEVER use the Standard Deviation:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Number of observations</td>
<td>998</td>
</tr>
<tr>
<td>Mean of independent variable</td>
<td>5.910134</td>
</tr>
<tr>
<td>Mean of dependent variable</td>
<td>1.911906</td>
</tr>
<tr>
<td>Standard dev. of ind. variable</td>
<td>0.9854415</td>
</tr>
<tr>
<td>Standard dev. of dep. variable</td>
<td>0.2973683</td>
</tr>
<tr>
<td>Correlation coefficient</td>
<td>0.9997551</td>
</tr>
<tr>
<td>Regression coefficient (SLOPE)</td>
<td>0.3016876</td>
</tr>
<tr>
<td>Standard error of coefficient</td>
<td>0.0002115986</td>
</tr>
<tr>
<td>t-value for coefficient</td>
<td>1425.754</td>
</tr>
<tr>
<td>Regression constant (INTERCEPT)</td>
<td>0.1288919</td>
</tr>
<tr>
<td>Standard error of constant</td>
<td>0.001267824</td>
</tr>
<tr>
<td>t-value for constant</td>
<td>101.6639</td>
</tr>
</tbody>
</table>

**Analysis of variance**

<table>
<thead>
<tr>
<th>Source</th>
<th>d.f</th>
<th>Sum of squares</th>
<th>Mean Square</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regression</td>
<td>1</td>
<td>188.11943</td>
<td>88.11943</td>
<td>2032775</td>
</tr>
<tr>
<td>Residual</td>
<td>996</td>
<td>0.04317594</td>
<td>8.334934e-05</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>997</td>
<td>88.16261</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ y = 1.1376 \times x^{0.30169} \]

Regression of set 0 results to set 1

**estimate**: 0.3017(2)

**true value**: 0.313686(8)
The exponent

$$\theta = 0.313686(8)$$

is the same in all realizations of DP.
It only depends on the dimension $d$.

DP stands for a **universality class**
of non-equilibrium phase transitions.

DP is the *'Ising model'* of non-equilibrium.
UNIVERSALITY

- All long-range properties, especially critical exponents and scaling functions, are universal, i.e., they are the same for all models in the DP universality class.

- Short-range properties and critical threshold ($p_c$) are non-universal.

→ Examples of different DP models?
→ Can we characterize the range of DP models?
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DP Lattice Models

- Directed bond percolation
- Directed site percolation
- Domany-Kinzel model
- Contact process
- ZGB-model for catalytic reactions

..... and many others
Domany-Kinzel Cellular Automaton

Transition probabilities:

\[ P[1|0, 0] = 0 \]
\[ P[1|0, 1] = P[1|1, 0] = p_1 \]
\[ P[1|1, 1] = p_2 \]
Domany-Kinzel Cellular Automaton

Algorithm:

For all $i$ generate a random number $z_i \in [0, 1]$ and set:

$$s_i(t + 1) = \begin{cases} 
1 & \text{if } s_{i-1}(t) \neq s_{i+1}(t) \text{ and } z_i(t) < p_1, \\
1 & \text{if } s_{i-1}(t) = s_{i+1}(t) = 1 \text{ and } z_i(t) < p_2, \\
0 & \text{otherwise}.
\end{cases}$$
### Domany-Kinzel Cellular Automaton

#### Special cases:

<table>
<thead>
<tr>
<th>case</th>
<th>restriction</th>
<th>$p_{1,c}$</th>
<th>$p_{2,c}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wolfram 18</td>
<td>$p_2 = 0$</td>
<td>$0.801(2)$</td>
<td>0</td>
</tr>
<tr>
<td>Site DP</td>
<td>$p_2 = p_1(2 - p_1)$</td>
<td>$0.70548515(20)$</td>
<td>$0.70548515(20)$</td>
</tr>
<tr>
<td>Bond DP</td>
<td>$p_1 = p_2$</td>
<td>$0.644700185(5)$</td>
<td>$0.873762040(3)$</td>
</tr>
<tr>
<td>Compact DP</td>
<td>$p_2 = 1$</td>
<td>$1/2$</td>
<td>1</td>
</tr>
</tbody>
</table>
Domany-Kinzel Model: Phase Diagram

- Inactive Phase
- Compact DP
- Bond DP
- Site DP
- Active Phase
- Wolfram rule 18
Domany-Kinzel Model: Phase Diagram

- **Compact DP** is **not** DP but it is the same as Glauber-Ising at $T = 0$.
- All the rest of the transition line belongs to DP.
Two-dimensional Domany-Kinzel model
End of Part I