Dynamics of the Ising model

- So far we have only discussed the properties of the canonical (thermal) state of the Ising model
- here the probability to find the system in a microstate $\{S_i\} \equiv \underline{S}$ given by
$$p_{th}(\underline{S}) = \frac{e^{-\beta E\{S_i\}}}{Z} = \frac{e^{-\beta E(\underline{S})}}{Z}$$

where $E\{S_i\}$ is the energy of the microstate / spin configuration and Z the partition function
- Statistical mechanics does not have a prescription concerning the dynamics, unlike quantum mechanics, where the Hamiltonian determines both the energetics and the temporal evolution

- a way for modelling the dynamics of the thermal Ising model is through a rate equation of the form (so called Markovian master equation)

$$\frac{\partial p(\underset{\sim}{S},t)}{\partial t} = \sum_{\underset{\sim}{S}'} \left[W_{\underset{\sim}{S}\underset{\sim}{S}'}\, p(\underset{\sim}{S}',t) - W_{\underset{\sim}{S}'\underset{\sim}{S}}\, p(\underset{\sim}{S},t) \right]$$

- here $W_{\underset{\sim}{S}\underset{\sim}{S}'}$ is the transition rate between two microstates $\underset{\sim}{S}$ and $\underset{\sim}{S}'$, eg.

$$\underbrace{\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow}_{\underset{\sim}{S}} \xrightarrow{W_{\underset{\sim}{S}\underset{\sim}{S}'}} \underbrace{\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow}_{\underset{\sim}{S}'}$$

which corresponds to a single spin flip

- the stationary state of the master equation is defined by $\frac{\partial p(\underset{\sim}{S},t)}{\partial t} = 0$

$$\hookrightarrow \sum_{\underset{\sim}{S}'} \left[W_{SS'}\, p(\underset{\sim}{S}',t) - W_{\underset{\sim}{S}'\underset{\sim}{S}}\, p(\underset{\sim}{S},t) \right] = 0,$$

which needs to be satisfied for all microstates $\underset{\sim}{S}$

- note, that stationarity merely requires the sum over all terms to be zero, i.e. the net flow of probability between each microstate $\underline{s}'$ and all other states vanishes
- a particular solution is given by the case in which all terms of the sum exactly cancel

$\hookrightarrow$ $$w_{\underline{s}\underline{s}'}\, p_{eq}(\underline{s}') = w_{\underline{s}'\underline{s}}\, p_{eq}(\underline{s}) \quad \text{for all } \underline{s}, \underline{s}'$$

- this condition is called detailed balance, and a state (probability distribution) that satisfies

$$\frac{p_{eq}(\underline{s})}{p_{eq}(\underline{s}')} = \frac{w_{\underline{s}\underline{s}'}}{w_{\underline{s}'\underline{s}}}$$

is called an equilibrium state

- therefore, in order to obtain a stationary state, that is the canonical state, we have to choose the rates according to

$$\frac{w_{\underline{s}\underline{s}'}}{w_{\underline{s}'\underline{s}}} = \frac{p_{th}(\underline{s})}{p_{th}(\underline{s}')} = \frac{e^{-\beta E(\underline{s})}}{e^{-\beta E(\underline{s}')}} = e^{-\beta(E(\underline{s}) - E(\underline{s}'))}$$

- this condition fixes only the ratio of the rates
- therefore, there is a lot of freedom in choosing the rates; e.g. we can multiply them by a constant or even a function of the spin configuration, and still the stationary state would remain (in principle) the same
- the simplest dynamics is the so-called <u>Glauber dynamics</u> which consists of single spin flips

↳

$$\downarrow \underset{k}{\uparrow} \downarrow \quad \underset{\Gamma_k^+}{\overset{\Gamma_k^-}{\rightleftarrows}} \quad \downarrow \underset{k}{\downarrow} \downarrow$$

with rates: $$\Gamma_k^{\pm} = \frac{e^{\pm\beta\varepsilon(S_{k-1}+S_{k+1})}}{e^{\beta\varepsilon(S_{k-1}+S_{k+1})}+e^{-\beta\varepsilon(S_{k-1}+S_{k+1})}}$$

$$= \frac{1}{2}\left(1 \pm \tanh\left(\beta\varepsilon(S_{k-1}+S_{k+1})\right)\right)$$

possible, because $S_{k\pm1}$ only take values -1 and $+1$ $\longrightarrow$ $$= \frac{1}{2}\left(1 \pm \frac{1}{2}(S_{k-1}+S_{k+1})\tanh(2\beta\varepsilon)\right)$$

- when $T \to 0$, i.e. $\beta \to \infty$ these rates become particularly simple:

$$\Gamma_k^{\pm} \xrightarrow{\beta\to\infty} \frac{1}{2}\left(1 \pm \frac{1}{2}(s_{k-1}+s_{k+1})\right)$$

- here only spin flips, that lower or conserve the energy can take place

$$\uparrow\downarrow\uparrow \quad \underset{\not\longleftarrow}{\longrightarrow} \quad \uparrow\uparrow\uparrow$$

$$\uparrow\downarrow\downarrow \quad \rightleftarrows \quad \uparrow\uparrow\downarrow$$

- let us now investigate, how the dynamics of observables, such as the magnetisation or correlation functions can be calculated with the help of the master equations
- to this end it is actually convenient to introduce a bra-ket notation like usually in quantum mechanics
- introducing the probability vector

$$|p\rangle = \sum_{s_1 \dots s_N = \pm 1} p_{s_1 s_2 \dots s_N} |s_1\rangle |s_2\rangle \dots |s_3\rangle \quad \text{, with } |s_j\rangle = \begin{cases} |1\rangle \\ |-1\rangle \end{cases}$$

allows us to write the master equation as

$\partial_t |p\rangle = W|p\rangle$, where W is the so-called dynamical or master operator

- an important role in this formulation plays the reference vector

$$|\mathbb{1}\rangle = \sum_{s_1 \dots s_N = \pm 1} |s_1\rangle \dots |s_N\rangle = (|1\rangle_1 + |-1\rangle_1)(|1\rangle_2 + |-1\rangle_2) \dots (|1\rangle_N + |-1\rangle_N)$$

with the help of which we can write the normalisation condition $\langle \mathbb{1}|p\rangle = 1$ (sum over all probabilities is one)

- this also implies $\underbrace{\partial_t \langle \mathbb{1}|p\rangle}_{0} = \langle \mathbb{1}|W|p\rangle \rightarrow \langle \mathbb{1}|W|p\rangle = 0$

and hence $\langle \mathbb{1}|W = 0$, i.e. $\langle \mathbb{1}|$ is a left-eigenvector of W with eigenvalue 0 (all columns of W sum up to zero)

- the expectation value of a quantity X is calculated according to $\langle X \rangle = \langle \mathbb{1}|X|p\rangle$

- the dynamical operator of the 1d Ising model under Glauber dynamics is

$$W = \sum_{k=1}^{N} \left[\Gamma_k^+ \left(\overbrace{\sigma_k^+}^{\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}} - \overbrace{\sigma_k^- \sigma_k^+}^{\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}} \right) + \Gamma_k^- \left(\overbrace{\sigma_k^-}^{\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}} - \overbrace{\sigma_k^+ \sigma_k^-}^{\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}} \right) \right]$$

$$= \sum_{k=1}^{N} \begin{pmatrix} -\Gamma_k^- & \Gamma_k^+ \\ \Gamma_k^- & -\Gamma_k^+ \end{pmatrix}_k, \quad \text{with } \Gamma_k^{\mp} = \frac{1}{2}\left(1 \pm \frac{1}{2}\left(\sigma_z^{k-1} + \sigma_z^{k+1}\right) \tanh(2\beta\varepsilon)\right)$$

- the time evolution of the expectation value of the magnetisation of the m-th spin is then calculated according to

$$\langle \mathbb{1} | \sigma_z^m \partial_t | p) = \partial_t \langle \sigma_z^m \rangle = \partial_t M_m$$

$$= \langle \mathbb{1} | \sigma_z^m W | p \rangle$$

$$= \underbrace{\langle \mathbb{1} | \sigma_z^m \begin{pmatrix} 0 & 1 \\ 0 & -1 \end{pmatrix}_m}_{\langle \mathbb{1} | (1 - \sigma_z^m)} \Gamma_m^+ | p) + \underbrace{\langle \mathbb{1} | \sigma_z^m \begin{pmatrix} -1 & 0 \\ 1 & 0 \end{pmatrix}_m}_{- \langle \mathbb{1} | (1 + \sigma_z^m)} \Gamma_m^- | p \rangle$$

$$= - \underbrace{\langle \sigma_z^m \rangle}_{M_m} + \frac{1}{2} \underbrace{\langle (\sigma_z^{m-1} + \sigma_z^{m+1}) \rangle}_{M_{m-1} + M_{m+1}} \tan(2\beta\epsilon)$$

- at $T = 0$ this becomes

$$\partial_t M_m(t) = - M_m(t) + \frac{1}{2} \left(M_{m-1}(t) + M_{m+1}(t) \right)$$

which describes the evolution of the magnetisation as a function of time

$$\langle \mathbb{1} | \sigma_z^m W | p \rangle = \sum_k \langle \mathbb{1} | \sigma_z^m \Gamma_k^+ (\sigma_k^+ - \sigma_k^- \sigma_k^+) | p \rangle$$

$$+ \sum_k \langle \mathbb{1} | \sigma_z^m \Gamma_k^- (\sigma_k^- - \sigma_k^+ \sigma_k^-) | p \rangle$$

$$= \sum_{k \neq m} \underbrace{\langle \mathbb{1} | \Gamma_k^+ (\sigma_k^+ - \sigma_k^- \sigma_k^+)}\, \sigma_z^m | p \rangle + \sum_{k \neq m} \langle \mathbb{1} | \Gamma_k^- (\sigma_k^- - \sigma_k^+ \sigma_k^-) \sigma_z^m | p \rangle$$

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix}_1^T \otimes \dots \otimes \underbrace{\begin{pmatrix} 1 \\ 1 \end{pmatrix}_k^T \begin{pmatrix} 0 & \Gamma_k^+ \\ 0 & -\Gamma_k^+ \end{pmatrix}_k}_{0} \otimes \dots \otimes \begin{pmatrix} 1 \\ 1 \end{pmatrix}^T \sigma_z^m \otimes \dots \otimes | p \rangle$$

$$+ \langle \mathbb{1} | \sigma_z^m \underbrace{\Gamma_m^+ (\sigma_m^+ - \sigma_m^- \sigma_m^+)} | p \rangle + \langle \mathbb{1} | \sigma_z^m \Gamma_m^- (\sigma_m^- - \sigma_m^+ \sigma_m^-) | p \rangle$$

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix}^T \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & \Gamma_m^+ \\ 0 & -\Gamma_m^+ \end{pmatrix}}$$

$$\begin{pmatrix} 1 \\ -1 \end{pmatrix}^T \begin{pmatrix} 0 & \Gamma_m^+ \\ 0 & -\Gamma_m^+ \end{pmatrix} = \begin{pmatrix} 0 \\ 2\Gamma_m^+ \end{pmatrix}^T = \begin{pmatrix} 1 \\ 1 \end{pmatrix}^T \begin{pmatrix} 0 & 0 \\ 0 & 2\Gamma_m^+ \end{pmatrix}$$

$$= \begin{pmatrix} 1 \\ 1 \end{pmatrix}^T (\mathbb{1} - \sigma_z^m) \Gamma_m^+$$

$$= \langle \Gamma_m^+ \rangle - \langle \sigma_z^m \Gamma_m^+ \rangle - \langle \Gamma_m^- \rangle - \langle \sigma_z^m \Gamma_m^- \rangle$$

$$= \frac{1}{2} \langle \sigma_z^{m-1} + \sigma_z^{m+1} \rangle \tanh(2\beta\varepsilon) - \frac{1}{2} \langle \sigma_z^m + \sigma_z^m \rangle$$

$$= - \langle \sigma_z^m \rangle + \frac{1}{2} \left(\langle \sigma_z^{m-1} \rangle + \langle \sigma_z^{m+1} \rangle \right) \tanh(2\beta\varepsilon)$$

Coarsening in the Ising model

- having access to the time depence of observables of the Ising model allows to consider non-equilibrium situations
- interesting is for instance to understand the evolution of a paramagnet after the temperature is suddenly changed to below T_c (this is called a quench)
- the stationary state should be magnetized, but how this state is assumed from a paramagnetic initial condition is surprisingly interesting
- the phenomenon occurring here is called coarsening
- this means that after the quench domains of locally uniform magnetisation are grown in a self-similar way
- the typical size of the magnetic domains, L, follows a power-law as a function of time, i.e $L \propto t^n$, with the power n being dependent on the considered dynamics e.g. Glauber dynamics

- we study this phenomenon using the correlation $C(|i-j|,t) = \langle \sigma_z^i \sigma_z^j \rangle(t)$
- this function follows the equation of motion

$$r \neq 0 : \quad \partial_t C(r,t) = C(r+1,t) - 2C(r,t) + C(r-1,t)$$

$$r = 0 : \quad C(0,t) = 1 \qquad \text{for all times}$$

- in order to solve this equation we consider the continuum limit, i.e. we assume, that the separation r between spins is a continuous variable
- we can then approximate:

$$C(r\pm 1,t) \approx C(r,t) \pm \frac{\partial}{\partial r} C(r,t) + \frac{1}{2}\frac{\partial^2}{\partial r^2} C(r,t)$$

$$\hookrightarrow \partial_t C(r,t) = \partial_r^2 C(r,t)$$

- this is the diffusion equation, which indeed has a so-called scaling solution, in which time and space are connected via a power law: $C(r,t) = f(\underbrace{r t^{-1/2}}_{x})$

- inserting the scaling ansatz into the differential equation leads to

$$\partial_x^2 f(x) = -\frac{x}{2}\partial_x f(x)$$

- integrating with the boundary conditions $f(0)=1$ and $f(\infty)=0$ leads to

$$C(r,t) = \operatorname{erfc}\left(\frac{r}{2t^{1/2}}\right) \; ; \; \overbrace{\operatorname{erfc}(x)}^{\text{complementary error function}} = 1 - \frac{2}{\sqrt{\pi}}\int_0^x d\tau\, e^{-\tau^2}$$

- this is the time dependence of the correlation function in the domain growth / coarsening regime
- under the Glauber dynamics the typical domain size L therefore follows

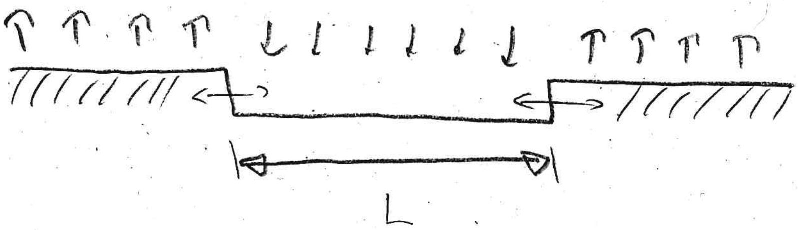
$$L \propto t^{1/2}$$

- the same result can actually be found with the following simple considerations:
- at $T=0$ only the following two processes have a non-zero rate

domain wall diffusion

domain wall annihilation

- the borders (walls) of a domain of length L

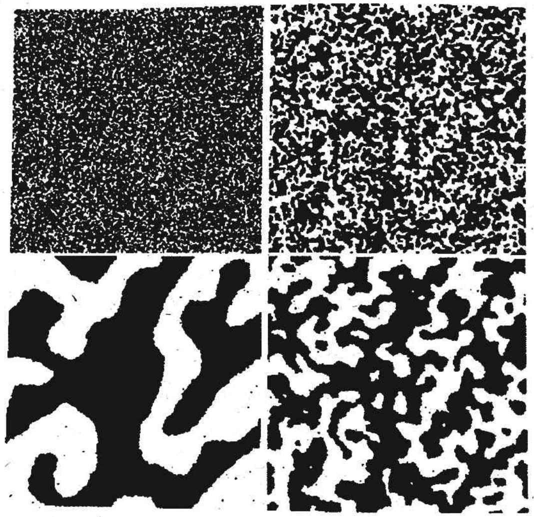


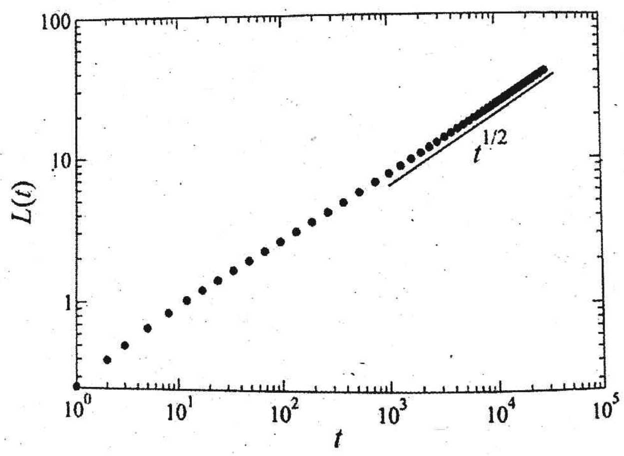
perform a random walk, and in order for both walls to meet and annihilate on average L^2 time steps (spin flips) are required

- therefore: $t_{\text{annihilation}} \propto L^2$, which confirms the previously found scaling
- this result is a direct consequence of the fact that at zero temperature the Glauber dynamics leads to domain wall diffusion
- So one would expect that a different type of dynamics could lead to different scaling behaviour

Glauber dynamics

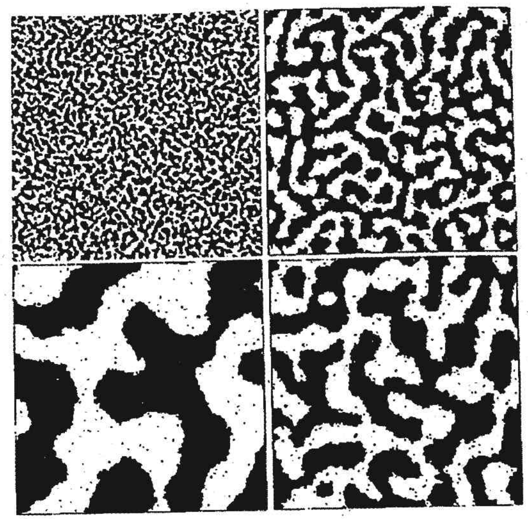
- 1000 x 1000 sites
- Quench from infinite T to $T=0.661\,T_c$
- $T=10, 10^2, 10^3, 10^4$

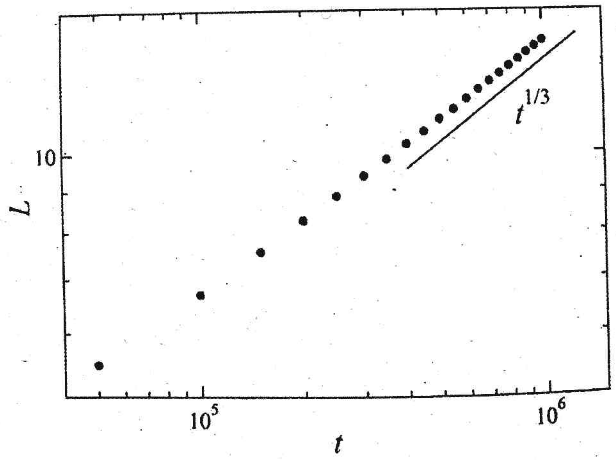




Kawasaki dynamics

- 256 x 256 sites
- Quench from infinite T to $T=0.661\,T_c$
- $T=10^2, 10^4, 10^5, 10^6$





- this is indeed the case, and we will study this using the so-called <u>Kawasaki spin-exchange dynamics</u>
- this dynamics conserves the magnetisation, i.e. the number of up and down spins is not changed under the dynamics
- the dynamical rules are as follows:

		energy change
$\downarrow\downarrow\downarrow\uparrow\downarrow\downarrow\downarrow$	particle diffusion,	$\Delta E = 0$
$\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow$	hole diffusion,	$\Delta E = 0$
$\uparrow\uparrow\uparrow\downarrow\uparrow\downarrow\downarrow$	particle attachment,	$\Delta E < 0$
$\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow$	particle detachment,	$\Delta E > 0$

- let us now consider the dynamics of a domain configuration of the following form:

$$\underbrace{\uparrow\uparrow\uparrow\uparrow\uparrow}_{\sim L}\underbrace{\downarrow\downarrow\downarrow\downarrow\downarrow}_{L}\underbrace{\uparrow\uparrow\uparrow\uparrow}_{\sim L}$$

- the first difference to the Glauber dynamics is that at $T=0$ nothing can move
- i.e. we need a finite temperature, so that the first spin can detach: $\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow \to \uparrow\uparrow\uparrow\downarrow\uparrow\downarrow$

- this is happening on a time scale $\tau_0 \sim e^{2\beta\varepsilon}$, since the rate is $\sim e^{-2\beta\varepsilon}$

- suppose that such detachment is happening, then an up spin has to move by L sites in order to travel from one to the other domain of up-spins
- this happens with probability $p(L)$, and thus the time for one spin moving from one $\uparrow\uparrow$-domain to the other is

$$\tau_0 \approx e^{2\beta\varepsilon}/p(L)$$

- to estimate the time at which one $\uparrow\uparrow$-domain has completely moved over to the other $\uparrow\uparrow$-domain, one needs to realise that in fact the $\downarrow\downarrow$-domain needs to move by L sites in order for that to happen
- this is a random walk which requires on average L^2 steps
- hence the timescale for the merging of the $\uparrow\uparrow$-domains is $t(L) \approx e^{\beta\varepsilon_0} \dfrac{L^2}{p(L)}$

- the probability $p(L)$ can be calculated as follows:

$$p(L) = p(L-1) \times \frac{1}{2}$$ = (probability of hopping $L-1$ sites) $\times$ (probability to hop to the final site)

$$+ \; p(L-1) \times \frac{1}{2} \times (1-p(L-1)) \times \frac{1}{2}$$ = (prob. of hopping $L-1$ sites) $\times$ (prob of not hopping to final site) $\times$ (prob. of not hopping back to the other domain) $\times$ (prob. of hopping to final site)

$$+ \; p(L-1) \times \frac{1}{2} \times (1-p(L-1)) \times \frac{1}{2} \times (1-p(L-1)) \times \frac{1}{2}$$

$$+ \; \dots$$

$$= \frac{p(L-1)}{2} \sum_{n=0}^{\infty} \left[\frac{1-p(L-1)}{2} \right]^n = \frac{p(L-1)}{1+p(L-1)}$$

$$\hookrightarrow \; p(L) = \frac{p(L-1)}{1+p(L-1)} \longrightarrow p(L) = \frac{1}{L}$$

- hence, the time scale for the merging of the $\uparrow\uparrow$-domains is

$$t(L) \approx e^{\beta E_0} L^3 \longrightarrow L \sim t^{1/3}$$

- the power law for the scaling regime of the coarsening dynamics is different to the Glauber dynamics

- This difference in the scaling behaviour is in fact a consequence of the conservation law of the Kawasaki dynamics

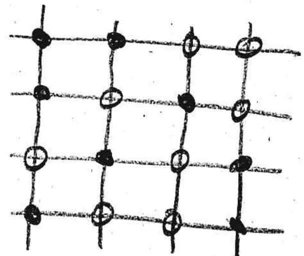
Out-of-equilibrium processes and phase transitions

- we will now consider phase transitions in many-body systems which cannot be described within the framework of equilibrium statistical mechanics
- for these out-of-equilibrium processes we cannot formulate a canonical partition function
- they are described merely through their dynamics, which may be formulated by a Markovian master equation
- paradigmatic examples are given by dynamical processes that feature an absorbing state, for instance some cellular automata
- an absorbing state is a microstate that can be entered dynamically, but which cannot be left anymore (this violates detailed balance)

- an example is given by the

<u>contact process</u>

- it is defined on a d-dimensional square lattice, whose sites are labelled by k
- each site can either be empty ($s_k = 0$; healthy) or occupied ($s_k = 1$; infected)
- the state of the lattice is updated, i.e. propagated in time, via the following rules:



∘ healthy
• infected

- probability for going from infected to healthy

$$\omega(1 \rightarrow 0) = \Gamma \qquad \bullet \longrightarrow \circ$$

↳ an infected site can spontaneously heal

- probability for going from healthy to infected

$$\omega(0 \rightarrow 1) = \frac{\lambda}{2d} \times (\text{number of infected neighbors})$$

$$\bullet\circ \longrightarrow \bullet\bullet$$

↳ a site can only be infected if at least one of its neighbors is infected

→ the state in which all sites are healthy is absorbing, i.e. once it is reached one cannot escape

- we can cast this dynamics into a master equation by introducing the operators

$n_k = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{\sigma_z^k + 1}{2}$, which projects on the infected state of site k

- using furthermore the spin raising and lowering operators, $\sigma_k^{\pm}$, we find for the contact process in 1 dimension the following equation:

$$\partial_t |p\rangle = \overbrace{\sum_k \underbrace{r\left[\sigma_k^- - n_k\right]}_{\text{spontaneous healing}} + \underbrace{\frac{\lambda}{2}(n_{k-1}+n_{k+1})\left[\sigma_k^+ - (1-n_k)\right]}_{\text{infection due to infected neighbours}}}^{W \text{ (dynamical operator)}} |p\rangle$$

- we can now calculate the time evolution of the local density of infected sites,

$$\partial_t \langle n_m \rangle = \langle \mathbb{1} | n_m \partial_t | p \rangle = -r \langle n_m \rangle + \frac{\lambda}{2} \langle (n_{m-1}+n_{m+1})(1-n_m) \rangle$$

- this is not a closed equation, because the right-hand-side depends on the correlation functions $\langle n_{m-1} n_m \rangle$, which themselves are subjects to an equation of motion

$$\partial_t \langle n_{m-1} n_m \rangle = \langle \mathbb{1} | n_{m-1} n_m W | p \rangle \propto \langle n_{m-1} n_m n_{m+1} \rangle + \ldots$$

- this hierarchy of coupled equations never closes

- for an approximate solution we employ a mean field approximation:

$\langle n_{m-1} n_m \rangle \approx \langle n_{m-1} \rangle \langle n_m \rangle$ multi-site correlations are neglected

$\langle n_{m-1} \rangle \approx \langle n_m \rangle = \rho$ the density of infected sites is assumed to be homogeneous

- this leads to the following mean field equation: $\partial_t \rho = \lambda \rho (1-\rho) - r\rho = (\lambda - r)\rho - \lambda \rho^2$

- realising, that $\dfrac{d\rho}{\lambda\rho\left(\frac{\lambda-r}{\lambda} - \rho\right)} = \dfrac{d\rho}{(\lambda-r)\,\rho} + \dfrac{d\rho}{(\lambda-r)\left[\frac{\lambda-r}{\lambda} - \rho\right]}$

the mean field equation can be integrated

- using the initial condition $\rho(0) = 1$ (initially the lattice is filled with infected sites) we find the solution

$$\rho(t) = \frac{\lambda - r}{\lambda - e^{-(\lambda-r)t}\, r}$$

density of infected sites

$$(\lambda-r)t = c + \log \rho - \log\left(\frac{\lambda-r}{\lambda} - \rho\right)$$

$$= c + \log \frac{\rho}{\frac{\lambda-r}{\lambda} - \rho}$$

$$\hookrightarrow c' e^{(\lambda-r)t} = \frac{\rho}{\frac{\lambda-r}{\lambda} - \rho}$$

$$t=0 \to \rho = 1$$

$$\hookrightarrow c' = \frac{1}{\frac{\lambda-r}{\lambda} - 1} \to c' = \frac{1}{-\frac{r}{\lambda}} = -\frac{\lambda}{r}$$

$$\hookrightarrow -\frac{\lambda}{r} e^{(\lambda-r)t}\left(\frac{\lambda-r}{\lambda} - \rho\right) = \rho$$

$$-\frac{\lambda-r}{r} e^{(\lambda-r)t} + \frac{\lambda}{r}\rho e^{(\lambda-r)t} = \rho$$

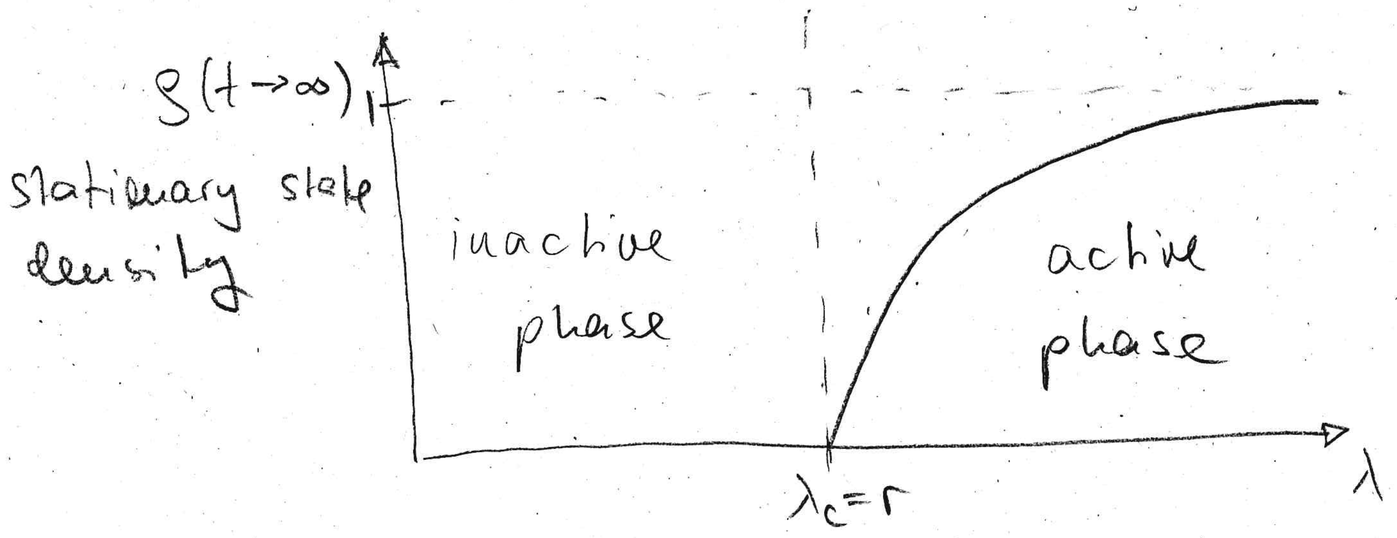
$$\frac{\lambda-r}{r} e^{(\lambda-r)t} = \rho\left(\frac{\lambda}{r} e^{(\lambda-r)t} - 1\right)$$

$$\hookrightarrow \rho = \frac{\lambda-r}{r} \frac{e^{(\lambda-r)t}}{\frac{\lambda}{r} e^{(\lambda-r)t} - 1} = \frac{\lambda - r}{\lambda - r e^{-(\lambda-r)t}}$$

- if the infection rate λ is smaller than the recovery rate, we find that the density of infected sites tends to zero: $\rho(t \to \infty) = 0 \quad , \lambda < r$

- Conversely, when $\lambda > r$, we find that
$$\rho(t \to \infty) = \frac{\lambda - r}{\lambda}$$

- apparently, $\lambda_c = r$ marks a critical value of the infection rate, below which the system goes to the (inactive) absorbing state
- above λ_c the system is in the so-called active phase in which it maintains a finite density of infected sites



- the transition between the inactive and active phase is continuous
- it can be characterised by a set of critical exponents, which define the so-called <u>directed percolation universality</u> class
- one exponent is obtained by studying the stationary state density ρ, near stationarity

$$\rho(t \to \infty) = \frac{1}{\lambda}(\lambda - r) = \frac{1}{\lambda}(\lambda - \lambda_c) \propto (\lambda - \lambda_c)^{\beta}$$

$$\hookrightarrow \beta = 1$$

- another exponent can be found by investigating the time dependence at criticality:

$$\lim_{\lambda \to r} \rho(t) = \frac{1}{1 + rt} \xrightarrow{rt \gg 1} t^{-\delta}$$

$$\hookrightarrow \delta = 1$$

- furthermore, we can identify an exponent by analysing the correlation time in the inactive phase

$$\rho(t) \overset{rt\gg 1}{\approx} (r-\lambda)\exp\left[-\frac{t}{\xi_{\parallel}}\right]$$, with $\xi_{\parallel}$ being the correlation time

$\hookrightarrow$ $\xi_{\parallel} \sim (\lambda-\lambda_c)^{-\nu_{\parallel}}$ with $\nu_{\parallel} = 1$

- the exponents we have obtained so far are mean field exponents
- the actual exponents have to be calculated numerically
- just like for the Ising model, they depend on dimensionality

	mean field	1d	2d	3d
β	1	0.276	0.584	0.81
δ	1	0.159	0.451	0.73
$\nu_{\parallel}$	1	1.734	1.295	1.11
$\nu_{\perp}$	1/2	1.097	0.451	0.73

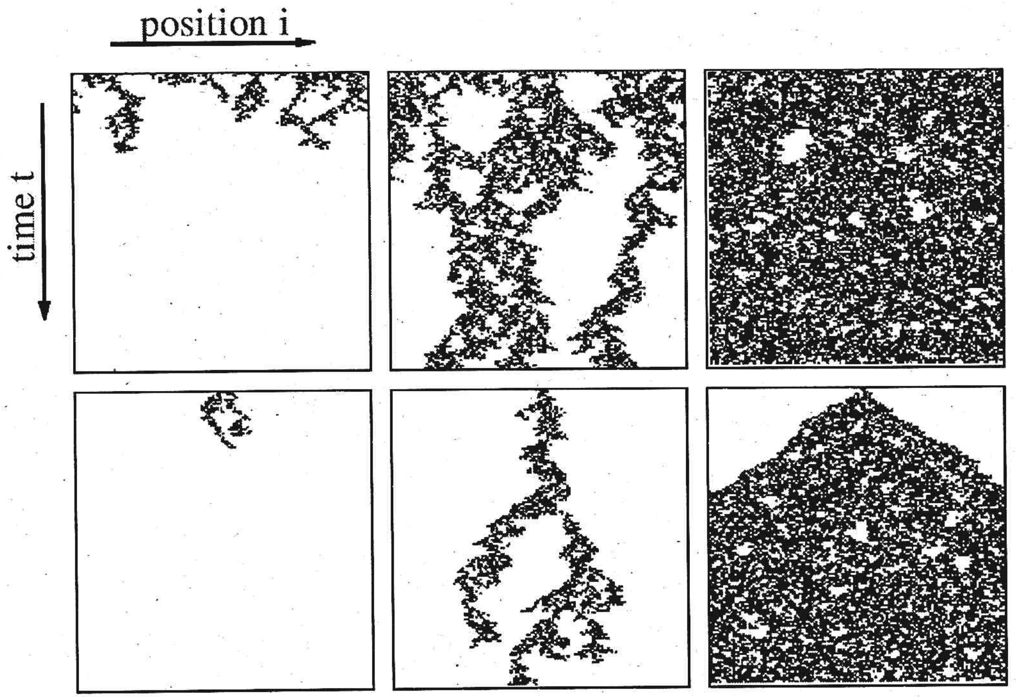
correlation length in space

- the actual critical point in 1d is $\lambda_c = 3.298\, r$

- note, that in contrast to the Ising model there is a phase transition already in one dimension

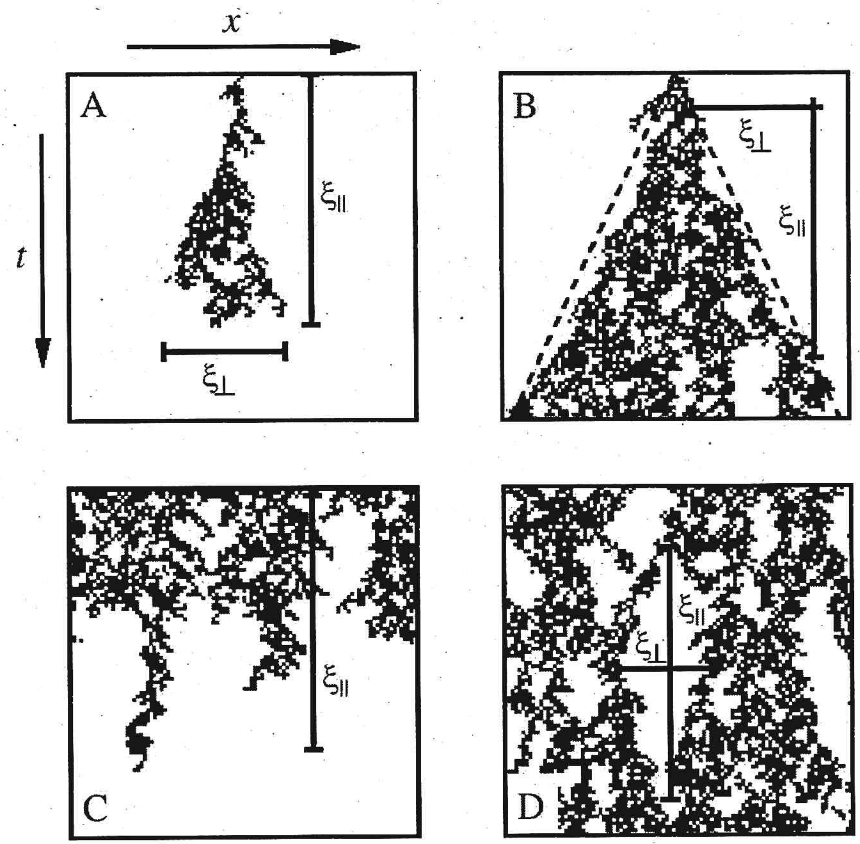
Phase transition in the contact process

- Inactive and active phase



$\lambda < \lambda_c$ $\lambda = \lambda_c$ $\lambda > \lambda_c$

- Correlation lengths

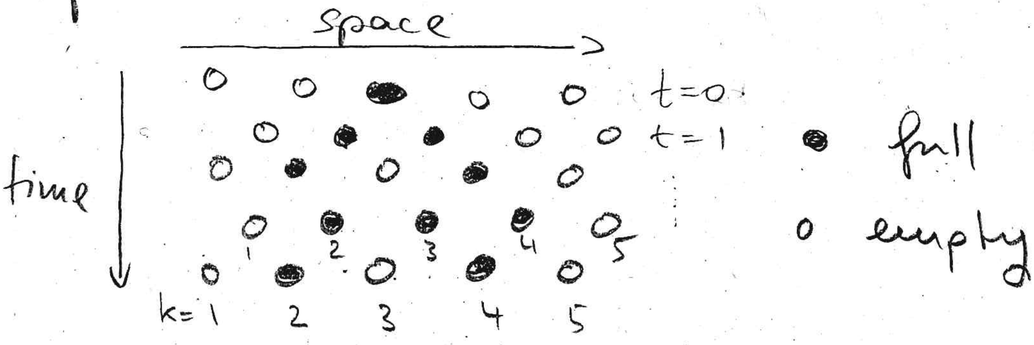


$\lambda < \lambda_c$ $\lambda > \lambda_c$

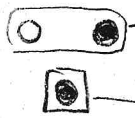
Domany-Kinzel cellular automata

- many basic models of nonequilibrium phase transitions can be formulated as dynamical processes of particles moving on a lattice
- cellular automata are a particular class:
  - each lattice site can at most be occupied by a single particle (exclusion)
  - the dynamical rules are local, i.e. state changes of a particle depend only on particles in the direct neighbourhood
  - the dynamics is Markovian, i.e. the configuration at time $t+1$ depends only on configuration at time t
- deterministic cellular automata were introduced at the beginning of the 20th century by John von Neumann
- Domany and Kinzel introduced stochastic (probabilistic) cellular automata in the 1980s, which serve as an important paradigm for non-equilibrium processes

- DK models are defined on a tilted square lattice whose sites are either empty or full



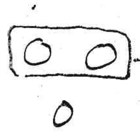
- the horizontal | vertical directions are space | time
- all sites of the lattice are initially empty, except for the first line, which contains the initial state
- the propagation in time proceeds line by line, where the line corresponding to time t is updated depending on the state of line $t-1$
- the update rules are


— configuration at $t-1$

— fill site at time t with probability p


— fill with probability p


— fill with probability q


— don't do anything if there are two empty sites at time t

- the DK models have (at least) one absorbing state, which is the empty state ○ ○ ○ ○ ○ ○
- therefore, it is not really surprising that there is an extremely close link to the contact process and the directed percolation universality class
- this can be seen by considering the evolution of the density of filled sites $\langle n_k^t \rangle$; $n_k^t = | \bullet \underset{k}{X} \bullet |_t$

↳ the dynamical rules lead to the following equation:

$$\langle n_k^{t+1} \rangle = p \langle n_k^t (1-n_{k+1}^t) \rangle + p \langle (1-n_k^t)\, n_{k+1}^t \rangle + q \langle n_k^t n_{k+1}^t \rangle$$

- employing a mean field treatment as we have done already in case of the contact process, and denoting $\rho_t = \langle n_k^t \rangle = \langle n_{k+1}^t \rangle$, one finds for the density of filled sites the following difference equation:

$$\rho_{t+1} - \rho_t = 2p\,\rho_t (1-\rho_t) + q\,\rho_t^2 - \rho_t$$

- turning this into a differential equation, using $\varrho_{t+1} - \varrho_t \approx \partial_t \varrho$ and rearranging the terms, yields

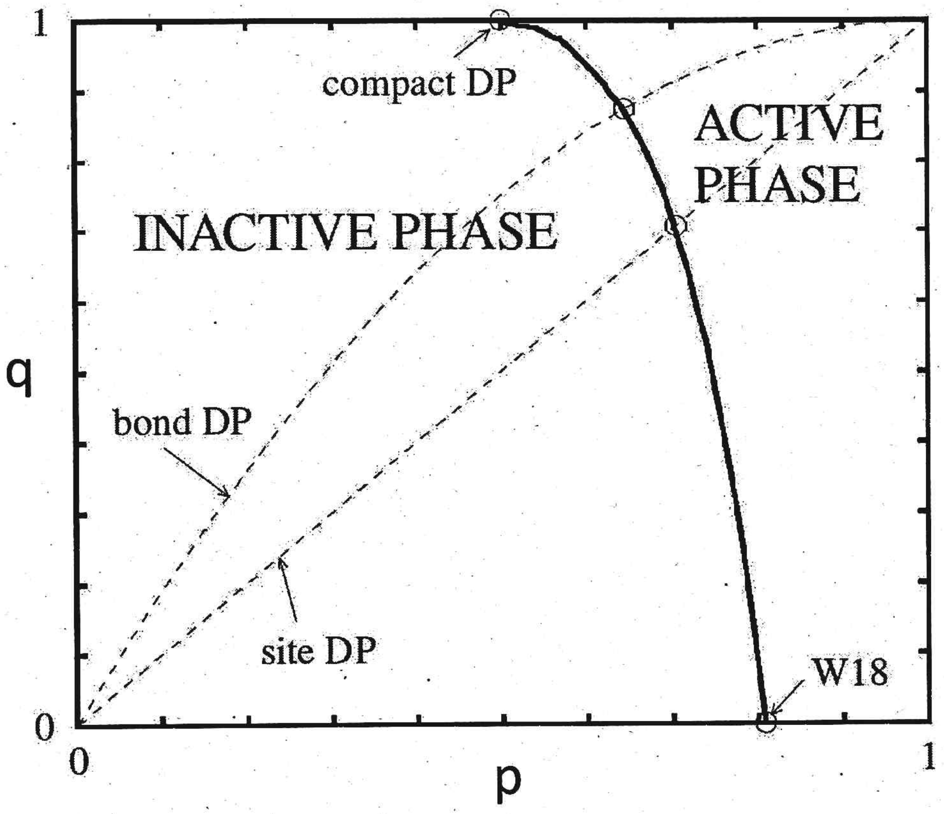
$$\partial_t \varrho(t) = (2p-1)\,\varrho(t) - (2p-q)\,\varrho^2(t)$$

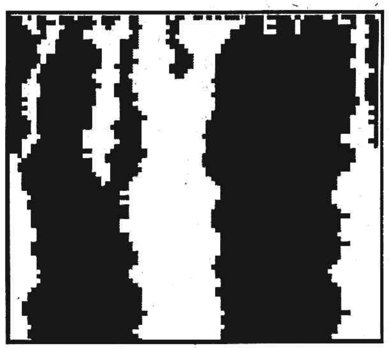
- this is precisely the same mean field equation that we obtained for the contact process
- in fact it turns out that also the DK cellular automata feature a phase transition between an absorbing state and an active phase which is in the directed percolation universality class, i.e. the critical exponents are the same
- <u>except</u>, when $q = 1$!
- here the mean field equation becomes

$$\partial_t \varrho(t) = (2p-1)\,\varrho(t)\,[1 - \varrho(t)]$$ and

apparently both, the empty state ($\varrho = 0$) and the completely filled state ($\varrho = 1$) are stationary states of the dynamics

Phase diagram of the Domany-Kinzel cellular automaton



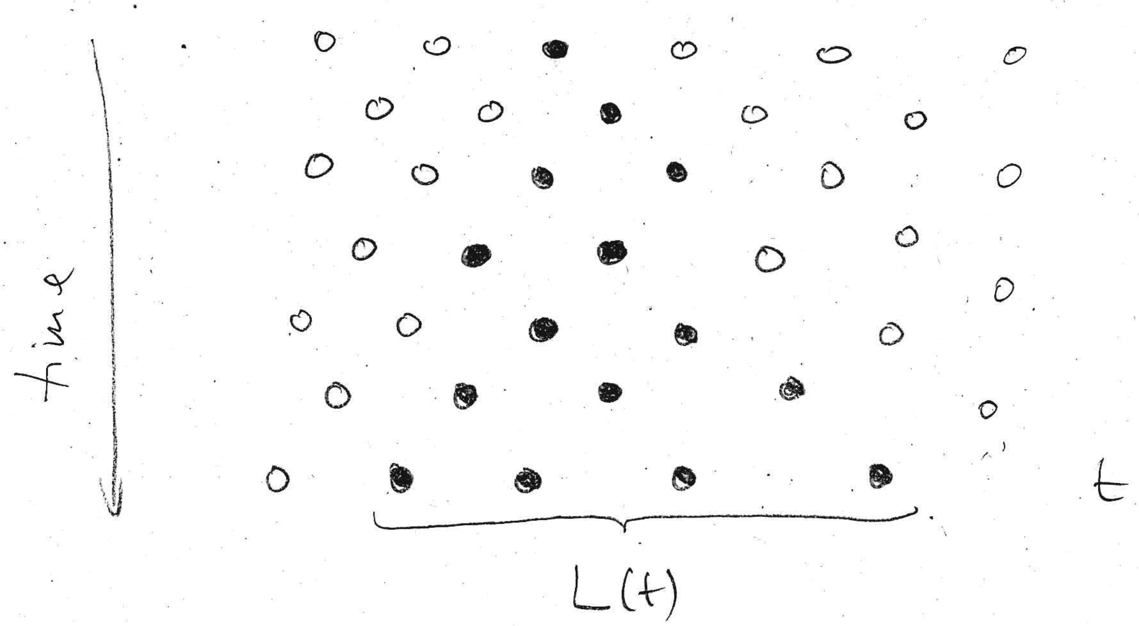


compact DP

bond DP

Wolfram rule 18

- this dynamics has a higher symmetry than the contact process because it is invariant under the exchange of healthy and infected sites • <—> o
- this is a so-called particle-hole symmetry, which not only leads to two absorbing states (oooo and ••••) but results also in different universal behaviour near the transition between the active and the inactive phase
- the universality class in this case goes under the name <u>compact directed percolation</u>
- the name stems from the fact that the dynamics creates compact clusters, i.e. clusters of infected sites without holes



- the phase transition point can be directly inferred from the particle-hole symmetry
- we have

	●●	●○	○●	○○
	●	●	●	●
with probability	1	p	p	0

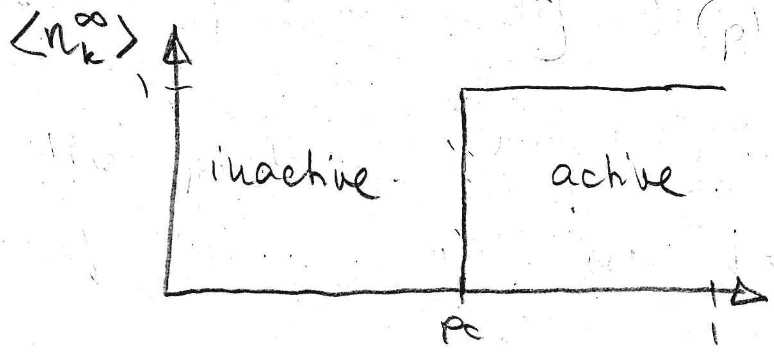
and

	●●	●○	○●	○○
	○	○	○	○
with probability	0	$1-p$	$1-p$	1

- however, we can exchange hole and particles, such that for the critical value of p it must hold that: $p_c = 1 - p_c$

$$\hookrightarrow p_c = \frac{1}{2}$$

- below the critical point the stationary state is the empty one: ○ ○ ○ ○ ○ ○
- by symmetry, however, the stationary state must be the completely filled one: ● ● ● ● ●
- therefore, the stationary state density of occupied sites, $\langle n_k^\infty \rangle$, follows



- this behaviour is markedly different with respect to the contact process
  ↳ near the critical point the density of filled sites behaves as

$$\langle n_k^\infty \rangle \propto (p-p_c)^\beta \quad \text{with } \beta = 0$$

- this „critical exponent" is clearly different to that of the directed percolation universality class
- we can find another critical exponent by studying the survival probability $P(p)$ of a seed; $\circ\ \circ\ \circ\ \underbrace{\bullet}_{L(t)}\ \circ\ \circ\ \circ$, as a function of p
- in each time step the size $L(t)$ of the cluster of filled sites can either grow, shrink or remain constant:

$$L(t+1) = \begin{cases} L(t)+1, & \text{with probability } p^2 \\ L(t), & \text{with probability } 2p(1-p) \\ L(t)-1, & \text{with probability } (1-p)^2 \end{cases}$$

- hence, $L(t)$ performs an asymmetric random walk with a probability

$$r = \frac{p^2}{p^2 + (1-p)^2}$$ to move to the right

and probability $1-r$ to move to the left (the probability for maintaining the length is not important here, as it merely changes the duration of an effective time step)

- in order to calculate $P(p)$ we need to compute the probability that $L(t=\infty) = \infty$, knowing that $L(0) = 1$ and that there is an absorbing barrier at $L = 0$ (here the system enters the absorbing state 00000)

- this problem is actually known as the "Gambler's ruin": here $L(t)$ is the amount of Euros the gambler possesses and in each time step he/she can win or lose 1 Euro

- bankruptcy therefore corresponds to $L = 0$, and the survival probability $P(p)$ is thus just the probability winning ω Euros with $\omega \to \infty$, starting with 1 Euro

- the probability of winning w Euros, starting from n Euros shall be denoted by R_n

↳ $R_0 = 0$, started with 0 Euros makes it impossible to win

$R_w = 1$, having w Euros wins

- the gambler starts with n Euros and wins the first bet with probability r
- he/she then has $n+1$ Euros and thus the probability to reach w Euros is R_{n+1}
- conversely, if he/she loses with probability $1-r$, he/she remains with $n-1$ Euros and the probability to win w Euros is R_{n-1}

↳ this leads to the recurrence relation

$$R_n = r\, R_{n+1} + (1-r)\, R_{n-1} \quad (0 < n < w)$$

with boundary conditions

$R_0 = 0$ and $R_w = 1$

- the equation is solved with the ansatz $R_n = x^n$
- this yields the so-called characteristic equation

$$r x^2 - x + (1-r) = 0$$

- its solutions are

$$x = \begin{cases} \frac{1-r}{r} \\ 1 \end{cases}$$

- the solution of the recurrence relation is thus $R_n = a \cdot \left(\frac{1-r}{r}\right)^n + b \cdot 1^n$,

where a and b have to be determined through the boundary conditions

$$\hookrightarrow \quad \begin{aligned} 0 &= a + b \\ 1 &= a\left(\tfrac{1-r}{r}\right)^{\omega} + b \end{aligned} \quad \longrightarrow \quad a = \frac{1}{\left(\frac{1-r}{r}\right)^{\omega} - 1}$$

$$b = -a$$

- substituting back, this yields

$$R_n = \frac{\left(\frac{1-r}{r}\right)^n - 1}{\left(\frac{1-r}{r}\right)^{\omega} - 1}$$

- we are now interested in the limit $\omega \to \infty$ (cluster grows to infinity) and $r > \frac{1}{2}$.

↳ $\lim_{\omega \to \infty} R_n = -\left(\frac{1-r}{r}\right)^n + 1$

- the survival probability we are after is then given by R_1

↳ $P(p) = \lim_{\omega \to \infty} R_1 = 1 - \left(\frac{1-r}{r}\right)$

$$= \frac{2}{p^2}\left(p - \frac{1}{2}\right)$$

- close to criticality, i.e. $p = p_c + \varepsilon$, we thus find the scaling

$$P(p) \propto (p - p_c)^{\beta'} \quad \text{with } \beta' = 1$$

- the β'-exponent can also be determined for processes in the directed percolation universality class
- here $\beta = \beta'$, which is the consequence of the so-called rapidity reversal symmetry

- for compact directed percolation, our exact solution shows that $\beta \neq \beta'$, and thus we find further confirmation that this universality class is different to directed percolation