Nucleation in the Ising Model

Abraham Hinteregger

University of Vienna

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Chapter

History

- 1924: Ernst Ising - *Beitrag zur Theorie des Ferromagnetismus*[1]

  "Es entsteht ... [durch] ... die Beschränkung der Wechselwirkung auf diejenige benachbarter Elemente [...] kein Ferromagnetismus."

- 1936: Rudolph Peierls - *On Ising's model of ferromagnetism*[2]

  "[...] for sufficiently low temperatures the Ising model in two [or more] dimensions shows ferromagnetism [...].

[1] Zeitschrift für Physik Februar–April 1925, Volume 31, Issue 1, pp 253-258
[2] Cambridge Philosophical Society 1936 / Volume 32 / Issue 03 / October

Lattice

Figure: Lattice in 1 dimension

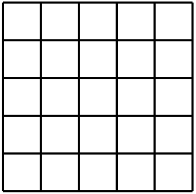

Figure: Lattice in 2 dimensions

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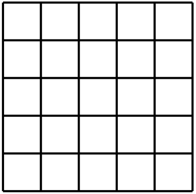

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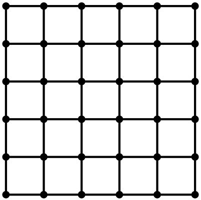

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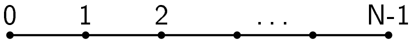

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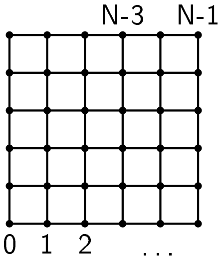

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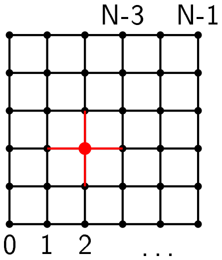

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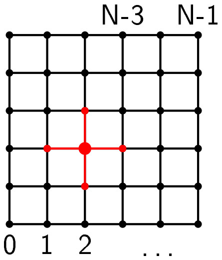

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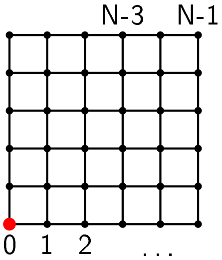

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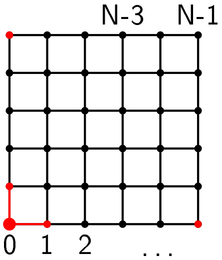

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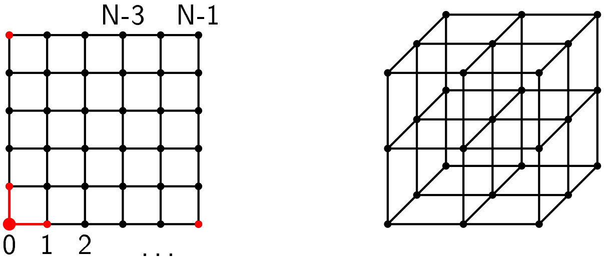
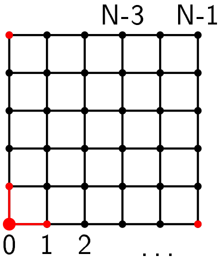
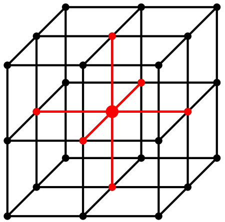


Figure: Lattice in 2 and 3 dimensions

Lattice

Figure: Lattice in 1 dimension





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Lattice Sites

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- Assignment of states $s = (s_0, s_1, s_2, \ldots, s_{N-1})$ to the lattice sites is called a configuration
- Therefore 2^N unique configurations for a lattice with N lattice sites.

Energy

- Each configuration has a corresponding energy - the Hamiltonian H

$$H(s) = H(s_0, s_1, \ldots, s_{N-1}) = -J \sum_{<\mathrm{i,j}>} s_i \cdot s_j - h \sum_{\mathrm{i}} s_i$$

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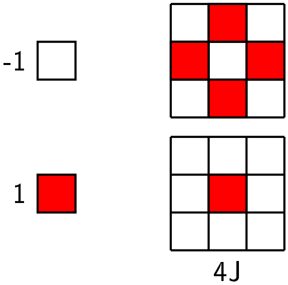

Figure: Energy contribution (from nearest neighbor interaction) of the central lattice site

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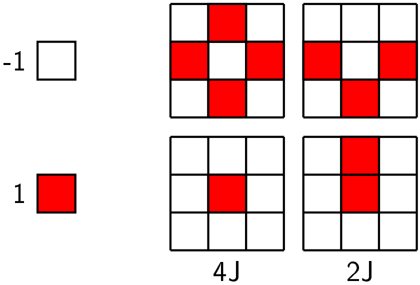

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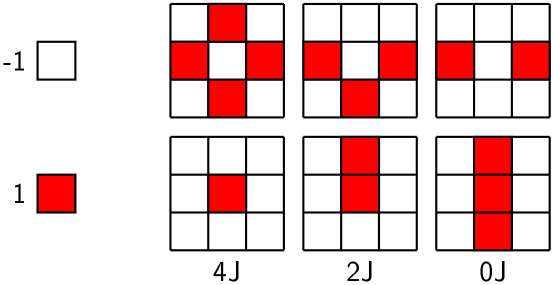

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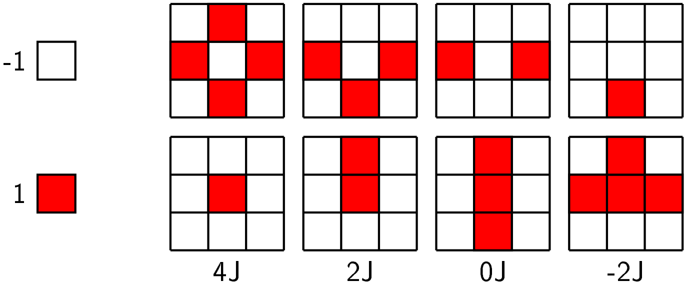

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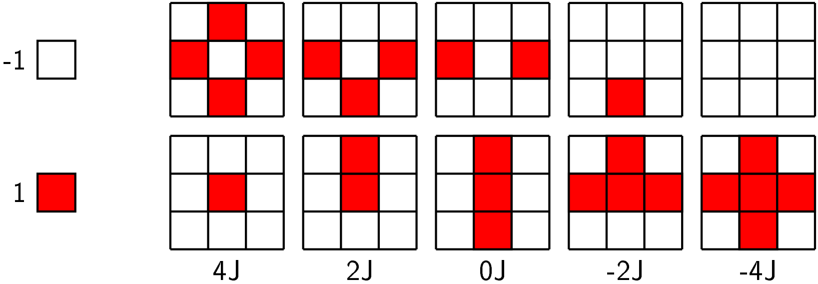

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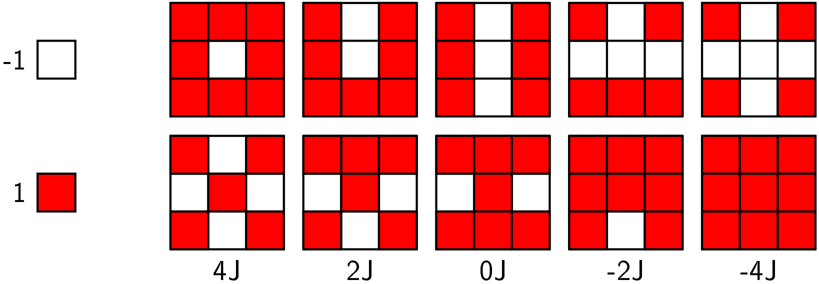

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Single Flip Monte Carlo (Metropolis- Hastings Algorithm)

- Current configuration is s_t
  - first configuration arbitrary
- Flip one lattice site $\rightarrow s_f$
  - has to be chosen randomly - suitable RNG necessary
- Calculate energy difference $\Delta H = H(s_f) - H(s)$
- Calculate acceptance probability P

$$P = \min\left(1, e^{-\beta \cdot \Delta H}\right), \qquad \beta = 1/kT > 0$$

- Generate random number $r \in [0, 1[$
  - $r < P \rightarrow s_{t+1} = s_f$
  - $r > P \rightarrow s_{t+1} = s_t$

Temperature in the Ising Model

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- $\Delta H < 0 \rightarrow P = 1$
- high temperature leads to higher acceptance probability $\rightarrow$ unordered (low magnetization, Curie Temperature T_c)
- critical temperature T_c when $\left\langle \sum_i^N s_i \right\rangle / N \approx 0$

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  - $kT_c/J = 2.269$

Summary - Ising Model

- molecules on a lattice - each with with one of two possible states
- (magnetic) moments prefer to align
- low temperatures: ordered
- high temperatures: disordered

Chapter

Nucleation

- is a phase transformation process
- phase transformation grows from small nucleus

Examples

- cloud chamber
- supercooled water

Nucleation

- Homogeneous nucleation
  - in a uniform substance
  - no nucleation until nucleus with critical size "appears" (due to stochastic processes)
  - higher supersaturation leads to smaller critical radius.
  - rarely occurs in nature
- Heterogeneous Nucleation
  - begins at some preferable interface and grows from there
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Chapter

Homogeneous Nucleation in the Ising Model

- Necessary modifications:
  - none
- Problems
  - long time until nucleus of critical size appears
  - inefficient to simulate billions of cycles until phase change takes place

Cluster size

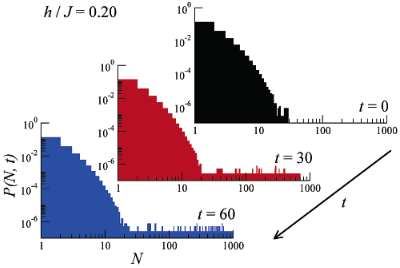

Figure: Propability of finding a cluster of size N at different times[3]

[3] Pan, Rappl, Chandler, Balsara: J. Phys. Chem. B 2006

Transition Path Sampling (TPS) - "shooting" method[4]

- needs two stable states (A & B)
- path through configuration space connecting these
- change the path a little at a random point between A and B
- sample new path and accept if it connects A with B

[4] aaDellago, Bolhuis, Chandler: Advances in Chemical Physics 123 (1998)

Transition Path Sampling

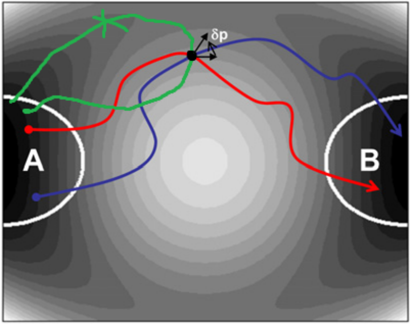

Figure: First path (red), slightly changed and accepted path (blue), rejected path (green)[5]

[5] Esobedo, Borrero, Araque - J. Phys.: Condens. Matter 21 (2009)

Heterogeneous Nucleation

- Necessary modifications:
  - handle boundaries in heterogeneous nucleation

$$H(s) = -J \sum_{<i,j>} s_i \cdot s_j - h \sum_{i} s_i - J_s \sum_{<i,j>}^{||} s_i \cdot s_j$$

  - implement walls/surfaces with fixed spins

Nucleation in and out of Pores[6]

$$H(s) = -0.8 \sum_{<i,j>} s_i \cdot s_j - 0.05 \sum_{i} s_i - 0 \overset{||}{\sum_{<i,j>}} s_i \cdot s_j, \qquad kT = 1$$

- nucleation near surfaces 10^{12} times faster
- fastest in pores
- nucleation in 2 steps
- diversified pore sizes lead to fastest reaction as probability of existence optimal pore size is higher

[6] Page, Sear - Heterogeneous Nucleation in and out of Pores PRL 97, 065701 (2006)

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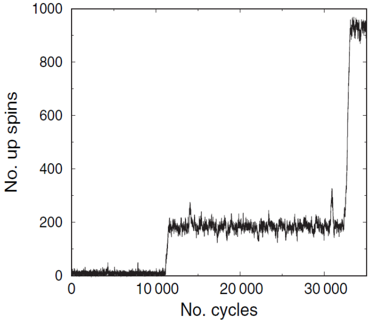

Figure: 2 phases of nucleation

[6]Page, Sear - Heterogeneous Nucleation in and out of Pores PRL 97, 065701 (2006)

Problems

- phase transitions are rare events (with realistic values for the coupling constant, ...)
- nonequilibrium systems therefore TPS (transition path sampling) not applicable.

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- $\rightarrow$ Forward Flux Sampling

Forward Flux Sampling

- Similar to TIS (transition interface sampling - a modified TPS)
  - initial state A: $\lambda < \lambda_A = \lambda_0$
  - final state B: $\lambda > \lambda_B = \lambda_n$
  - path has to pass every λ_i in increasing order (can go backwards in between too) until it reaches λ_n (B)
- after reaching a new interface (λ_{i+1}) configuration is stored
- stored configurations used as starting point for new trial runs
- trial runs continued until path reaches A ($\rightarrow$ failure) or a new interface λ_{i+1} ($\rightarrow$ success)

(Direct) Forward Flux Sampling[7]

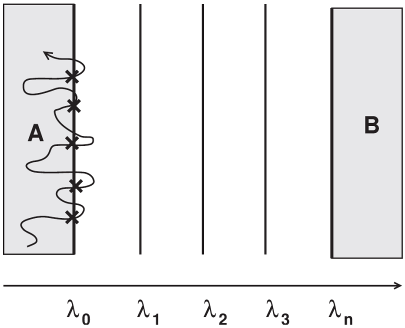

Figure: Sampling path starting in A - store configurations where the path leaves A (X)

[7] Allen, Valeriani, Rein ten Wolde: 2009 J. Phys.: Condens. Matter 21

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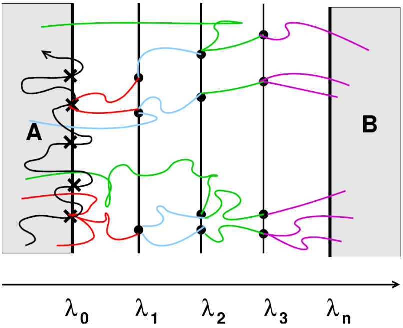

Figure: Sampling new paths from every stored configuration. Discard if path goes back to A

[7] Allen, Valeriani, Rein ten Wolde: 2009 J. Phys.: Condens. Matter 21

Chapter

Possible Adjustments to the Ising Model

- next-nearest neighbor interaction or even higher range
- forces from the outside, e.g. gravity
- Multi Hit Swendsen Wang algorithm
- Kawasaki Dynamics (alternative Metropolis algorithm with fixed state ratios and amounts)
  - choose any (A-B) bond
  - $(A - B) \rightarrow (B - A)$
  - calculate new energy
  - ...

Potts Model

- states not only $-1 \wedge 1$ but (discrete) angles.
- $H = -J_c \sum_{i,j} cos\left(\theta_i - \theta_j\right) + \dots$
- Applications
  - percolation (Wu: "Percolation and the Potts Model" (1978))
  - flow of foam (Sanyal, Soma: "Viscous instabilities in flowing foams" (2006))
  - cancerous tumors (Sun, Chang, Cai: "A Discrete Simulation of Tumor Growth Concerning Nutrient Concentration" (2004))

- Page, Sear - Heterogenous Nucleation in and out of Pores (2006): PRL 97, 065701
- Allen, Valeriani, Rein ten Wolde - Forward Flux Sampling for rare event simulations (2009): J. Phys.: Condens. Matter 21 (2009) 463102 (21pp)
- Allen, Frenkel, Rein ten Wolde - Forward Flux Sampling-type schemes for simulating rare events: Efficiency analysis (2008): http://arxiv.org/abs/cond-mat/0602269v1
- Escobedo, Borrero, Araque - Transition path sampling and forward flux sampling. Applications to biological systems 2009 J. Phys.: Condens. Matter 21 333101

- Sourcefiles and binaries on my github
  https://github.com/oerpli/Ising2D