AP3082 Presentation: XY-Model

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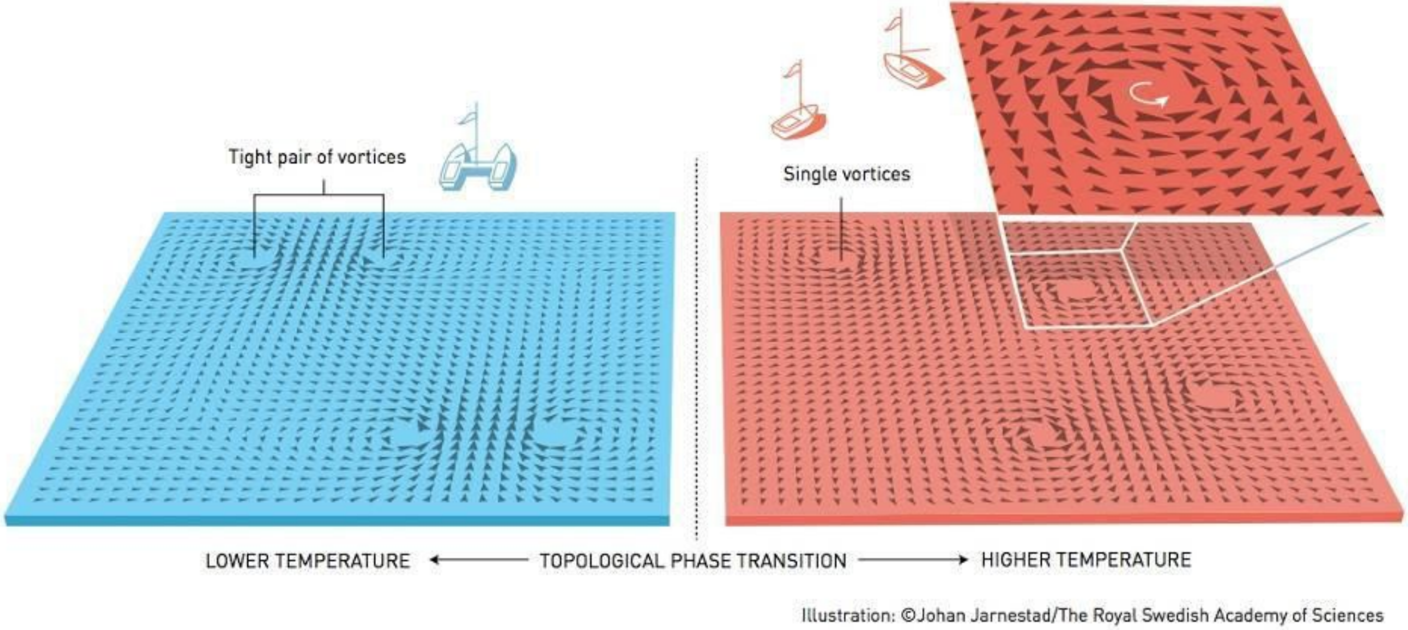
The XY model

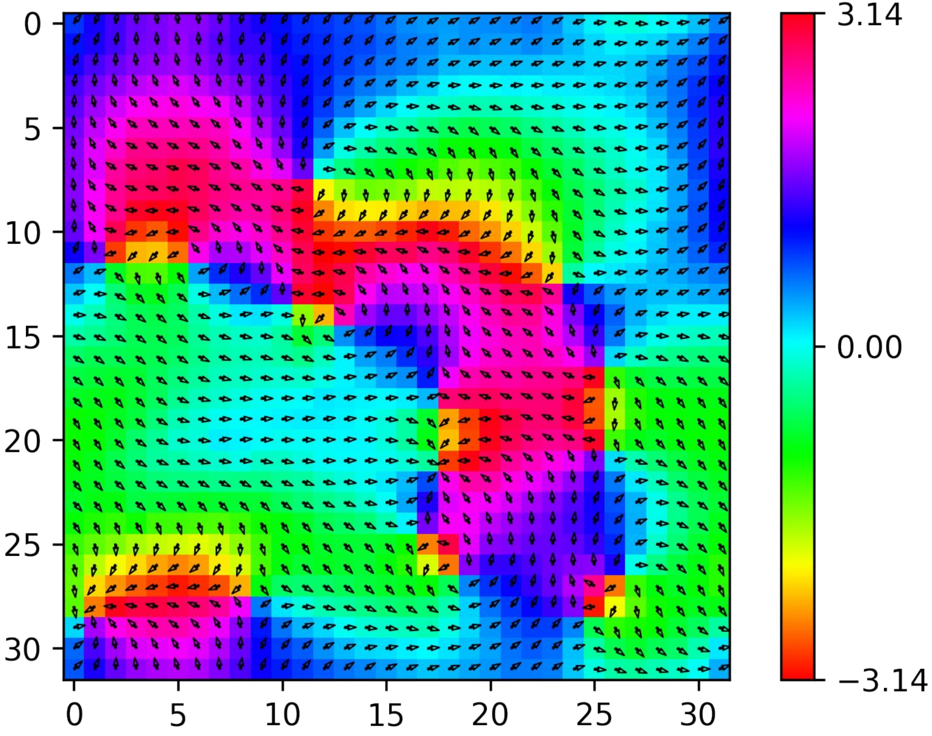


Research questions

- What is the order parameter that describes the system?
- What is the behaviour of the system under different algorithms?

The XY model

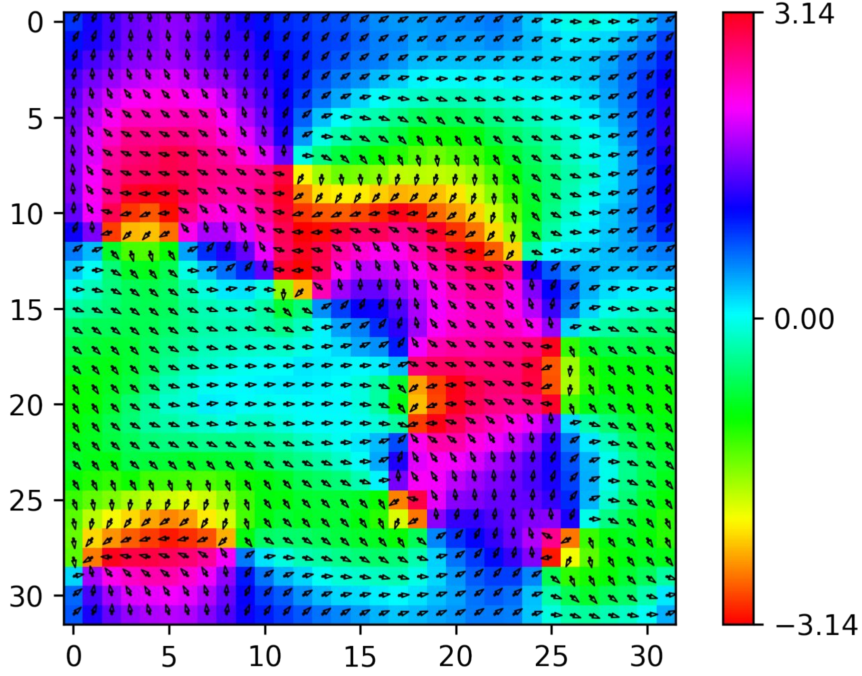
- Two-dimensional.
- Ferromagnetic, $J > 0$.
- Nearest-neighbour model.
- Periodic boundary condition.



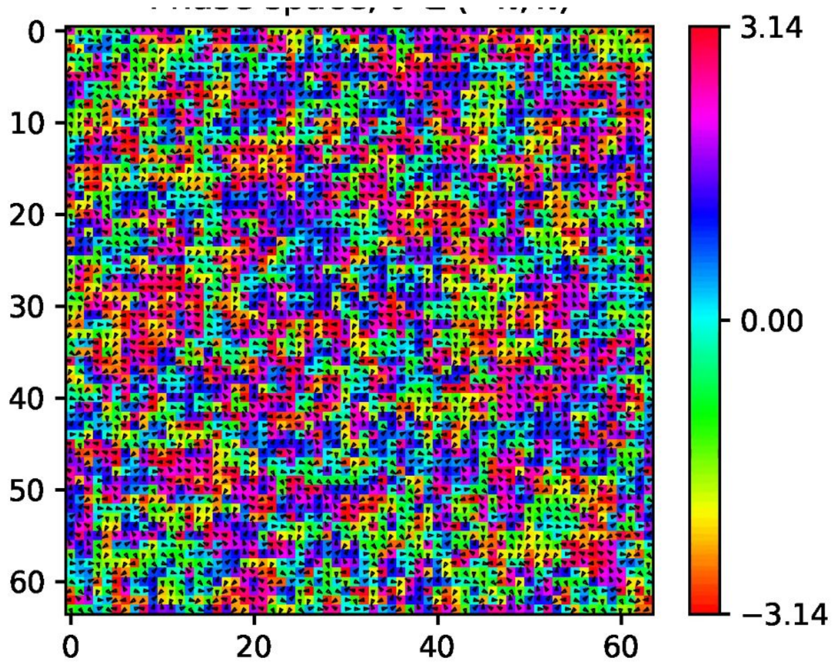
$$H = -J \sum_{\langle i,j \rangle} \cos\left(\phi_i - \phi_j\right), \quad \phi \in (-\pi, \pi]$$

Temperature phases?

Low temperature



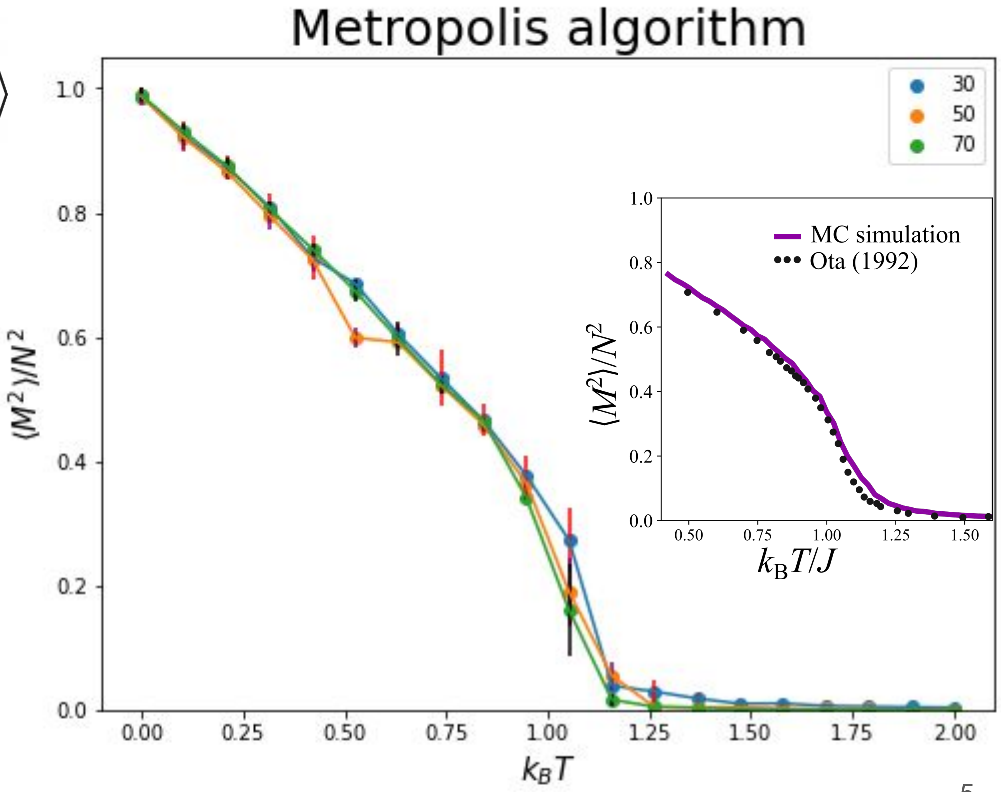
High temperature



Magnetization vs Temperature

$$\frac{\langle M^2 \rangle}{L^4} = \frac{1}{L^4}\left\langle \left(\sum_{i=1}^{N} \cos\theta_i\right)^2 + \left(\sum_{i=1}^{N} \sin\theta_i\right)^2 \right\rangle$$

- Smooth transition from low to high temperature.
- Absence of long-range order.
- Consistent behaviour under different algorithms.



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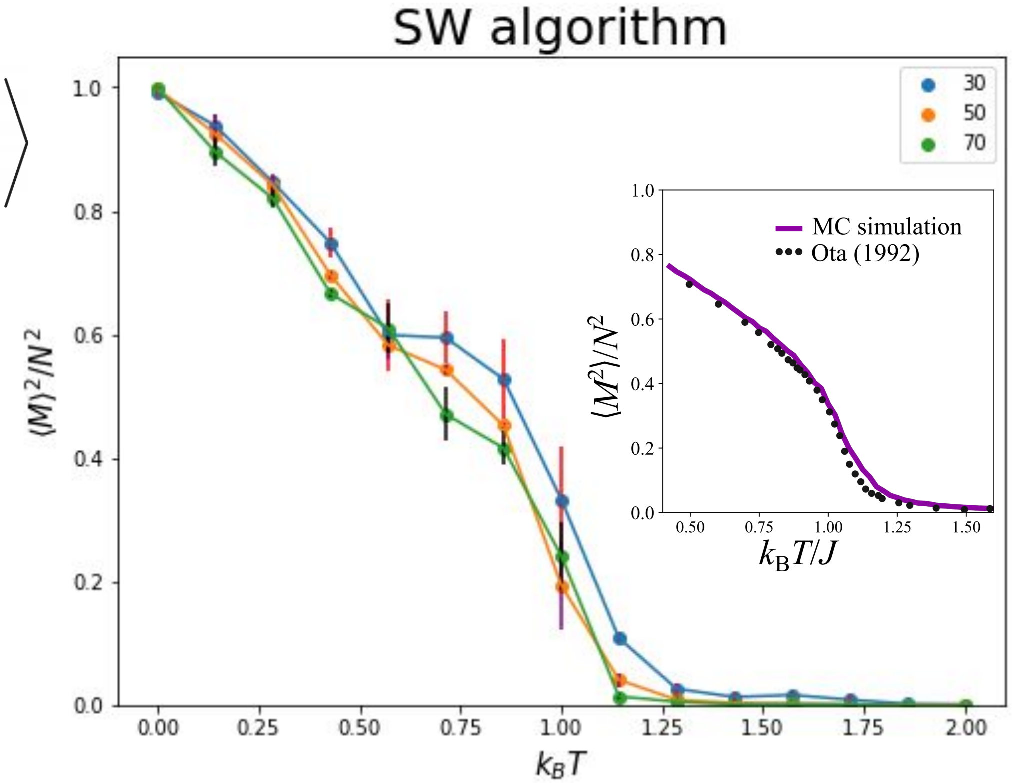

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- Absence of long-range order.
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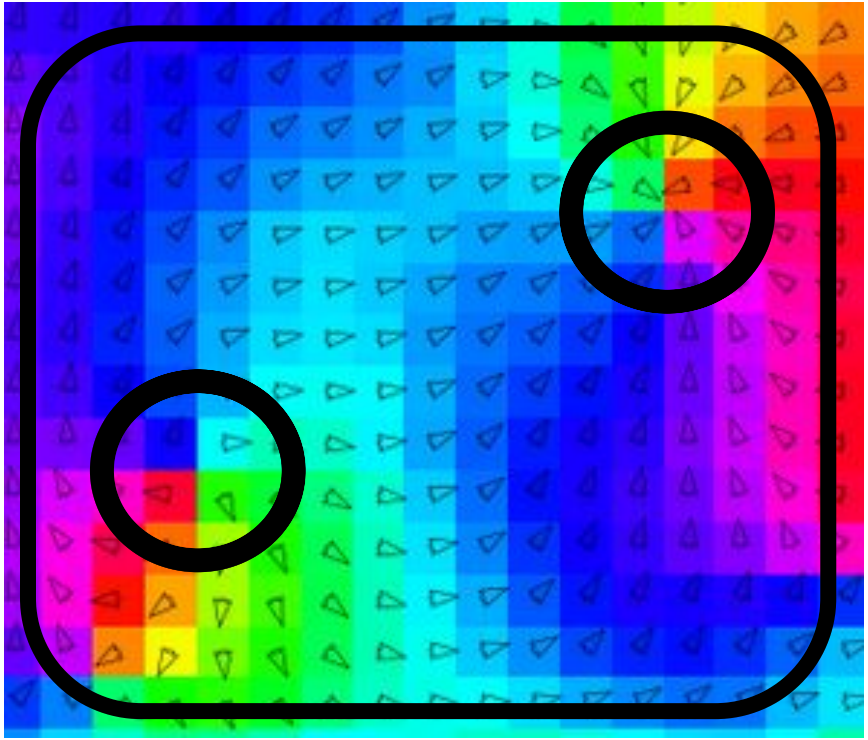
Is there a phase transition?

Vortices and anti-vortices



- They are sources (sinks) of winding spins.
- Vorticity is a path integral around a vortex.

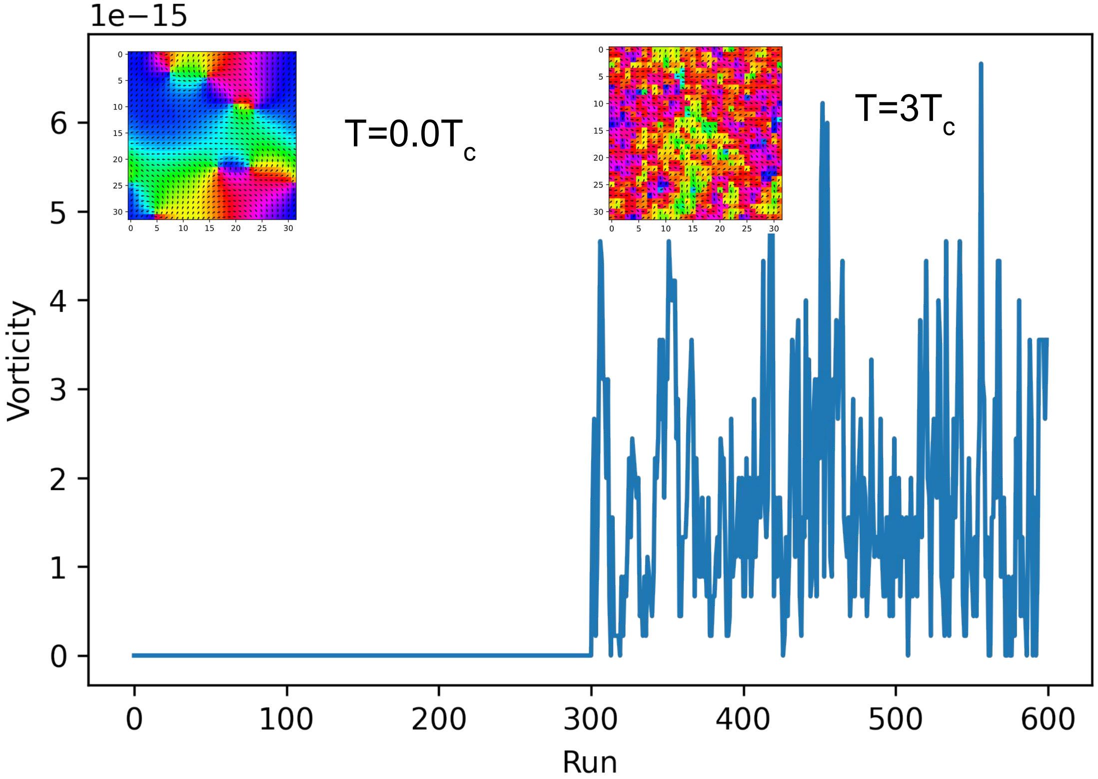
$$2\pi n_\nu = \oint d\vec{l} \cdot \vec{\nabla}\theta(x,y) \approx \sum_C \vec{n}_C \cdot \vec{\nabla}\theta_C$$

Vortices and anti-vortices

- Low temperature phase: Pairs of vortices

- High temperature phase: Unbinded vortices

Vorticity can be used as an order parameter in the XY model.



L=32, τ_{relax} = 500000, τ_{extra} = 2000

Vortices and anti-vortices

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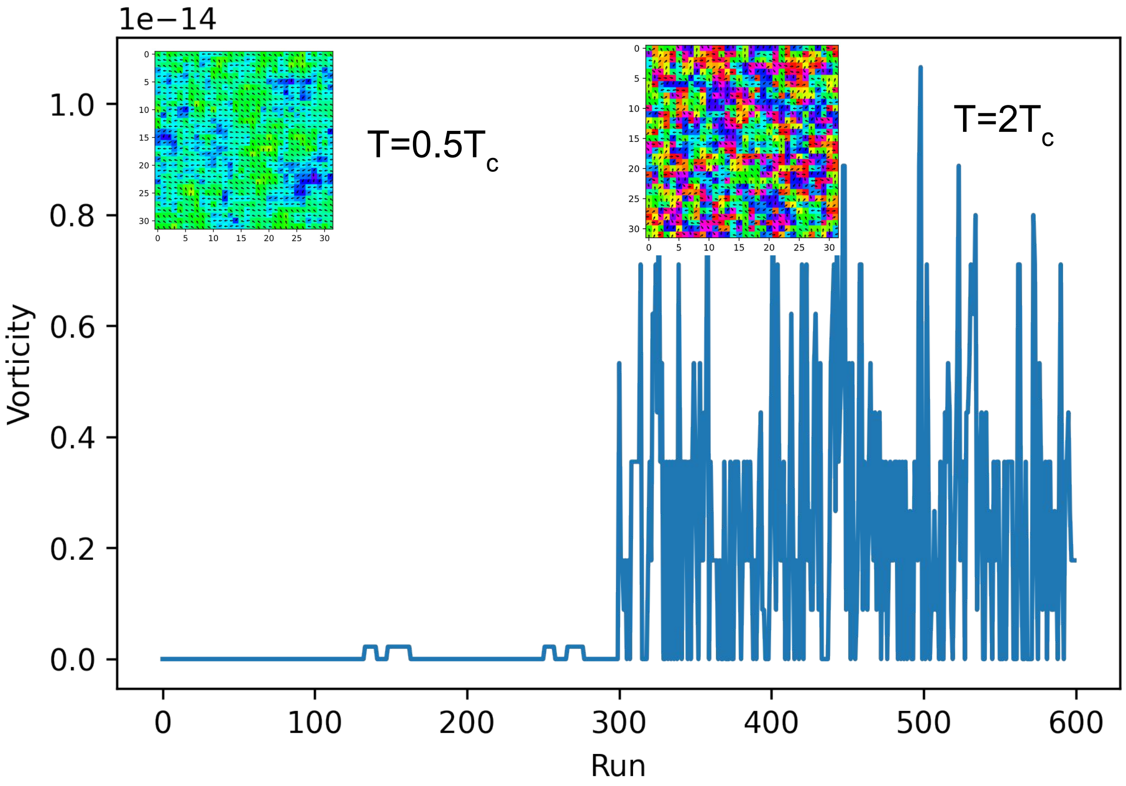
Vorticity can be used as an order parameter in the XY model?



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Vortices and anti-vortices

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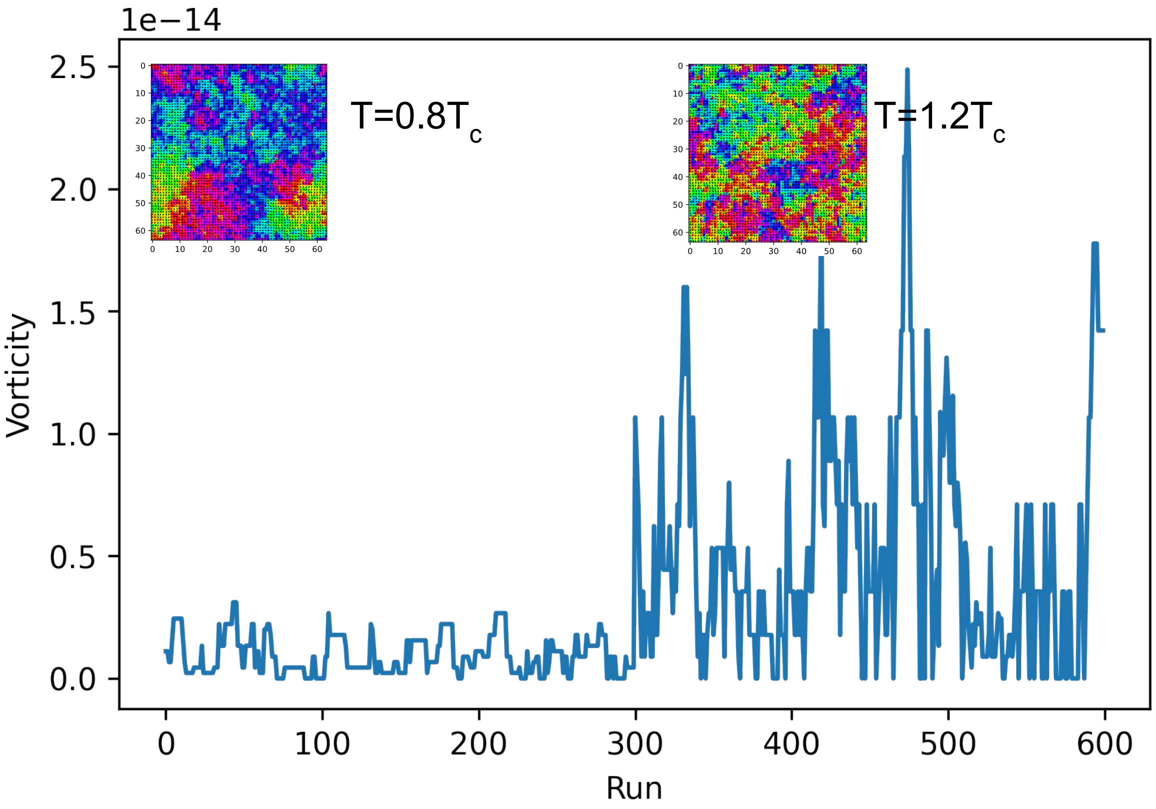
Vorticity can be used as an order parameter in the XY model?

No! Problem with our code.



L=64, τ_{relax} = 600000, τ_{extra} = 2000

Cluster algorithm: Swendsen-Wang algorithm

Procedure:

- Create clusters of similarly aligned spins with probability:

$$P(\vec{s}_i, \vec{s}_j) = 1 - e^{-2\beta(\vec{s}_i \cdot \vec{r})(\vec{s}_j \cdot \vec{r})}$$

- Flip all clusters with ½ probability.

Cluster formation: Each color represents a different cluster made of similarly aligned spins

Cluster algorithm: Swendsen-Wang algorithm

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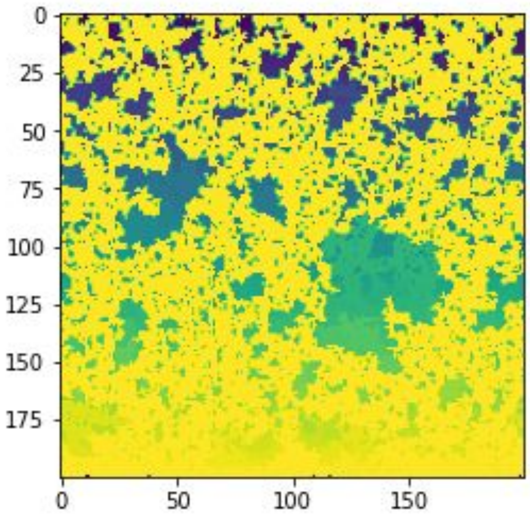


Cluster algorithm: Invaded cluster (not implemented)

Obtain the critical temperature of the system with no a-priori information by inducing percolation in the spin clusters.

Simulation validation $\langle M^2(T)\rangle/N^2$

T	[1]	[2]	SW	Error	Met	Error
0.5	0.71	0.71	0.77 ± 0.12	8%	0.69 ± 0.03	2.8%
0.9	0.44	0.44	0.3 ± 0.004	32%	0.42 ± 0.02	4.5%
1.	0.3	0.33	0.1 ± 0.004	66%	0.17 ± 0.06	48%
1.1	0.11	0.12	0.001 ± 0.0004	99%	0.08 ± 0.03	33%
1.2	0.05	0.05	0.00 ± 0.0	-	0.01 ± 0.01	80%

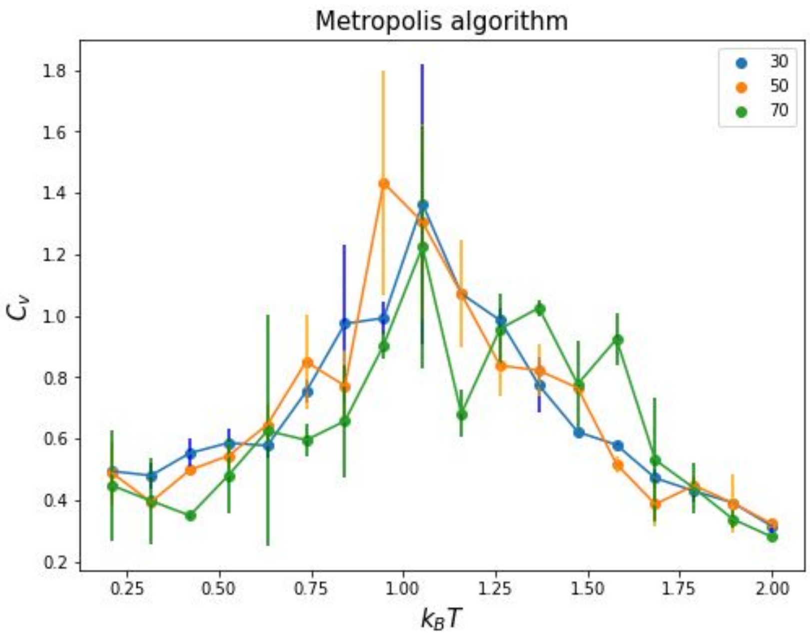
[1]: https://doi.org/10.1143/PTP.60.1669 Miyashita et al 1978

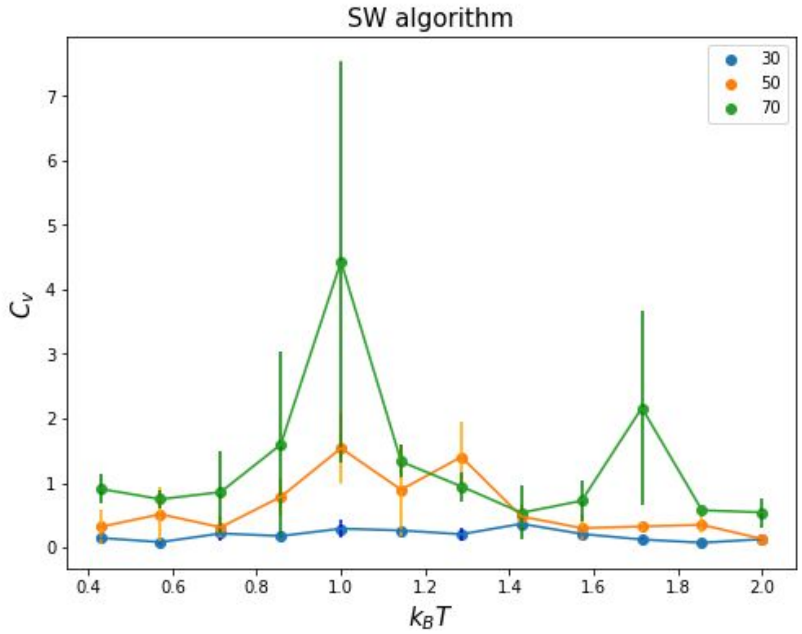
[2]: https://doi.org/10.1088/0953-8984/4/24/011 Ota et al 1992

MT: $\tau_{relax} = \tau_{wait} = 5$ E5. SW: $\tau_{relax} = \tau_{wait} = 10$. Size: L =64. Error calculation: data blockage method.

Specific heat vs Temperature

$$c / k_{\mathrm{B}} = \frac{\left\langle E^2 \right\rangle - \left\langle E \right\rangle^2}{L^2 \left(k_{\mathrm{B}} T \right)^2}$$



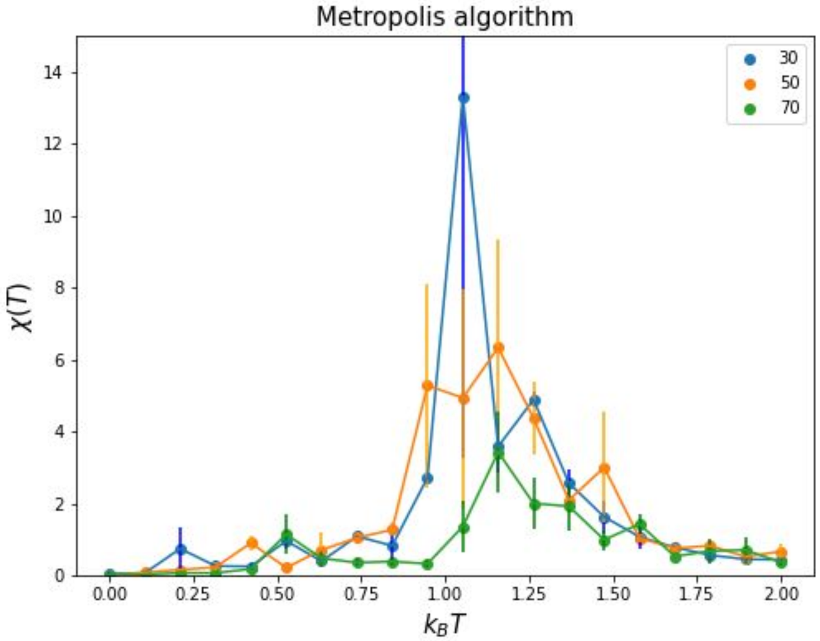


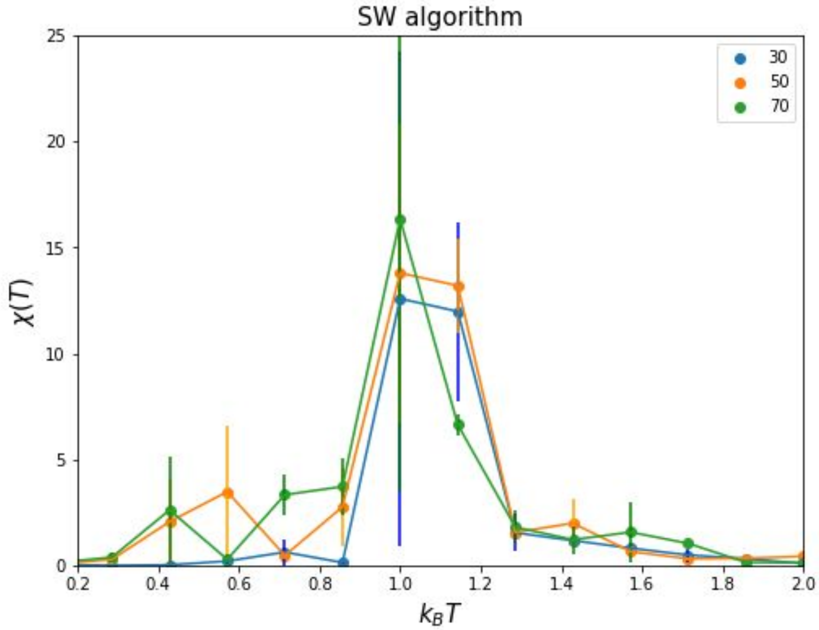
MT: t_relax = t_wait = 5 E5. SW: t_relax = 10, t_wait = 8.

Error calculation: data blockage method.

Susceptibility vs Temperature

$$\chi(T) = \frac{N^2}{k_B T}(\langle M^2 \rangle - \langle M \rangle^2)$$





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Error calculation: data blockage method.

Numba

- Designed to be used with NumPy
- Decorator to functions
- Translates to machine code
- Leads to high-speed (C++)

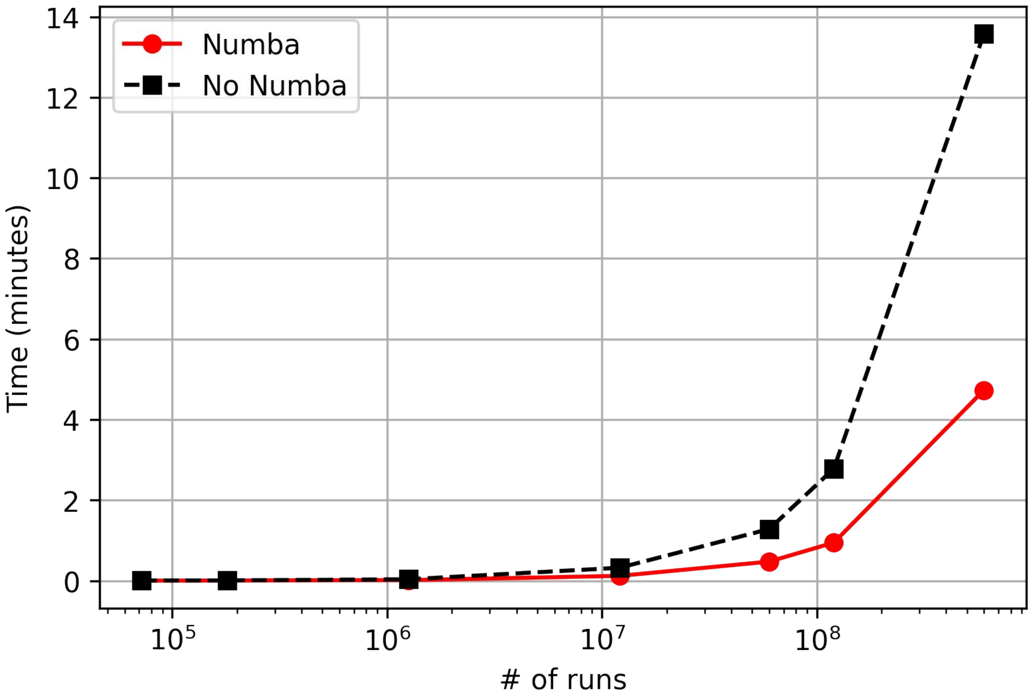
```
from numba import jit
import random

@jit(nopython=True)
def monte_carlo_pi(nsamples):
    acc = 0
    for i in range(nsamples):
        x = random.random()
        y = random.random()
        if (x ** 2 + y ** 2) < 1.0:
            acc += 1
    return 4.0 * acc / nsamples
```

Source: http://numba.pydata.org/

Performance: Numba vs no Numba

- Small # of runs
  - No difference
- Large # of runs
  - Large difference



Conclusion: Research questions

- What is the order parameter that describes the system?

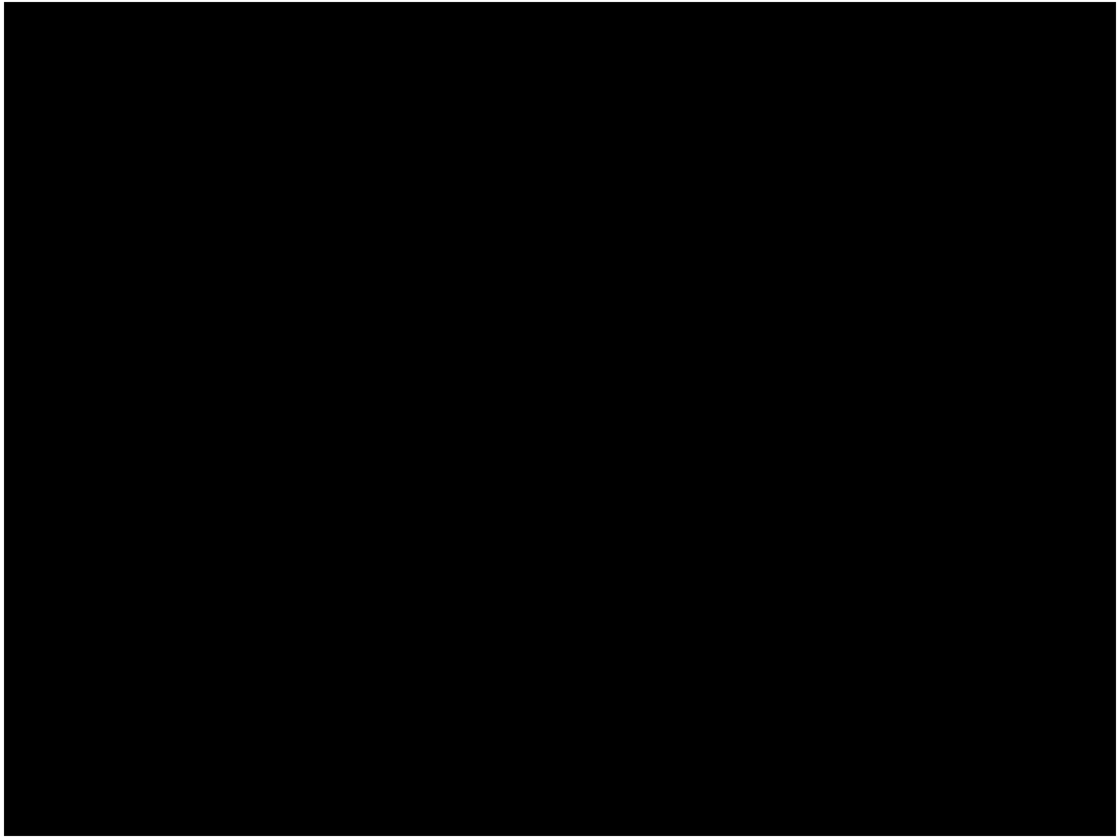
The vorticity describes the topological phase transition of the system, however we did not manage to implement it.

- What is the behaviour of the system under different algorithms?

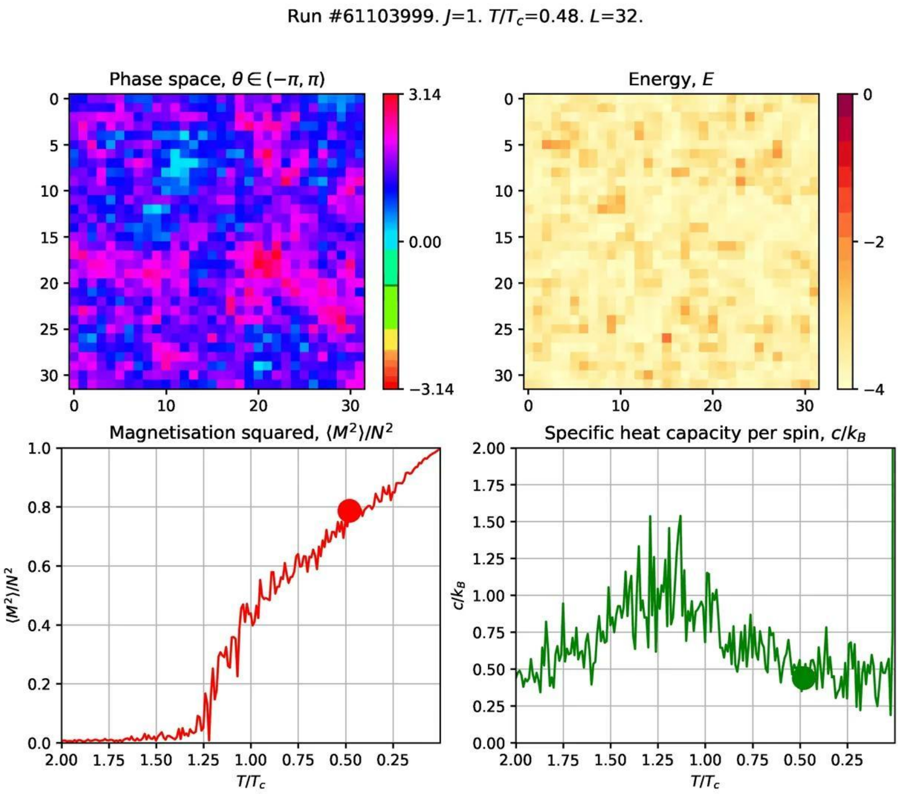
Our simulation results are in agreement with the literature. Errors are larger as temperature increase.

Thank you for your attention!
Questions?

Appendix: Slow quench



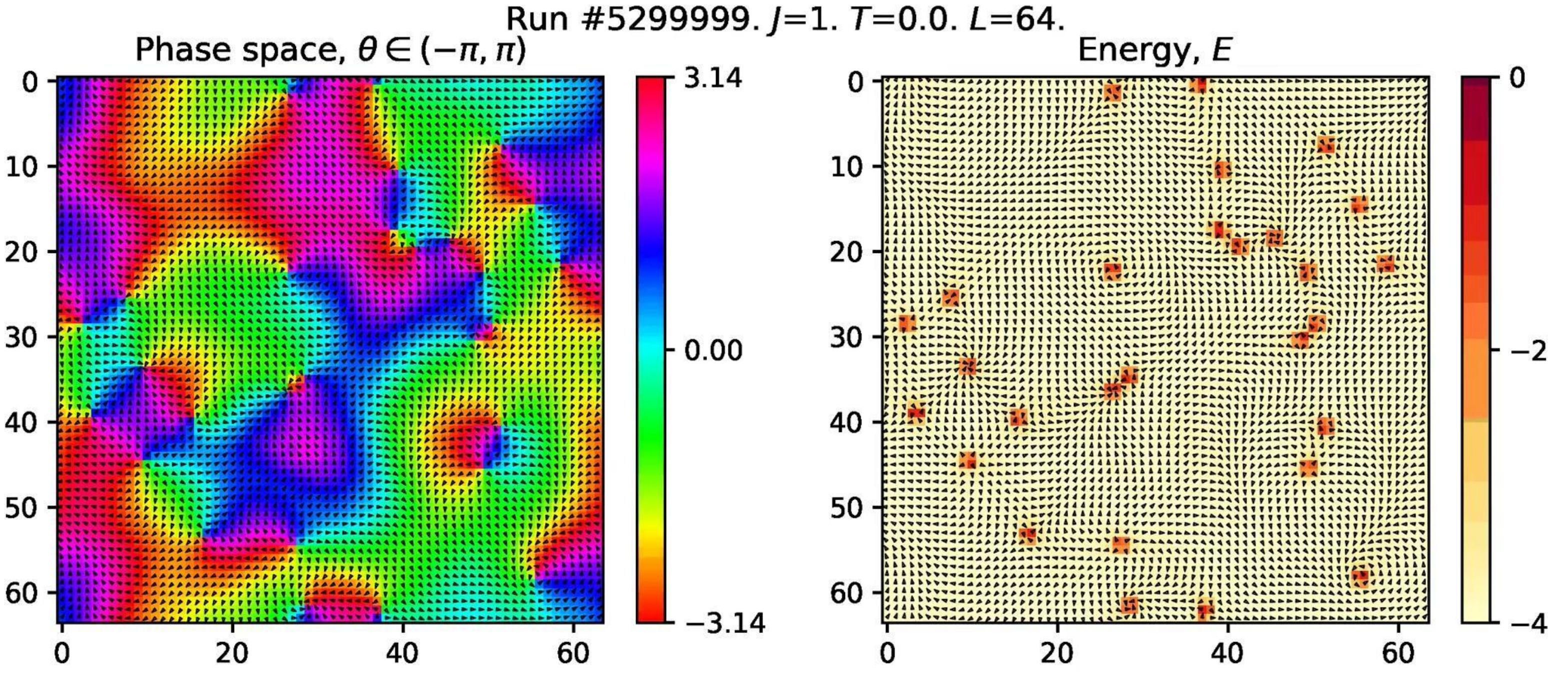
Appendix: Slow quench



- Magnetisation
  - Sharp change at $T/T_c=1$.

- Specific heat capacity
  - KT theory -
    $T_c <$ peak

Appendix: Fast quench



Appendix: Metropolis algorithm (brief recap)

- Choose a random spin as trial spin.
- Rotate it by random amount.
- Calculate $\Delta E = E_{trial} - E_{old}$.
- If $\Delta E \leq 0$
  - Take trial spin as the new spin.
- Else
  - If $r < \exp(-\Delta E/T)$, $r \in [0,1]$
    - Take trial spin as the new spin.
  - Else
    - Continue without changes.