The Transverse Field Ising Model

Monte-Carlo simulation of Quantum Phase Transitions

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22/12/2023

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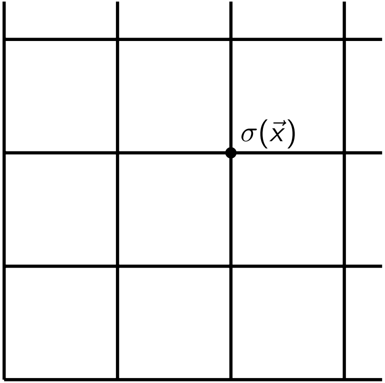
$\mathbb{Z}_2$ gauge theory

- $\mathbb{Z}_2$ gauge theory Hamiltonian on a 2D lattice

$$H_{\mathbb{Z}_2} = -g \sum_{\vec{x},j} \sigma_j^x(\vec{x})$$

$$-\frac{1}{g} \sum_{\vec{x}} \sigma_1^z(\vec{x})\sigma_2^z(\vec{x}+e_1)\sigma_1^z(\vec{x}+e_2)\sigma_2^z(\vec{x}),$$



$\mathbb{Z}_2$ gauge theory

- $\mathbb{Z}_2$ gauge theory Hamiltonian on a 2D lattice

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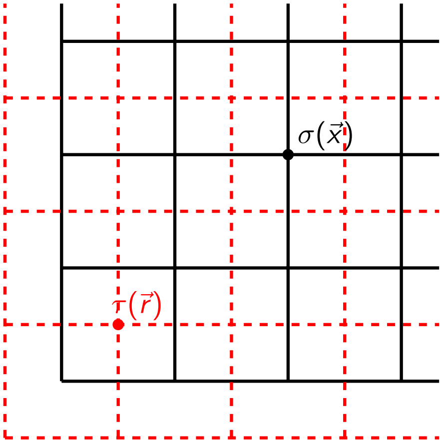
- Duality with a Transverse Field Ising model on the 2D dual lattice

$$H = -g \sum_{\vec{r},j} \tau^z(\vec{r})\tau^z(\vec{r}+e_j) - \frac{1}{g} \sum_{\vec{r}} \tau^x(\vec{r}).$$



The Transverse Field Ising model

$$H = -J \sum_{\langle i,j \rangle} S_i^z S_j^z - \Gamma \sum_i S_i^x$$

$$[S^z, S^x] = iS^y, \qquad S^z |\pm 1\rangle = \pm |\pm 1\rangle, \qquad S^x |\pm 1\rangle = |\mp 1\rangle$$

A quantum Hamiltonian requires a quantum treatment!

Classical Mapping: a proof in 1D

From the Hamiltonian

$$H = -J \sum_{i=1}^{N} S_i^z S_{i+1}^z - \Gamma \sum_{i=1}^{N} S_i^x ,$$

compute the partition function

$$Z = \mathrm{Tr} \exp\left(-\beta H\right) = \mathrm{Tr} \exp\left(-\beta \left(H_0 + V\right)\right) .$$

Classical Mapping: a proof in 1D

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With the Trotter formula [3]

$$\exp\left(A_1 + A_2\right) = \lim_{M\to\infty}\left[\exp\left(A_1/M\right)\exp\left(A_2/M\right)\right]^M,$$

expand the partition function

$$Z = \sum_{\{S_1^1,\cdots,S_N^1\}} \langle S_1^1,\cdots,S_N^1|\, e^{-\beta H_0/M} e^{-\beta V/M} \times \cdots \times e^{-\beta H_0/M} e^{-\beta V/M}\, |S_1^1,\cdots,S_N^1\rangle\,.$$

$$
\begin{aligned}
Z &= \sum_{\{S_1^1,\cdots,S_N^1\}} \langle S_1^1,\cdots,S_N^1|\, e^{-\beta H_0/M} e^{-\beta V/M} \times \cdots \times e^{-\beta H_0/M} e^{-\beta V/M}\, |S_1^1,\cdots,S_N^1\rangle \\
&= \sum_{\{S\}} \prod_{k=1}^{M} \langle S_1^k,\cdots,S_N^k|\, e^{-\beta H_0/M} e^{-\beta V/M}\, |S_1^{k+1},\cdots,S_N^{k+1}\rangle
\end{aligned}
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&= \sum_{\{S\}} \prod_{k=1}^{M} \langle S_1^k, \cdots, S_N^k | \, e^{-\beta H_0/M} e^{-\beta V/M} \, | S_1^{k+1}, \cdots, S_N^{k+1} \rangle \\
&= \left(\frac{1}{2} \sinh(2\beta\Gamma/M) \right)^{MN/2} \sum_{\{S\}} \exp \Bigg[-\frac{\beta}{M} \Bigg(-J \sum_{i=1}^{N} \sum_{k=1}^{M} S_i^k S_{i+1}^k \\
&\qquad - \frac{M}{2\beta} \ln \coth \left(\frac{\beta\Gamma}{M} \right) \sum_{i=1}^{N} \sum_{k=1}^{M} S_i^k S_i^{k+1} \Bigg) \Bigg]
\end{aligned}
$$

Classical mapping in 1D

$$H = -J \sum_{i=1}^{N} S_i^z S_{i+1}^z - \Gamma \sum_{i=1}^{N} S_i^x,$$

$$\Updownarrow$$

$$H_{\text{eff}} = -J \sum_{i=1}^{N} \sum_{k=1}^{M} S_i^k S_{i+1}^k - \frac{M}{2\beta} \ln\coth\left(\frac{\beta\Gamma}{M}\right) \sum_{i=1}^{N} \sum_{k=1}^{M} S_i^k S_i^{k+1},$$

Classical mapping in 1D

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Classical thermal phase transitions in $d+1$ dimensions

$\downarrow$

Quantum phase transitions in d dimensions

Classical mapping in 2D

The quantum Hamiltonian on a 2D $N_x \times N_y$ lattice

$$H = -J \sum_{i,j} S^z_{i,j} \left(S^z_{i+1,j} + S^z_{i,j+1} \right) - \Gamma \sum_{i,j} S^x_{i,j},$$

can be mapped to a classical anisotropic Ising model on a 3D $N_x \times N_y \times N_z$ lattice

$$H_{\text{eff}} = -\sum_{k=1}^{N_z} \sum_{i,j} \left[J S_{i,j,k} \left(S_{i+1,j,k} + S_{i,j+1,k} \right) + K_{N_z}(\beta) S_{i,j,k} S_{i,j,k+1} \right].$$

Phase transitions

Two phases

- $\Gamma/J \ll 1$: ferromagnetic phase

$$H \simeq -J \sum_{\langle i,j \rangle} S_i^z S_j^z$$

- $\Gamma/J \gg 1$: paramagnetic phase

$$H \simeq -\Gamma \sum_i S_i^x$$

Observables

- Magnetisation per spin

$$m = \frac{1}{N} \sum_{\mathrm{i,j,k}} S_{i,j,k}$$

- Magnetic susceptibility

$$\chi = \frac{\partial m}{\partial \Gamma} = \beta \left(\langle m^2 \rangle - \langle m \rangle^2 \right)$$

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Metropolis-Hasting algorithm

1. Start from an initial configuration.
2. Sweep through the lattice: flip random spins
   - If $\mathrm{d}E < 0$: accept this new configuration.
   - Else: accept with probability $\exp\left(-\beta \mathrm{d}E\right)$.
3. Repeat sweeps until the required number of configurations have been generated.
4. Ditch the first N_{eq} configurations generated before reaching equilibrium.

From [2]

Monte-Carlo sweeps

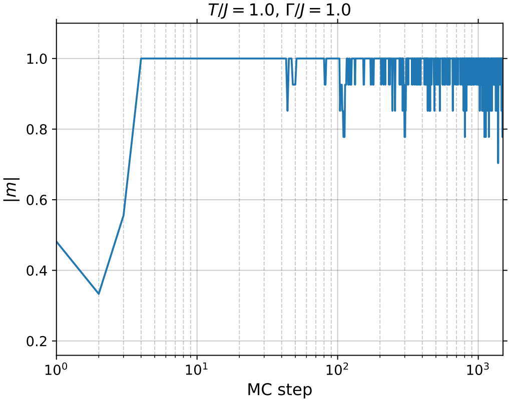

Figure: Magnetisation per spin as our Monte-Carlo process goes on at $T/J = 1$ and $\Gamma/J = 1$ for a $3 \times 3 \times 3$ lattice. One MC step represents a whole sweep of the lattice.

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Trotter dimension size

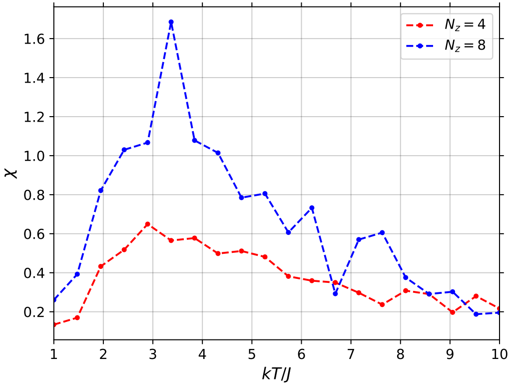

Figure: Susceptibility as a function of temperature for $\Gamma/J = 1$ for a $2 \times 2 \times N_z$ lattice.

Thermal phase transition

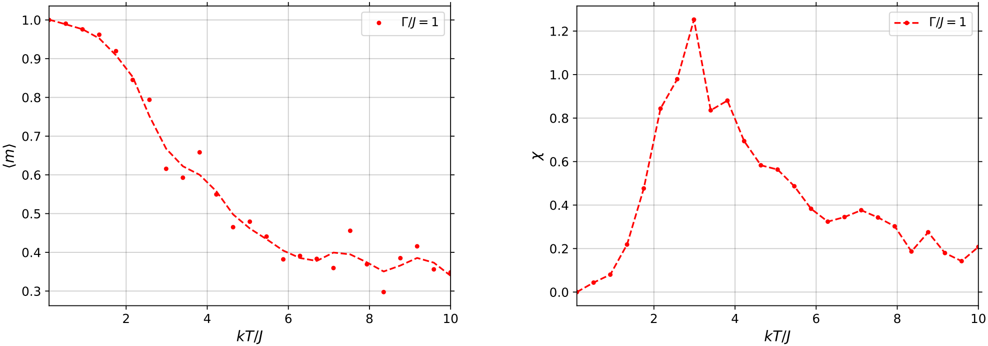

Figure: $3 \times 3 \times 4$ lattice at $\Gamma/J = 1$

Quantum phase transitions

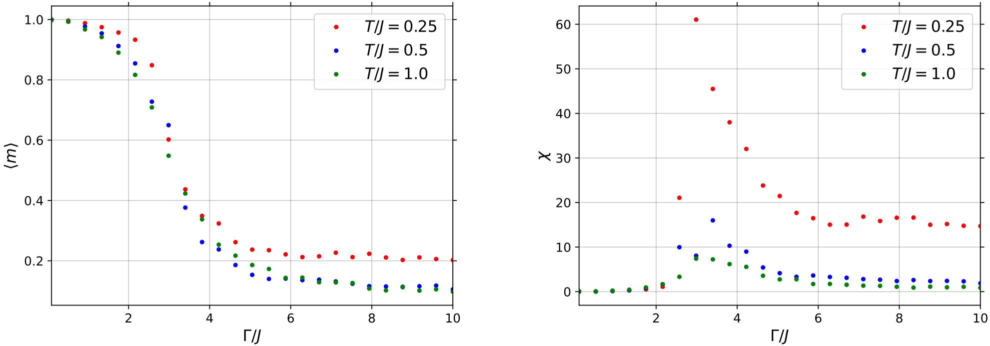

Figure: $4 \times 4 \times 10$ lattice

Closing remarks

- A quantum system can be mapped to a classical one with one additional dimension.
- The size of the additional dimensions has to be large for the mapping to work $\Rightarrow$ limitations due to the slowness of our algorithm.
- There are numerous other methods for probing $T = 0$ phase transitions.
- There exists a nice link between gauge theories on the lattice and classical statistical mechanics.

References

[1] Eduardo Fradkin. *Field Theories of Condensed Matter Physics*. 2nd ed. Cambridge University Press, 2013. DOI: 10.1017/CBO9781139015509.

[2] *Monte Carlo Simulation in Statistical Physics: An Introduction*. Cham: Springer International Publishing, 2019.

[3] H.F. Trotter. "On the product of semi-groups of operators". In: *Proc. Amer. Math. Soc.* *10* (1959), pp. 545–551.