Gauge Theory, Duals and Monte Carlo

Exploring the Ising model under the singlet constraint

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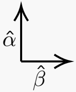
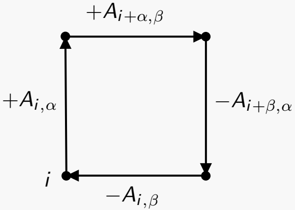
Maxwell ED on a 2D lattice

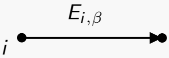
$$\vec{E} \xrightarrow{\text{discrete}} \vec{E}_i = (E_{i,\alpha}, E_{i,\beta})$$

$$B = (\vec{\nabla} \times \vec{A})_z \xrightarrow{\text{discrete}} B_i = A_{i,\beta} + A_{i+\beta,\alpha} - A_{i+\alpha,\beta} - A_{i,\alpha}$$





Magnetic (discrete curl)

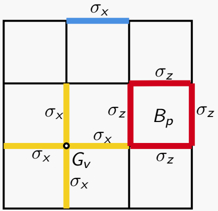


Electric (edge)

$\mathbb{Z}_2$ Lattice Gauge Theory

Hamiltonian of the pure $\mathbb{Z}_2$ lattice gauge theory:

$$H = -J \sum_p \underbrace{\prod_{e \in p} \sigma_e^z}_{B_p} - h \sum_e \sigma_e^x .$$



Gauge transformation (Local symmetry):

$$G_v = \prod_{e \in +_v} \sigma_e^x, \qquad [G_v, H] = 0,$$

$$G_v^2 = \mathbb{1} \implies G_v = \pm 1.$$

$\mathbb{Z}_2$ Lattice Gauge Theory (contd.)

Constraints:

- To probe the low energy subspace, we choose the charge-free sector (Gauss' law constraint)

$$G_v = +1, \; \forall \; v.$$

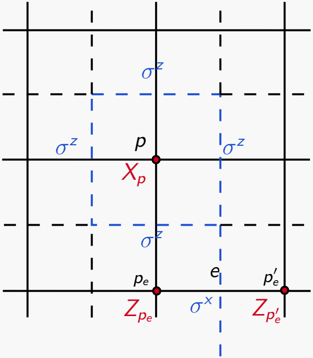
$$\left[G_v \sim e^{i(\vec{\nabla}\cdot\vec{E})_v} = +1 \implies (\vec{\nabla}\cdot\vec{E})_v = 0.\right]$$

- On a torus,

$$\prod_p B_p = \mathbb{1}.$$

Dual transformation:

$$\sigma_e^x = \sigma_{p_e\, p'_e}^x \longrightarrow Z_{p_e} Z_{p'_e},$$
$$\prod_{e \in p} \sigma_e^z = B_p \longrightarrow X_p.$$



The dual Hamiltonian is given by:

$$H = -J \sum_p B_p - h \sum_e \sigma_e^x$$

$$\Downarrow$$

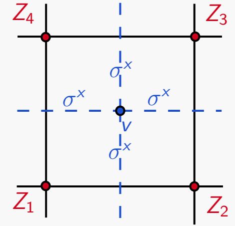
$$\boxed{H_{\text{dual}} = -J \sum_p X_p - h \sum_e Z_{p_e} Z_{p'_e}}$$

The singlet constraint

Constraints from $\mathbb{Z}_2$ gauge theory:

- Gauss' law constraint is automatically satisfied

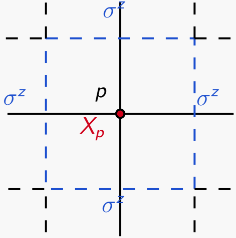
$$G_v = \prod_{e \in +_v} \sigma_l^x = \prod_{\langle ij \rangle \in \square_v} Z_i Z_j \equiv \mathbb{1}.$$



- The periodic boundary conditions of the $\mathbb{Z}_2$ lattice lead to

$$\prod_p B_p = \boxed{\prod_i X_i \stackrel{!}{=} \mathbb{1}.}$$

This is known as the **singlet constraint**.



Path Integral quantum Monte Carlo

The singlet-Ising model in d-dimensions:

$$\hat{H} = -J \sum_p \hat{X}_p - h \sum_e \hat{Z}_{p_e} \hat{Z}_{p'_e}, \qquad \prod_p \hat{X}_p \overset{!}{=} \mathbb{1}$$

The singlet Hilbert space is defined as:

$$\mathcal{H}_s = \{\text{span } \hat{P} \,|\{\sigma\}\rangle \text{ where } |\{\sigma\}\rangle = |\pm 1\rangle \otimes |\pm 1\rangle \ldots \otimes |\pm 1\rangle\}$$

and $\hat{P}$ is the singlet sector projector:

$$\hat{F} \equiv \prod_p \hat{X}_p \quad \Longrightarrow \quad \hat{P} = \frac{\hat{\mathbb{1}} + \hat{F}}{\sqrt{2}}$$

Partition function:

$$\mathcal{Z} = \mathrm{tr}\, e^{-\beta \hat{H}} = \sum_{\{\sigma\}} \langle \{\sigma\} | \hat{P}\, e^{-\beta \hat{H}}\, \hat{P} | \{\sigma\} \rangle$$

Trotterization process:

$$e^{-\beta H} = \underbrace{e^{-\Delta\tau H} e^{-\Delta\tau H} \ldots e^{-\Delta\tau H}}_{N_\tau \text{ times}} \text{ and insert } \mathbb{1}_s.$$

$$\implies \mathcal{Z} = \left(\prod_{\ell=0}^{N_\tau - 1} \sum_{\{\sigma(\ell)\}} \right) \prod_{\ell=0}^{N_\tau - 1} \langle \{\sigma(\ell+1)\} | \hat{P}\, e^{-\Delta\tau H}\, \hat{P} | \{\sigma(\ell)\} \rangle$$

where $N_\tau = \beta / \Delta\tau$.

Path Integral quantum Monte Carlo (contd.)

In the limit $N_\tau \to \infty$,

$$\mathcal{Z} = \left(\prod_{\ell=0}^{N_\tau - 1} \sum_{\{\sigma(\ell)\}} \right) e^{-S[\sigma]} \sim \int [\mathcal{D}\sigma] \, e^{-S[\sigma]}$$

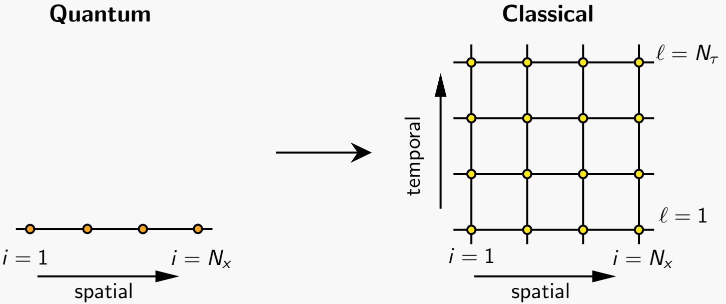
Effective classical action of the singlet theory:

$$S[\sigma] = -h\Delta\tau \sum_{\ell} \sum_{e} \sigma_{p_e}(\ell)\sigma_{p'_e}(\ell) - \sum_{\ell} \ln\cosh\left[K \sum_{p} \sigma_p(\ell+1)\sigma_p(\ell) \right]$$

where $K = -1/2 \ln\tanh(J\Delta\tau)$.

A generalized classical Ising model in $d+1$-dimensions.

Starting from 1-dimension



The resulting classical Ising model is now $(1+1)$-dimensional.

$$\boxed{S[\sigma] = -h\Delta\tau \sum_{\ell=1}^{N_\tau} \sum_{i=1}^{N_x} \sigma_i(\ell)\sigma_{i+1}(\ell) - \sum_{\ell=1}^{N_\tau} \ln\cosh\left[K \sum_{i=1}^{N_x} \sigma_i(\ell+1)\sigma_i(\ell)\right]}$$

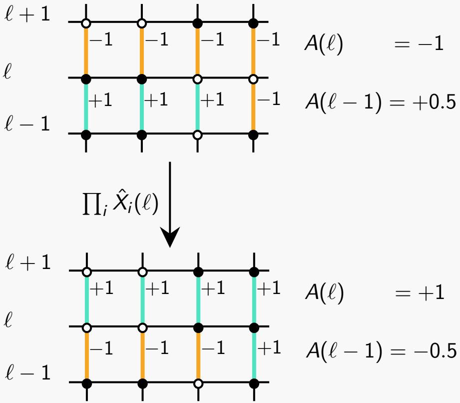
Subsystem Symmetry

Define a local "Alignment" observable:

$$A(\ell) \equiv \frac{1}{N_x} \sum_{i=1}^{N_x} [\sigma_i(\ell)\, \sigma_i(\ell+1)]$$

$$= \frac{1}{N_x}[N_a(\ell) - N_o(\ell)]$$

$$\in [-1, 1]$$



If spins are flipped along layer ℓ,

$$\implies A(\ell) \to -A(\ell), \qquad A(\ell-1) \to -A(\ell-1)$$

Flip operation:

- $\ln\cosh[-KN_x\, A(\ell)] = \ln\cosh[KN_x\, A(\ell)]$
- $[-\sigma_i(\ell)][-\sigma_{i+1}(\ell)] = \sigma_i(\ell)\sigma_{i+1}(\ell)$

$\implies$ S is invariant under the flip operation $\prod_i \hat{X}_i(\ell)$ (subsystem symmetry).

A direct consequence of the singlet constraint.

$$S[\sigma] = -h\Delta\tau \sum_{\ell=1}^{N_\tau}\sum_{i=1}^{N_x} \sigma_i(\ell)\sigma_{i+1}(\ell) - \sum_{\ell=1}^{N_\tau} \ln\cosh\left[KN_x\, A(\ell)\right]$$

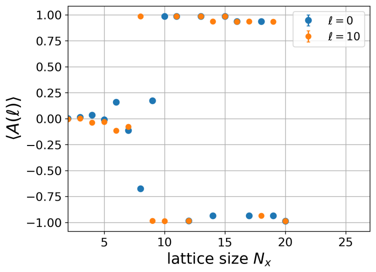
Metropolis Monte Carlo simulations

A single MC sweep consists of repeating the below $N_x N_\tau$ times:

(i) Select a random lattice site (i_0, ℓ_0).

(ii) Calculate ΔS due to $\sigma_{i_0}(\ell_0) \to -\sigma_{i_0}(\ell_0)$.

(iii) Accept the flip with probability $= \min[1, e^{-\Delta S}]$.



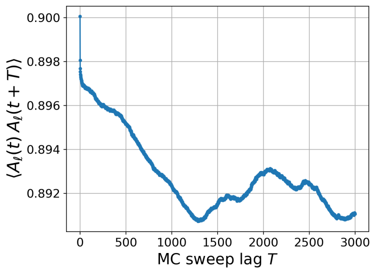


Figure: Subsystem symmetry-breaking with $N_\tau = 40$, $K = h = \Delta\tau = 1$.

Fixing subsystem symmetry-breaking

Central idea:

$f N_x$ **random spin flip proposals** $+$ **random** $A(\ell)$ **flip operation**.

Flip operation: $A(\ell) \to -A(\ell) \Rightarrow S \to S \implies \Delta S = 0$.

A single Monte Carlo sweep now involves:

- $N_x N_\tau$ random spin flip proposals.
- $\lfloor N_\tau / f \rfloor$ random alignment flips.

where $f \in \mathbb{R}^+$.

Monte Carlo with alignment flips

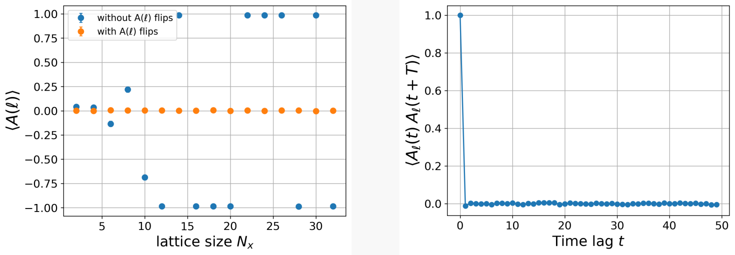


Figure: Introducing $A(\ell)$ flips with $N_\tau = 40,\ K = h = \Delta\tau = 1$.

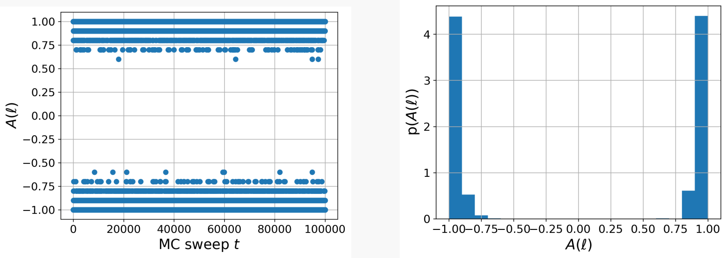


Figure: Alignment measurements.

Mapping quantum operators to classical observables

For singlet compatible operators $\hat{Q} : \mathcal{H}_s \longrightarrow \mathcal{H}_s$,

$$\hat{F}\,\hat{Q}\,\hat{F} \stackrel{!}{=} \hat{Q}$$

Expectation value of an operator $\hat{Q}$:

$$\langle \hat{Q} \rangle_{\text{th}} = \frac{\text{tr}(e^{-\beta \hat{H}}\,\hat{Q})}{\mathcal{Z}} \to \frac{1}{\mathcal{Z}} \int [\mathcal{D}\sigma]\, e^{-S[\sigma]}\, O_Q \approx \langle O_Q \rangle_{\text{MC}}$$

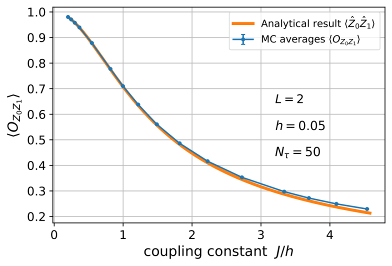
- $\hat{Z}_i \hat{Z}_j \longrightarrow O_{Z_i Z_j} = \frac{1}{N_\tau} \sum_{\ell=0}^{N_\tau - 1} \sigma_\ell^i \sigma_\ell^j$
- $\hat{X}_i \to O_{X_i} = \frac{1}{N_\tau} \sum_{\ell=0}^{N_\tau - 1} \left[\frac{\cosh\left(2K\sigma_\ell^i \sigma_{\ell+1}^i - K \sum_{j=0}^{N_x - 1} \sigma_{\ell+1}^j \sigma_\ell^j\right)}{\cosh\left(K \sum_{j=0}^{N_x - 1} \sigma_{\ell+1}^j \sigma_\ell^j\right)} \right]$

2-site problem

Analytically calculated quantum expectation values for $N_x = 2$:

$$\langle \hat{Z}_0 \hat{Z}_1 \rangle = \frac{h}{\sqrt{h^2 + J^2}} \tanh\left(2\beta\sqrt{h^2 + J^2}\right)$$

$$\langle \hat{X}_0 \rangle = \langle \hat{X}_1 \rangle = \frac{J}{\sqrt{h^2 + J^2}} \tanh\left(2\beta\sqrt{h^2 + J^2}\right)$$



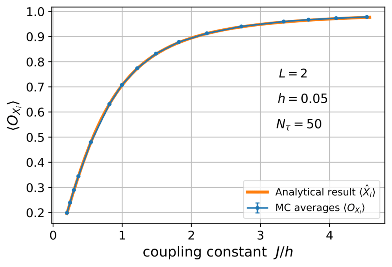


Figure: Comparing MC with analytical results at $h = 0.05$, $N_\tau = 50$ $(\beta h = 2.5)$.

Comparing against Exact Diagonalization

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta \hat{H}} \hat{\mathcal{O}} \right) = \frac{\sum_i \langle E_i | \hat{\mathcal{O}} | E_i \rangle \; e^{-\beta E_i}}{\sum_i \langle E_i | E_i \rangle \, e^{-\beta E_i}}.$$

Diagonalize the Hamiltonian in the singlet basis.

Results for $N_x = 13$.

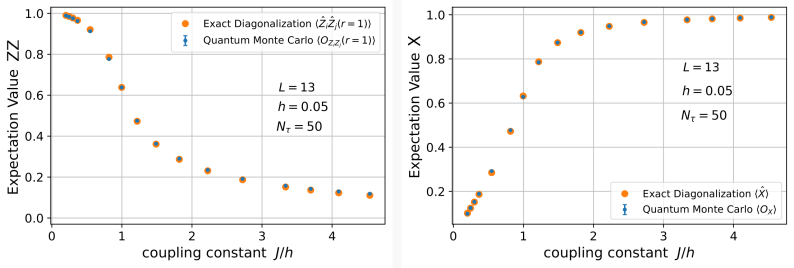


Figure: Comparing MC with ED at $h = 0.05$, $N_\tau = 50$ $(\beta h = 2.5)$.

Finite temperature $\longrightarrow$ $\beta h < 1$.

βh acts like a temperature "scale".

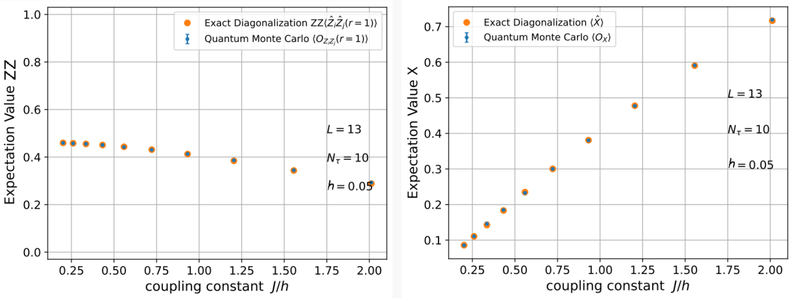


Figure: Comparing MC with ED at $h = 0.05$, $N_\tau = 10$ $(\beta h = 0.5)$.

Critical properties

Magnetization $\hat{m} \equiv \sum_i \hat{Z}_i$ isn't singlet compatible.

However, $\hat{m}^{2n}$ (for $n \in \mathbb{Z}^+$) are singlet compatible, and we can *still* define a Binder cumulant.

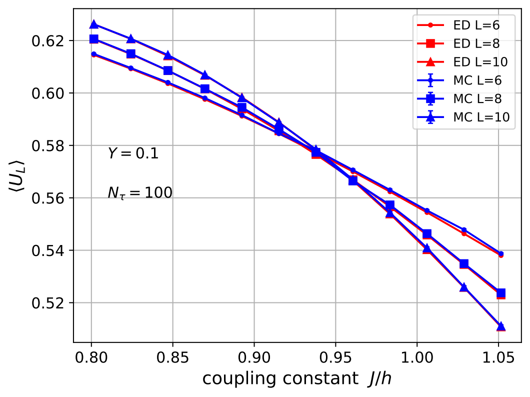
$$\hat{m}^{2n} \longrightarrow O_{m^{2n}} = \frac{1}{N_\tau} \sum_{\ell=0}^{N_\tau - 1} [\tilde{m}(\ell)]^{2n}$$

where $\tilde{m}(\ell) \equiv \dfrac{1}{N_x} \displaystyle\sum_{i=0}^{N_x - 1} \sum_i \sigma_\ell^i$.

$$\implies U_L \equiv 1 - \frac{1}{3} \frac{\langle \hat{m}^4 \rangle}{\langle \hat{m}^2 \rangle^2}$$

Critical point

Binder cumulant plots for small lattice sizes:



$(J_c/h_c)_{\text{MC}} = 0.935$ $\quad$ $(J_c/h_c)_{\text{ED}} = 0.937$

Need to try for larger system sizes...

Summary

- Study of $\mathbb{Z}_2$ lattice gauge theory $\xrightarrow{\text{dual}}$ TFIM under the singlet constraint $\xrightarrow{\text{PIQMC}}$ a generalized classical Ising model.
- Singlet constraint manifests itself as a subsystem symmetry in the classical model.
- SSB of an order parameter (magnetization) might not be necessary to characterize phases.
- Phases of $\mathbb{Z}_2$ lattice gauge theory $\sim$ Phases of TFIM.

References

- D. Horn, M. Weinstein, S. Yankielowicz. *Hamiltonian approach to $Z(N)$ lattice gauge theories.* Phys. Rev. D **19**, 3715. doi: 10.1103/PhysRevD.19.3715.
- John B. Kogut. *An introduction to lattice gauge theory and spin systems.* Rev. Mod. Phys. **51**, 659. doi:10.1103/RevModPhys.51.659.
- A. W. Sandvik, A. Avella, F. Mancini. *Computational Studies of Quantum Spin Systems.* AIP Conference Proceedings. AIP, 2010. doi: 10.1063/1.3518900.