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Quantum Simulations of Gauge Theories

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Pure \mathbb{Z}_2 Gauge Theory and the Transverse Field Ising Model

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1 Introduction

2 Theoretical background

2.1 The \mathbb{Z}_2 gauge theory and its Quantum Ising dual

The Ising gauge theory, theory with a discrete \mathbb{Z}_2 gauge symmetry in $2 + 1$ -dimensions [1]

$$H_{\mathbb{Z}_2} = -g \sum_{\vec{x}, j} \sigma_j^x(\vec{x}) - \frac{1}{g} \sum_{\vec{x}} \sigma_1^z(\vec{x}) \sigma_2^z(\vec{x} + e_1) \sigma_1^z(\vec{x} + e_2) \sigma_2^z(\vec{x}), \quad (1)$$

where \vec{x} refers to a position on the lattice, $j = 1, 2$ the two possible directions of a link, $\sigma_j^{x/z}(\vec{x})$ are the Pauli matrices, living on the links of the lattice. The local operator

$$Q(\vec{x}) \equiv \sigma_1^x(\vec{x}) \sigma_1^x(\vec{x} - e_1) \sigma_2^x(\vec{x}) \sigma_2^x(\vec{x} - e_2) \quad (2)$$

commutes with $H_{\mathbb{Z}_2}$. It generates local gauge transformations. One can check that $Q^2 = \mathbb{1}$, so that the local symmetry of our problem is indeed \mathbb{Z}_2 . The operator

$$\tau^z(\vec{r}) = \prod_{(\vec{x}, j) \text{ pierced by } \gamma(\vec{r})} \sigma_j^x(\vec{x}), \quad (3)$$

called the magnetic charge, is a gauge invariant quantity. γ is an open path on the dual lattice. Since

$$\{W_p^2(\vec{r}), \tau_z^2(\vec{r})\} = 0 \text{ and } W_p^2(\vec{r}) = \tau_z^2(\vec{r}) = \mathbb{1}, \quad (4)$$

one can identify W_p with the Pauli matrix τ^x on the dual lattice.

$$H = - \sum_{i=1}^N \tau_i^z \tau_{i+1}^z - g \sum \tau_j^x. \quad (5)$$

where i, j run over the dual lattice sites.

2.2 The classical mapping of the Quantum Ising Model

Our transverse Ising Model is not diagonal in the eigen-basis of S^z and requires a quantum treatment. Luckily for us, a combination of clever tricks allows us to map the transverse field Ising Hamiltonian in d dimensions to a classical anisotropic Ising Hamiltonian in $d + 1$ dimensions [2]. Let us demonstrate this in the case of the $1 - D$ Quantum Ising model for simplicity. Its Hamiltonian simply reads

$$H = -J \sum_{i=1}^N S_i^z S_{i+1}^z - \Gamma \sum_{i=1}^N S_i^x. \quad (6)$$

The thermodynamical properties of this system can all be derived through its partition function $Z = \text{Tr} \exp(-\beta H)$, with $\beta = 1/k_B T$. Everything starts with the Trotter formula [3]:

$$\exp(A_1 + A_2) = \lim_{M \rightarrow \infty} [\exp(A_1/M) \exp(A_2/M)]^M. \quad (7)$$

Writing our Hamiltonian as $H = H_0 + V$, where H_0 is the spin-spin interaction and V the action of the magnetic field, one can expand the partition function as follows (keeping the large M limit implicit for neatness):

$$\begin{aligned} Z &= \text{Tr} e^{-\beta(H_0+V)} \\ &= \text{Tr} \left[e^{-\beta H_0/M} e^{-\beta V/M} \right]^M \\ &= \sum_{\{S_1^1, \dots, S_N^1\}} \langle S_1^1, \dots, S_N^1 | e^{-\beta H_0/M} e^{-\beta V/M} \dots \\ &\quad \times e^{-\beta H_0/M} e^{-\beta V/M} | S_1^1, \dots, S_N^1 \rangle, \end{aligned}$$

where $|S_i^1\rangle = |\pm 1\rangle_i$ is an eigenstates of S_i^z . The sum runs over all possible configurations for the lattice. Now, between each pair of exponential we can insert the identity in the form

$$\mathbb{1} = \sum_{\{S_1^k, \dots, S_N^k\}} |S_1^k, \dots, S_N^k\rangle \langle S_1^k, \dots, S_N^k|. \quad (8)$$

The k index, which simply labels one complete set of eigenstates of S_z , can be regarded as an additional dimension to our lattice (often referred to as the Trotter dimension). The spin S_i^k can be understood the spin living on the (i, k) site of a 2 dimensional lattice. Then

$$Z = \sum_{\{S\}} \prod_{k=1}^M \langle S_1^k, \dots, S_N^k | e^{-\beta H_0/M} e^{-\beta V/M} | S_1^{k+1}, \dots, S_N^{k+1} \rangle, \quad (9)$$

where we introduced periodic boundary conditions in the Trotter dimension, $|S_1^{M+1}, \dots, S_N^{M+1}\rangle = |S_1^1, \dots, S_N^1\rangle$ so as to match the bracket sandwiching of the trace. We have use the shorthand $\sum_{\{S\}} = \sum_{\{S_1^1, \dots, S_N^1\}} \dots \sum_{\{S_1^M, \dots, S_N^M\}}$, which is just a sum over all possible configurations of our 2D lattice. Now, the H_0 exponential is diagonal in the $|S_1^k, \dots, S_N^k\rangle$ basis, so that, using its hermiticity

$$\langle S_1^k, \dots, S_N^k | e^{-\beta H_0/M} = \exp \left[\frac{\beta J}{M} \sum_{i=1}^N S_i^k S_{i+1}^k \right] \langle S_1^k, \dots, S_N^k|. \quad (10)$$

The second exponential now reads

$$\begin{aligned} \langle S_1^k, \dots, S_N^k | e^{-\beta V/M} | S_1^{k+1}, \dots, S_N^{k+1} \rangle &= \langle S_1^k, \dots, S_N^k | \exp \left[\frac{\beta \Gamma}{M} \sum_{i=1}^N S_i^x \right] | S_1^{k+1}, \dots, S_N^{k+1} \rangle \\ &= \prod_{i=1}^N \langle S_i^k | e^{\beta \Gamma S_i^x / M} | S_i^{k+1} \rangle. \end{aligned}$$

Here comes a trick, keeping in mind that S^x just flips the spin and that $(S^x)^2 = \mathbb{1}$:

$$\begin{aligned}
\langle S | e^{aS^x} | S' \rangle &= \langle S | \left(\sum_{n=0}^{\infty} \frac{a^{2n} (S^x)^{2n}}{n!} + \sum_{n=0}^{\infty} \frac{a^{2n+1} (S^x)^{2n+1}}{n!} \right) | S' \rangle \\
&= \cosh a \langle S, S' \rangle + \sinh a \langle S | S^x | S' \rangle \\
&= \cosh a \langle S, S' \rangle + \sinh a \langle S, -S' \rangle \\
&= \begin{cases} \cosh a & \text{if } S = S', \\ \sinh a & \text{if } S = -S'. \end{cases}
\end{aligned}$$

Now, simply note that

$$\begin{aligned}
\left(\frac{1}{2} \sinh 2a \right)^{1/2} \exp \left[\frac{SS'}{2} \ln \coth a \right] &= \sqrt{\sinh a \cosh a} \times \begin{cases} \exp \left[\frac{1}{2} \ln \coth a \right] & \text{if } S = S' \\ \exp \left[-\frac{1}{2} \ln \coth a \right] & \text{if } S = -S' \end{cases} \\
&= \sqrt{\sinh a \cosh a} \times \begin{cases} \sqrt{\cosh a / \sinh a} & \text{if } S = S' \\ \sqrt{\sinh a / \cosh a} & \text{if } S = -S' \end{cases} \\
&= \begin{cases} \cosh a & \text{if } S = S' \\ \sinh a & \text{if } S = -S' \end{cases} \\
&= \langle S | e^{aS^x} | S' \rangle
\end{aligned}$$

This was a long road, but we can finally put everything together.

$$\begin{aligned}
Z &= \sum_{\{S\}} \prod_{k=1}^M \prod_{i=1}^N \exp \left[\frac{\beta J}{M} S_i^k S_{i+1}^k \right] \left(\frac{1}{2} \sinh 2\beta\Gamma/M \right)^{1/2} \exp \left[\frac{S_i^k S_{i+1}^{k+1}}{2} \ln \coth(\beta\Gamma/M) \right] \\
&= \left(\frac{1}{2} \sinh(2\beta\Gamma/M) \right)^{MN/2} \sum_{\{S\}} \exp \left[-\frac{\beta}{M} \left(-J \sum_{i=1}^N \sum_{k=1}^M S_i^k S_{i+1}^k - \frac{M}{2\beta} \ln \coth \left(\frac{\beta\Gamma}{M} \right) \sum_{i=1}^N \sum_{k=1}^M S_i^k S_{i+1}^{k+1} \right) \right] \\
&= C \operatorname{Tr} \left[e^{-\beta_{\text{cl}} H_{\text{eff}}} \right],
\end{aligned}$$

with the classical temperature $\beta_{\text{cl}} = \beta/M$. Let us also abbreviate $K_M = \frac{1}{2\beta} \ln \coth \left(\frac{\beta\Gamma}{M} \right)$. In the large M limit, the prefactor vanishes, so that it drops out of any physical observables (obtained by differentiating the logarithm of the partition function). One recognizes in H_{eff} the Hamiltonian of a classical (since the S_i^k are just numbers) anisotropic Ising model without any magnetic field. The weird thing is that the coupling constant of the spin-spin interactions depend on the lattice size in the Trotter dimension and even on the temperature for the interactions along the Trotter dimension. The quantum Ising model dual to our \mathbb{Z}_2 gauge Hamiltonian is two dimensional, the above result therefore needs to be generalized to higher dimensions. The quantum Ising model on a two dimensional $N_x \times N_y$ lattice

$$H = -J \sum_{i,j} S_{i,j} (S_{i+1,j}^z + S_{i,j+1}^z) - \Gamma \sum_{i,j} S_{i,j}^x, \quad (11)$$

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

$$H_{\text{eff}} = - \sum_{k=1}^{N_z} \sum_{i,j} [J S_{i,j,k} (S_{i+1,j,k} + S_{i,j+1,k}) + K_{N_z} S_{i,j,k} S_{i,j,k+1}] \quad (12)$$

3 Metropolis-Hasting Monte-Carlo algorithm

We have derived a classical Ising Hamiltonian which shares, up to a constant, the same partition function with the quantum model. We should therefore be able to study its thermodynamical properties, mainly its phase transitions, through a simple Monte-Carlo algorithm, which naively works as follows:

Metropolis-Hasting algorithm

1. Generate a random configuration.
2. Spin one randomly chosen spin on the lattice and compute the change in energy dE .
 - If $dE < 0$: accept this new configuration.
 - Else: accept the configuration with probability $\exp(-\beta dE)$, otherwise reject it.
3. Repeat until the required number of configurations have been generated.
4. Ditch the first N_{eq} generated configurations before reaching equilibrium

The Metropolis procedure was specifically designed to generate a sample configurations according to their probability distribution. One can then compute averages without worrying about computing the partition function of the system:

$$\langle O \rangle = \frac{1}{N_{\text{sample}}} \sum_{\text{sample}} O. \quad (13)$$

A few subtleties have to be taken into account. The time taken by the Metropolis algorithm to reach equilibrium -that is to say the number of steps required to generate configurations with the proper probability distribution- is not easy to guess, and has to be adjusted "by hand" quite qualitatively. One can for example plot the evolution of desired observables as the Monte-Carlo sampling goes on. We can however expect typical behaviours.

- The bigger the lattice, the more steps will be required to thoroughly explore the space of configurations (of which there are $2^{N_x N_y N_z!}$). This is troublesome in our case since the classical mapping only holds in the large N_z limit. This can be partially solved by the means of cluster methods, where the Metropolis update consists of flipping whole chunks of spins at the same time. Computing the change in energy will however naively requires going through the whole lattice, with complexity $\mathcal{O}(N_x N_y N_z)$, which might be too costly for thousands of Metropolis updates.
- Disordered phases (for example at high temperatures) will naively require less steps to reach equilibrium, since we can expect the initial random configuration to quite likely with respect to the actual distribution.

4 Results

4.1 Phase transitions

5 Closing remarks and perspectives

References

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