2023 LATTICE

Thermodynamics of non-Abelian D_4 lattice gauge theory via Quantum Metropolis Sampling

Lorenzo Maio

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Collaborators

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Overlook

Introduction 1

Classical Lattice simulations, based on Markov Chain Monte Carlo (MCMC) algorithms, proved **successful** in computing for example the **hadron spectrum** and the non-trivial **QCD vacuum structure**. They are also crucial in first principle computation of many phenomenologically interesting observables: such as the $(g-2)_\mu$, **elements of the CKM matrix**,...

However, they are subject to limitations which most of times are due to the lack of statistical interpretation (the well known **sign problem**). This prevents us from the (direct) study of **real-time dynamics**, the QCD properties with **non-zero baryonic chemical potential** or **topological theta term**; and from the (direct) computation of **transport coefficients** and **scattering amplitudes with more than one hadron** in the initial or final state, and so on.

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Introduction 2

Our collaboration is particularly interested in the study of thermodynamic properties of lattice gauge theories: for this reason we are testing a variety of strategies to perform numerical computations of thermal averages on Quantum Computers.

$$\langle \mathcal{O} \rangle_\beta = \frac{1}{Z(\beta)} \mathrm{Tr}\left[\mathcal{O} e^{-\beta \hat{H}}\right]$$

where

$$\beta = \frac{K_B}{T} \qquad \text{and} \qquad Z(\beta) = \lim_{N\to\infty} \sum_{\{x_\tau\}} \langle x_0 | \, e^{-\frac{\beta}{N}\hat{H}} \, |x_1\rangle \langle x_2| \cdots |x_{N-1}\rangle \langle x_N| \, e^{-\frac{\beta}{N}\hat{H}} \, |x_0\rangle$$

In classical simulations, one can make use of the path-integral formulation to compute such observables, but in many cases, the sign problem arises. In this context, Quantum Computers represent a promising technology as it is possible to devise MCMC quantum algorithms which **do not suffer for the sign problem**.

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Introduction 3

In his talk (Today), G. Clemente already introduced some of the main approaches (that we are exploring) for thermal average estimations: quantum MCMC, quantum annealing, variational-based approaches.

In my talk I am going to focus on the **Quantum Metropolis Sampling (QMS)** algorithm, first introduced by K. Temme et al. **[Nature 471 (2011) 87]**. We applied it to a simple toy model: a $(2+1)$D gauge theory on a two-points lattice with periodic boundary conditions and D_4 symmetry groups. (Details later).

Quantum Metropolis Sampling 1

Quantum Metropolis Sampling **follows the same scheme of a classical Metropolis algorithm**: it consists in a Markov Chain that extracts the Hamiltonian eigenstates $|\phi_k\rangle$ with probability $e^{-\beta E_k}/Z(\beta)$ (where E_k is the eigenvalue of $|\phi_k\rangle$)

In its original formulation, the algorithm requires 4 quantum registers:

$$|acc\rangle_4 |E_{new}\rangle_3 |E_{old}\rangle_2 |\phi\rangle_1$$

The state of the system $|\phi\rangle_1$ have to be initialized to an Hamiltonian eigenstate, $|\phi_k\rangle$. This can be easily done by initializing it to $|\mathbf{0}\rangle$, and then performing a Quantum Phase Estimation (QPE) between registers 1 and 2 (which generally requires a Trotterization **[M. Troyer and U. J. Wiese (2005)]**) followed by a measure on the energy register, obtaining the starting state

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Quantum Metropolis Sampling 2

1. Metropolis proposal

From a set of unitary operators $\mathcal{C}$ (which must respect some properties that will be outlined later), it is classically drawn an element C which is applied to the state register. Then a phase estimation is performed between registers 1 and 3.

$$|0\rangle_4 |\mathbf{0}\rangle_3 |E_k\rangle_2 |\phi_k\rangle_1 \rightarrow^{C} \sum_p x_{k,p}^{(C)} |0\rangle_4 |\mathbf{0}\rangle_3 |E_k\rangle_2 |\phi_p\rangle_1 \rightarrow^{QPE} \sum_p x_{k,p}^{(C)} |0\rangle_4 |E_p\rangle_3 |E_k\rangle_2 |\phi_p\rangle_1$$

2. Acceptance evaluation

Apply an oracle $W(E_p, E_k)$ between the energy registers and the acceptance qubit

$$\sum_p x_{k,p}^{(C)} |0\rangle_4 |E_p\rangle_3 |E_k\rangle_2 |\phi_p\rangle_1 \rightarrow^{W(E_p,E_k)} \sum_p x_{k,p}^{(C)} |\mathcal{W}_{k,p}\rangle_4 |E_p\rangle_3 |E_k\rangle_2 |\phi_p\rangle_1$$

$$|\mathcal{W}_{k,p}\rangle_4 = \sqrt{f(\Delta E_{p,k})}\,|1\rangle_4 + \sqrt{1 - f(\Delta E_{p,k})}\,|0\rangle_4 \quad \text{and} \quad f(\Delta E_{p,k}) = \min(1, e^{-\beta \Delta E})$$

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Quantum Metropolis Sampling 3

3. Accept/Reject

In this step, a measurement on the register $|\mathcal{W}_{k,p}\rangle_4$ is performed with two possible results:

- 1: the proposed state is **accepted**, E_{new} is measured and the resulting eigenstate is used at step 1.
- 0: the proposal is **rejected**. The system state must be reverted trying to project back to the old eigenstate (**to a state with the old energy is sufficient**).

Notes

- it is possible to use only one quantum register for the energies, using a classical register to store E_{old} and slightly modifying the oracle W;
- in the case of lattice gauge theories, **the set $\mathcal{C}$ and measurements must obey a further condition: to respect gauge invariance**;
- the set $\mathcal{C}$ should contain as many operators as necessary to ensure ergodicity and detailed balance. However it is possible to demonstrate that 2 non-commuting operators are sufficient to generate the whole unitary group representing the transition between physical states.

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Simulations and related studies

Of course, this algorithm cannot be ran on current Quantum Computers. Our study is based on simulations without noise. For our simulations we used **SUQA** (**S**imulator of **U**niversal **Q**uantum **A**lgorithms) **[https://github.com/QC-PISA/suqa.git]**.

Some of us already verified the applicability of this algorithm to a simple toy model (which is affected by the sign problem in classical simulations): a system of three spins in a frustrated configuration **[G. Clemente et al., PRD 101 (2020) 7]**. In this study, some of my collaborators et al., showed that QMS is able to reproduce correct results and studied its systematic errors.

In a new study, we studied in more details the systematics of this algorithm on the same toy model, comparing it with the Quantum-Quantum Metropolis Algorithm **[M.-H. Yung and A. Aspuru-Guzik, PNAS USA 109 754 (2012)]**. Results can be found at **[arXiv:2308.01279]**

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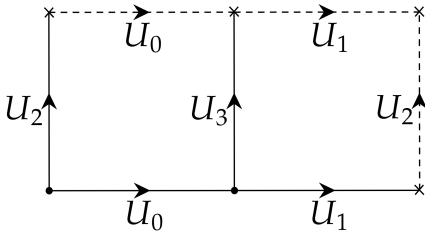
The model we study

We tested this algorithm on a pure-gauge D_4 lattice gauge theory, using the same toy model used by Lamm et al. in **[Phys. Rev. D 100 (2019) no.3, 034518]**.



The model live on a 2D lattice with 2 points and periodic boundary conditions. Four links connect the points among each other along the two directions.

The Hamiltonian of the system, in the basis of the links, reads $\hat{H} = \hat{H_V} + \hat{H_K}$

$$H_V = \frac{1}{g^2} \sum_{\vec{U}} V(\vec{U}) \, |\vec{U}\rangle \, \langle \vec{U}| \qquad \left(|\vec{U}\rangle = |U_3\rangle \, |U_2\rangle \, |U_1\rangle \, |U_0\rangle \right)$$

$$H_K = -\mathrm{Log} \, T_K \quad \text{where} \quad \langle \vec{U}| \, T_K \, |\vec{U}\rangle \cong \prod_{i=0}^{3} e^{\frac{1}{g^2} \mathrm{Tr}\left[\rho(U_i')^{-1} \rho(U_i)\right]}.$$

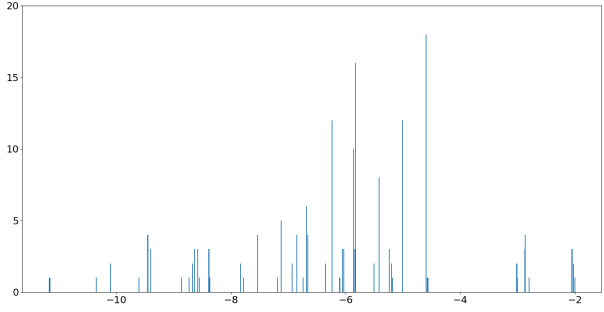
The model we study

Due to gauge invariance with respect to local transformations **[see A. Mariani's talk]**

$$\dim \mathcal{H}_{phys} = \sum_{S \in conj.classes} \left(\frac{|G|}{|S|} \right)^{|E|-|V|} = 176$$

However we had to use a 12-qubits state.

The spectrum of the theory can be analytically computed



Results

We fixed $\frac{1}{g^2} = 0.8$ and performed different simulations using several values of temperatures, and number of qubits in the energy register (n_{qe}). Our goal is to study the deviation of the sampled spectrum. Each simulation required to run QMS on $12 + n_{qe} + 1$ qubits.

We also measured plaquette distributions in separate runs to verify that non-commuting observables are correctly sampled. Also, the measurement could cause further systematics.

The explored values are summarized in the following:

$$\beta = 10^{-7}, \quad 0.1, \quad 0.5$$

$$n_{qe} = 3, \quad 4, \quad 5, \quad 6, \quad 7$$

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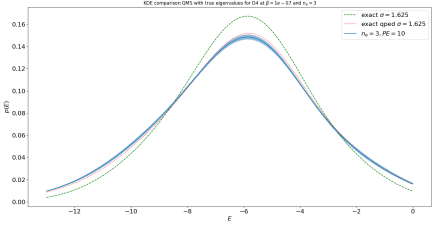
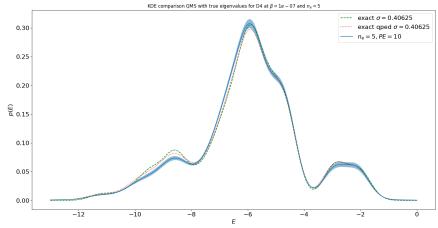
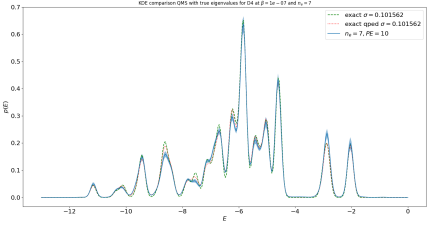
$$\beta = 0,\ n_{qe} = 3, 5, 7$$



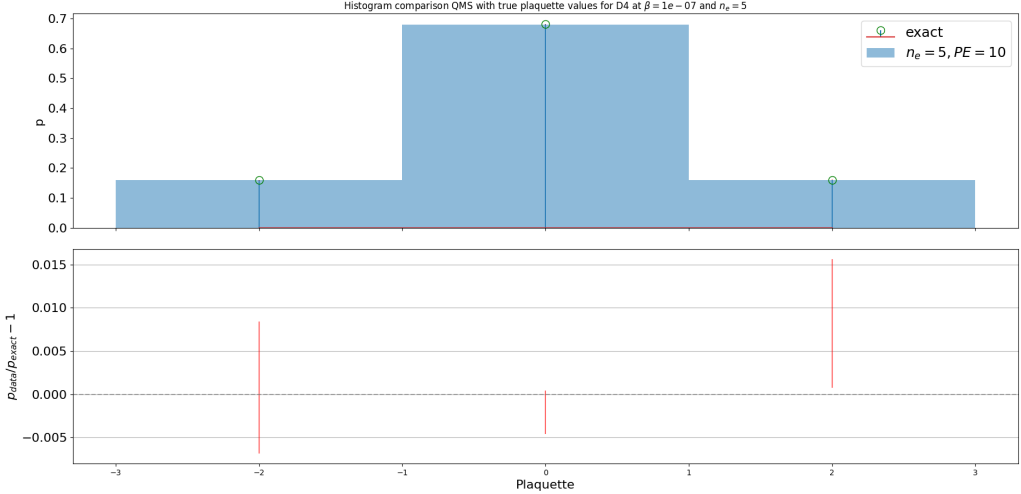




At $\beta = 0$, the measured spectrum reproduces really well the smeared real spectrum. The maximum distances between points and QPEd-smeared distribution is 2σ at the most.

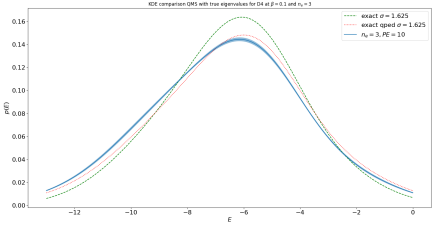
results

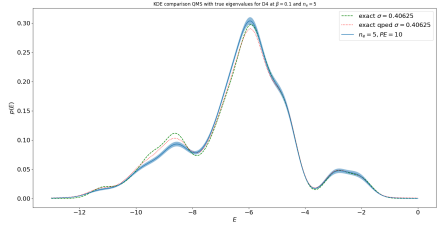
$$\beta = 0,\ n_{qe} = 5$$



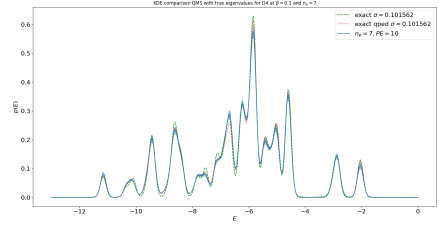
results

$$\beta = 0.1,\ n_{qe} = 3, 5, 7$$





At $\beta = 0.1$ the distribution of energy measurements reproduces quite well the smeared spectrum (for high numbers of qubits).



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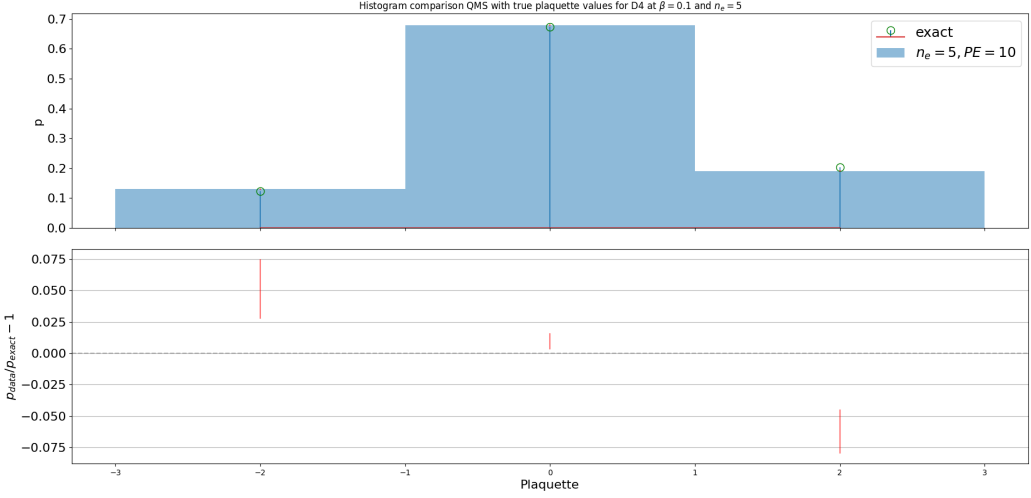
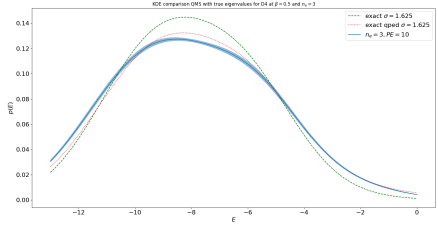
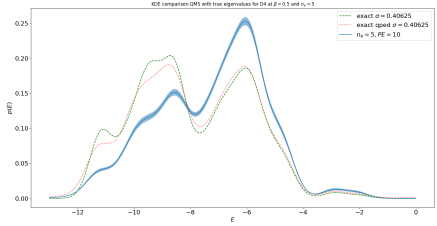
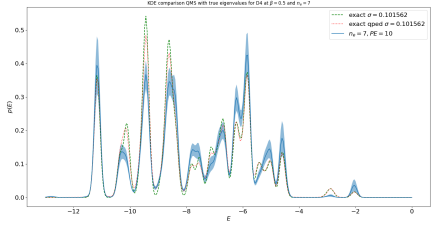


results

$$\beta = 0.5,\ n_{qe} = 3, 5, 7$$







At $\beta = 0.5$ the measured energy distribution is clearly non-reliable for higher n_{qe}.

results

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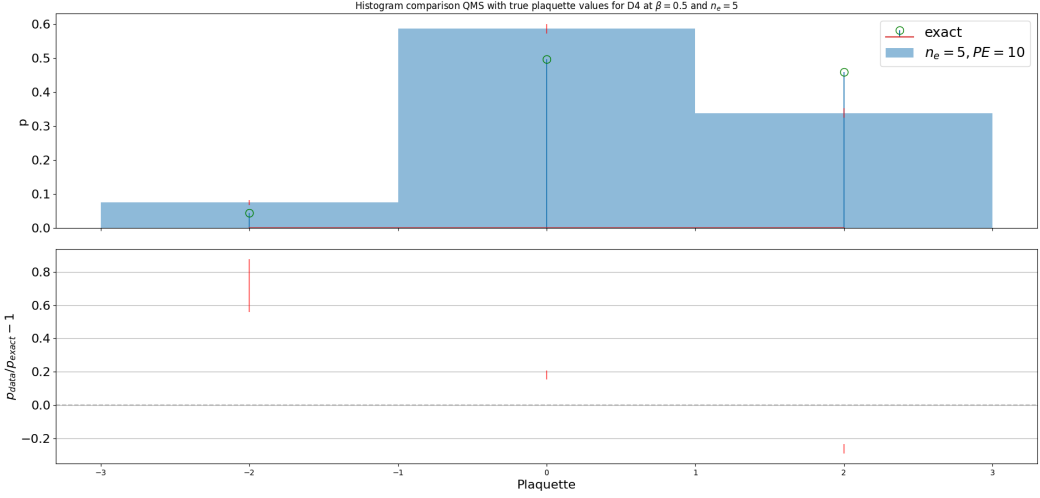

Observation

QMS runs return good results for $\beta = 0$ and 0.1.

Simulations at higher β are more biased with respect to those at lower β, both in the spectrum and the plaquette estimation.

This could be due to a drop in the acceptance: $e^{-\beta \Delta E}$ becomes smaller and smaller as β increases. Together with the spectrum discreteness, this could generate an effective ergodicity loss.

Possible way to fix it: randomized state initialization.

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Conclusions

We described the algorithm we use and how to represent the non-Abelian discrete gauge group D_4 in a 2 point $(2+1)D$ lattice with periodic boundary conditions.

Gauge preserving moves and measurements must be performed in order to explore physical states only.

It is possible to find a set of moves $\mathcal{C}$ that permits to obtain an ergodic Markov Chain among physical states, and it substantially requires two operators.

For the first time, a quantum MCMC algorithm has been tested on a non-Abelian group to study thermal averages.

Results of the simulations are in good agreement with analytical expectations at lower β, while a divergence can be observed at higher values.

Thank you!