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

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The possibility to use fault-tolerant Quantum Computers in the "Beyond the NISQ era" is a promising perspective: it could bring the implementation of Markov Chain Monte Carlo (MCMC) quantum algorithms on real machines. Then, it would be possible to exploit the quantum properties of such devices to study the thermodynamic properties of the system. This also allows us to avoid the infamous sign problem, which plagues classical Monte Carlo simulations of several interesting systems - such as QCD in the presence of an external electric field or a finite chemical potential. In this work, we discuss the effectiveness of Quantum Metropolis Sampling in the study of thermodynamic properties of a non-Abelian gauge theory, based on the discrete D_4 symmetry group. This is the first study of a non-Abelian Lattice Gauge Theory by means of a quantum MCMC algorithm: we simulate the behavior of an ideal quantum Computer, aiming to demonstrate the feasibility of such simulations.

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1. Introduction

Numerical computations represent a crucial step in the study of natural phenomena at every scale, and the invention of digital electronic computers, together with the development of suitable algorithms, brought a boost in numerical techniques. Such invention represented a revolution in science, as well as in every field of human activities. Concerning the impact of this technology on Theoretical Particle Physics, let us limit ourselves to cite the Markov Chain Monte Carlo (MCMC) algorithms, that allowed us to investigate the properties of strong interactions, as, e.g., the hadron spectrum, or the QCD vacuum structure, through lattice simulations, relying on first principles only; and they are still successfully applied in frontier research representing a crucial step in the computation of observables such as the muon $g-2$ or the elements of the CKM Matrix.

However, these powerful methods are subject to limitations which, most of the times, are due to a lack of statistical interpretation: the infamous *sign problem*. Such restriction prevents us to compute directly (i.e., without relying on any *escamotage*) many observables, such as (to list a few important examples): real-time dynamics, QCD properties at finite density or with a finite theta term, transport coefficients or scattering amplitudes with more than one hadron in the initial or final state. Fortunately, nowadays, we are to the verge of a new technological revolution, as quantum computers have been available to researchers for a few years and their compute capabilities are steady growing. Soon, they could represent a new powerful tool, capable of facing computations which cannot be addressed with classical computers and, in particular, restricting to the interests of the authors, they can run MCMC algorithms that do not suffer for the sign problem.

We are especially interested in the study of thermodynamic properties of lattice gauge theories, hence we are exploring a variety of strategies and algorithms to compute thermal averages: quantum MCMC [1], quantum annealing [2], variational-based approaches. In this contribution we focused on the Quantum Metropolis Sampling (QMS) algorithm, first introduced in [3], a quantum MCMC algorithm that we applied to a simple toy model: a $(2+1)$D gauge theory on a two sites lattice with periodic boundary conditions and D_4 symmetry group. This represents the first application of a quantum MCMC algorithm to the study of thermodynamic properties of a non-Abelian Lattice Gauge Theory. In Section 2 of this contribution we introduce the QMS, in Section 3 the details on the system and the simulations are presented and in Sections 4 and 5 we discuss our results and present the conclusions. More details on this work can be found in Ref. [4].

2. The QMS algorithm

As previously stated, our main interest is the study of thermodynamic properties of lattice gauge theories, thus a mandatory step is the computation of thermal averages

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

where $\hat{H}$ is the Hamiltonian operator, β the inverse temperature and

$$Z(\beta) = \mathrm{Tr}\, e^{-\beta \hat{H}}. \tag{2}$$

In classical simulations, one can use a MCMC algorithm using the path-integral formulation to compute such observables, but, in many cases, the sign problem arises, as the trace appears as a

sum of non-positive terms when rewritten in a computational basis which is easily accessible by a classical computer. In this context, Quantum Computers could be exploited to run MCMC quantum algorithms that do not suffer for the sign problem.

QMS follows the same logic of a classical Metropolis algorithm [5], as it generates a Markov Chain that returns a sequence of states distributed according to the Boltzmann distribution, on which one can compute Eq. (1). The main difference lies in the fact that we can use Quantum Computers properties to directly access the eigenstates of the Hamiltonian, $|\phi_j\rangle$, thus Eqs. (1) and (2) can be rewritten as

$$\langle O\rangle_\beta = \frac{1}{Z(\beta)} \langle\phi_j| O |\phi_j\rangle e^{-\beta E_j}, \qquad Z(\beta) = \sum_j e^{-\beta E_j}, \tag{3}$$

where E_j is the eigenvalue of $|\phi_j\rangle$. It is clear that, in such formulation, the sign problem cannot arise.

In our implementation, the algorithm only requires 3 quantum registers:

$$|\text{acc}\rangle_3 |E\rangle_2 |\phi\rangle_1 , \tag{4}$$

where the first register encodes the quantum state, the second one encodes the energy of such state, and the third one is a single-qubit register that encodes the result of the Metropolis test executed on the energy register and a classical register, as it is explained below. The state register has to be initialized to a Hamiltonian eigenstate, $|\phi_j\rangle$. Such initialization can be easily accomplished by initializing it to $|\mathbf{0}\rangle$, and then performing a Quantum Phase Estimation (QPE), between registers 1 and 2 (that generally requires a Trotterization [6]) and measuring the second register to make the state collapse on an initial eigenspace. Thus, the initial state of the algorithm is the following

$$|0\rangle_3 |E_j\rangle_2 |\phi_j\rangle_1 , \tag{5}$$

then the energy is copied on a classical register, and the algorithm runs. It consists of three steps:

1. **Metropolis proposal**. From a set of unitary operators C (whose properties are outlined below) it is classically and randomly drawn an element C, which is applied to the state register. Then, a new phase estimation is performed between registers 1 and 2, but no measure on the energy register is performed this time. In formulae:

$$|0\rangle_3 |E_j\rangle_2 |\phi_j\rangle_1 \xrightarrow{C} \sum_p x^{(C)}_{j,p} |0\rangle_3 |E_j\rangle_2 |\phi_p\rangle_1 \xrightarrow{\text{QPE}} \sum_p x^{(C)}_{j,p} |0\rangle_3 |E_p\rangle_2 |\phi_j\rangle_1 , \tag{6}$$

   where $x^{(C)}_{j,p} = \langle\phi_p| C |\phi_j\rangle$.

2. **Acceptance evaluation**. An oracle $W(E_p, E_j)$ is applied between the registers 2 and 3. Such oracle stores the condition for acceptance or rejection on the third register, according to the acceptance probability of transition between eigenstates, given by

$$p_{\phi_j \to \phi_p} = \min\left(1,\ e^{-\beta \Delta E_{pj}}\right), \tag{7}$$

   where ΔE_{pj} is the energy difference between the states p and j, and the oracle makes use of the second quantum register and the classically stored initial energy to compute it. Thus the

state can be now written as

$$\sum_p x_{j,p}^{(C)} |0\rangle_3 |E_p\rangle_2 |\phi_j\rangle_1 \xrightarrow{W(E_p,E_j)} \sum_p x_{j,p}^{(C)} |\mathcal{W}_{pj}\rangle_3 |E_p\rangle_2 |\phi_j\rangle_1 , \tag{8}$$

where $|\mathcal{W}_{pj}\rangle_3 = \sqrt{p_{\phi_j \to \phi_p}} |1\rangle_3 + \sqrt{1 - p_{\phi_j \to \phi_p}} |0\rangle_3$.

3. **Accept/reject**. A measurement on the $|\mathcal{W}_{pj}\rangle_3$ register is performed, with two possible outcomes: 1 or 0. In the first case, the proposed state has been accepted, then a measurement on the energy register is performed, the result is copied in the classical register of the old energy, and the algorithm is repeated from step 1. In the case 0 is measured in the acceptance register, the proposal is refused and the state must be reverted trying to project it back on the old eigenstate. In [3] an iterative procedure is proposed to accomplish such objective.

The iteration of such algorithm gives rise, after a certain number of thermalization steps, to a sequence of states distributed according to the desired probability distribution, hence it is possible to perform the measurements in Eq. (3). However, to measure hermitian operators that do not commute with $\hat{H}$, one must corrupt the system state $|\phi\rangle_1$, hence the Markov Chain has to be thermalized again before taking another measurement. Moreover, in the case of lattice field theories, one should preserve gauge invariance at every step in the chain. For this reason the measurements and the set C of "kick operators" should preserve gauge invariance[1]. Finally, concerning the properties of the latter, it should contain as many operators as necessary to ensure ergodicity and detailed balance: it is possible to demonstrate that 2 non-commuting operators are sufficient to generate the whole unitary group representing the transition between physical states (further details, including the demonstration, can be found in Ref. [4]).

3. System and Simulation details

We tested this algorithm on a pure-gauge non-Abelian D_4 lattice gauge theory, using the same toy model introduced in [7] and shown in Fig. 1. It lives on a $2D$ lattice with 2 sites and periodic boundary conditions (PBC) in both directions, thus the sites are connected to each other (and to themselves) by 4 links. Defining the system state as $|\vec{U}\rangle = |U_3\rangle |U_2\rangle |U_1\rangle |U_0\rangle$, the Hamiltonian of such a system can be written as

$$\hat{H} = \hat{H}_V + \hat{H}_K, \tag{9}$$

where

$$\hat{H}_V = \frac{1}{g^2} \sum_{\vec{U}} V(\vec{U}) |\vec{U}\rangle \langle\vec{U}| \qquad \text{and} \qquad H_K = -\mathrm{Ln}\, T_K, \tag{10}$$

where Ln is the matrix logarithm and T_K is the transfer matrix, defined element-wise as

$$\langle\vec{U}| T_K |\vec{U}\rangle = \prod_{i=0}^{3} e^{\frac{1}{g^2}\mathrm{Tr}\left[\rho(U_i')^{-1}\rho(U_i)\right]}, \tag{11}$$

where ρ denotes a fundamental (2-dimensional, irreducible) representation of D_4.

[1]The original formulation of the QMS requires that the algorithm restarts from step 0 after a measurement, hence the measurement can spoil the gauge invariance. However, in our implementation, a more efficient rethermalization procedure, which does not reset the state, is applied [1], thus gauge invariance must be preserved.

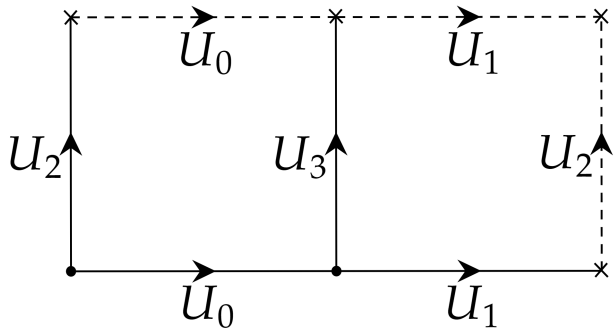

Figure 1: The toy model we studied: it consists of 2 lattice sites connected by 4 link variables with PBC in a 2 dimensional space.

The extended dimension of this system is $|D_4|^{|E|} = 8^4 = 4096$ (where $|E|$ is the number of links in the model), hence a 12-qubits register is needed to describe it. However, due to gauge invariance with respect to local transformations, the physical Hilbert space of this system can be computed as [8]

$$\dim \mathcal{H}_{\text{phys}} = \sum_{S \in \text{ conj. classes}} \left(\frac{|D_4|}{|S|} \right)^{|E|-|V|} = 176, \tag{12}$$

where $|S|$ and $|V|$ are, respectively, the cardinality of each conjugacy class and the number of vertices of the lattice, hence the spectrum of the theory only counts 176 physically distinct states. Such spectrum has been analytically computed, and we use this result to compute energy density to compare with QMS results.

Of course, QMS cannot run on current Quantum Computers, as it involves long circuits and indefinitely long while cycles, that are out of reach for today technologies. Thus, we simulated such algorithm using SUQA [9], a simulator of quantum algorithms developed by one of the authors (GC), and used by our collaboration also in other studies [1, 2, 4].

In the next session we briefly present our results. Our goal is to study the deviation of the sampled energy density distribution and of the measurement from the analytical expectation. Such measurements are plagued by different caveats, that need to be kept under control. For example, the Quantum Phase Estimation has a finite resolution, hence it distorts the spectrum affecting both the energy measurements and the sampled distribution. Another aspect to take care of is the fact that the plaquette measurement spoils the state, hence it could bias the sampled distribution if the Markov Chain does not get properly re-thermalized.

4. Results

To perform simulations, we fixed $\frac{1}{g^2} = 0.8$ and performed different simulations using several values of temperatures β, and number of qubits in the energy register (n_e). We performed measurements of the energy and of a plaquette operator (the trace of the product of the links along the closed square in the left in Fig. 1). Each simulation required to run QMS on $1 + n_e + 12$ qubits.

In Fig. 2 we show the results obtained for the energy density at $\beta = 10^{-7}$, 0.1 and 0.5, and limit ourselves to the simulations performed with $n_e = 5$, more details can be found in Ref. [4]. In each

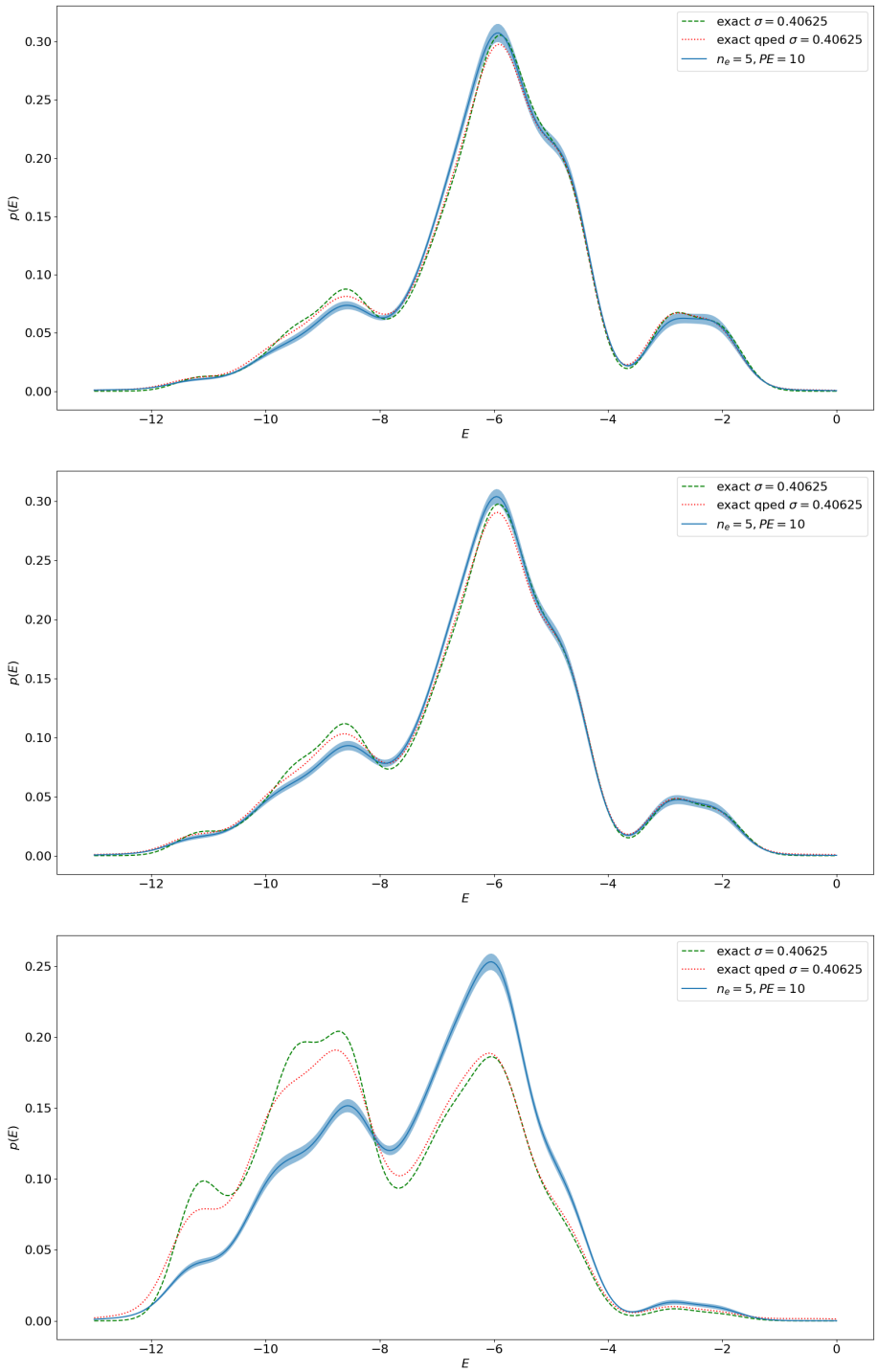

Figure 2: Results for the energy density distribution, computed at (from top to bottom) $\beta = 10^{-7}$, 0.1 and 0.5, using $n_e = 5$. All the curves are subject to a Gaussian KDE smearing with $\sigma \sim 0.4$. Green and orange lines represent the exact analytical result, and the distortion caused by QPE. The blue band represents the statistical error on the simulated results.

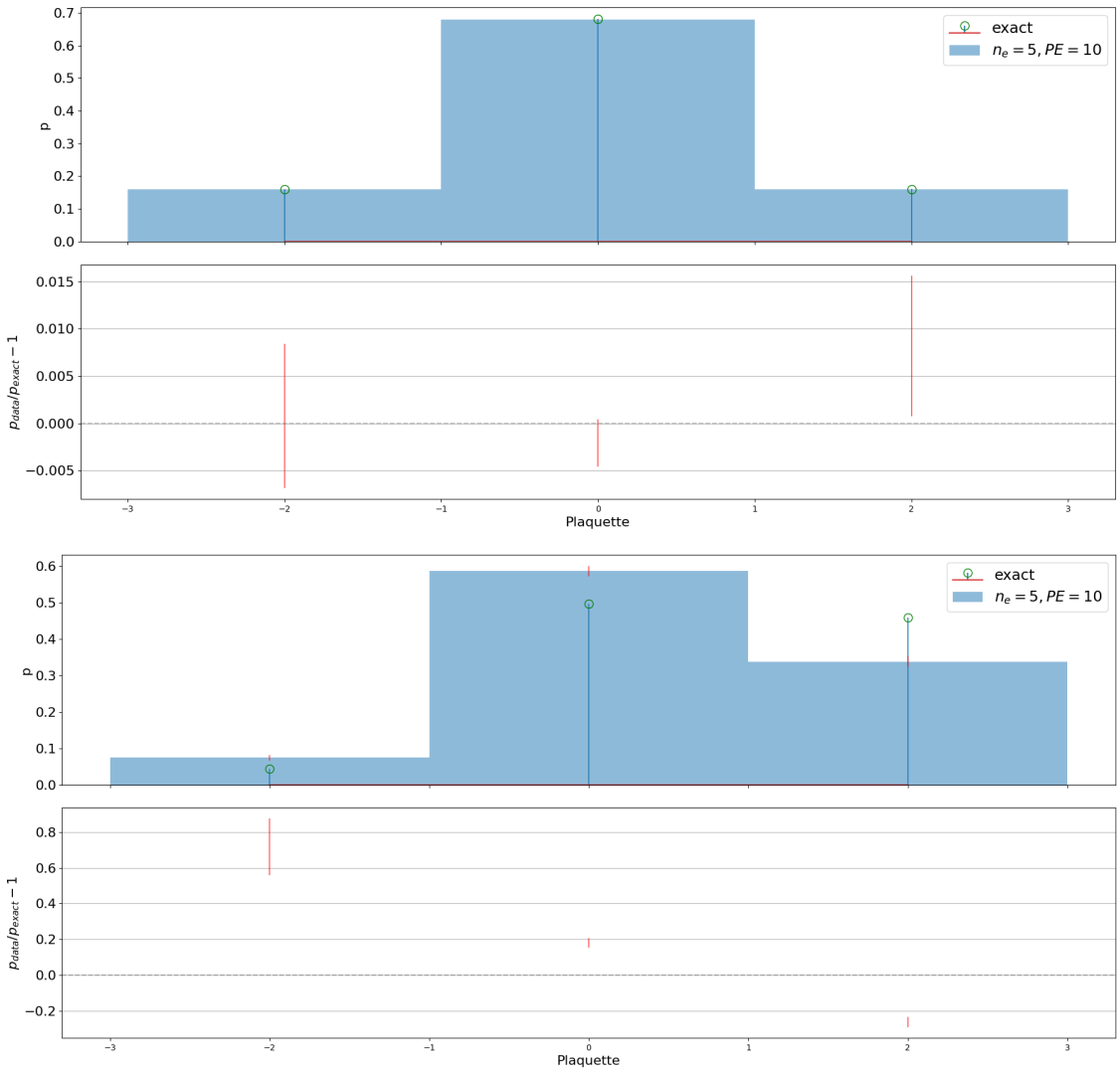

Figure 3: Results for the distribution of the plaquette values at (from top to bottom) $\beta = 10^{-7}$ and 0.5, using $n_e = 5$. In top panels we present the histogram together with the theoretical expectation; in the lower panel it is shown the relative discrepancy of results and expectation

graph, the exact distribution, the effect of the QPE distortion on it and the results of the simulation, are shown after a Kernel Density Estimation (KDE) with a Gaussian kernel and smearing radius $\sigma \sim 0.4$, in order to avoid the usual histogram instabilities due to low statistics and to obtain a fair comparison between results and theoretical expectations. It can be observed that at $\beta = 0$ and 0.1, our results reproduce quite well the expected behavior, and the QPE distortion is enough to explain the deviation from the exact distribution. However, at $\beta = 0.5$, the sampled distribution fails in reproducing the exact behavior. This is probably due to a lower acceptance probability in the Metropolis test $e^{-\beta\Delta E}$, which could result in an effectively non-ergodic set of moves.

In Fig. 3, we show the results for the occurrence of the possible values of the plaquette operator, compared with the analytical expected result, for $\beta = 10^{-7}$ and 0.5 (as the $\beta = 0.1$ case

is qualitatively equal to the former one). Also for the plaquette measurement we can see that at lower β the results are in agreement with theoretical expectation, while such accordance is spoiled at higher β values.

5. Conclusions

We used a quantum MCMC algorithm, named QMS, to study a simple Lattice Gauge Theory based on the discrete non-Abelian group D_4, living on a $2D$ and 2 sites lattice with PBC along both directions. We found that in our implementation of the algorithm, measurements should respect gauge invariance. This request should be obeyed also by the set C of moves, from which one randomly draws the kick operator for the Monte Carlo step. Moreover, it can be demonstrated that 2 non-commuting operators suitably chosen, are sufficient to generate a proper set C of kick operators.

We simulated the QMS for different values of β, using different numbers of qubits in the energy register n_e. The algorithm is found to work extremely well at lower values of β, where the acceptance probability is higher, while the accuracy fades off at higher β, both for the energy density distribution and the plaquette distribution. We refer the interested reader to Ref. [4], where we discuss in more details all the technical issues. More details on the QMS can be also found in Refs. [1, 2].

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