Perfect Sampling for Quantum Gibbs States

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We show how to obtain perfect samples from a quantum Gibbs state on a quantum computer. To do so, we adapt one of the "Coupling from the Past"-algorithms proposed by Propp and Wilson. The algorithm has a probabilistic run-time and produces perfect samples without any previous knowledge of the mixing time of a quantum Markov chain. To implement it, we assume we are able to perform the phase estimation algorithm for the underlying Hamiltonian and implement a quantum Markov chain that satisfies certain conditions, implied e.g. by detailed balance, and is primitive. We analyse the expected run-time of the algorithm, which is linear in the mixing time and quadratic in the dimension. We also analyse the circuit depth necessary to implement it, which is proportional to the sum of the depth necessary to implement one step of the quantum Markov chain and one phase estimation. This algorithm is stable under noise in the implementation of different steps. We also briefly discuss how to adapt different "Coupling from the Past"-algorithms to the quantum setting.

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1. Introduction

Markov chain Monte Carlo methods are ubiquitous in science. They have a similar structure: the solution to a problem is encoded in the stationary distribution of a Markov chain that can be simulated. The chain is then simulated for a "long enough" time until the current state of the chain is "close enough" to a sample of the stationary distribution of interest.

It is expected that with the advent of quantum computers one could use similar methods to develop algorithms to simulate quantum many-body systems that do not suffer from the sign problem[25], and many quantum algorithms have been proposed [31, 20, 5, 11, 33, 23, 30, 3, 13].

However, as for classical Monte Carlo methods, it is in general difficult to obtain rigorous bounds on how long is "long enough", as the huge literature dedicated to Markov chain mixing attests [16]. This prompted research on an algorithm that would "decide for itself" when the current state of the Markov chain is close to or is even a perfect sample of the stationary distribution, without any prior knowledge of the mixing properties of the chain.

One of the first algorithms to do so was developed in [17]. Later Propp and Wilson proposed the "Coupling from the Past" (CFTP)-algorithm [21] and showed how it can be applied to efficiently obtain perfect samples for the Ising model. They also showed how to sample perfectly from the stationary distribution of an unknown Markov chain for which we can only observe transitions on a subsequent paper [22] and many perfect sampling algorithms have been developed since ¹. There are also proposals of quantum speedups to these algorithms [9].

In this article, we will generalize some of these algorithms to get perfect samples from a Gibbs state of a Hamiltonian with non-degenerate spectrum on a quantum computer. By this we mean that we are able to perform any measurement and observe the same statistics for the outcomes as if we were measuring the actual Gibbs state.

To implement them, we will need to be able to perform the phase estimation algorithm[14] for the underlying Hamiltonian. We assume we can also implement a quantum Markov chain that drives the system to the desired Gibbs state and fulfills certain assumptions, such as reversibility of the chain, which we elaborate on below. We also comment on which of the current proposals to prepare Gibbs states on quantum computers may be adapted for our purposes.

Like it is the case for the classical algorithms, our quantum algorithms do not require any previous knowledge about the mixing properties of the quantum Markov chain. They "decide for themselves" when the current state of the system corresponds to a perfect sample of the target Gibbs state and their run-time is probabilistic.

We will focus on adapting the "voter CFTP" algorithm. Our version of this algorithm will turn out to have the same expected run-time as its classical counterpart. That is, for voter CFTP the expected run-time quadratic in the dimension of the system and

¹The website http://dimacs.rutgers.edu/~dbwilson/exact/, maintained by Wilson, contains a comprehensive list of references concerning the topic and other related material.

linear in the mixing time. We also briefly discuss how to generalize other variations of CFTP.

These algorithms are stable under noise and we give bounds on their stability. One potential advantage of the "voter CFTP" in comparison to other methods proposed in the literature is that it only requires the implementation of a quantum circuit of low depth a (potentially prohibitive) number of times and significant classical post-processing to obtain a perfect sample without any prior knowledge of the mixing time. Other methods require the implementation of a circuit of (potentially prohibitive) length one time to obtain an approximate sample, but only under previous knowledge of or assumptions on the mixing time. These algorithms are therefore also qualitatively different from ours.

2. Preliminaries

2.1. Notation and basic concepts

We begin by introducing some basic concepts we will need and fixing the notation. Throughout this paper, \mathcal{M}_d will denote the space of $d \times d$ complex matrices and $[d] = \{1, \ldots, d\}$. We will denote by \mathcal{D}_d the set of d-dimensional quantum states, i.e. positive semidefinite matrices $\rho \in \mathcal{M}_d$ with trace 1. We will call a hermitian operator $H \in \mathcal{M}_d$ a Hamiltonian. For an inverse temperature $\beta > 0$, we define $\mathcal{Z}_\beta = \operatorname{tr}[e^{-\beta H}]$ to be its partition function and $e^{-\beta H}/\mathcal{Z}_\beta$ its Gibbs state. A quantum channel $T: \mathcal{M}_d \to \mathcal{M}_d$ is a trace preserving completely positive map. A state $\sigma \in \mathcal{D}_d$ is a stationary state of T if we have $T(\sigma) = \sigma$. The channel is called primitive if we have $\forall \rho \in \mathcal{D}_d : \lim_{n \to \infty} T^n(\rho) = \sigma$ and $\sigma > 0$. One can also give an equivalent spectral of characterization to primitive quantum channels. A quantum channel is primitive if $\sigma > 0$ is the only eigenvector corresponding to eigenvalues of modulus 1 of the channel[4]. In particular, this implies that the property of being primitive is stable under small perturbations of the channel.

A collection of self-adjoint operators $\{F_i\}_{i\in I}$ is called a POVM (positive-operator valued measure) if the $F_i \in \mathcal{M}_d$ are all positive semidefinite and $\sum_{i\in I} F_i = 1$. Here $1 \in \mathcal{M}_d$ is the identity matrix. A state $\rho \in \mathcal{D}_d$ and a POVM $\{F_i\}_{i\in I}$ induce a probability distribution p through $p(i) = \operatorname{tr}[F_i\rho]$. All the algorithms we will discuss have as their goal to produce exact samples of the distribution p generated by an arbitrary POVM in the case that ρ is a Gibbs state.

The following class of quantum channels will be one of the backbones of the algorithms we will present later.

Definition 2.1 (Eigenbasis preserving quantum channels). A quantum channel $T: \mathcal{M}_d \to \mathcal{M}_d$ is called eigenbasis preserving for a Hamiltonian $H = \sum_i E_i |\psi_i\rangle\langle\psi_i|$ with non-degenerate spectrum and inverse temperature $\beta > 0$ if we have that for all $i, j \in [d]$ the commutator

$$[T(|\psi_i\rangle\langle\psi_i|), |\psi_j\rangle\langle\psi_j|] = 0$$

and
$$T\left(\frac{e^{-\beta H}}{\mathcal{Z}_{\beta}}\right) = \frac{e^{-\beta H}}{\mathcal{Z}_{\beta}}$$
.

By the commutator property, we can model the dynamics under T on states that commute with $e^{-\beta H}/\mathcal{Z}_{\beta}$ as a classical Markov chain. One should not take this condition to imply that the dynamics under T are classical, as will become clear in subsection 3.2, where we present some examples of eigenbasis preserving channels. We will first suppose

that we can implement these channels exactly, but will later relax this condition and discuss the influence of noise in Section 3.4.

We will also need some distinguishability measures for quantum states and channels and convergence speed measures for primitive quantum channels. One of the main ones is through the Schatten 1-Norm $||X||_1 = \operatorname{tr}[|X|]$ for $X \in \mathcal{M}_d$. This is justified by the clear operational interpretation given by its variational expression [18, p. 404]. If we denote by \mathcal{P}_d the set of orthogonal projections in \mathcal{M}_d , we have for $\rho, \sigma \in \mathcal{D}_d$

$$\frac{\|\rho - \sigma\|_1}{2} = \sup_{P \in \mathcal{P}_d} \operatorname{tr}[P(\rho - \sigma)]. \tag{1}$$

That is, $\|\rho - \sigma\|_1/2$ expresses the maximal probability of correctly distinguishing two states σ, ρ by a projective measurement. This norm also induces the $1 \to 1$ norm on operators $T: \mathcal{M}_d \to \mathcal{M}_d$:

$$||T||_{1\to 1} = \sup_{X \in \mathcal{M}_d} \frac{||T(X)||_1}{||X||_1}.$$
 (2)

As a measure of the convergence speed of a quantum channel we define the l_1 -mixing time threshold of a primitive quantum channel $T: \mathcal{M}_d \to \mathcal{M}_d$ with unique stationary state σ , which is given by

$$t_{mix} = \min\{n \in \mathbb{N} : \sup_{\rho \in D_d} ||T^n(\rho) - \sigma||_1 \le 2e^{-1}\}.$$

A crucial ingredient for our sampling algorithm is the phase estimation algorithm, discovered originally in [14]. There are now many variations of it [1, 6, 26] and it is still the subject of active research. We will neither discuss in detail how to implement it nor its complexity and refer to [26] for that. For our purposes, we will just suppose that for a given Hamiltonian H acting on \mathbb{C}^d we may implement a unitary U on $\mathbb{C}^d \otimes (\mathbb{C}^2)^{\otimes m}$ for some $m \in \mathbb{N}$ that acts as follows:

For $|\psi_i\rangle$ an eigenstate of a Hamiltonian H with $H|\psi_i\rangle = E_i|\psi_i\rangle$ we have $U|\psi_i\rangle\otimes|0\rangle = |\psi_i\rangle\otimes|E_i\rangle$, where $|E_i\rangle$ is the binary expansion of E_i in the computational basis of $(\mathbb{C}^2)^{\otimes m}$. We will first assume that we may implement U exactly, but later also discuss how imperfections in the implementation of the phase estimation algorithm influence the output of the sampling algorithm in Section 3.4.

We will now fix some notation and terminology for classical Markov chains. A sequence X_0, X_1, X_2, \ldots of random variables taking values in a (finite) set S, referred to as the state space, is called a Markov chain if we have

$$P(X_{n+1} = j | X_n = i) = \pi(i, j)$$

for a $|S| \times |S|$ matrix π . π is called the transition matrix of the chain. We will always denote by π the transition matrix of a Markov chain that should be clear from context. A probability distribution μ on S is called stationary if we have that $\pi\mu = \mu$. A Markov chain is said to be irreducible if

$$\forall i, j \in S \ \exists n : \pi^n(i, j) > 0.$$

It is aperiodic if

$$\forall i \in S : \gcd\{n \in \mathbb{N} \setminus \{0\} : \pi^n(i, i) > 0\} = 1.$$

It is a well known fact that if a Markov chain is aperiodic and irreducible there exists a unique stationary distribution μ such that for any other distribution ν on S we have that $\lim_{n\to\infty}\pi^n\nu=\mu$. We also define the variational distance between probability distributions ν , μ as

$$\|\nu - \mu\|_1 = \frac{1}{2} \sum_{i \in S} |\mu(i) - \nu(i)|. \tag{3}$$

With a slight abuse of notation we will also denote the l_1 -mixing time threshold in variation distance for a Markov chain by

$$t_{mix} = \min\{n \in \mathbb{N} : \sup_{\nu} \|\pi^n \nu - \mu\|_1 \le e^{-1}\}.$$
 (4)

Notice that we incorporated the 1/2 factor into the definition of the norm in Equation (3), which explains its absence in (4). Let

$$C = \min\{T | \forall i \in S \exists 1 \le k \le T \text{ s.t. } X_k = i\}.$$

We will denote by $E_i(C)$ the expected time it takes to observe all states starting from $X_0 = i$ and by $T_C = \max_{i \in S} E_i(C)$ the cover time of the chain. We refer to e.g. [16, Chapter 1] for a review of these concepts.

2.2. (Classical) Voter CFTP

We will briefly describe a perfect sampling algorithms based on CFTP for Markov chains introduced in [22], called "voter CFTP". We mostly stick to their terminology and notation. The goal of this algorithm is to produce perfect samples of the stationary distribution μ of some Markov chain. One of the main advantages of this algorithm is that we only need to be able to observe valid transitions of this Markov chain to obtain perfect samples of the target distribution.

One should note that this is in general not the most efficient algorithm for perfect sampling [22], but arguably the simplest to understand. Besides the pedagogical motivation to present it, it turns out that this version is of interest in the quantum case, as we will see later. For this algorithm we suppose we have access to a randomized procedure $\mathbf{RandomSuccessor}: S \to S$ such that $P(\mathbf{RandomSuccessor}(i) = j) = \pi(i, j)$, where π is a transition matrix having μ as a stationary measure. We also let G be a vertex-labeled graph with vertices $-\mathbb{N}_0 \times S$ and labels S. We will define the labels and edges as the algorithm runs and denote by G(k,i) the label of the vertex (k,i). Pseudocode for the algorithm is provided below in Algorithm 1.

One does not need to add the edge on Step 7. This only helps to visualize the process. The expected run-time of this algorithm and its complexity of course depend on properties of **RandomSuccessor**: $S \to S$. We will discuss these when we analyze the same questions for our algorithm in the quantum case. We now provide a proof that Algorithm 1 indeed produces a perfect sample if it terminates almost surely.

Theorem 2.1. Suppose Algorithm 1 terminates with probability 1 and denote the output by Y. Then $P(Y = i) = \mu(i)$.

Proof. Let $\epsilon > 0$. As the algorithm terminates with probability 1, there is a N_{ϵ} s.t.

 $P(\text{algorithm terminates after at most } N_{\epsilon} \text{ steps}) \geq 1 - \epsilon.$

Algorithm 1 Voter CFTP[22]

```
1: procedure Voter CFTP
       Set G(0, i) = i and k = 0.
 2:
       while \exists j, i \in S s.t. G(k, i) \neq G(k, j) do
 3:
           for i \in S do
 4:
              Let j = \mathbf{RandomSuccessor}(i).
 5:
              Set G(k-1, i) = G(k, j).
 6:
              Add the edge \{(k-1, i), (k, j)\}
 7:
           end for
 8:
           Set k \to k-1
 9:
       end while
10:
11: return G(k, i_0) for some i_0 \in S
12: end procedure
```

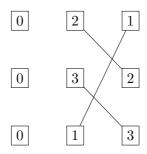


Figure 1: Possible first two columns of the graph after running the for-loop in the fourth step one time for d = 3. Notice that the third column has still not been labeled.

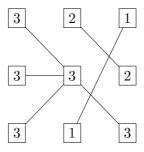


Figure 2: Possible graph after running the for-loop one more time. Notice the algorithm has terminated and outputs the sample 3.

Denote by A_{ϵ} the event that the algorithm terminates after at most N_{ϵ} steps. Define a Markov chain $X_{-M}, X_{-M+1}, X_{-M+2}, \ldots, X_0$ for some $M \in \mathbb{N}$ and choose X_{-M} according to μ , i.e. $P(X_{-M} = i) = \mu(i)$. The transitions are defined by the graph, which we suppose has been labeled for all (k,i) with k > -M. Given $X_k = j$ we set $X_{k+1} = i$, where $\{(k,j),(k+1,i)\}$ is an edge of the graph G. As we chose X_{-M} according to μ and **RandomSuccessor** has μ as a stationary distribution, $P(X_k = i) = \mu(i)$ for all $-M \le k \le 0$. We have

$$P(X_0 \neq Y) = P(X_0 \neq Y | A_{\epsilon}) P(A_{\epsilon}) + P(X_0 \neq Y | A_{\epsilon}^C) P(A_{\epsilon}^C).$$

One can check that the label on the graph at (-M,i) is nothing but the value of X_0 . Thus, if we assume that the algorithm has terminated, the value of X_0 does not depend on the initial value and will always be equal to Y. Therefore $P(X_0 \neq Y | A_{\epsilon}) = 0$ if $-M \leq N_{\epsilon}$. Also, by construction, $P(X_0 \neq Y | A_{\epsilon}^C)P(A_{\epsilon}^C) \leq \epsilon$. We then conclude $P(X_0 \neq Y) \leq \epsilon$ and so the value of Y and X_0 coincide, as ϵ was arbitrary. As X_0 is distributed according to μ , so is Y.

3. CFTP for quantum Gibbs states

3.1. Voter CFTP

Given a Hamiltonian $H \in \mathcal{M}_d$ with non-degenerate spectrum, an eigenbasis preserving quantum channel T for some inverse temperature $\beta > 0$ and a POVM $\mathcal{F} = \{F_i\}_{i \in I}$, the following algorithm allows us to obtain perfect samples from the distribution $p(i) = \operatorname{tr}\left[F_i\frac{e^{-\beta H}}{Z_\beta}\right]$. The algorithm uses three registers corresponding to the tensor factors $\mathbb{C}^d \otimes \mathbb{C}^m \otimes \mathbb{C}^m$, where m is large enough to perform phase estimation for H and tell apart the different eigenvalues of H. The first one will encode the current state of our system, while the other two will be used to record the output of two phase estimation algorithms. Also define a labeled graph G with vertices $V = -\mathbb{N}_0 \times \{1, \dots, d\}$ and labels given by $\{0, \dots, d\}$. We assume that G has no edges at the beginning of the algorithm and the vertices are labeled as

$$G(k,j) = \begin{cases} j & \text{if } k = 0\\ 0 & \text{otherwise} \end{cases}$$
 (5)

We assume we can prepare the maximally mixed state $\frac{1}{d}$. This can be done for example by picking a uniformly distributed integer between 1 and d and preparing the corresponding state of the computational basis. We will assume that the Hamiltonian has a spectral decomposition given by $H = \sum_i E_i |\psi_i\rangle\langle\psi_i|$. The number n denotes how many samples we wish to obtain in total and c will denote a counter for the number of samples we still wish to obtain. The pseudocode for the algorithm is below in Algorithm 2

We now prove it indeed outputs perfect samples.

Theorem 3.1. Let T be a primitive, eigenbasis preserving quantum channel for a Hamiltonian H and inverse temperature $\beta > 0$. Then Algorithm 2 terminates with probability 1 and generates n perfect samples of the distribution p defined above.

Algorithm 2 Voter CFTP for quantum Gibbs states

```
1: procedure QUANTUM VOTER CFTP
        Set S = \emptyset and c = n.
 2:
        while c \neq 0 do
 3:
            Prepare the state \frac{1}{d} \otimes |0\rangle\langle 0| \otimes |0\rangle\langle 0|
 4:
            Run phase estimation on the first and second register.
 5:
            Measure the second register in the computational basis.
 6:
            if i \in S then
 7:
                Measure \mathcal{F} on the first register.
 8:
                Update c to c-1.
 9:
            else
10:
                Apply T \otimes id_m \otimes id_m to the system.
11:
                Run phase estimation on the first register and third register.
12:
13:
                Measure the third register in the computational basis. Let the result be
    j.
                For the largest k s.t. G(k,i) = 0 we add the edge \{(k,i), (k+1,j)\}.
14:
                if G(k+1,j) \neq 0 then
15:
                   Change the labels on all the vertices (k', i') with k' < k for which there
16:
    is a path to (k, i) from 0 to G(k + 1, j).
                end if
17:
                if There is k_0 \in -\mathbb{N} and l \in [d] s.t. \forall i \in [d] G(k_0, i) = l then
18:
                   Append l to S.
19:
                   Erase all edges to the vertices (k_0, i) and set the labels to G(k_0, i) = i
20:
    and G(k, i) = 0 for k < k_0.
                end if
21:
            end if
22:
23:
        end while
24: end procedure
```

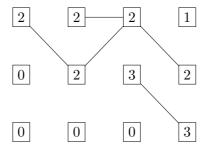


Figure 3: Possible first four columns of the graph after running the while-loop in step 3 five times for d = 3.

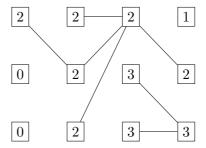


Figure 4: Possible graph after running the while-loop two more times. Notice the algorithm has terminated and outputs the sample 2.

Proof. We will first show that with probability 1 there is a $k \in -\mathbb{N}$ and $l \in [d]$ s.t. $\forall i \in [d] \ G(k,i) = l$. The probability that we observe an eigenstate $|\psi_i\rangle$ at step 6 is $\frac{1}{d}$, so with probability 1 we will observe it if we run the loop at step 3 often enough. This implies that we will assign a label different to 0 to arbitrary vertices of the graph G if we run the while-loop at step 3 for long enough. Observe that as T is an eigenbasis preserving quantum channel, the dynamics on the eigenbasis of H under T is just a classical Markov chain. As T is primitive and the stationary state has full rank, this Markov chain is aperiodic and irreducible [4]. Because of that, the probability that we will obtain a k s.t. $G(k,i) = l \ \forall i \in [d]$ is 1, using the same argument as the one given in [22] for the classical case. By the same argument, the probability that this label is l is given by $\frac{e^{-\beta E_l}}{Z_\beta}$, as this is also the stationary distribution of the underlying classical Markov chain. As before, we will observe $|\psi_l\rangle|E_l\rangle|0\rangle$ at step 6 with probability 1 if we run the while-loop at step 3 often enough and this will then be a perfect sample by the previous discussion.

Note that we could also check if the measurement outcome we observe at step 13 is one of the desired outcomes to increase our probability of observing it.

3.2. Examples of eigenbasis preserving channels

In order to run Algorithm 2, we need to be able to implement a primitive eigenbasis preserving quantum channel for the Gibbs state we want to sample from. In recent years many algorithms have been proposed to approximately prepare quantum Gibbs states on a quantum computer [31, 20, 5, 11, 33, 23, 30, 3, 13]. We will here briefly discuss how some of them provide us with eigenbasis preserving quantum channels for Gibbs states.

One class of eigenbasis preserving channels are quantum dynamical semigroups with Davies generators. These are Markovian approximations for a quantum system weakly coupled to a thermal reservoir. A detailed description of the derivation and structure of Davies generators is beyond the scope of this article and can be found in [10, 7]. Under some conditions on the Hamiltonian and the coupling of the system to the bath, the Davies semigroup is primitive. The exact speed of this convergence is the subject of current research. We refer to [29] for a discussion of the conditions under which the Davies generators are primitive and some bounds on the convergence speed. In [13] Davies generators are also proposed as a way of preparing thermal states on a quantum computer.

For our purposes, their main property is that if the underlying Hamiltonian has a non-degenerate spectrum, the dynamics in the eigenbasis of the Hamiltonian does not couple diagonal terms to off-diagonal terms. They are therefore eigenbasis preserving. This has been observed by many authors since the beginning of their study [7, 8, 24] and we again refer to those for a proof of this claim.

Another example is given by the Quantum metropolis algorithm proposed in [30], as the quantum channel implemented at each step also maps eigenstates of H to eigenstates of H. However, it can be simplified for our purposes. As in the usual Metropolis algorithm, at each step we have to accept or reject a move that has been made. One of the main difficulties to implement the quantum algorithm is reversing the evolution of the system if we reject the move. This is because, by the No-Cloning Theorem [32], we can't make a copy of the previous state of the system. But the information that we rejected the move is enough for our algorithm, as we may simply copy the previous label when labeling the vertices. We may therefore skip the procedure of reversing the move.

More generally, it can be shown that dynamical semigroups that satisfy a quantum version of the detailed balance condition and whose stationary state has a non-degenerate spectrum are always eigenbasis preserving [2]. Our two previous examples fall into that category. This gives us a simple sufficient criterion to check whether a given implementation is eigenbasis preserving.

Note, however, that it is not a priori clear that a quantum dynamical semigroup can be implemented efficiently or by only using local operations. We refer to [13, 15] for a discussion of these topics.

3.3. Expected run-time, Memory Requirements and Circuit Depth

We will now address the expected run-time of Algorithm 2. To this end, we will only consider the number of calls of the phase estimation and eigenbasis preserving channel and not the necessary classical post-processing, as we consider the quantum routines the more expensive resources.

In [22, Theorem 5], it was shown that the expected time to obtain a sample using Algorithm 1 is $\mathcal{O}(t_{mix}d^2)$ steps, where again t_{mix} is the time s.t. the chain is e^{-1} close to stationarity and d the size of our state space.

We will say that a column indexed by $k \in -\mathbb{N}$ of G is complete if $\forall i \in [d]$ $G(k,i) \neq 0$. In [22], it is shown that we need to complete on average $\mathcal{O}(t_{mix}d)$ columns of the graph G before the labels on a column become constant. As each step to complete a column need $\mathcal{O}(d)$ calls of **RandomSuccessor**, this leads to a total of $\mathcal{O}(t_{mix}d^2)$ calls of **RandomSuccessor**. The dynamics in the eigenbasis of H is essentially classical, so we may use the exact same reasoning to conclude that we will need an expected $\mathcal{O}(t_{mix}d)$

number of complete columns until we obtain one perfect sample.

But in our case we may need more uses of the channel and phase estimation, as we may not prepare an arbitrary eigenstate of H which might be necessary to complete a column deterministically. But preparing the initial states probabilistically does not significantly change the overall efficiency of the algorithm, as illustrated by the next theorem.

Theorem 3.2. Let $T: \mathcal{M}_d \to \mathcal{M}_d$ be a primitive eigenbasis preserving quantum channel for a Hamiltonian H with inverse temperature $\beta > 0$ with mixing time t_{mix} . Then the expected number of steps until Algorithm 2 returns a perfect sample is $\mathcal{O}(t_{mix}d^2n)$.

Proof. By Corollary A.1, proved in Appendix A, the expected number of measurements necessary to complete a column is $\mathcal{O}(d)$. From the result [22, Theorem 5] we know that we will need an expected number of $\mathcal{O}(t_{mix}d)$ number of complete columns to obtain a sample.

It should be clear from Theorem 3.2 that Algorithm 2 is considerably less efficient than other Algorithms such as Quantum Metropolis [30] if we are willing to settle for an approximate sample. After all, to obtain a sample that is e^{-1} close in trace distance to the Gibbs state, one only needs t_{mix} steps of the Metropolis algorithm instead of the $\mathcal{O}(t_{mix}d^2)$ needed for CFTP. It is therefore important to stress again that these algorithms are very different in nature. Algorithm 2 provides us with perfect, not approximate samples, and it is the first algorithm of this form for quantum Gibbs states to the best of our knowledge. It also provides a certificate that we are indeed sampling from the right distribution when it terminates, while most other algorithms require some mixing time bounds to obtain a sample that can be considered close to the target distribution. Moreover, it only requires us to be able to implement one step of the chain.

We now analyze the circuit depth and memory requirements to obtain a sample.

Theorem 3.3. Let C_{PT} and C_{T} be the circuit depth needed to implement the phase estimation for H and the eigenbasis preserving channel, respectively. Then one needs to implement a quantum circuit of depth $\mathcal{O}(C_{PT} + C_T)$ a $\mathcal{O}(t_{mix}d^2)$ number of times to obtain a sample and moreover an expected $\mathcal{O}(d)$ classical memory.

Proof. The circuit length part follows easily from just going through the steps of Algorithm 2, as to label the new vertex we need to implement two phase estimation steps and apply the eigenbasis preserving channel once.

To see the that we only need $\mathcal{O}(d)$ classical memory, notice that we only need to store the information contained in the last complete column to perform the later steps. This is because it contains all possible labels for future columns. By Corollary A.1, we have that the expected number of labels we obtain before completing a column is also $\mathcal{O}(d)$, and so we need a total classical memory of size $\mathcal{O}(d)$.

The quantum part of Algorithm 2 can also be easily parallelized, as we could use different quantum computers feeding a classical computer with valid transitions.

3.4. Stability under Noise

We will now address two possible sources of noise for Algorithm 2 and show it is stable under these two. First, in the implementation of the eigenbasis preserving channel and second in the phase estimation steps. One may quantify the stability of primitive quantum Markov chains with the following constant:

Definition 3.1. Let $T: \mathcal{M}_d \to \mathcal{M}_d$ be a primitive quantum channel with stationary state $\sigma \in \mathcal{D}_d$. We define

$$\kappa(T) = \sup_{X \in \mathcal{M}_d, tr(X) = 0} \frac{\|(id - T + T_{\infty})^{-1}(X)\|_1}{\|X\|_1}$$

with $T_{\infty}(X) = tr(X)\sigma$.

We refer to [28] for bounds on this constant and how it can be used to quantify the stability of a quantum Markov chain. Also note that due to the spectral characterization of primitive quantum channels [27], the set of primitive quantum channels is relatively open in the convex set of quantum channels.

Theorem 3.4. Let $T: \mathcal{M}_d \to \mathcal{M}_d$ be a primitive eigenbasis preserving channel for a Hamiltonian H and inverse temperature $\beta > 0$ and $T': \mathcal{M}_d \to \mathcal{M}_d$ a quantum channel satisfying

$$||T - T'||_{1 \to 1} \le \epsilon \tag{6}$$

for some $\epsilon > 0$ small enough for T' to be primitive too. For a POVM $\{F_i\}_{i \in I}$, let p and p' be probability distributions we obtain by measuring $\{F_i\}_{i \in I}$ on the output of Algorithm 2 using T and T' respectively. Then

$$||p - p'||_1 \le (\kappa(T) + 2)\epsilon. \tag{7}$$

Proof. Let $\{|\psi_j\rangle\}_{1\leq j\leq d}$ be the eigenbasis of H and define $Q:\mathcal{M}_d\to\mathcal{M}_d$ to be the quantum channel given by

$$Q(X) = \sum_{j} \operatorname{tr}(|\psi_{j}\rangle\langle\psi_{j}|X)|\psi_{j}\rangle\langle\psi_{j}|. \tag{8}$$

Note that as T is an eigenbasis preserving channel, QTQ is also an eigenbasis preserving channel with stationary state $\frac{e^{-\beta H}}{\mathcal{Z}_{\beta}}$. As T' is assumed to be primitive, QT'Q is primitive too, as $\|QT'Q - QTQ\|_{1\to 1} \le \|T' - T\|_{1\to 1}$. Denote by ρ the stationary state of the channel QT'Q. By the variational expression for the trace distance, we have that

$$||p - p'||_1 \le ||\frac{e^{-\beta H}}{\mathcal{Z}_{\beta}} - \rho||_1.$$
 (9)

From Theorem 1 in [28] it follows that

$$\|\frac{e^{-\beta H}}{\mathcal{Z}_{\beta}} - \rho\|_{1} \le \kappa(QTQ)\|Q(T - T')Q\|_{1 \to 1}.$$
 (10)

As Q is a quantum channel, it follows that $||Q||_{1\to 1} \le 1$ and so

$$||Q(T - T')Q||_{1 \to 1} \le ||T - T'||_{1 \to 1}. \tag{11}$$

Equation (7) would then follow from $\kappa(QTQ) \leq 2 + \kappa(T)$. Note that as T is primitive, we have that $||T - T_{\infty}|| < 1$, where the norm is the operator norm. Also, $QT_{\infty}Q = T_{\infty}$ and Q is a projection. Thus

$$||QTQ - T_{\infty}|| \le ||T - T_{\infty}|| < 1.$$

As T is an eigenbasis preserving channel, we have that

$$Q(T-T_{\infty})Q = (T-T_{\infty})Q$$

and so

$$(Q(T - T_{\infty})Q)^n = Q(T - T_{\infty})^n Q.$$

We therefore have

$$(\mathrm{id} - (Q(T - T_{\infty})Q))^{-1} = \sum_{n=1}^{\infty} \frac{(Q(T - T_{\infty})Q)^n}{n!} = (12)$$

$$id - Q + Q \left(\sum_{n=0}^{\infty} \frac{(T - T_{\infty})^n}{n!} \right) Q = id - Q + Q(id - (T - T_{\infty}))^{-1}Q.$$
 (13)

As $||Q||_{1\to 1}$, $||id||_{1\to 1} \le 1$ and from (12) we obtain

$$\kappa(QTQ) = \sup_{X \in \mathcal{M}_d, \text{tr}(X) = 0} \frac{\|[Q(\text{id} - (T - T_\infty))^{-1}Q + \text{id} - Q](X)\|_1}{\|X\|_1} \le$$
(14)

$$\sup_{X \in \mathcal{M}_d, \operatorname{tr}(X) = 0} \frac{\|Q(\operatorname{id} - (T - T_\infty))^{-1} Q(X)\|_1 + \|(\operatorname{id} - Q)(X)\|_1}{\|X\|_1} \le 2 + \kappa(T).$$

We will now analyze the errors stemming from phase estimation in a similar manner. We assume that with probability q we make an error preparing or measuring a state doing phase estimation, that this probability is the same for the second and first phase estimation procedure and that these errors occur independently. We will consider the case in which we misidentify the initial or final state. Under these conditions we have:

Theorem 3.5. Let q be defined as above and $\{F_i\}_{i\in I}$ a POVM. For a primitive eigenbasis preserving channel $T: \mathcal{M}_d \to \mathcal{M}_d$ for a Hamiltonian H and inverse temperature $\beta > 0$, let $p_i = tr\left(F_i \frac{e^{-\beta H}}{\mathcal{Z}_{\beta}}\right)$ and p'_i be the probability of observing F_i at the output of Algorithm 2 with faulty phase estimation. Then

$$||p - p'||_1 \le q + 2(\kappa(T) + 2)(1 - (1 - q)^2).$$

Proof. Define the stochastic matrix $(\xi)_{i,j} = \zeta_{i,j}$, where $\zeta_{i,j}$ is the probability of measuring E_i if the state of the system is described by $|\psi_j\rangle$. Also, let $(\pi)_{i,j} = \text{tr}[|\psi_i\rangle\langle\psi_i|T(|\psi_j\rangle\langle\psi_j|)]$. Then the transition matrix for the labels of the graph in Algorithm 2 is given by

$$\pi' = (1 - q)^2 \pi + q(1 - q)\xi \pi + q(1 - q)\pi \xi + q^2 \xi \pi \xi.$$
(15)

The term $(1-q)^2\pi$ corresponds to the situation in which we performed phase estimation twice without any errors, $q(1-q)\xi\pi+q(1-q)\pi\xi$ to one error in the first and second phase estimation steps respectively and $q^2\xi\pi\xi$ to errors on the two steps. This transition matrix will still be primitive for q sufficiently small. Let r be the stationary distribution of π and r' the one of π' . Observe that, as $\kappa(\pi) \leq \kappa(QTQ)$, we may use the bound $\kappa(QTQ) \leq 2 + \kappa(T)$ from the proof of Theorem 3.4 and obtain

$$||r - r'||_1 \le (\kappa(T) + 2) ||(1 - q)^2 \pi + q(1 - q)\xi \pi + q(1 - q)\pi \xi + q^2 \xi \pi \xi - \pi||_{1 \to 1}$$

$$\le 2 (\kappa(T) + 2) (1 - (1 - q)^2).$$
(16)

We would then be measuring the POVM on the state $\rho' = \sum_i r'(i)|\psi_i\rangle\langle\psi_i|$ if no error occurs at step 6. However, if an error occurs, we will be measuring the POVM on the state $\rho_{EM} = \sum_i (\xi r')(i)|\psi_i\rangle\langle\psi_i|$. As this happens with probability q, the state on which we measure our POVM is given by $\rho_M = q\rho_{EM} + (1-q)\rho'$. As ρ_{EM} commutes with ρ , we have from the previous discussion and Equation (16) that

$$\|\rho_M - \rho\|_1 \le q + 2(\kappa(T) + 2)(1 - (1 - q)^2).$$
 (18)

The claim then follows from the variational expression for the trace distance as in the proof of Theorem 3.4.

3.5. Adapting other Variations of CFTP

In [22] the authors also discuss other variations of CFTP that can be more efficient, such as the cover time CFTP algorithm. We will not discuss in detail how to also adapt these other proposals, but it should be straightforward to do so from the results in the last sections. In this section, we will just mention the main ideas. Note that the only thing necessary to implement all these variations is a valid **RandomSuccessor** function and the outputs of the measurements in steps 6 and 13 of Algorithm 2 do exactly that. This information could then be fed to a classical computer running a variation of CFTP. The only difference to the classical case is that we may not choose arbitrary initial states, but do so probabilistically. However, by waiting until each initial state is observed, we may circumvent this and do not have a significant overhead by the result of Corollary A.1.

For some variations of CFTP, like again the cover time CFTP, one also needs to iterate $\mathbf{RandomSuccessor}$. This is also straightforward. If we want to obtain a given number of iterations of $\mathbf{RandomSuccessor}$, we just apply an eigenbasis preserving channel T to the first register, repeated by a phase estimation step and a measurement in the computational basis. We then repeat this procedure to obtain the iterations.

One could then repeat the analysis done in this section and see that the run-time is again of the same order of magnitude as the classical version of the CFTP algorithm and obtain a perfect sampling algorithm with a run-time proportional to the cover time.

4. Conclusion and Open Problems

We have shown how to adapt perfect sampling algorithms for classical Markov chains to obtain perfect samples of quantum Gibbs states on a quantum computer. These algorithms have an average run-time which is similar to their classical counterparts and we also show that they are stable under noise. We argue that one of its main advantages is its short circuit depth. However, the scaling of the algorithm is still prohibitive for many-body applications and it would be interesting to investigate whether there is a class of models to which we can tailor the perfect sampling algorithms to be efficient, as was done with success for attractive spin systems [21].

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A. Expected number of observations to sample all possible outputs

To estimate the expected run-time of Algorithm 2, we need to determine how often, on average, we must measure some orthonormal basis $\{|\psi_i\rangle\}_{1\leq i\leq d}$ of \mathbb{C}^d on the state $\frac{1}{d}$ until we observe all possible elements of the basis. This corresponds to the time necessary to complete a column in Algorithm 2.

One can see that this corresponds to the problem of determining the expected time for d urns to be occupied (have at least one ball in them) if we place one ball in one urn chosen uniformly at random for each time unit and independently. This type of problem is usually referred to as an occupancy problem.

Theorem A.1. Suppose we put one ball in $d \in \mathbb{N}$ (initially empty) urns uniformly at random and independently for each time unit $t = 1, 2, \ldots$ Let Y be the random variable $Y = \min\{t | all \ urns \ contain \ at \ least \ one \ ball\}$. Then $E(Y) = \mathcal{O}(d)$.

Proof. One can show (see e.g. [19] or [12, Section 3.1]) that the probability of all the urns being occupied after we put n balls into them is given by

$$\sum_{k=0}^{d-1} (-1)^k \left(\frac{d-k}{d}\right)^n \tag{19}$$

for $n \ge d$ and 0 for n < d. We then have

$$P(Y \ge n) = \sum_{k=1}^{d-1} (-1)^{k+1} \left(\frac{d-k}{d}\right)^{n-1}$$
 (20)

by (19) for $n \ge d$. As $E(Y) = \sum_{n=1}^{\infty} P(Y \ge n)$ we obtain

$$E(Y) = d + \sum_{n=d+1}^{\infty} \sum_{k=1}^{d-1} (-1)^{k+1} \left(\frac{d-k}{d}\right)^{n-1}.$$
 (21)

We will now show that $\sum_{n=d+1}^{\infty} \sum_{k=1}^{d-1} (-1)^k \left(\frac{d-k}{d}\right)^{n-1} = \mathcal{O}(d)$, which completes the proof. By the formula for the limit of a geometric series we have

$$\sum_{n=d+1}^{\infty} \sum_{k=1}^{d-1} (-1)^k \left(\frac{d-k}{d}\right)^{n-1} = d \sum_{k=1}^{d-1} \frac{(-1)^{k+1}}{k} \left(1 - \frac{k}{d}\right)^{d-1}.$$
 (22)

Define the sequence $\{\nu_d\}_{d\in\mathbb{N}}$ of measures on N as

$$\nu_d(k) = \begin{cases} \left(1 - \frac{k}{d}\right)^{d-1}, & \text{for } k \le d - 1\\ 0, & \text{else} \end{cases}$$
 (23)

It is then clear that $\{\nu_d\}_{d\in\mathbb{N}}$ converges weakly to ν with $\nu(k)=e^{-k}$. Define the ν -integrable and bounded function

$$f: \mathbb{N} \to \mathbb{R}, k \mapsto \frac{(-1)^{k+1}}{k}$$
 (24)

and observe that by the weak convergence we have

$$\int f d\nu_d \to \int f d\nu. \tag{25}$$

This means in particular that the sequence $\{a_d\}_{d\in\mathbb{N}}$ given by

$$a_d = \sum_{k=1}^d \frac{(-1)^{k+1}}{k} \left(1 - \frac{k}{d}\right)^{d-1} = \int f d\nu_d$$

is bounded. Denote by $C = \sup_{d \in \mathbb{N}} a_d$. We then have

$$E(Y) \le d + Cd = \mathcal{O}(d).$$

Corollary A.1. The expected time to label a whole column in Algorithm 2 is $\mathcal{O}(d)$.

Proof. Clear.

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