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# Adiabatic Quantum Simulators 

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#### Abstract

In his famous 1981 talk, Feynman proposed that unlike classical computers, which would presumably experience an exponential slowdown when simulating quantum phenomena, a universal quantum simulator would not. An ideal quantum simulator would be controllable, and built using existing technology. In some cases, moving away from gate-model-based implementations of quantum computing may offer a more feasible solution for particular experimental implementations. Here we consider an adiabatic quantum simulator which simulates the ground state properties of sparse Hamiltonians consisting of one- and two-local interaction terms, using sparse Hamiltonians with at most three-local interactions. Properties of such Hamiltonians can be well approximated with Hamiltonians containing only two-local terms. The register holding the simulated ground state is brought adiabatically into interaction with a probe qubit, followed by a single diabatic gate operation on the probe which then undergoes free evolution until measured. This allows one to recover e.g. the ground state energy of the Hamiltonian being simulated. Given a ground state, this scheme can be used to verify the QMA-complete problem LOCAL HAMILTONIAN, and is therefore likely more powerful than classical computing.


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## I. INTRODUCTION

Computer simulation of quantum mechanical systems is an indispensable tool in all physical sciences dealing with nanoscale phenomena. Except for specific and rare cases ${ }^{1}$, classical computers have not been able to efficiently simulate quantum systems, as in all known techniques at least one of the computational resources required to perform the simulation scales exponentially with the size of the system being simulated.

Numerous classical approximative methods, such as density functional theory ( $\mathrm{DFT}^{2}$ ) and quantum Monte Carlo ( $\mathrm{QMC}^{3}$ ) have been developed to address various aspects of the efficiency problem, but no known polynomially scaling methods are universally applicable. Each suffers from particular deficiencies such as the fermionic sign problem of QMC or the approximate exchangecorrelation functionals of DFT. Quantum computers on the other hand, as conjectured by Feynman ${ }^{4}$, may be used to simulate other quantum mechanical systems efficiently. Feynman's conjecture was subsequently expanded leading to the rapidly growing area of study known as quantum simulation ${ }^{5-13}$.

Quantum simulation is expected to be able to produce classically unattainable results in feasible run times, using only a modest number of fault tolerant (or error corrected) quantum bits. For example, calculating the ground state energy of the water molecule to the level of precision necessary for experimental predictions ( $\approx 1$ $\mathrm{kcal} / \mathrm{mol}$ ) - a problem barely solvable on current supercomputers ${ }^{14}$ - would require roughly 128 coherent quantum bits (before error correction) ${ }^{9}$, and on the order of billions of quantum gates ${ }^{15}$. To date, several experimental implementations of quantum simulation algo-
rithms have been done for small systems ${ }^{11,16,17}$.
Theoretical quantum simulation falls into two main categories: dynamic evolution and static properties. Both categories rely heavily on the Trotter decomposition to handle non-commuting terms in the Hamiltonian when mimicking the unitary time propagator of the system to be simulated. To approximate evolution under a Hamiltonian $H=\sum_{i=1}^{k} H_{i}$ consisting of $k$ noncommuting but local terms $\left\{H_{i}\right\}_{i=1}^{k}$, one applies the sequence of unitary gates $\left\{e^{-i H_{i} t / n}\right\}_{i=1}^{k}$ a total of $n$ times. As the number of repetitions $n$ tends to infinity the approximation error caused by the non-commutativity vanishes and the approximation converges to the exact result ${ }^{\frac{5}{5}}$. If each time slice requires a constant number of gates independent of the parameter $t / n$, then reducing the approximation error by repeating the sequence $n$ times can become expensive for high accuracy applications ${ }^{15}$.

Constructing a practical method of quantum simulation is a significant challenge. Gate-model based simulation methods (with quantum error correction) can provide a scalable solution but are well out of reach of present-day experiments, except for small systems. On the other hand, some experimental implementations seem to be well suited to operate as adiabatic processors. For these setups, moving away from the gate model may offer a less resource-intensive, and consequently a more feasible solution for simulating medium-sized quantum systems. This paper addresses the problem by presenting a hybrid model of quantum simulation, consisting of an adiabatically controlled simulation register coupled to a single gate-model readout qubit. Our scheme can simulate the constant observables of arbitrary spin graph Hamiltonians. It allows the measurement of the expec-
tation value of any constant $k$-local observable using a $k+1$-local measurement Hamiltonian. Fault tolerance of the adiabatic model of quantum computing is a topic of growing interest. Its robustness in the presence of noise has been studied in ${ }^{18,19}$. We only consider the simulation protocol here, and don't study the adiabatic error correction that would be required for a practical large scale implementation.

In most quantum computing architectures, the natural interactions are two-local. However, under certain conditions $k$-local interactions can be well approximated using techniques such as perturbative Hamiltonian gadgets ${ }^{20-23}$ or average Hamiltonian methods ${ }^{24}$ - this provides even the possibility of utilizing gate model fault tolerance to protect the slower adiabatic evolution, an approach that seems promising. We note that reference ${ }^{25}$ considered the mapping of a given $n$-qubit target Hamiltonian with $k$-local interactions onto a simulator Hamiltonian with two-local interactions.

Structure of this paper: We will continue by giving an overview of the simulator design, including initialization, adiabatic evolution and measurement. The following section investigates the performance of the method in simulating a small system in the presence of noise. Finally, we will present our conclusions. Appendix A further details the specifics of our method (including the numeric simulation of the technique).

## II. SIMULATOR OVERVIEW

We consider the simulation of systems represented by finite collections of spins acted on by a time-independent Hamiltonian described by a graph $G=(V, E)-$ e.g. the Heisenberg and Ising models. Each graph vertex $v \in V$ corresponds to a spin acted on by a local Hamiltonian $L_{v}$, and each edge $e \in E$ to a two-local interaction $K_{e}$ between the involved vertices. The Hamiltonian $H_{T}$ we wish to simulate is given by

$$
\begin{equation*}
H_{T}=\sum_{v \in V} L_{v}+\sum_{e \in E} K_{e} \tag{1}
\end{equation*}
$$

The simulator consists of an adiabatically controlled simulation register $S$ with Hamiltonian $H_{S}$, and a probe register $P$ which will be acted on by gate operations and measured projectively. We will engineer the probe $P$ such that it behaves as a controllable two-level system with the orthonormal basis $\left\{\left|p_{0}\right\rangle,\left|p_{1}\right\rangle\right\}$. Without loss of generality, the probe Hamiltonian can be expressed as $H_{P}=\delta\left|p_{1}\right\rangle\left\langle p_{1}\right|$, where $\delta$ is the spectral gap between the probe's ground and first excited states.

Initialization: We will first set the simulation register Hamiltonian $H_{S}$ to $H_{S, I}$ and prepare $S$ and $P$ in their respective ground states. The Hamiltonian $H_{S, I}$ has a simple ground state which can be (i) computed classically and (ii) prepared experimentally in polynomial time -
such as a classical approximation to the ground state of the simulated system. The simulator Hamiltonian is thus initially given by

$$
\begin{equation*}
H_{0}=H_{S, I} \otimes \mathbb{1}_{P}+\mathbb{1}_{S} \otimes H_{P} \tag{2}
\end{equation*}
$$

Adiabatic evolution: According to the adiabatic theorem $^{26}$, a quantum system prepared in an energy eigenstate will remain near the corresponding instantaneous eigenstate of the time-dependent Hamiltonian governing the evolution if there are no level crossings and the Hamiltonian varies slowly enough. By adjusting the simulator parameters, we adiabatically change $H_{S}$ from $H_{S, I}$ to $H_{S, T}$, the fully interacting Hamiltonian of the system to be simulated.

Let us denote the ground state of $H_{S, T}$ as $\left|s_{0}\right\rangle$. At the end of a successful adiabatic evolution $P$ is still in its ground state $\left|p_{0}\right\rangle$, and $S$ is in (a good approximation to) the ground state of the simulated system, $\left|s_{0}\right\rangle$. Hence the simulator is now in the ground state $|\mathrm{g}\rangle=\left|s_{0}\right\rangle \otimes\left|p_{0}\right\rangle$ of its instantaneous Hamiltonian

$$
\begin{equation*}
H_{1}=H_{S, T} \otimes \mathbb{1}_{P}+\mathbb{1}_{S} \otimes H_{P} \tag{3}
\end{equation*}
$$

The computational complexity of preparing ground states of quantum systems has been studied ${ }^{20-22}$. It is possible to prepare a desired ground state efficiently provided that the gap between the ground and excited states is sufficiently large ${ }^{26}$ (see alternative methods in ${ }^{27}$ ). This depends on the initial and final Hamiltonians and on the adiabatic path taken. In general, finding the ground state energy of a Hamiltonian, even when restricted to certain simple models, is known to be complete for QMA, the quantum analogue of the class $\mathrm{NP}^{20-22}$. In fact there are physical systems such as spin glasses in nature which may never settle into their ground states.

However, a host of realistic systems (e.g. insulators, molecular systems) can on physical grounds be expected to retain a large energy gap and should thus be amenable to quantum simulation algorithms which rely on adiabatic state preparation.

Measurement: The measurement procedure begins by bringing $S$ and $P$ adiabatically into interaction. The simulator Hamiltonian becomes

$$
\begin{equation*}
H_{2}=H_{1}+\underbrace{A \otimes\left|p_{1}\right\rangle\left\langle p_{1}\right|}_{H_{S P}}, \tag{4}
\end{equation*}
$$

where the operator $A$ corresponds to an observable of the simulated system that is a constant of motion, i.e., commutes with $H_{S, T}$. Hence the total energy itself can always be measured by choosing $A=H_{S, T}$. Other such observables depend on the particular system and often can be analytically constructed given the Hamiltonian.

Let us use $a_{\text {min }}$ to denote the lowest eigenvalue of $A$. If $a_{\text {min }}+\delta>0$, then $|\mathrm{g}\rangle$ is also the ground state of $H_{2}$ and in the absence of noise the transitions from the ground
state are perfectly suppressed during the adiabatic evolution (see Appendix Afor proof). Assuming that $A$ can be decomposed into a sum of two-local operators, the interaction term $H_{S P}$ involves three-local interactions. These terms can be implemented using either Hamiltonian gadget techniques or average Hamiltonians (see Appendix A for details).

After the adiabatic evolution, at time $t=0$, we apply a Hadamard gate to the measurement probe which puts it into a superposition of its two lowest states. This is no longer an eigenstate of $H_{2}$, and the system will evolve as

$$
\begin{equation*}
|\psi(t)\rangle=\frac{1}{\sqrt{2}}\left|s_{0}\right\rangle \otimes\left(\left|p_{0}\right\rangle+e^{-i \omega t}\left|p_{1}\right\rangle\right) \tag{5}
\end{equation*}
$$

where $\omega:=\left(a_{0}+\delta\right) / \hbar$, and $a_{0}:=\left\langle s_{0}\right| A\left|s_{0}\right\rangle$ is the expectation value we wish to measure. We have thus encoded the quantity $a_{0}$, a property of the ground state of $H_{S, T}$, into the time dependence of the probe $P$.

After a time $t$, we again apply a Hadamard gate to the probe, resulting in the state

$$
\begin{equation*}
|\psi(t)\rangle=\left|s_{0}\right\rangle \otimes\left(\cos (\omega t / 2)\left|p_{0}\right\rangle+i \sin (\omega t / 2)\left|p_{1}\right\rangle\right), \tag{6}
\end{equation*}
$$

and then measure the probe. The probability of finding it in the state $\left|p_{0}\right\rangle$ is

$$
\begin{equation*}
P_{0}(t)=\frac{1}{2}(1+\cos (\omega t))=\cos ^{2}(\omega t / 2) \tag{7}
\end{equation*}
$$

If we have non-demolition measurements (see e.g. ${ }^{28}$ ) at our disposal, then measuring the probe does not disturb the state of the simulator which can be reused for another measurement.

One repeats the measurement with different values of $t$ until sufficient statistics have been accumulated to reconstruct $\omega$ and hence $a_{0}$ - this is reminiscent of Ramsey spectroscopy ${ }^{29}$ and hence should seem natural to experimentalists. In essence, we have performed Kitaev's phase estimation algorithm ${ }^{30}$, using the interaction Hamiltonian $H_{S P}$ instead of a controlled unitary.

If the ground state subspace of $H_{S, T}$ is degenerate and overlaps more than one eigenspace of $A$, or the simulation register $S$ has excitations to higher energy states at the beginning of the measurement phase, the probability of finding the probe in the state $\left|p_{0}\right\rangle$ is given by a superposition of harmonic modes. For example, for a thermalized state with inverse temperature $\beta$, we obtain

$$
\begin{equation*}
P_{0}(t)=\frac{1}{2}\left(1+\frac{1}{\sum_{x y} e^{-\beta E_{x}}} \sum_{k l} e^{-\beta E_{k}} \cos \left(\omega_{k, l} t\right)\right) \tag{8}
\end{equation*}
$$

where the first summation index runs over the energy eigenstates and the second over the eigenstates of $A$ in which energy has value $E_{k}$, and $\omega_{k, l}=\left(a_{k, l}+\delta\right) / \hbar$.

## III. EFFECTS OF NOISE

Any large scale implementation of the proposed method would most likely require adiabatic error correction ${ }^{31-33}$. However, for small systems this might not be necessary indicating that our method is feasible for immediate experimental technologies. For this reason, we will examine how robust a small scale implementation of our protocol would be.

To assess the effects of noise on the simulation method, we performed a numerical simulation of the simplest nontrivial implementation of the hybrid simulator, consisting of two simulator qubits and one probe qubit, with a randomly chosen $H_{T}$. Each qubit was coupled to its own bosonic heat bath with an Ohmic spectral density using the Born-Markov approximation ${ }^{34}$. The qubit-bath couplings were chosen such that the resulting single-qubit decoherence times $T_{1}$ and $T_{2}$ are compatible with recent superconducting flux qubit experiments with fully tunable couplings (see for example ${ }^{35}$ ). The noise model is described further in Appendix A The observable $A$ was chosen to be $H_{S, T}$, the simulated Hamiltonian itself, which means that the ground state energy was being measured.

We simulated measurements on 40 evenly distributed values of the time delay $t$. At each $t_{i}$ we performed 50 measurements, and averaged the results to get an estimate of $P_{0}\left(t_{i}\right)$. An exponentially decaying scaled cosine function was then fitted to this set of data points to obtain an estimate for $\omega$ and thus for $s_{0}$. The fit was done using the MATLAB LSQNONLIN algorithm, guided only by fixed order-of-magnitude initial guesses for the parameter values.


FIG. 1. Measurement procedure under Markovian noise. The continuous curve represents the probability of finding the probe in the state $\left|p_{0}\right\rangle$, the circles averaged measurement results and the dotted line a least squares fit to them. $\hbar \omega_{0}=h \cdot 25 \mathrm{MHz}$ is the energy scale of the Hamiltonians involved.

The results of the simulation are presented in Fig. 1 . The noise, together with the slight nonadiabaticity of the
evolution, cause excitations out of the ground state which result in a signal consisting of multiple harmonic modes. However, the ground state mode still dominates and with a realistic level of noise and relatively modest statistics we are able to reconstruct $\omega$ to a relative precision of better than 0.01 . This includes both the uncertainty due to finite statistics, and the errors introduced by the environment through decoherence and the Lamb-Stark shift.

In an experimental implementation there may also be other noise sources not considered here related to the measurement process itself, as well as systematic (hardware) errors in the quantum processor (qubits, couplers etc.). Nonetheless, our results indicate that a simple experimental implementation of the simulation scheme could be possible using existing hardware. For future implementations, there exist fault tolerant constructions for adiabatic quantum computing ${ }^{27,31-33,36}$.

## IV. CONCLUSION

The presented simulation scheme differs significantly from existing gate-model methods. Instead of a series of coherent gate operations, it uses an adiabatic control sequence which may require less complicated control hardware. At the measurement stage we require singlequbit gate operations and measurements, but only on the probe qubit. These operations should be relatively simple to implement compared to a full Trotter decomposition of the simulated Hamiltonian. Without error correction our method has limited scalability, but it might outper-
form gate-model simulators in some small-to-mediumsized problems. A simple experimental implementation could be feasible with present-day technology. In order to simulate a system of $n$ qubits with a two-local Hamiltonian described by the graph $G$, ideally our scheme requires one probe qubit for the readout and $n$ simulation qubits. Additionally, if Hamiltonian gadgets are used to implement three-local interactions, one ancilla qubit is required for each two-local term in the simulated observable (represented by an edge in the corresponding graph). In practice the number of ancillas may be slightly higher if more involved types of gadgets are used to implement the three-local interactions. The total number of qubits required thus scales as $O(n)$ for sparse graphs and $O\left(n^{2}\right)$ for maximally connected ones.

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## Appendix A: Supporting material

Here we provide supplementary information on the adiabatic quantum simulation method. In addition, we have created a MATLAB-based numerical simulation of a simple instance of the hybrid simulator subject to Markovian noise. The full source code of the simulation is available on request.

## 1. Gadgets

One possible way to effect the 3-local Hamiltonians we require in our construction is to approximate them with 2-local interactions.

## a. Perturbative gadget

This Gadget Hamiltonian construction was proposed in ${ }^{20}$ and has since been used and extended by others ${ }^{21,22}$. These papers contain further background details including notation.

We label the working qubits $1-3$. The effective 3-local interaction is well approximated on qubits 1,2 and 3 (within $\epsilon$ ) in a low energy subspace - constructed by adding a penalty Hamiltonian to an ancillary (mediator) qubit $m$. The mediator qubit $m$ doubles the size of the state space and the penalty Hamiltonian splits the Hilbert space into low and high energy subspaces, separated by an energy gap $\Delta$ (which is inversely proportional to a polynomial in $\epsilon$ - in our case reduced to $\Delta \geq \epsilon^{-3}$ ). The details of the gadget we develop for use in this work follow.

We will apply a Hamiltonian $H_{p}$ to the mediator qubit $m$ as well as a Hamiltonian $V$ to qubits $1-3$ and $m$. The Hamiltonian $H_{p}+V$ has a ground state that is $\epsilon$-close to the desired operator $J A_{1} \otimes A_{2} \otimes A_{3} \otimes|0\rangle\langle 0|$.

$$
\begin{gather*}
H_{p}:=\Delta|1\rangle\left\langle\left. 1\right|_{m}\right.  \tag{A1}\\
V(J, \Delta(\varepsilon)):=\mathbf{y}+\Delta^{1 / 3}|0\rangle\left\langle\left. 0\right|_{m}-\Delta^{1 / 3} A_{1} \otimes A_{2}+\frac{\Delta^{2 / 3}}{\sqrt{2}}\left(A_{2}-A_{1}\right) \otimes \sigma_{x}+J A_{3} \otimes\left(\mathbf{1}-\Delta^{2 / 3}|1\rangle\left\langle\left. 1\right|_{m}\right)\right.\right. \tag{A2}
\end{gather*}
$$

where $\mathbf{y}$ is some Hamiltonian already acting on qubits $1-3$ as well as a possible larger Hilbert space. Note the gadget above assumes $A_{i}^{2}=\mathbf{1}, \forall i=1,2,3$.

The so called self-energy expansion (A3) under appropriate conditions is known to provide a series approximation to the low-lying eigenspace of an operator. To verify that the Hamiltonian $H_{p}+V$ gives the desired approximation, one relies on expansion of the self energy to $4^{t h}$ order (here the higher order terms give rise to effective interactions greater than second order):

$$
\begin{equation*}
\Sigma_{-}(z)=\langle 0| V|0\rangle+\frac{\langle 0| V|1\rangle\langle 1| V|0\rangle}{z-\Delta}+\frac{\langle 0| V|1\rangle\langle 1| V|1\rangle\langle 1| V|0\rangle}{(z-\Delta)^{2}}+\mathcal{O}\left(\frac{\|V\|^{4}}{\Delta^{3}}\right) \tag{A3}
\end{equation*}
$$

where the operator is written in the $\{|0\rangle,|1\rangle\}$ basis of $m$. One considers the range $|z| \leq 2|J|+\epsilon$ and notes that $\left\|\Sigma_{-}(z)-J A_{1} \otimes A_{2} \otimes A_{3}\right\|=\mathcal{O}(\epsilon)$ and applies the Gadget Theorem ${ }^{20}$.

Before concluding this section, we note that care must be taken when adiabatically evolving gadgets. Reference ${ }^{37}$ contains a proof that the linear path Hamiltonian is universal for adiabatic quantum computation. Universality (and hence a non-exponentially contracting gap) remains when the locality of the construction is reduced using perturbative gadgets ${ }^{21}$.

## b. Exact diagonal gadget

Modern experimental implementations of adiabatic quantum computers typically are limited to only being able to couple spins with one type of coupling (e.g. $\sigma_{z} \otimes \sigma_{z}$ ). In such a case, the standard gadget Hamiltonian approach will not work as these gadgets require multiple types of couplers ${ }^{23}$. We will now provide a new type of gadget Hamiltonian which creates an effective, exact $\sigma_{z} \otimes \sigma_{z} \otimes \sigma_{z}$ interaction in the low energy subspace using just $\sigma_{z} \otimes \sigma_{z}$ and local terms.

Let us first assume that we have access to a penalty function $H_{\text {AND }}\left(x_{*}, x_{1}, x_{2}\right)$, where $x_{i} \in\{0,1\}$ such that $H_{\mathrm{AND}}=0$ any time $x_{*}=x_{1} x_{2}$ and is greater than some large constant $\Delta$ for all $x_{*} \neq x_{1} x_{2}$. By solving a system of constraints, such a penalty function is possible to write as a sum of two-local terms:

$$
\begin{equation*}
H_{\mathrm{AND}}\left(x_{*}, x_{1}, x_{2}\right)=\Delta\left(3 x_{*}+x_{1} x_{2}-2 x_{*} x_{1}-2 x_{*} x_{2}\right) \tag{A4}
\end{equation*}
$$

The Boolean variables $\left\{x_{i}\right\}$ can be represented on qubits using the correspondence $x_{i} \simeq \hat{x}_{i}=|1\rangle\left\langle\left. 1\right|_{i}\right.$. Furthermore, we have $\sigma^{z}=\mathbf{1}-2|1\rangle\langle 1|$ as usual. This gives us

$$
\begin{align*}
& H=\sigma_{1}^{z} \sigma_{2}^{z} \sigma_{3}^{z}=\mathbf{1}-2 \hat{x}_{1}-2 \hat{x}_{2}-2 \hat{x}_{3}+4 \hat{x}_{1} \hat{x}_{2}+4 \hat{x}_{1} \hat{x}_{3}+4 \hat{x}_{2} \hat{x}_{3}-8 \hat{x}_{1} \hat{x}_{2} \hat{x}_{3} \\
& \quad \hat{=} \mathbf{1}-2 \hat{x}_{1}-2 \hat{x}_{2}-2 \hat{x}_{3}+4 \hat{x}_{1} \hat{x}_{2}+4 \hat{x}_{1} \hat{x}_{3}+4 \hat{x}_{2} \hat{x}_{3}-8 \hat{x}_{*} \hat{x}_{3}+H_{\mathrm{AND}}\left(x_{*}, x_{1}, x_{2}\right) \tag{A5}
\end{align*}
$$

where (A5) holds in the low energy subspace after the introduction of an ancilla qubit $*$. By writing the Boolean operators in terms of Pauli matrices, we obtain
$H=\left(\frac{3}{4} \Delta-1\right) \mathbf{1}+\left(2-\frac{\Delta}{2}\right) \sigma_{*}^{z}+\left(\frac{\Delta}{4}-1\right)\left(\sigma_{1}^{z}+\sigma_{2}^{z}\right)+\sigma_{3}^{z}-\frac{\Delta}{2} \sigma_{*}^{z}\left(\sigma_{1}^{z}+\sigma_{2}^{z}\right)-2 \sigma_{*}^{z} \sigma_{3}^{z}+\left(\frac{\Delta}{4}+1\right) \sigma_{1}^{z} \sigma_{2}^{z}+\left(\sigma_{1}^{z}+\sigma_{2}^{z}\right) \sigma_{3}^{z}$.
We have hence provided a method which allows one to create diagonal k-local couplings using one- and two-local couplings. This method opens the door to simulate a wider range of Hamiltonians using current and next generation quantum computing technology. In addition, it should also prove useful in future investigations into the fault tolerance of the proposed protocol, in a way similar to the comparison in ${ }^{10}$.

## 2. Average Hamiltonian Method

An alternate method of generating the special Hamiltonians we require is to make use of the time average of a series of simpler generating Hamiltonians ${ }^{24}$. It has long been known that by regularly switching between a set of fixed Hamiltonians $\left\{H_{i}\right\}$, it is possible to approximate time evolution under any other Hamiltonian $H$, provided that $H$ is contained within the algebra generated by $\left\{H_{i}\right\}$. This fact lies at the heart of both average Hamiltonian theory and geometric control theory. Over the years many methods have been developed for making the approximations accurate to high order, however here we will focus only on approximations correct to first order.

In order to construct an average Hamiltonian we will make use of a first order approximation to the Baker-CampbellHausdorff formula:

$$
\begin{equation*}
\log \left(e^{A} e^{B}\right) \approx A+B+\frac{1}{2}[A, B] \tag{A6}
\end{equation*}
$$

From this we obtain formulae for approximating the exponential of both the sum and the Lie bracket of $A$ and $B$ to first order.

$$
\begin{align*}
& e^{A+B} \approx e^{A} e^{B}  \tag{A7}\\
& e^{[A, B]} \approx e^{A} e^{B} e^{-A} e^{-B} . \tag{A8}
\end{align*}
$$

These equations can be related to time evolution under some Hamiltonians, $H_{i}$, by replacing A and B with operators of the form $i H_{i} t / \hbar$. Clearly by applying these rules recursively, it is possible to generate any Hamiltonian in the Lie algebra generated by the initial set of static Hamiltonians. We note that the combination of any pairwise entangling Hamiltonian, such as an Ising Hamiltonian together with tunable local Z and X fields is sufficient to generate the full Lie algebra $\mathfrak{s u}\left(2^{N}\right)$ for an N qubit system, and so can be used to approximate an arbitrary Hamiltonian.

Although the time-varying Hamiltonian means that the system does not have a ground state in the normal sense, the average energy of the system is minimized when the system is within $O(t)$ of the ground state of the target average Hamiltonian. As a result of this, if the time scale for switching between Hamiltonians is small compared to the time scale for the adiabatic evolution of the system, the system will behave as if it was experiencing the average Hamiltonian.

## 3. Noise model

The noise model used in our MATLAB simulation consists of a separate bosonic heat bath coupled to each of the qubits. The baths have Ohmic spectral densities,

$$
\begin{equation*}
J(\omega)=\hbar^{2} \omega \Theta(\omega) \Theta\left(\omega_{c}-\omega\right) \tag{A9}
\end{equation*}
$$

where the cutoff $\omega_{c}$ was chosen to be above every transition frequency in the system, and are assumed to be uncorrelated. Each bath is coupled to its qubit through an interaction operator of the form

$$
\begin{equation*}
D=\lambda\left(\cos (\alpha) \sigma_{z}+\sin (\alpha) \sigma_{x}\right) \tag{A10}
\end{equation*}
$$

Using the Born-Markov approximation we obtain an evolution equation which is of the Lindblad form ${ }^{34}$. Denoting the level splitting of a qubit by $\hbar \Delta$, we obtain the following uncoupled single-qubit decoherence times:

$$
\begin{align*}
& T_{1}^{-1}=\lambda^{2} \sin ^{2}(\alpha) 2 \pi \Delta \operatorname{coth}(\beta \hbar \Delta / 2)  \tag{A11}\\
& T_{2}^{-1}=\frac{1}{2} T_{1}^{-1}+\lambda^{2} \cos ^{2}(\alpha) 4 \pi /(\hbar \beta) \tag{A12}
\end{align*}
$$

where $\beta=\frac{1}{k_{B} T}$. Given $T_{1}, T_{2}, T$ and $\Delta$, we can solve the bath coupling parameters $\lambda$ and $\alpha$ separately for each qubit, and then use the same noise model in the fully interacting case. The values used for the parameters are presented in Table The single-qubit decoherence times $T_{1}$ and $T_{2}$ were chosen to be compatible with recent coupled-qubit experiments with fully tunable couplings such as ${ }^{35}$. The bath temperature $T$ and the energy scale $\hbar \omega_{0}$ of $H_{T}$, the Hamiltonian to be simulated, were likewise chosen to match the temperatures and coupling strengths found in contemporary superconducting qubit experiments. To simulate manufacturing uncertainties, the actual values of the $T_{1}$ and $T_{\phi}$ parameters for the individual qubits were drawn from a Gaussian distribution with a small standard deviation.

TABLE I. Noise model parameters

| $T_{1}$ | $\sim N(1.0,0.1) \mu \mathrm{s}$ |
| :--- | ---: |
| $T_{\phi}$ | $\sim N(1.3,0.1) \mu \mathrm{s}$ |
| $T_{2}^{-1}$ | $=\frac{1}{2} T_{1}^{-1}+T_{\phi}^{-1}$ |
| $T$ | 20 mK |
| $\omega_{c}$ | $20 \omega_{0}$ |
| $\omega_{0}$ | $2 \pi \cdot 25 \mathrm{MHz}$ |

## 4. Measurement

The pre-measurement system Hamiltonian is

$$
\begin{equation*}
H_{1}=H_{S, T} \otimes \mathbb{1}+\mathbb{1} \otimes H_{P} . \tag{A13}
\end{equation*}
$$

The operators $H_{S}$ and $H_{P}$ can be expanded in terms of their eigenvalues and eigenstates using the (possibly degenerate) spectral decomposition

$$
\begin{equation*}
H_{S}=\sum_{k j} s_{k}\left|s_{k, j}\right\rangle\left\langle s_{k, j}\right|, \quad s_{0}<s_{1}<\ldots \tag{A14}
\end{equation*}
$$

and correspondingly for $H_{P}$.
Let the states of systems $S$ and $P$ begin in their ground state subspaces, the full normalized state $|\mathrm{g}\rangle$ of the simulator belonging to the ground state subspace of the non-interacting Hamiltonian $H_{1}$ :

$$
\begin{equation*}
|\mathrm{g}\rangle \in \operatorname{span}\left\{\left|s_{0, k}\right\rangle \otimes\left|p_{0, l}\right\rangle\right\}_{k, l} . \tag{A15}
\end{equation*}
$$

$S$ and $P$ are brought adiabatically into interaction with each other. The Hamiltonian becomes

$$
\begin{equation*}
H_{2}=H_{1}+\underbrace{A \otimes\left(\mathbb{1}_{P}-\Pi_{p_{0}}\right)}_{H_{S P}} \tag{A16}
\end{equation*}
$$

where the operator $A$ corresponds to an observable of the simulated system that commutes with $H_{S}$, and

$$
\begin{equation*}
\Pi_{p_{0}}=\sum_{m}\left|p_{0, m}\right\rangle\left\langle p_{0, m}\right| \tag{A17}
\end{equation*}
$$

is the projector to the ground state subspace of $H_{P}$. Because $A$ and $H_{S}$ commute, they have shared eigenstates:

$$
\begin{align*}
H_{S}\left|s_{k, j}\right\rangle & =s_{k}\left|s_{k, j}\right\rangle  \tag{A18}\\
A\left|s_{k, j}\right\rangle & =a_{k, j}\left|s_{k, j}\right\rangle \tag{A19}
\end{align*}
$$

a. Ground state lemma

We will now show that Hamiltonians $H_{1}$ and $H_{2}$ have the same ground state subspace given that $a_{\text {min }}+p_{1}-p_{0}>0$ where $a_{\text {min }}$ is $A$ 's lowest eigenvalue.

Lemma 1. Let $H_{1}$ and $H_{2}$ be the finite dimensional Hamiltonians defined previously in (A13) and (A16), and $a_{\text {min }}+$ $p_{1}-p_{0}>0$. Now, iff $H_{1}|\star\rangle=\lambda|\star\rangle$, where $\lambda$ is the smallest eigenvalue of $H_{1}$, then $H_{2}|\star\rangle=\kappa|\star\rangle$, where $\kappa$ is the smallest eigenvalue of $\mathrm{H}_{2}$.

Proof. Firstly, we have

$$
\begin{aligned}
\langle g| H_{1}|g\rangle & =s_{0}+p_{0} \\
\langle g| H_{S P}|g\rangle & =0
\end{aligned}
$$

Now, expanding an arbitrary normalized state $|\phi\rangle$ in the eigenbases of $H_{S}$ and $H_{P}$,

$$
|\phi\rangle=\sum_{x y i j} c_{x y i j}\left|s_{x, i}\right\rangle\left|p_{y, j}\right\rangle,
$$

we get

$$
\begin{aligned}
\langle\phi| H_{1}|\phi\rangle & =\sum_{x y i j}\left|c_{x y i j}\right|^{2}\left(s_{x}+p_{y}\right) \\
& \geq \sum_{x y i j}\left|c_{x y i j}\right|^{2}\left(s_{0}+p_{0}\right)=s_{0}+p_{0}, \\
\langle\phi| H_{S P}|\phi\rangle & =\langle\phi| \sum_{x y i j} c_{x y i j} A\left|s_{x, i}\right\rangle\left(\mathbb{1}_{P}-\Pi_{p_{0}}\right)\left|p_{y, j}\right\rangle \\
& =\langle\phi| \sum_{x i j} \sum_{y \geq 1} c_{x y i j} a_{x, i}\left|s_{x, i}\right\rangle\left|p_{y, j}\right\rangle \\
& =\sum_{x i j} \sum_{y \geq 1}\left|c_{x y i j}\right|^{2} a_{x, i} \\
& \geq a_{\min } \sum_{x i j} \sum_{y \geq 1}\left|c_{x y i j}\right|^{2} \geq 0 \quad \text { if } \quad a_{\min } \geq 0 .
\end{aligned}
$$

Hence, if $A$ 's lowest eigenvalue $a_{\min } \geq 0$ then $|g\rangle$ is the ground state of $H_{2}=H_{1}+H_{S P}$ as well. If $A$ is not nonnegative, we can perform the transformation

$$
\begin{aligned}
H_{S}^{\prime} & =H_{S}+a_{\min } \mathbf{1} \\
H_{P}^{\prime} & =H_{P}-a_{\min } \Pi_{p_{0}} \\
A^{\prime} & =A-a_{\min } \mathbf{1}
\end{aligned}
$$

This leaves $H_{2}$ invariant, but makes $A^{\prime}$ nonnegative. As long as $a_{\text {min }}+p_{1}-p_{0}>0$ then $\left\{\left|p_{0, m}\right\rangle\right\}_{m}$ still span the ground state subspace of $H_{P}^{\prime}$ and the above analysis remains valid.

## b. Ground state degeneracy and excitations

If the ground state subspace of $H_{S, T}$ is degenerate and overlaps more than one eigenspace of $A$, or the simulation register $S$ has excitations to higher energy states at the beginning of the measurement phase, we need a more involved analysis of the measurement procedure. Assume the pre-measurement-phase state of the simulator is given by

$$
\rho_{0}=\left(\sum_{k l m n} c_{k l m n}\left|s_{k, l}\right\rangle\left\langle s_{m, n}\right|\right) \otimes\left(\begin{array}{cc}
a & 0  \tag{A20}\\
0 & 1-a
\end{array}\right) .
$$

All three terms in $H_{2}$ commute given that $\left[H_{S}, A\right]=0$. Hence

$$
\begin{align*}
e^{q H_{2}} & =\left(e^{q H_{S}} \otimes \mathbb{1}_{P}\right)\left(\mathbb{1}_{S} \otimes e^{q H_{P}}\right)\left(e^{q H_{S P}}\right) \\
& =\left(e^{q H_{S}} \otimes e^{q H_{P}}\right)\left(e^{q A} \otimes\left(\mathbb{1}_{P}-\Pi_{p_{0}}\right)+\mathbb{1}_{S} \otimes \Pi_{p_{0}}\right) \tag{A21}
\end{align*}
$$

As a result of the measurement procedure right before the actual measurement the state is given by

$$
\begin{align*}
\rho_{1}(t) & =\mathbb{H}_{P} e^{-i t H_{2} / \hbar} \mathbb{H}_{P} \rho_{0} \mathbb{H}_{P} e^{i t H_{2} / \hbar} \mathbb{H}_{P} \\
& =\mathbb{H}_{P} e^{-i t H_{S P} / \hbar}\left(\sum_{k l m n} c_{k l m n} e^{-i t\left(s_{k}-s_{m}\right) / \hbar}\left|s_{k, l}\right\rangle\left\langle s_{m, n}\right|\right) \otimes \frac{1}{2}\left(\begin{array}{cc}
1 & e^{i t \delta / \hbar}(2 a-1) \\
e^{-i t \delta / \hbar}(2 a-1) & 1
\end{array}\right) e^{i t H_{S P} / \hbar} \mathbb{H}_{P} \\
& =\sum_{k l m n}\left(c_{k l m n} e^{-i t\left(s_{k}-s_{m}\right) / \hbar}\left|s_{k, l}\right\rangle\left\langle s_{m, n}\right|\right) \otimes \frac{1}{2} \mathbb{H}_{P}\left(\begin{array}{cc}
1 & e^{i t \omega_{m, n}}(2 a-1) \\
e^{-i t \omega_{k, l}}(2 a-1) & \left.e^{-i t\left(a_{k, l}-a_{m, n}\right) / \hbar}\right)
\end{array}\right) \mathbb{H}_{P}, \tag{A22}
\end{align*}
$$

where $\omega_{k, l}=\left(a_{k, l}+\delta\right) / \hbar$ and $\mathbb{H}_{P}$ is the Hadamard gate operating on the probe. Projecting the probe to the ground state subspace, we get $\Pi_{p_{0}} \rho_{1}(t) \Pi_{p_{0}}=$

$$
\begin{equation*}
=\sum_{k l m n}\left(c_{k l m n} e^{-i t\left(s_{k}-s_{m}\right) / \hbar}\left|s_{k, l}\right\rangle\left\langle s_{m, n}\right|\right) \otimes \frac{1}{4}\left(1+e^{-i t\left(a_{k, l}-a_{m, n}\right) / \hbar}+2 \cos \left(\omega_{m, n} t\right)(2 a-1)\right)|0\rangle\langle 0| \tag{A23}
\end{equation*}
$$

Thus the probability of finding the probe in the ground state subspace is given by a superposition of harmonic modes:

$$
\begin{equation*}
P_{0}(t)=\operatorname{Tr}\left(\Pi_{p_{0}} \rho_{1}(t) \Pi_{p_{0}}\right)=\frac{1}{2}\left(1+\sum_{k l} c_{k l k l} \cos \left(\omega_{k, l} t\right)(2 a-1)\right) \tag{A24}
\end{equation*}
$$

[^0]
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    1 F. Verstraete, V. Murg, and J. I. Cirac, Advances in Physics 57, 143 (2008)
    ${ }^{2}$ R. G. Parr and W. Yang, Density-Functional Theory of Atoms and Molecules (Oxford University Press, 1989).
    ${ }^{3}$ W. A. Lester Jr., L. Mitas, and B. Hammond, Chem. Phys. Lett. 478, 1 (2009)
    ${ }_{5}^{4}$ R. Feynman, Int. J. Theor. Phys. 21, 467 (1982)
    ${ }^{5}$ S. Lloyd, Science 273, 1073 (1996)
    ${ }^{6}$ D. A. Lidar and H. Wang, Phys. Rev. E 59, 2429 (1999)
    ${ }^{7}$ R. Somma, G. Ortiz, J. E. Gubernatis, E. Knill, and R. Laflamme, Phys. Rev. A 65, 042323 (2002)
    ${ }^{8}$ C. Negrevergne, R. Somma, G. Ortiz, E. Knill, and R. Laflamme, Phys. Rev. A 71, 032344 (2005).
    9 A. Aspuru-Guzik, A. D. Dutoi, P. Love, and M. Head-Gordon, Science 309, 1704 (2005)
    ${ }^{10}$ K. R. Brown, R. J. Clark, and I. L. Chuang, Phys. Rev. Lett. 97, 050504 (2006)
    ${ }^{11}$ B. P. Lanyon, J. D. Whitfield, G. G. Gillet, M. E. Goggin, M. P. Almeida, I. Kassal, J. D. Biamonte, M. Mohseni, B. J. Powell, M. Barbieri, A. Aspuru-Guzik, and A. G. White, Nature Chemistry 2, 106 (2009)

    12 J. D. Whitfield, J. Biamonte, and A. Aspuru-Guzik, Molecular Physics 109, 735 (2010) arXiv:1001.3855
    ${ }_{13}$ X.-s. Ma, B. Dakic, W. Naylor, A. Zeilinger, and P. Walther, Nature Physics 7, 399 (2011) arXiv:1008.4116v1 [quant-ph]
    ${ }^{14}$ G. K.-L. Chan and M. Head-Gordon, J. Chem. Phys. 118, 8551 (2003)
    ${ }^{15}$ C. R. Clark, T. S. Metodi, S. D. Gasster, and K. R. Brown, Phys. Rev. A 79, 062314 (2009)
    16 A. Friedenauer, H. Schmitz, J. T. Glueckert, D. Porras, and T. Schaetz, Nature Physics 4, 757 (2008)
    ${ }_{17}^{17}$ R. Gerritsma, G. Kirchmair, F. Zähringer, E. Solano, R. Blatt, and C. F. Roos, Nature 463, 68 (2009) arXiv:0909.0674
    18 A. M. Childs, E. Farhi, and J. Preskill, Phys. Rev. A 65, 012322 (2001)
    ${ }^{19}$ M. H. S. Amin, P. J. Love, and C. J. S. Truncik, Phys. Rev. Lett. 100, 060503 (2008)
    ${ }^{20}$ J. Kempe, A. Kitaev, and O. Regev, SIAM J. Comput. 35, 1070 (2006)
    ${ }^{21}$ R. Oliveira and B. M. Terhal, Quant. Inf. Comp. 8, 0900 (2008), arXiv:quant-ph/0504050v6.
    22 J. D. Biamonte and P. J. Love, Phys. Rev. A 78, 012352 (2008)
    23 J. D. Biamonte, Phys. Rev. A 77, 052331 (2008)
    24 J. Waugh, L. Huber, and U. Haeberlen, Phys. Rev. Lett. 20, 180 (1968)
    ${ }^{25}$ S. Bravyi, D. P. DiVincenzo, D. Loss, and B. M. Terhal, Phys. Rev. Lett. 101, 070503 (2008)
    ${ }^{26}$ E. Farhi, J. Goldstone, S. Gutmann, and M. Sipser, Quantum Computation by Adiabatic Evolution, Report MIT-CTP-2936 (MIT, 2000) arXiv:quant-ph/0001106
    ${ }^{27}$ D. Bacon and S. T. Flammia, Phys. Rev. Lett. 103, 120504 (2009).
    ${ }^{28}$ I. Siddiqi, R. Vijay, F. Pierre, C. M. Wilson, L. Frunzio, M. Metcalfe, C. Rigetti, R. J. Schoelkopf, M. H. Devoret, D. Vion, and D. Esteve, Phys. Rev. Lett. 94, 027005 (2005)
    ${ }^{29}$ N. Ramsey, Molecular Beams (Oxford University Press, 1963).
    ${ }^{30}$ A. Kitaev, "Quantum measurements and the Abelian stabilizer problem," (1995), arXiv:quant-ph/9511026
    ${ }^{31}$ S. P. Jordan, E. Farhi, and P. W. Shor, Phys. Rev. A 74, 052322 (2006)
    ${ }^{32}$ D. A. Lidar, Phys. Rev. Lett. 100, 160506 (2008)
    ${ }^{33}$ M. H. S. Amin, D. V. Averin, and J. A. Nesteroff, Phys. Rev. A 79, 022107 (2009)
    ${ }_{35}^{34}$ H.-P. Breuer and F. Petruccione, The theory of open quantum systems (Oxford University Press, 2002).
    ${ }^{35}$ A. O. Niskanen, K. Harrabi, F. Yoshihara, Y. Nakamura, S. Lloyd, and J. S. Tsai, Science 316, 723 (2007).
    ${ }^{36}$ I. J. Crosson, D. Bacon, and K. R. Brown, Phys. Rev. E 82, 031106 (2010) arXiv: 1006.4388 [cond-mat.stat-mech]
    ${ }^{37}$ D. Aharonov, W. van Dam, J. Kempe, Z. Landau, S. Lloyd, and O. Regev, SIAM J. Computing 37, 166 (2007)

