Effects of Noise, Correlations and errors in the preparation of initial states in Quantum Simulations

Nayeli Zuniga-Hansen, Yu-Chieh Chi, Mark S. Byrd
Physics Department and Computer Science Department, Southern Illinois University, Carbondale, Illinois 62901-4401

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In principle a quantum system could be used to simulate another quantum system. The purpose of such a simulation would be to obtain information about problems which cannot be simulated with a classical computer due to the exponential increase of the Hilbert space with the size of the system and which cannot be measured or controlled in an actual experiment. The system will interact with the surrounding environment, with the other particles in the system and be implemented using imperfect controls making it subject to noise. It has been suggested that noise does not need to be controlled to the same extent as it must be for general quantum computing. However the effects of noise in quantum simulations and how to treat them are not completely understood. In this paper we study an existing quantum algorithm for the one-dimensional Fano-Anderson model to be simulated using a liquid-state NMR device. We calculate the evolution of different initial states in the original model, and then we add interacting spins to simulate a more realistic situation. We find that states which are entangled with their environment, and sometimes correlated but not necessarily entangled have an evolution which is described by maps which are not completely positive. We discuss the conditions for this to occur and also the implications.

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I. INTRODUCTION

Simulating quantum systems with quantum systems is one of the primary reasons there is a great deal of interest in building a quantum computing device. The difficulty of simulating quantum systems on a classical computer, mainly due to the exponential increase of the Hilbert space with system size, was Richard P. Feynman’s motivation for proposing the idea that a quantum system might perform this task much more efficiently [1]. Lloyd showed later that some quantum systems could be manipulated to represent the evolution of other quantum systems using only local interactions [2].

There are many problems of interest in quantum mechanics which have no known analytical solution. Thus for a wide range of physical systems simulation is a valuable tool for solving quantum mechanical problems. Classical simulation of such systems can quickly become intractable as the number of particles increases. The resources that are required to perform such a task increase exponentially with the size of the system. For example, in order to represent the state of \( N \) 2-state particles a \( 2^N \) vector is required and for its evolution the unitary will be a \( 2^N \times 2^N \) matrix [2,3]. However, only \( N \) particles would be necessary to simulate such a system [2,4]. In this sense, a quantum simulator is conjectured to provide exponential speedup over classical simulation [5]. But that is not the only advantage; other problems such as the sign problem from Quantum Monte Carlo algorithms for fermionic systems, or the exchange-correlation functionals in Density Functional Theory [6,7] will not be present in a quantum simulation. Therefore, many difficult problems in particle physics, condensed matter systems, and chemistry, among others, could be tackled [5,6,8,20].

Quantum simulations have received a great deal of recent attention since they are feasible without the need for a universal quantum computing device. The question of the universality of Hamiltonians has been addressed to a great extent [21–30] and algorithms have been developed to simulate specific systems [1,6,12,19,31–40]. In addition, experiments have been designed and implemented [16,41–47]. However, a great deal of work remains to be done. Currently available quantum simulating devices have relatively few controllable particles. They are, after all, quantum systems that inevitably interact with the surrounding environment and therefore are subject to noise. Just as with quantum computing, this is an important issue when it comes to scalability. It is therefore necessary to study how the interactions affect a quantum simulation.

The purpose of the present work is to study effects of noise in an existing algorithm proposed for a quantum simulation and to take away from this example as much general understanding as we can. The primary noise considered is prior unknown correlations or entanglement within the system and between the simulated system and the environment. We study the evolution of different initial states, including ideal ones and states in which errors are present due to mistakes in preparation and/or interactions with particles in the system and find the dynamical maps that represent the evolution. The algorithm we explore was proposed and developed by Ortiz et al. [6] to simulate the one-dimensional Fano-Anderson model. To examine various behaviors of the system with initial correlations, we first provide a background for the
quantum simulation in Section I A which focuses on the
different sources of noise that can affect the experiments.
Section I B provides a brief review of open system quan-
tum dynamics, and discusses dynamical maps and their
main characteristics, including requirements for positiv-
ity and complete positivity; the purpose is to use dy-
amical maps to describe general errors in simulations.
Section II contains a brief explanation of the algorithm
used, including the modifications we made to represent
noise in the system. Finally, our results, given in Section
IV are divided in two parts: those states for which the
Bloch vector only has a component along the \( z \) direc-
tion, and those which have some small component along
\( x \) and a main one along \( z \). We will also discuss why this is
important. These two last subsections are subsequently
divided into simulations performed with no external noise
and simulations with noise. For the purpose of compar-
ison, the parameters of the system were obtained from
Ref. [6] and were used for all the considered scenarios.

A. Quantum simulations

There are two classifications of quantum simulators. The
Universal Quantum Simulator (UQS) [48] (also re-
ferred to as Digital [49]), is a quantum computer repres-
ented by the standard circuit model with the set of uni-
versal gates that act on a collection of two-state systems
[22, 50, 51]. The term universal implies that the quantum
computer would be able to simulate any arbitrary quan-
tum system [52] which implies universal quantum comput-
ation is possible. However, a fully functioning quantum
computer has not been built yet. So researchers have
designed and implemented devices consisting of smaller
and controllable quantum systems specifically intended
for simulations. This is the other type of quantum sim-
ulators, referred to as Specialized Quantum Simulators
(SQS) [48, 55] or analogue quantum simulators [49, 50] since
they are not able to be used to simulate any quan-
tum device or computation. Rather, they are able to sim-
ulate a smaller, but interesting class of physical systems.
Examples of such systems include: ultracold atoms, ion
traps, quantum dots, atoms in optical lattices, coupled
cavities, photons, electrons floating on He films and NMR
devices [4, 10, 18, 19, 32, 12, 13, 17, 39, 53, 54]. In the
SQS, universality for all quantum systems is not required,
thus many interesting advances and simple simulations
have already been performed [16, 18, 38, 41, 42, 44–
46, 54, 67, 59].

Just as is the case with any other quantum system,
unwanted interactions with an environment can have a
detrimental effect on the outcome. Error correction
and/or prevention is usually required for accurate imple-
mentation. However, inaccurate unitary transformations
are also a source of noise and the evolution of the sys-
tem under a specific Hamiltonian is the main problem of
interest [3, 69].

All steps, preparation, evolution and measurement,
state of the system, which could provide useful information about the effects of noise and interactions in quantum simulations. Furthermore, there are many sets of operators in the operator-sum decomposition which give rise to the same map. This is true of completely positive maps \([93, 94]\) as well as maps which are not completely positive \([95]\).

**B. Noise in Quantum Systems, Completely and Non Completely Positive Maps**

The density matrix, or density operator, represents our knowledge of the quantum state of a system. In general any density operator must satisfy the following conditions in order to represent a physical state \([96]\):

\[
    \rho = \rho^\dagger, \text{ it is Hermitian,} \tag{1}
\]

\[\rho \geq 0, \text{ it is positive semi-definite,} \tag{2}\]

\[\text{Tr}(\rho) = 1, \text{ it has trace } 1, \tag{3}\]

The evolution of a closed system is described by a unitary transformation, as

\[
    \psi(t) = U\psi(0),
\]

where \(U = \exp iHt\). It follows that

\[
    \rho(t) = U\rho(0)U^\dagger.
\]

The density operator is often written as an expansion of pure states

\[
    \rho = \sum_j p_j \ket{j}\bra{j},
\]

where the \(p_j\) are the probabilities associated to each of the states \(\ket{j}\). If one of the probabilities is equal to 1 and the rest are 0, then the state is pure. For two-state systems we can write the density operator in terms of the 2 \(\times\) 2 unit matrix and the Pauli operators,

\[
    \rho = \frac{1}{2} (I + \vec{a} \cdot \vec{\sigma}),
\]

where the coefficients \(a_i\) are the projections along the \(x\), \(y\) and \(z\) directions of the so-called Bloch vector. This provides a representation of the quantum state in the well-known Bloch sphere, which is a geometric representation of the states of a qubits in terms of a sphere with radius 1. (For higher dimensional systems, this is referred to as the polarization vector, coherence vector, or generalized block vector. See \([97, 103]\) and references therein.) The magnitude of the Bloch vector is constrained by the condition \(\sqrt{a_x^2 + a_y^2 + a_z^2} \leq 1\), and \(|\vec{a}| = 1\) represents a pure state. Thus any state on the surface of the Bloch sphere is a pure state. A mixed state is represented by a vector with \(|\vec{a}| < 1\). With this notation it is possible to have a visual representation of the quantum states at different times.

A system \(S\) that is coupled to an environment \(E\) with Hilbert spaces \(\mathcal{H}_S\) and \(\mathcal{H}_E\), respectively, can be considered a larger isolated system whose initial state is described by \(\rho_{SE}(0)\). The time evolution of this system is then given by the joint evolution of the system and environment \([92]\):

\[
    \rho_{SE}(t) = U\rho_{SE}(0)U^\dagger.
\]

We are often only interested in the evolution of the system, \(S\). Tracing out the environmental degrees of freedom provides us with the reduced dynamics of the system

\[
    \rho_S(t) = \text{Tr}_E[\rho_{SE}(t)] = \text{Tr}_E [U_{SE}(t)\rho_{SE}(0)U_{SE}^\dagger].
\]

With the reduced dynamics of \(S\), we can find the map that transforms the initial state \(\rho(0)\), into the final state \(\rho(t)\). To obtain the “dynamical map” it is convenient to write the \(N \times N\) density operator \(\rho\) as a \(N^2 \times 1\) column vector that is transformed into another \(N^2 \times 1\) column vector through the \(N^2 \times N^2\) supermatrix \(A\):

\[
    \rho_{s,s'}(t) = A_{s,s',rs}\rho_{rs}(0), \tag{4}
\]

where \(A\) describes the most general evolution of \(\rho\) \([104]\). In matrix notation

\[
    \rho' = A\rho. \tag{5}
\]

Because \(\rho\) must be mapped to another positive \(\rho'\) the following conditions are imposed on \(A\) \([96]\):

\[
    A_{r,s',rs} = (A_{s',sr,r})^*, \text{ is Hermitian,} \tag{6}
\]

\[
    \sum_{r,sr,s'} x^s_r x_{sr} A_{rs,r's'} y^s_{r'} y_{s'} \geq 0, \text{ } A \text{ is positive,} \tag{7}
\]

\[
    \sum_r A_{rr',rs'} = \delta_{r',r}, \text{ } A \text{ is Trace Preserving.} \tag{8}
\]

These conditions ensure the conditions Eqs. \([1]-[3]\) on the density operator are satisfied.

By interchanging indices of \(A\), we obtain another \(N^2 \times N^2\) supermatrix \(B\) \([96]\):

\[
    B_{rr',ss'} = A_{rs,r's'}. \tag{9}
\]

The \(1 \times N^2\) rows of \(A\) become the \(N \times N\) block matrices of \(B\). The following conditions are imposed on \(B\) so that it represents a physical map:

\[
    B_{rr',ss'} = (B_{r',sr,s})^*, \text{ } B \text{ is Hermitian.} \tag{10}
\]
\[ \sum_{r \neq s, s', s''} x'_r y_r B_{r r', s s'} x_s y'_s \geq 0, \quad B \text{ is positive semi-definite,} \]
\[ \sum_{r} B_{r r', r s} = \delta_{r s}, \quad B \text{ is trace preserving.} \tag{12} \]

From these we may write
\[ \rho(t) = B [\rho(0)]. \tag{13} \]

If \( B \) is decomposed into its eigenvectors and eigenvalues, the action of the map can be represented as follows
\[ B [\rho(0)] = \sum_{\alpha} \lambda_{\alpha} \rho(0) \zeta_{\alpha}, \]
where \( \lambda_{\alpha} \in \mathbb{R} \) are the eigenvalues. The hermiticity of \( \rho' \) is guaranteed by the restriction given in Eq. \( [10] \) [107], so that \( B \) must be Hermitian. The matrix \( A \) is required to transform \( \rho(0) \) into another Hermitian state \( \rho(t) \), but \( A \) is not necessarily Hermitian itself. The complete positivity of the map implies that the final state will be positive. The eigenvalues of \( B \) must all be positive for it to be guaranteed to be a completely positive map. If \( B \) has a negative eigenvalue but still transforms any positive \( \rho(0) \) into a positive \( \rho(t) \), then \( B \) is a positive but not necessarily completely positive map.

Non-completely positive maps have been measured using quantum process tomography (QPT) [105, 106] which has caused the specifics of QPT to be questioned [107]. But the possibility that a map which is not a completely positive map can transform a valid quantum state into another valid state has brought a great deal of interest in studying the conditions for complete positivity. This is in addition to the interest in it due to the partial transpose as an indicator of entanglement [108, 109].

In 1994, Pechukas showed that complete positivity constrains a system to product states of the form \( \rho_{SE} = \rho_S \otimes \rho_E \), where \( \rho_E \) is a fixed state of the bath [91, 110] which excludes correlations and does not represent many physical situations. Alicki in Ref. [111] argued that there is no general definition for the reduced quantum dynamics beyond the weak coupling regime, therefore, when the system is in an initially correlated state with the environment, linear assignment maps have no unique definition [107], and linearity would only be preserved for states that are invariant under the transformation [111]. Pechukas replied in Ref. [110], and agreed that open system reduced dynamics can be non-linear. However, Rodriguez-Rosario et al. examine the assignment maps in [107] and argue against giving up linearity by noting that the assignment maps can be linear if the conditions of consistency or positivity are relaxed, and favor relaxing the positivity condition. A quantum system that interacts with the environment before our prescribed \( t = 0 \) can be described by completely positive dynamics if the environment does not re-act on the system [104], i.e. the coupling is weak and/or the initial state is in a particular form [91].

As mentioned above, when the map is completely positive the eigenvalues of \( B \) in Eq. \( [13] \) can be taken to all be positive. When they are, Eq. \( [13] \) can be rewritten as
\[ \rho(t) = B [\rho(0)] = \sum_{\alpha} \lambda_{\alpha} \rho(0) \zeta_{\alpha} = \sum_{\alpha} C_{\alpha} \rho(0) C^\dagger_{\alpha}, \tag{14} \]
where \( C_{\alpha} = \sqrt{\lambda_{\alpha}} \zeta_{\alpha} \). Eq. \( [14] \) is sometimes known as the Kraus representation or operator-sum decomposition [112], although it was originally discussed in this context by Sudarshan, Mathews, and Rau [93]. Jordan, et al. demonstrated that entanglement in the initial state of the system can lead to non-completely positive maps that still transform a positive \( \rho \) into another positive \( \rho \) [113]. Rodriguez-Rosario, et al. found that for purely classical correlations, the “quantum discord” (defined below) vanishes, and this is a sufficient condition for completely positive reduced dynamics [114]. Later, Shabani and Lidar demonstrated that the quantum discord was also a necessary condition for complete positivity [115]. Quantum discord was introduced by Ollivier and Zurek in 2001, it is defined as a ‘measure of the quantumness of the correlations’ [116], and is calculated as follows:
\[ \delta(S : E) = - \text{Tr} (\rho_E \log(\rho_E)) + \text{Tr} (\rho_{SE} \log(\rho_{SE})) - \sum_j \text{Tr}(\Pi^E_j \rho_{SE} \Pi^E_j \rho_{SE}) \frac{\Pi^E_j \rho_{SE} H^E_j \rho_{SE} \Pi^E_j \rho_{SE}}{\text{Tr}(\Pi^E_j \rho_{SE})}, \tag{15} \]
where \( H(x) = H(\rho_x) = - \text{Tr}(\rho_x \log(\rho_x)) \) is the Von Neumann entropy and \( - \sum_j \text{Tr}(\Pi^E_j \rho_{SE}) \frac{\Pi^E_j \rho_{SE} H^E_j \rho_{SE} \Pi^E_j \rho_{SE}}{\text{Tr}(\Pi^E_j \rho_{SE})} \) is the conditional entropy, defined as the entropy of the system with respect to a set of projective measurements performed on the environment. Quantum discord provides a measure of the nature of correlations, it vanishes for classical correlations and is maximum when there is entanglement.

**II. BACKGROUND**

As mentioned before, the extent to which the noise from the environment can be included in a quantum simulation is dependent on both the simulating and simulated systems. Of course it would useful to have some previous knowledge of the system-bath interactions. However, this is often not the case. Here we study effects of unwanted noise in a quantum simulation using an algorithm [6] that simulates the one dimensional Fano-Anderson model. In this case we have a realistic model of the interaction and use the dynamical maps of the system to describe the noisy evolution. Starting with different initial states of the system and bath, we reduce the dynamics to a two-particle model system. The algorithm requires the two particles to be initialized in a particular state. Due to interactions with external qubits in the simulating device, these initial conditions may be imperfect. In addition, if the particles are allowed to interact for some small period of time before the beginning of the
actual algorithm, the particles could begin in a correlated or entangled state. We consider the possibility of errors in the preparation of one of the particles in the system as well as the possibility of correlations between particles. We added a visualization of the evolution of the Bloch vector in order to provide an intuitive picture of the differences in the initial states and how they evolve. It is useful to note that, regardless of the non-complete positivity of some of the maps obtained, the final state is a physical state and the system is a realistic physical model with realistic couplings. The significance of these results will be discussed in the conclusions. We now describe our methods and results.

A. Quantum Algorithm

Ortiz, et al. proposed an algorithm for the quantum simulation of the one-dimensional Fano-Anderson model [13]. This model consists of an impurity described by an energy $\epsilon$ surrounded by a ring of $n$ spinless fermions having energies $\epsilon_k$. The fermions interact with the impurity, which is also a spinless fermion, through a hopping potential $V$ [6] [15]. The spinless fermion Hamiltonian is given by [6] [15]

$$H = \sum_{i=0}^{n} \epsilon_k c_i^\dagger c_i + \epsilon b^\dagger b + V \sum_{i=0}^{n-1} (c_{i+1}^\dagger b + b^\dagger c_i) \delta_{k,0}. \quad (16)$$

The system is mapped via Jordan-Wigner transformation to the spin system to obtain [6]

$$\tilde{H} = \frac{\epsilon}{2} \sigma_z^1 + \frac{\epsilon_{k,0}}{2} \sigma_z^2 + \frac{V}{2} (\sigma_x^1 \sigma_x^2 + \sigma_y^1 \sigma_y^2). \quad (17)$$

Ortiz, et al. consider an NMR device for their simulation as do we, but the model is certainly not limited to this type of device. The simulator has an NMR drift Hamiltonian of the form [6]

$$H_d(t) = \frac{1}{2} \left[ \frac{(\epsilon + \epsilon_{k,0})}{2} - \sqrt{\left( \frac{\epsilon - \epsilon_{k,0}}{2} \right)^2 + V^2} \right] \sigma_z^1 + \frac{1}{2} \left[ \frac{(\epsilon + \epsilon_{k,0})}{2} + \sqrt{\left( \frac{\epsilon - \epsilon_{k,0}}{2} \right)^2 + V^2} \right] \sigma_z^2. \quad (18)$$

The control Hamiltonian for spins in the system is

$$H_c(t) = \sum_{i,j} \alpha_{x,i,j} \sigma_z^i + \sum_{i,j} \alpha_{y,i,j} \sigma_z^i, \quad (19)$$

where the $\alpha$ are controllable. The last term is considered controllable because it can be turned on/off with the $x$ and $y$ rotations.

To obtain the representation of the Hamiltonian in Eq. (17), the following control sequence can be applied to Eq. (18) [6]

$$U = e^{i \frac{\epsilon}{2} \sigma_z^2} e^{-i \frac{\epsilon}{2} \sigma_y^1 e^{-i \frac{\epsilon_{k,0}}{2} \sigma_z^1 e^{i \frac{\epsilon}{2} \sigma_z^1} e^{i \frac{\epsilon}{2} \sigma_z^1}} e^{-i \frac{\epsilon_{k,0}}{2} \sigma_z^1 e^{i \frac{\epsilon}{2} \sigma_z^1} e^{i \frac{\epsilon}{2} \sigma_z^1}}. \quad (20)$$

The goal is to see if the initial state of the impurity has changed over time and, if so, how much. For this purpose, we use the time correlation function $C(t) = b(t)b(0)$, which in spin operator representation becomes $C(t) = e^{i \theta t} \sigma_z^1 e^{-i \theta t} \sigma_z^1$, where $\sigma_{+} = \sigma_x + i \sigma_y$ and $\sigma_{-} = \sigma_x - i \sigma_y$. The time correlation function provides information about the overlap of the initial and final states of the impurity.

We use the same form of the Hamiltonian in Eq. (17) to perform the unitary evolution on different initial states of the system and perform the same operation regardless of prior interactions. We then obtain the reduced dynamics of the state of the impurity site (qbit 1) and then obtain the dynamical map that describes the evolution. We also calculate the time correlation function for the purpose of comparing the results of the different situations to those of an ideal scenario. In this way we observe the effects of the noise and possible errors in the outcome of the simulation.

B. Simulation with Noise

To include other qbits in the environment surrounding the system of interest we modified the control Hamiltonian in two different ways:

1. First, we added two extra spins and had them interacting via $zz$ coupling with the particle that represents the state of the fermion site (qbit 2):

$$H_{NMR} = \frac{1}{2} \left( \frac{(\epsilon + \epsilon_{k,0})}{2} - \sqrt{\left( \frac{\epsilon - \epsilon_{k,0}}{2} \right)^2 + V^2} \right) \sigma_z^1 + \frac{1}{2} \left( \frac{(\epsilon + \epsilon_{k,0})}{2} + \sqrt{\left( \frac{\epsilon - \epsilon_{k,0}}{2} \right)^2 + V^2} \right) \sigma_z^2 + J_{zz} \sigma_z^2 \sigma_z^3 + J_{zz} \sigma_z^2 \sigma_z^4 + J_{zz} \sigma_z^3 \sigma_z^4. \quad (21)$$

2. Next, we added an extra particle, which interacts in the same fashion ($zz$ coupling) with both particles that represent the system of interest: the resonant impurity and the fermion site:

$$H_{NMR} = \frac{1}{2} \left( \frac{(\epsilon + \epsilon_{k,0})}{2} - \sqrt{\left( \frac{\epsilon - \epsilon_{k,0}}{2} \right)^2 + V^2} \right) \sigma_z^1 + \frac{1}{2} \left( \frac{(\epsilon + \epsilon_{k,0})}{2} + \sqrt{\left( \frac{\epsilon - \epsilon_{k,0}}{2} \right)^2 + V^2} \right) \sigma_z^2 + J_{zz} \sigma_z^1 \sigma_z^3 + J_{zz} \sigma_z^2 \sigma_z^4 + J_{zz} \sigma_z^3 \sigma_z^4, \quad (22)$$
where $J_{zz}$ represents the $zz$ coupling constant. We used the same control sequence from Eq. (20) to obtain Eq. (17), to represent a situation in which the extra qubits are environmental and thus are taken to be unknown.

III. RESULTS

In this section we describe the results of the simulations for the two different modifications to the Hamiltonian as well as different initial states.

A. States with Bloch vector in the $z$ direction

We first consider states with only a $z$ component to their Bloch vectors. These form a special class of states due to the commutativity of the $zz$ Hamiltonian with these initial states.

1. Noiseless Quantum Simulation

Here we consider the cases where no bath is present, but different initial states are considered. Three cases are considered corresponding to three types of different initial states used in the simulation:

A.1 Pure states

$$|\psi(0)\rangle = |00\rangle, |01\rangle, |10\rangle, |11\rangle.$$

Density operator calculated as $\rho(0) = |\psi(0)\rangle \langle \psi(0)|$.

A.2 Entangled states

$$|\psi(0)\rangle = \alpha_0 |01\rangle + \alpha_1 |10\rangle,$$

where $\alpha_0^2 + \alpha_1^2 = 1$, and the density operator is given by $\rho(0) = |\psi(0)\rangle \langle \psi(0)|$.

A.3 Correlated states

$$\rho(0) = (1-p)(\rho_1^I \otimes \rho_2^I) + p(\rho_1^{II} \otimes \rho_2^{II}),$$

where $\rho_1^I$ and $\rho_2^I$ are the density operators corresponding to some initial state of the impurity (“spin-down”/occupied) and fermion (“spin-up”/unoccupied), respectively, and $\rho_1^{II}$ and $\rho_2^{II}$ correspond to the other initial state of the impurity (“spin-up”/unoccupied) and fermion (“spin-up”/unoccupied).

We represented the initial state of the impurity in terms of its $x$, $y$ and $z$ projections of the Bloch vector. The magnitude of each component of the projections, $a_i$, can be obtained by performing the partial trace over everything else except qbit 1, as $a_i = \text{Tr}[\sigma_i(\rho(0))].$

First consider an initial density operator

$$\rho_S(0) = \frac{1}{2} (1 + \mathbf{a}_i \cdot \mathbf{\sigma}_i).$$

In this case, case A.1,

$$\rho_S(0) = \frac{1}{2} (1 + a_3 \sigma_z),$$

where $a_3$ represents a real constant that is equal to, or less than, the radius of the Bloch sphere (i.e. $0 \leq a_3 \leq 1$). It represents the projection along the $z$ axis. The final state was obtained through the reduced dynamics of $\rho_S$ after the evolution:

$$\rho_S(t) = \text{Tr}[\rho_S(0) \{ U \rho(0) U^\dagger \}].$$

When the initial states $\rho_S(0)$ only had a $z$ component, the final states $\rho_S(t)$ only had a $z$ component as well

$$\rho_S(t) = \frac{1}{2} (1 + b_3 \sigma_z),$$

where $b_3$ is another real constant that is subject to $0 \leq b_3 \leq 1$. The value of $b_3$ depends on $a_3$ and on the parameters $\epsilon, \xi_k, V$ and $t$. When states with only a $z$ component are input, the final states also only have a $z$ component. This is consistent with the hopping model where the “spin-down” corresponds to the state being occupied. The evolution is described by the dynamical map

$$B = \begin{pmatrix}
\frac{1+b_3}{2} & 0 & 0 & 0 \\
0 & \frac{1+b_3}{2} & 0 & 0 \\
0 & 0 & \frac{1-b_3}{2} & 0 \\
0 & 0 & 0 & \frac{1-b_3}{2}
\end{pmatrix}.\tag{26}$$
The parameters are \( \epsilon = 8, \varepsilon = -2, \) and \( V = 4, \) for the time interval \( \Delta t \in [0.1, 0.9]. \)

The eigenvalues of the map are plotted as functions of time in Figure 2.

The case of a maximally entangled state case A.2 also has a similar form with only a \( z \) component in the initial and final states of the system. Thus there is only this standard interpretation of the hopping model Hamiltonian when there is no external noise.

2. Simulation with noise from spin bath

In this section we present the results for systems governed by the Hamiltonians in Eqs. (21) and (22). The goal is to simulate a two body problem, so we used the same control sequence in Eq. (20). However, the initial state of a “bath” of two particles was included in the total system Hamiltonian. As in the simulation that had no external noise, we chose different initial configurations, Explicitly, including the bath qubits these are:

A.4 Pure states

\[
|\psi(0)\rangle = |0011\rangle, |0111\rangle, |1011\rangle, |1111\rangle,
\]

and density operator \( \rho(0) = |\psi(0)\rangle \langle \psi(0)|. \)

A.5 Entangled states

\[
|\psi(0)\rangle = \alpha_0 |0111\rangle + \alpha_1 |1011\rangle
\]

Where \( \alpha_0^2 + \alpha_1^2 = 1, \) and the density operator is given by \( \rho(0) = |\psi(0)\rangle \langle \psi(0)|. \)

A.6 Correlated states

\[
\rho(0) = ((1 - p)(\rho_1^I \otimes \rho_2^I) + p(\rho_1^{II} \otimes \rho_2^{II}))(|1\rangle \langle 1| \otimes |1\rangle \langle 1|). \tag{29}
\]

The fact that the states only had a component in the \( z \) direction and only interact with the bath via \( zz \) couplings resulted in results that were very similar to the ones in the previous section. The initial state of qbit 1 (the impurity) can again be written in Pauli notation as:

\[
\rho_S(0) = \text{Tr}_E \rho(0) = \frac{1}{2}(1 + a_3 \sigma_z). \tag{30}
\]

The final state is obtained by tracing over the bath degrees of freedom

\[
\rho_1(t) = \text{Tr}_E(U \rho(0) U^\dagger) = \frac{1}{2}(1 + b_3 \sigma_z), \tag{31}
\]

\( b_3 \) is another real constant that can be positive or negative, depending on the direction of the Bloch vector of the final state along the \( z \) axis.

The most general dynamical map has the same form as the map in Eq. (26),

\[
B = \frac{1+b_3}{2} \begin{pmatrix} 1+b_3 & 0 & 0 & 0 \\ 0 & 1+b_3 & 0 & 0 \\ 0 & 0 & 1-b_3 & 0 \\ 0 & 0 & 0 & 1-b_3 \end{pmatrix}. \tag{32}
\]

We observed that the coupling \( J_{zz} \) has an effect in the rate of change of the state of qbit 1, which is presented in the results for the calculation of the time correlation function. For purposes of comparison, the parameters of the system were the same as the results above. In Figs. 3 and 4, the eigenvalues of \( B \) are plotted with the couplings to the particles of the spin bath being \( J_{zz} = 8 \) and \( J_{zz} = \frac{1}{2} \) respectively.

Figs. 2, 3 and 4 show the evolution of the same initial state but each has a different environment. Being states initially in the \( z \) direction, the dynamics are completely positive since the interaction with the bath is a \( zz \) coupling. However, it does change the hopping rate. In Fig. 3 this is particularly noticeable due to the choice of the coupling. The state of the impurity does not transfer as easily due to the strong correlations generated by the interaction with the spin bath. In Fig. 4 the situation is different. In this case the eigenvalues remained the same regardless of the strength of the coupling with the environment. Having a single extra particle interacting with both qbits with the same strength would mean they both have the same interaction with the bath.

B. Arbitrary initial direction of the Bloch vector

Noise in the initialization of the state could result in a direction for the Bloch vector which is not in the \( z \) direction. States that have an \( x \) or a \( y \) component to their
Larmor precession will be present. This is often observed in a NMR device under general circumstances and leads to noise in the system. Here we consider an initial state with a component of the Bloch vector in the $x$ direction. Clearly a $y$ component is not necessary, and only specifies a different initial condition for the angle since the system will precess.

1. **Noiseless Quantum Simulation**

The initial states were chosen to have a component in the $x$ direction; the components in $x$ and $z$ were selected such that the magnitude of the Bloch vector is close to 1 emulating a small error in the initialization. Explicitly, the different initial configurations were:

$$
\rho_1(0) = \frac{1}{2}(1 + a_1 \sigma_x + a_3 \sigma_z),
$$

or

$$
\rho_2(0) = \frac{1}{2}(1 + a_1 \sigma_x - a_3 \sigma_z),
$$

where $\rho_1$ is the state of the impurity, $\rho_2$ is the state of the fermion and the $a_i$ are subject to $0 \leq \sqrt{a_1^2 + a_3^2} \leq 1$. Therefore, the total initial state is

$$
\rho(0) = \rho_1(0) \otimes \rho_2(0).
$$

The final state of the impurity was, once again, obtained by doing a partial trace over the degrees of freedom of the fermion

$$
\rho(t) = \text{Tr}_E \left( U \rho(0) U^\dagger \right) = \frac{1}{2} (1 + b_1 \sigma_x + b_2 \sigma_y + b_3 \sigma_z). \quad (33)
$$

The map $B$ is given by

$$
B = \left( \begin{array}{cccc}
\frac{1+b_2}{2} & 0 & 0 & \frac{-ib_2}{a_1} \\
0 & \frac{1+b_1}{2} & \frac{b_1 a_1}{a_3} & 0 \\
0 & \frac{b_1 a_3}{a_1} & \frac{1+b_3}{2} & 0 \\
\frac{ib_2}{a_1} & 0 & 0 & \frac{1-b_2}{2}
\end{array} \right). \quad (34)
$$

The eigenvalues of $B$ are given by

$$
\lambda_1 = \frac{a_1 - \sqrt{4b_1^2 + a_1^2 b_3^2}}{2a_1}, \quad \lambda_2 = \frac{a_1 + \sqrt{4b_1^2 + a_1^2 b_3^2}}{2a_1},
$$

$$
\lambda_3 = \frac{a_1 - \sqrt{4b_3^2 + a_1^2 b_1^2}}{2a_1}, \quad \lambda_4 = \frac{a_1 + \sqrt{4b_3^2 + a_1^2 b_1^2}}{2a_1}, \quad (35)
$$

where
\[
\begin{align*}
  b_1 &= \left\{ \cos\left(\frac{1}{2} t (\epsilon + \epsilon_{k_0})\right) \cos\left(\frac{1}{2} t \sqrt{4V^2 + (\epsilon - \epsilon_{k_0})^2}\right) - \sin\left(\frac{1}{2} t (\epsilon + \epsilon_{k_0})\right) \frac{(\epsilon - \epsilon) \sin\left(\frac{1}{2} t \sqrt{4V^2 + (\epsilon - \epsilon_{k_0})^2}\right)}{\sqrt{4V^2 + (\epsilon - \epsilon_{k_0})^2}} \right\} a_1, \\
  b_2 &= \left\{ -\sin\left(\frac{1}{2} t (\epsilon + \epsilon_{k_0})\right) \cos\left(\frac{1}{2} t \sqrt{4V^2 + (\epsilon - \epsilon_{k_0})^2}\right) - \cos\left(\frac{1}{2} t (\epsilon + \epsilon_{k_0})\right) \frac{(\epsilon - \epsilon) \sin\left(\frac{1}{2} t \sqrt{4V^2 + (\epsilon - \epsilon_{k_0})^2}\right)}{\sqrt{4V^2 + (\epsilon - \epsilon_{k_0})^2}} \right\} a_1 \\
  &\quad + 2(-1 + a_3)V^2 + a_3(\epsilon - \epsilon)^2 + (1 + a_3)V^2 \cos\left(\frac{1}{2} t \sqrt{4V^2 + (\epsilon - \epsilon)^2}\right) \\
  b_3 &= \frac{4V^2 + (\epsilon - \epsilon)^2}{2(-1 + a_3)V^2 + a_3(\epsilon - \epsilon)^2 + (1 + a_3)V^2 \cos\left(\frac{1}{2} t \sqrt{4V^2 + (\epsilon - \epsilon)^2}\right)}.
\end{align*}
\]

Note that if \( a_1 \to 0 \), then \( b_1 \) and \( b_2 \) are 0. The factor \( a_1 \) in the denominator of the eigenvalues is eliminated using Von Neumann’s rule, and that yields

\[
\begin{align*}
  \lambda_1 &= \frac{1 - b_3}{2}, \\
  \lambda_2 &= \frac{1 + b_3}{2}, \\
  \lambda_3 &= \frac{1 - b_3}{2}, \\
  \lambda_4 &= \frac{1 + b_3}{2},
\end{align*}
\]

which are the same as the eigenvalues of the map in Eq. (36). The eigenvalues of \( B \) when \( a_1 > 0 \) are shown in Figure (6). In Fig. (6), the dynamics of the system are positive but not completely positive. This system is not in contact with a bath or reservoir, but it consists of two particles. This is a case of initial correlations between particles in the system, which are errors for this model since correlations should not be present in initial state preparation. The general observation was that when the initial state has a component of the Bloch vector in \( x \) or \( y \) as well as one in \( z \), the result is a non completely positive map.

2. Simulation with noise from spin bath

The results in this subsection are generated from adding the qubits in the spin bath, and using the following initial states

\[
\rho(0) = \rho_1(0) \otimes \rho_2(0) \otimes (|1\rangle \langle 1|) \otimes (|1\rangle \langle 1|),
\]

where

\[
\rho_1(0) = \frac{1}{2} (\mathbb{1} + a_3 \sigma_z + a_3 \sigma_z),
\]

and

\[
\rho_2(0) = \frac{1}{2} (\mathbb{1} + a_3 \sigma_z - a_3 \sigma_z).
\]

The reduced dynamics of \( S \) are given by

\[
\rho(t) = \text{Tr}_E (U \rho(0) U^\dagger) = \frac{1}{2} (\mathbb{1} + b_1 \sigma_x + b_2 \sigma_y + b_3 \sigma_z),
\]

with a \( B \) map of the same for as that in Eq. (34),

\[
B = \begin{pmatrix}
    \frac{1+b_4}{2} & 0 & 0 & -ib_3 \\
    0 & \frac{1+b_4}{2} & \frac{b_1}{a_1} & 0 \\
    0 & \frac{b_2}{a_1} & \frac{1-b_4}{2} & 0 \\
    \frac{b_3}{a_1} & 0 & 0 & \frac{1+b_4}{2}
\end{pmatrix}.
\]

Once again, the noise, which has the form of purely \( zz \) couplings, caused variations in the parameters, mostly in the rate of change of the state of qbit 1. The eigenvalues for a system with two spins interacting with the fermion only and for one spin interacting with both particles in the system are presented in Figs. 7 and 8.

In Figs. 7 and 8, the reduced dynamics are not completely positive. This is due to the initial state of the impurity site (qbit 1) having a component of its Bloch vector in the \( x \) direction. The algorithm was designed to have an initial state where one of the two state systems is in the up state and the rest are in the down state. Dynamical maps obtained through quantum process tomography can present discrepancies if the initial states are prepared through different experimental methods. Thus the \( x \) component represents a preparation error which gives rise to a non-completely positive map like in the previous case.

C. Time correlation function

Ortiz et al. calculated the time correlation function

\[
C(t) = \langle b(t) b(0) \rangle,
\]

and plotted the result as \( |G|^2 = \text{Tr} (\rho(t) \rho(0)) \) as a function of time. Since we want to calculate the effects of noise and different initial state, we followed the same procedure for the different situations. The results are summarized in graphs, Figs. 9, 10 and 11. In Fig. 9, there is a slight difference between the results of the original system compared to those under which errors could arise due to noise and unknown initial states. The coupling to the environment affects how fast or slow qbit 1 evolves. However, if the coupling to the bath is weak, these errors are not as prominent. There was one case in which there was no effect on the speed of change by spins in the bath.

When the initial state had a component in \( x \) the resulting correlation functions were very close to the original
FIG. 5: Animation of the evolution of the Bloch Vector of the reduced dynamics of qbit 1 in the initial state $\rho_1 = \frac{1}{2}(\mathbb{1} + 0.2\sigma_x + 0.97\sigma_z)$

FIG. 6: Eigenvalues for the dynamical map of the reduced dynamics of qbit 1. The initial state of the system is $\rho_1 = \frac{1}{2}(\mathbb{1} + 0.2\sigma_x + 0.97\sigma_z)$, $\rho_2 = \frac{1}{2}(\mathbb{1} - \sigma_z)$. The parameters of the system are $\epsilon = -8$, $\varepsilon = -2$, $V = 4$. Evaluated in the time interval $t \in [0.1, 0.9]$.

FIG. 7: Eigenvalues of the dynamical map for the reduced dynamics of qbit 1. The initial state of the system is $\rho_1 = \frac{1}{2}(\mathbb{1} + 0.2\sigma_x + 0.97\sigma_z)$, $\rho_2 = \frac{1}{2}(\mathbb{1} - \sigma_z)$, $\rho_3 = \frac{1}{2}(\mathbb{1} - \sigma_z)$, $\rho_4 = \frac{1}{2}(\mathbb{1} - \sigma_z)$. The system parameters are $\epsilon = -8$, $\varepsilon = -2$, $V = 4$, $J_{zz} = \frac{1}{10}$ evaluated in the time interval $t \in [0.1, 0.9]$.

The $x$ component of the Bloch vector is increased, we can see shifts in the time correlation function. The greater $a_1$ is, the larger the observed shift. This could be useful for detecting possible errors in state preparation.

IV. CONCLUSIONS

Interactions of quantum systems with a surrounding environment are undesirable for reliable quantum simul-
The interaction of the system with the environment is clearly necessary for implementing the appropriate noise control method. Understanding and controlling or suppressing the noise from the environment is one of the most important objectives of studying open system quantum dynamics. Lloyd’s suggestion to use the noise to simulate the interaction of the system with the environment is clearly useful only in special cases. For some analog simulators, isolation has nearly been achieved, but that will not be the case for many devices. For the cases where noise suppression is required, understanding the noise will be necessary for implementing the appropriate noise control method.

FIG. 8: Eigenvalues of the dynamical map for the reduced dynamics of qubit 1. The initial state of the system is \( \rho_1 = \frac{1}{2} (1 + 0.2\sigma_x + 0.97\sigma_z) \), \( \rho_2 = \frac{1}{2} (1 - \sigma_z) \), \( \rho_3 = \frac{1}{2} (1 - \sigma_x) \). The system parameters are \( \epsilon = -8 \), \( \epsilon = -2 \), \( V = 4 \), \( J_{zz} = \frac{1}{10} \) evaluated in the time interval \( t \in [0.1, 0.9] \).

FIG. 9: Time correlation function of the reduced dynamics of qubit 1. The system parameters are \( \epsilon = -8 \), \( \epsilon = -2 \), \( V = 4 \) and time interval \( t \in [0.1, 0.9] \). The results represent the closed system and the system that interacts with two additional qubits, coupled only to qubit 2. The initial state of qubit 1 is \( \rho = |0\rangle \langle 0| \) for one set of results, and \( \rho = \frac{1}{2} (1 + 0.2\sigma_x + 0.97\sigma_z) \) for the other.

FIG. 10: Time correlation function of the reduced dynamics of qubit 1. The system parameters are \( \epsilon = -8 \), \( \epsilon = -2 \), \( V = 4 \) in the time interval \( t \in [0.1, 0.9] \). The results correspond to the closed system and the system that interacts with two additional qubits, coupled only to qubit 2. The initial state of qubit 1 is \( \rho = |0\rangle \langle 0| \) for one set of results, and \( \rho = \frac{1}{2} (1 + 0.2\sigma_x + 0.97\sigma_z) \) for the other.

FIG. 11: Time correlation function of the reduced dynamics of qubit 1. The system parameters are \( \epsilon = -8 \), \( \epsilon = -2 \), \( V = 4 \) evaluated in the time interval \( t \in [0.1, 0.9] \). The result represents the time correlation function of the closed system compared to the correlation function of the reduced dynamics of qubit 1 in the initial state \( \rho = \frac{1}{2} (1 + a_1\sigma_x + a_3\sigma_z) \) for different values of \( a_1 \) and \( a_3 \).
It is known that interactions with the environment can lead to correlations that can result in non completely positive maps. We found that such non completely positive maps are not rare in our study of a very simple model of a quantum system of fermions which can readily be simulated on a quantum computing device, or a dedicated quantum simulator. This Fano-Anderson model exhibits maps which are not completely positive for a variety of initial states, some of which were entangled and some with other non-trivial quantum correlations in the sense of non-zero quantum discord. They were shown to arise for even a fairly small transversal component to an initial density matrix which is supposed to have its Bloch vector aligned along the z axis. Thus fairly small experimental errors can lead to maps which are not completely positive in a rather simple experiment. These noises also cause relatively small errors in the final outcome of the measurement.

Initially correlated states, if they are not so identified, but are instead identified improperly as arising from completely positive maps, may encourage an experimenter to try to employ dynamical decoupling controls to eliminate errors. These controls will be ineffective in these cases.

We have used a very specific and simple model to illustrate the effects of noise on the system including the presences of maps which are not completely positive. However, it is important to emphasize that these effects are quite general and will be present in some form in many other quantum systems including a wide class of quantum simulations.

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