Simulating Open Quantum Systems on Near Term Quantum Computers

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Abstract

The simulation of quantum systems is poised to be one of the first and most impactful applications of quantum computers. This thesis focuses on such simulation with a particular emphasis on simulating open quantum systems, i.e. systems which can exchange energy, particles, information, or more with their surroundings. Chapter 1 introduces the fundamentals of quantum computing and quantum information. In chapter 2 we review the basics of quantum dynamics, and open quantum systems. Chapter 3 explores errors in actual quantum computers and discusses techniques to optimize results when running on currently available quantum hardware. Chapter 4 comes from the paper “Simulation of Thermal Relaxation in Spin Chemistry Systems on a Quantum Computer Using Inherent Qubit Decoherence”[1] in which we show how to use qubit decoherence to our advantage to simulate an open spin chemistry system undergoing thermal relaxation on IBM’s quantum computers. Chapter 5 originates from the paper “Driven-dissipative quantum mechanics on a lattice: Simulating a fermionic reservoir on a quantum computer”[2] where we show how to simulate the dynamics of a driven dissipative Hubbard model on IBM’s quantum computers without reset gates. Chapter 6 is derived from the paper “Demonstrating robust simulation of driven-dissipative problems on near-term quantum computers”[3]. This paper extends the work presented in chapter 5 with the introduction of selective reset gates - allowing us to simulate Trotterized time evolution further than had previously been achieved on any digital quantum computer. We also calculate the current through
the system and prepare the thermal state of atomic limit of the same model. Finally, chapter 7 contains concluding remarks.

INDEX WORDS: Quantum Information, Quantum Computing, Open Quantum Systems, Dissipation
DEDICATION

To my amazing wife Nhật Nguyên without whom I wouldn’t have been able to get here. Thank you for all your patience, support and love.
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1.1 Introduction

The invention and ubiquitous adoption of the computer during the last century has arguably been the most transformative thing to ever occur for our species. The scale, scope, and efficiency with which mankind is now able to compute and communicate is completely unprecedented in our history. Nevertheless, there remain classes of problems for which our awesome computing power is woefully inadequate. It has been proven there are certain problems which computers cannot solve at all[4]. Modern encryption relies in part on the fact that computers are painfully slow at factoring large numbers[5]. Advances in physics, chemistry, and more are hindered by the difficulty of simulating the behavior of quantum mechanical systems on computers.

In the 1980s, scientists began to speculate about using quantum hardware to build quantum computers which would be fundamentally more powerful than their classical counterparts[6, 7]. In the 1990s, the first quantum algorithms were discovered that gave provable speed-ups over the best classical algorithms[8, 9, 10, 11, 12, 13, 14, 15]. Among those are Shor’s famous polynomial-time integer factoring algorithm[9], Grover’s famous quadratic speed-up for unstructured search[12], and Lloyd’s efficient method for simulating quantum Hamiltonian dynamics[13]. Today it is still an open problem to classify which classes of problems can be solved efficiently on classical hardware, on quantum hardware, and which can be simulated more efficiently
on quantum hardware vs. classical hardware. Despite the failings of our colleagues working in the field of computational complexity, today we have quantum algorithms for a wide variety of problems which are more efficient than the best known classical algorithms; a comprehensive catalog is kept in Ref. [16]. In the remainder of this chapter we will explore the differences between classical and quantum information and how these differences can be exploited to more efficiently solve certain problems.

1.2 Classical Versus Quantum Information

Classical information and computing centers around manipulating bits. Bits are objects that can exist in only one of two states, which we will call state $|0\rangle$ and state $|1\rangle$. Practically bits are often realized by using high/low voltage, presence/absence of an electron, or up/down magnetization of a magnetic domain, but any system with two distinguishable states is sufficient. Information is stored via a binary encoding, e.g. $a \leftrightarrow 101$. Information is processed by reading and flipping bits according to some algorithm, e.g. if the first bit is $|1\rangle$, then flip the second bit otherwise do nothing. It will be useful for introducing quantum information to formulate the ideas of classical information in terms of linear algebra.

We can do this by representing states of bits as vectors and manipulations of bits as matrices (i.e. linear transformations or linear operators). For classical computation, only permutation matrices are valid gates. Note that this actually defines reversible classical computation, which reduces to the standard model of computation if we simply discard some of the bits at the end. We begin with the following definitions for our bit states

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (1.1)$$
and introduce the notation $\langle v \equiv |v|^\dagger$ such that

$$\langle v | w \rangle = v^\dagger w : \text{inner product} \quad \text{and} \quad |v\rangle\langle w| = vw^\dagger : \text{outer product} \quad (1.2)$$

The state of multiple bits is given as a tensor product of the individual bit states. That is, if I have a two-bit computer with its bits in the states $b_1 = |v\rangle$ and $b_2 = |w\rangle$ -- then I say the state of the computer is $|v\rangle \otimes |w\rangle \equiv |vw\rangle$.

Putting everything together, the operation (call it $cX$) described above, “if the first bit is $|1\rangle$, then flip the second bit otherwise do nothing" is given by

$$cX = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X \quad \text{with} \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \rightarrow XX |0\rangle = X |1\rangle = |0\rangle. \quad (1.3)$$

where $I$ is the identity operator. Applying this to the state $|vw\rangle$ gives

$$cX |vw\rangle = |0\rangle\langle 0| \otimes I |w\rangle + |1\rangle\langle 1| \otimes X |w\rangle \quad (1.4)$$

Because $|0\rangle$ and $|1\rangle$ are orthonormal we have $\langle s|v\rangle = \delta_{sv}$ giving

$$cX |vw\rangle = \delta_{0v} |vw\rangle + \delta_{1v} |v\bar{w}\rangle \quad (1.5)$$

which tells us if $|v\rangle$ (the first bit) is in $|1\rangle$ we get $|v\bar{w}\rangle$ i.e. flip the second bit. If $|v\rangle$ is in $|0\rangle$ we get $|vw\rangle$ i.e. do nothing – exactly as desired. All classical computations (A computation on one or two bits can still be achieved by adding one or two ancilla bits and discarding them at the end) can be efficiently recast using this formalism[17]. We begin all bits in state $|0\rangle$ and use only the $X$ gate (from Eq. 1.3) and the Toffoli gate

$$T(a, b, c) = (|00\rangle\langle 00|_{ab} + |01\rangle\langle 01|_{ab} + |10\rangle\langle 10|_{ab}) \otimes I_c + |11\rangle\langle 11|_{ab} \otimes X_c \quad (1.6)$$

where $a$, $b$, and $c$ are indices of the bits on which we operate and $I$ is applied to all bits $\notin \{a, b, c\}$. This is sufficient to implement all classical logic. It further implies that the
state of our bits will always be a product state, i.e. in the form $|b_0\rangle \otimes |b_1\rangle \otimes |b_2\rangle \otimes \cdots \otimes |b_n\rangle$ with $b_i \in \{0, 1\}$.

It turns out that all quantum computation can also be described by this formalism[18]. The only difference is quantum computation allows more general gates than classical computation. In particular, reversible classical computation allows only gates which are permutation matrices. This makes perfect sense because reversible transformations are formally permutations[19]. Quantum computation, on the other hand, allows gates which are arbitrary unitary matrices. This is a much more general class of gates and gives rise to the power of quantum computing.

Why should it make sense that quantum operations are general unitaries unlike their classical counterparts? One motivating explanation is to simply inspect the Schrödinger equation

$$i\partial_t |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \quad \text{with} \quad \hbar = 1$$

(1.7)

where $\hat{H}$ is the system’s Hamiltonian and $|\psi(t)\rangle$ is the state of the quantum bits (qubits) at time $t$. Let’s assume we have quantum hardware that can apply an arbitrary (time-independent) physical Hamiltonian to the qubits for a fixed duration $\tau$. This is a stronger assumption than is actually needed but simplifies the explanation here. If our qubits were in a state $|\psi_0\rangle$ initially, we find the state of the qubits after time $\tau$ to be

$$|\psi_f\rangle = e^{-i\hat{H}\tau} |\psi_0\rangle = U |\psi_0\rangle .$$

(1.8)

Because $\hat{H}$ is an arbitrary Hamiltonian, $U$ is an arbitrary unitary operator.

Note that I’ve casually introduced the idea of a qubit in the preceding paragraph, without much explanation. That is because it is the same as the description of the classical bit given above. The only difference is allowing general unitaries to act on the bit vectors results in fundamentally quantum states which classical bits cannot
occupy. General unitaries give rise to the ideas of superposition and entanglement. Consider using the gate \( G \) defined below with the \( cX \) from Eq. 1.3 on two qubits in the \( |00\rangle \) state:

\[
G = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ -i & -1 \end{pmatrix} \rightarrow cX \cdot (G \otimes I) |00\rangle = \frac{1}{\sqrt{2}} (|00\rangle - i |11\rangle). \tag{1.9}
\]

We see that the qubits are now in a superposition (i.e. linear combination) of \( |00\rangle \) and \( |11\rangle \) with complex coefficients. Furthermore they are entangled, meaning neither qubit has a well-defined state independent of the other. Put another way, this two-qubit state cannot be expressed as a product of the individual qubit states. To see this, let’s suppose each qubit did have a well-defined state. We’ve just seen that qubits can exist in complex superpositions, so our most general state for each qubit is \( a |0\rangle + b |1\rangle \) with \( |a|^2 + |b|^2 = 1 \) because unitary transformations preserve vector norms. So we are looking for complex numbers \( a, b, c, \) and \( d \) such that

\[
(a |0\rangle + b |1\rangle) \otimes (c |0\rangle + d |1\rangle) = \frac{1}{\sqrt{2}} (|00\rangle - i |11\rangle). \tag{1.10}
\]

Expanding this out tells us that \( ac = -ibd = 1/\sqrt{2} \) and \( ad = bc = 0 \). By inspection, these equations have no solutions since the first two imply none of \( a, b, c, \) or \( d \) are 0 while the last two imply at least one of \( a \) or \( d \), and one of \( b \) or \( c \) are 0. This tells us that the qubits literally have no well-defined individual states – only the composite state of the pair is defined.

At its heart, this is the basis for the extra power quantum computers have compared to classical ones. Because classical bits always have a well defined state, the state of a classical computer is describable by specifying the state of each bit. So \( n \) bits are specified by \( n \) boolean values, e.g. 1101001001 ... 1001. On the other hand, a
maximally entangled \( n \)-qubit state requires \( N \equiv 2^n \) amplitudes to specify
\[
\alpha_1 |0\ldots00\rangle + \alpha_2 |0\ldots01\rangle + \alpha_3 |0\ldots10\rangle + \alpha_4 |0\ldots11\rangle + \\
\alpha_{N-3} |1\ldots00\rangle + \alpha_{N-2} |1\ldots01\rangle + \alpha_{N-1} |1\ldots10\rangle + \alpha_N |1\ldots11\rangle.
\] (1.11)

Unfortunately, that’s not the end of the story. The postulates of quantum mechanics tell us that we cannot directly access the state of the quantum computer[17], call it \( |\Psi\rangle \). Instead, when we observe the quantum computer, it collapses into one of the states in the superposition with a probability given by the squared norm of the amplitude
\[
|\Psi\rangle = \sum_{i=1}^{N} \alpha_i |\psi_i\rangle \xrightarrow{\text{observe}} |\psi_k\rangle \quad \text{with} \quad \text{prob} = |\alpha_k|^2,
\] (1.12)
making it tricky to leverage the exponentially large information content inside the quantum computer. Figuring out how to take advantage of entangled qubits is what quantum algorithms research is all about and is still an open and active field.

While the above gives the general formalism for thinking about quantum operators, it’s important to note that, like classical computers, digital quantum computers come with a finite set of gates. Despite this, it is sufficient to (approximately) implement any arbitrary unitary gate efficiently[20]. One common universal gate set is \( cX \), \( H \), and \( T \) where
\[
H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad \text{and} \quad T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}.
\] (1.13)

Other common gates include \( X \), \( Y \), and \( Z \), the Pauli matrices, where \( X \) is defined in Eq. 1.3 and
\[
Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\] (1.14)

Or the more general \( R_{\hat{n}}(\theta) = e^{-i(\hat{n} \cdot \vec{P})\theta/2} \) where \( \hat{n} \) is a unit vector and \( \vec{P} = \{X, Y, Z\} \).
A quantum computation is then represented by a series of gates acting on a set of qubits initialized to a known state (usually the all $|0\rangle$ state), with the qubits being measured at the end. More complicated, hybrid quantum/classical protocols also exist where qubits are measured or reset (non-unitary operations) mid-circuit and subsequent gates can be applied conditionally based on the measurement results. This is the circuit model of quantum computation, and while other models exist, it is by far the most popular in the literature and in actual physical implementations of digital quantum computers. We can pictorially show such a computation (Fig. 1.1) by letting horizontal lines represent qubits, boxes or other common symbols representing gates, with the horizontal position corresponding to time flowing from left to right.

\[
\begin{align*}
|q_1\rangle &= |0\rangle \\
|q_2\rangle &= |0\rangle \\
|q_3\rangle &= |0\rangle \\
|q_4\rangle &= |0\rangle \\
U_{\text{full}} |\Psi_{\text{final}}\rangle
\end{align*}
\]

(a) Quantum computation as a single unitary transformation, followed by measurements.

\[
\begin{align*}
|0\rangle \\
|0\rangle \\
|0\rangle \\
|0\rangle \\
U_1 U_2 U_3 U_4 U_5 U_6 U_7 U_8 U_9 U_a U_b U_c U_d |\Psi_{\text{final}}\rangle
\end{align*}
\]

(b) Same computation broken down into elementary one- and two-qubit gates.

**Figure 1.1: Quantum circuit structure.** Two equivalent quantum computations. One using a single unitary and one in terms of elementary gates.

### 1.3 Simulating Quantum Dynamics

One area where it is more straightforward how to take advantage of a quantum computer is in the simulation of quantum physics itself. Assuming we can efficiently specify the Hamiltonian and prepare the system's initial state of the system, storing and evolving the system is efficient. On a classical computer, simply storing the state of an entangled quantum system is exponentially expensive in the size of the system. Manipulating it is likewise exponentially costly. Thus, Hamiltonian simulation is believed
to be exponentially harder on a classical computer – if it weren’t, classical computers would be able to efficiently simulate quantum computers, rendering the whole field moot.

The efficient simulation of Hamiltonian dynamics is useful for a wide variety of applications, as it is the main subroutine in most algorithms computing correlation functions and energy spectra[21, 22]. From these we can find e.g. densities, transport properties, scattering properties, susceptibilities, conductivity, and more.[21, 22, 23, 24, 25, 26].

The naive method (1st order product formula) for simulating quantum dynamics involves

1. Preparing your qubits in the desired initial state. This step is highly non-trivial for most states of interest, especially ground states / low temperature thermal states. Devising techniques for this step is an active research area.

2. Writing your Hamiltonian in terms of Pauli operators. Techniques for this are well-known and relatively straightforward[27, 28]. We will use the Jordan-Winger as an example below.

\[ \hat{H}(t) = \sum_{\gamma} \alpha_{\gamma}(t)P_{\gamma} \quad \text{with} \quad P_{\gamma} = p_0 \otimes p_1 \otimes \cdots \otimes p_n \quad (1.15) \]

where \( p_i \in \{I, X, Y, Z\} \) is a Pauli operator acting on the \( i \)th qubit.

3. For time-dependent Hamiltonians or Hamiltonians with non-commuting terms (i.e. almost all non-trivial problems), rewrite the time evolution operator as a product of small time-steps, \( \Delta t = t/r \). This process is referred to as Trotterization.

\[ U(t) \approx \prod_{k=1}^{r} e^{-i\Delta t\hat{H}(k\Delta t)} = \prod_{k=1}^{r} e^{-i\Delta t \sum_{\gamma} \alpha_{\gamma}(k\Delta t) P_{\gamma}} \quad (1.16) \]
4. Break exponents of sums into products of exponents. Note this is not an exact operation when different $P_{\gamma}$s do not all mutually commute and so incurs a Trotter error of $O(\Delta t^2)$[13].

\[ U(t) \approx \prod_{k=1}^{r} \prod_{\gamma} e^{-i\Delta t \alpha_{\gamma}(k \Delta t) P_{\gamma}} \]  

(1.17)

5. Decompose the terms $e^{-i\Delta t \alpha_{\gamma}(k \Delta t) P_{\gamma}}$ into quantum gates. This is generally difficult but because physical Hamiltonians tend to be local and sparse, this step is often reasonably straightforward and efficient.

6. Run on a quantum computer to produce the desired time evolved state.

1.3.1 Hubbard Model Example

As is consistent with the literature, we will skip step 1 above and assume we have the desired state on the qubits to begin with. Chapter 6 gives some ideas about how to prepare thermal states of the Hubbard model.

**Fermionic Transformations**

For step 2, we note qubits are naturally suited to deal with spins, but not to deal with Fermions. So to run computations on a quantum computer it is important to find efficient transformations from Fock space to Hilbert space and from $c$ and $c^\dagger$ to $\sigma^+ \equiv (X - iY)/2$, $\sigma^- \equiv (X + iY)/2$ and $\sigma^z \equiv Z$. The next subsection shows a worked example of using the simple Jordan Wigner encoding, however more efficient encodings are possible such as the Bravyi-Kitaev encoding[27] among others.

**Jordan Wigner**

A simple way of doing this is the Jordan Wigner transformation. Here the transformation from Fock space to Hilbert space is trivial, with qubit $j$ storing the occupation
of site $j$ as $q_j = f_j$ where $f_j \in \{0, 1\}$. Note we’re assuming a linear ordering to the sites, for a $d \geq 2$ dimensional grid an ordering must be selected. E.g. for an $N \times N$ 2D grid, one could take $(i, j) \mapsto j + N(i - 1)$. We further note that each qubit only has two states whereas each Hubbard site has four, necessitating using two qubits per site. This can be accomplished by letting site $i$ be represented by qubits $2i - 1$ and $2i$. Here we will represent site $i$, for a lattice with $N$ total sites, with qubits $i$ (for spin up) and $i+N$ (for spin down).

To convert $c$ into Pauli matrices, we note that $c \mapsto \sigma^-$ recovers the local anticommutation relations $\{\sigma^+_j, \sigma^-_j\} = \{c^+_{ij}, c_j\} = 0$ but the non-local ones are incorrect: $\{c^+_{ij}, c_j\} = 1$ whereas $\{\sigma^+_i, \sigma^-_j\} = 2\sigma^+_i\sigma^-_j$ for $i \neq j$. This is fixed by including a phase in the mapping such that the phase for qubit $j$ is 1 if there are an even number of qubits in the $|1\rangle$ state on sites 1 to $j - 1$ and -1 otherwise. This makes intuitive sense. For example, consider a state with up-spin electrons on sites 1 and 3, and a down-spin on site 2. In 2nd quantization this state is given as

$$|\psi\rangle = c^+_1 c^+_3 c^+_2 |0\rangle .$$

If we then add a down-spin on site 1, we have

$$|\psi'\rangle = +c^+_1 c^+_1 c^+_3 c^+_2 |0\rangle = -c^+_1 c^+_1 c^+_3 c^+_2 |0\rangle = +c^+_1 c^+_3 c^+_2 |0\rangle$$

and we can see we pick up a factor of $-1$ for each occupied spin-site (qubit in the $|1\rangle$ state) we cross. Mathematically we can write this as

$$c_j = e^{i\pi \lambda_j} \sigma^-_j \quad \text{with} \quad \lambda_j = \sum_{k=1}^{j-1} \sigma^+_k \sigma^-_k \quad \text{and so} \quad c^+_j = e^{-i\pi \lambda_j} \sigma^+_j$$

using the fact that $[\sigma^+_j, \sigma^+_k \sigma^-_k] = 0$ for $j \neq k$. This allows us to rewrite Hamiltonians in terms of Pauli matrices. An $N$ site Hubbard model Hamiltonian, in terms of Fermionic operators, reads

$$\hat{H}_f = \sum_{i,j=1}^{2N} \tilde{t}_{ij} c^+_i c_j + U \sum_i c^+_i c_{i+N} c_{i+N}$$
where $U$ is the on-site interaction and $\tilde{t}_{ij} = -t$ if spin-sites $i$ and $j$ are nearest neighbors and 0 otherwise. We immediately see we have to deal with operators of the form $c_i^\dagger c_j$ and $c_i^\dagger c_i$. The latter is easily evaluated,

$$c_i^\dagger c_i = e^{-i\pi \lambda_i} c_i^\dagger e^{i\pi \lambda_i} = \sigma_i^+ \sigma^-,$$

(1.22)

again using the fact that $[\sigma_j^+, \sigma_k^+ \sigma_k^-] = 0$ for $j \neq k$. The term $c_i^\dagger c_j$ is slightly more involved.

When $j = i \pm 1$ (the only terms for a 1D chain without periodic boundary conditions) we again find

$$c_i^\dagger c_{i+1} = e^{-i\pi \lambda_i} c_i^\dagger e^{i\pi \lambda_{i+1}} \sigma_{i+1}^- = \sigma_i^+ e^{-i\pi \sigma_i^+} \sigma_i^- = \sigma_i^+ \sigma^-,$$

$$c_i^\dagger c_{i-1} = e^{-i\pi \lambda_i} c_i^\dagger e^{i\pi \lambda_{i-1}} \sigma_{i-1}^- = \sigma_i^+ e^{-i\pi \sigma_i^+} \sigma_i^- = \sigma_i^+ \sigma^-.$$  

(1.23)

Where we’ve used $\sigma^+ \sigma^+ = \sigma^- \sigma^- = 0$ and $e^{-i\pi \sigma_i^+} \sigma^- = \sum_{n=0}^{\infty} \frac{(-i\pi \sigma_i^+ \sigma^-)^n}{n!}$ meaning only the $n = 0$ term survives.

When we have periodic boundary conditions and/or a $d \geq 2$ dimensional grid, non-local hopping terms appear and the phases no longer cancel nicely. We have

$$c_i^\dagger c_j = \sigma_i^+ e^{-i\pi \lambda_i} e^{i\pi \lambda_j} \sigma_j^- = \sigma_i^+ \exp \left\{ \pm i\pi \sum_{k=(i \land j)+1}^{(i \lor j)-1} \sigma_k^+ \sigma_k^- \right\} \sigma_j^-$$

(1.24)

where $\cdot \land \cdot$ and $\cdot \lor \cdot$ are the min and max functions respectively. Because every term in the sum commutes with every other, this can be rewritten as

$$c_i^\dagger c_j = \prod_{k=(i \land j)+1}^{(i \lor j)-1} e^{\pm i\pi \sigma_k^+ \sigma_k^-} \sigma_j^- = \prod_{k=(i \land j)+1}^{(i \lor j)-1} Z_k \sigma_j^- = \sigma_j^+ \prod_{k=(i \land j)+1}^{(i \lor j)-1} Z_k$$

(1.25)

where we’ve used $\sigma^- = (X + iY)/2$, $X^2 = Y^2 = 1$ and $iYX = Z$. For $i-1 \leq j \leq i+1$ we can see this immediately recovers Eqs. 1.22, 1.23.

Putting everything together, our rewritten Hamiltonian is

$$\hat{H}_\sigma = \sum_{i,j=1}^{2N} \frac{\tilde{t}_{ij}}{4} (X_i - iY_i) (X_j + iY_j) \prod_{k=(i \land j)+1}^{(i \lor j)-1} Z_k + \frac{U}{4} \sum_{i=1}^{N} (1 - Z_i)(1 - Z_{i+N}).$$

(1.26)
This can be further simplified by noting that $\tilde{t}_{ij}$ is symmetric by definition (if $i$ and $j$ are neighbors so are $j$ and $i$). Expanding out $(X_i - iY_i)(X_j + iY_j)$ and using $[X_i, Y_j] = 0$ for $i \neq j$ we get $X_iX_j + Y_iY_j + i(X_iY_j - X_jY_i)$. Exchanging $i$ and $j$ gives back $X_iX_j + Y_iY_j - i(X_iY_j - X_jY_i)$. Therefore, in the sum each pair $(i, j)$ and $(j, i)$ will cancel their $XY$ terms, leaving only $XX$ and $YY$ terms. We can thus multiply by two and set $i \leq j$, finally giving,

$$
\hat{H}_\sigma = \sum_{i \leq j = 1}^{2N} \frac{\tilde{t}_{ij}}{2} (X_iX_j + Y_iY_j) \prod_{k=i+1}^{j-1} Z_k + \frac{U}{4} \sum_{i=1}^{N} (1 - Z_i)(1 - Z_{i+N}).
$$

(1.27)

**Trotterization**

Armed with our Hamiltonian in terms of Pauli operators over qubits (Eq. 1.27), we now focus on how to evolve the qubits under the action of this Hamiltonian. Because the Hamiltonian is time independent, the time evolution operator is simply given by the formal solution to the Schrödinger equation (Eq. 1.7), $U(t) = e^{-i\hat{H}t} = e^{-i\sum \hat{H}_\ell t}$.

Unfortunately, not all the terms in our Hamiltonian are mutually commuting, e.g. $[X_iX_j, Z_i] \neq 0$. This means that $e^{-i\sum \hat{H}_\ell t} \neq \prod \hat{H}_\ell$. This is unfortunate because it is typically very difficult to break the unitary $e^{-i\sum \hat{H}_\ell t}$ into any realistic gateset a quantum computer might have. Alternatively, the unitaries $e^{-i\hat{H}_\ell t}$ are much more manageable.

We get around this by using the identities given in Eqs. 1.16, 1.17. For our case, Trotterization takes the form

$$
e^{-i\hat{H}_\sigma t} = \prod_{k=1}^{r} e^{-i\hat{H}_\sigma \Delta t} \quad \text{with} \quad \Delta t = \frac{t}{r}
$$

(1.28)

with which we can make $\Delta t$ arbitrarily small by choosing a large enough $r$. Then we have

$$
e^{-i\hat{H}_\sigma t} = e^{-i\sum \hat{H}_\ell \Delta t} = \prod_{\ell} e^{-i\hat{H}_\ell \Delta t} + O(\Delta t^2).
$$

(1.29)
Which can be made arbitrarily accurate by increasing $r$ to shrink $\Delta t$. This technique is known as Trotterization and is based on the Lie-Trotter formula[29]. More general versions exist using higher order expansions as well as other methods of Hamiltonian simulation unrelated to product formulas, however they are beyond the scope of the current discussion.

**Quantum Gates**

To finally simulate time evolution on a quantum computer, we need to re-express the terms $e^{-i\alpha \hat{H}_\ell}$ where

$$\hat{H}_\ell \in \{1, Z_i, Z_iZ_j, X_iZ_{i+1} \cdots Z_{j-1}X_j + Y_iZ_{i+1} \cdots Z_{j-1}Y_j\}.$$  \hspace{1cm} (1.30)

Because global phases are not physically meaningful, the term where $\hat{H}_\ell = 1$ is the identity and need not be implemented. $\hat{H}_\ell = Z_i$ corresponds, by definition, to an $R_z(\theta) = HR_z(\theta)H$ gate on qubit $i$. $\hat{H}_\ell = Z_iZ_j$ creates the gate $e^{-iaZ_iZ_j}$. This can be implemented as shown in Fig. 1.2a. Finally we have the case where $\hat{H}_\ell = X_iZ_{i+1} \cdots Z_{j-1}X_j + Y_iZ_{i+1} \cdots Z_{j-1}Y_j$. Although not immediately obvious, it is easily checked that this gate is implemented by the gate sequence shown in Fig. 1.2b.

Equipped with these gates, the Hubbard model is then simulated by repeated applying them to build up the unitary $e^{-i\hat{H}t}$ as per Eqs. 1.28 and 1.29. By first preparing the qubits in some desired state $|\psi_0\rangle$ (using a separate protocol not covered here), we then get the time evolved state $|\psi_f\rangle = e^{-i\hat{H}t} |\psi_0\rangle$ as desired.
\[ |q_1\rangle - H - R_x(2\alpha) - H = e^{-i\alpha Z_i Z_j} \]

(a) Quantum circuit for the gate \( e^{-i\alpha Z_i Z_j} \)

\[ |q_i\rangle - H - R_x(\pi/2) - H - R_x(2\alpha) - H - R_x(-\pi/2) - H = e^{-i\alpha (Z_i Z_{i+1} \cdots Z_{j-1} X_j + Y_i Z_{i+1} \cdots Z_{j-1} Y_j)} \]

(b) Quantum circuit for the gate \( e^{-i\alpha (X_i Z_{i+1} \cdots Z_{j-1} X_j + Y_i Z_{i+1} \cdots Z_{j-1} Y_j)} \)

**Figure 1.2:** Quantum circuits for Hubbard terms using basis gates. The two non-trivial unitaries for the Hubbard model using only \( R_x(\theta) \), \( H \), and \( cX \) gates.
2.1 Motivation

In nature, nothing is ever truly isolated from the rest of the universe; every system interacts in some way with its surroundings. This is especially true here on Earth where we do most of our experiments. Whether it’s stray photons, fluctuating magnetic fields, heat transfer, or something else - a perfectly accurate description of any system must account for the dynamics internal to the system itself as well as influences from the systems environment. A theoretical system which is completely isolated (e.g. its the only thing in the universe or it sits in a magical box which protects it completely from outside influence) is called a closed system or isolated system. In contrast, any system which is not closed, i.e. interacts with its surroundings is called an open system.

Clearly because all real-world systems are open, understanding their behavior is important to science. At the same time, open systems are more complex than closed ones by definition; an open system is just a closed system plus environmental influences. This makes their study more challenging. Indeed, a fully accurate description of a system’s environment is tantamount to taking into consideration the entirety of the cosmos. Such an approach is clearly impractical and unnecessarily detailed. The goal in finding useful descriptions of open quantum systems is, like for complex closed systems, to find simplified models of environments and their interactions which
account for observed behavior of interest. Identifying and solving these useful models is difficult, and an active area of scientific inquiry.

In addition to being more technically correct, many systems of interest are fundamentally open in that a large part of their behavior comes from trading energy, information, particles,...etc. with their surroundings. Such systems will be the focus of this thesis. In particular we will consider the behavior of quantum systems which are driven (i.e. we pump energy into the system) and dissipative (i.e. the system may dump energy into or absorb energy from its environment). Such systems are interesting to study for multiple reasons, including but not limited to:

1. Their behavior is poorly understood.

2. They describe physically interesting dynamics that isolated systems cannot (e.g. heating/cooling, depolarization, noise, equilibration,...etc.)

3. Their steady states can be interesting phases of matter (e.g. Bose-Einstein condensates[30], η-condensates[31], superconducting/superfluid states[32], topological phases[33],...etc.).

4. Their steady states may contain yet to be discovered states of matter.

5. Many of these systems can be efficiently simulated on a quantum computer but not on a classical computer (exponential gain in speed and resources).

2.2 Overview

The majority of work done to date in both quantum mechanics and quantum computing has been done for closed quantum systems, largely due to the fact that they are much simpler than their open counterparts. Closed quantum systems follow Hamiltonian dynamics also known as coherent dynamics, or unitary dynamics. The state of
a closed quantum system at all times is fully determined by its Hamiltonian $\hat{H}$ and state at any time $t$, $|\psi(t)\rangle$, by the Schrödinger equation ($\hbar = 1$ throughout)

$$i\partial_t |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$ (2.1)

In contrast, an open quantum system does follow the Schrödinger equation, its dynamics are not represented by a Hamiltonian, it does not evolve in a unitary fashion, and the state at a time $t$ only determines its state for times $t' \geq t$. Despite these differences, we can use the well established formalism for closed quantum systems to investigate open quantum systems. We do this by realizing that an open system is a subsystem of a larger closed system. Simply consider both the environment and the open system together as one larger, closed quantum system. This larger system, as a whole, behaves as we expect. What we are interested in is how the subsystem (our open system) behaves as a part of a larger closed system. We’ll find that these open systems are not adequately described using standard pure states (e.g. $|\psi(t)\rangle$ in Eq. 2.1) and we’ll need to use the more general density operator to describe the states of an open quantum system. To motivate this we begin by looking at a simple composite (bipartite) quantum system.

2.3 Density Operators

Motivation for this section comes in part from the contents of Ref. [34]. As the simplest example, let’s consider 2 identical two-level quantum systems (e.g. 2 qubits, 2 atoms with 2 energy levels each, 2 spin-1/2 systems,...etc.). Let $A$ denote the first system with basis states $|0\rangle_A$ and $|1\rangle_A$. Likewise let $B$ denote the second system with basis states $|0\rangle_B$ and $|1\rangle_B$. The basis for our composite space, $AB$, is then given by states of the form $|i\rangle_A \otimes |j\rangle_B \equiv |ij\rangle$ where $i, j \in \{0, 1\}$. To further motivate the connection to open quantum systems, let’s say that we have full access to $A$ (system of interest)
and no access to $B$ (environment). This means that we can manipulate and make measurements on $A$ but we cannot directly influence or measure $B$. We know that the composite system, $AB$, will obey the Schrödinger equation. However, what can we say about how $A$ alone behaves when it is a part of $AB$?

Let’s say $AB$ is in the pure state $|\psi\rangle_{AB} = \alpha |00\rangle + \beta |11\rangle$. What is the state of $A$? To answer this let’s rewrite this using vector notation with

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

so that

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \rightarrow |\psi\rangle_{AB} = \begin{pmatrix} \alpha \\ 0 \\ 0 \\ \beta \end{pmatrix}$$

(2.3)

So now we’re looking for $|\psi\rangle_A$ such that

$$|\psi\rangle_A \otimes |\psi\rangle_B = |\psi\rangle_{AB} \rightarrow \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} \otimes \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix} = \begin{pmatrix} \alpha \\ 0 \\ 0 \\ \beta \end{pmatrix}$$

(2.4)

This has no solution as the first and last line imply none of $a, b, c, d$ is 0 while the middle two imply at least 2 are 0. This in turn means that $A$ alone has no definitive state, only $AB$ does. This is equivalent to saying that $A$ and $B$ are entangled, or correlated. We cannot specify the state of $A$ independent from the state of $B$. However, we have no access to $B$ and thus limited information about $AB$. We would like a way to talk about the state of $A$ even when it not in a pure state, as above.
So what can we say about $A$? Well let’s say we want to measure an observable over $A$ say $M_A$. When we apply $M_A$ to $A$, we implicitly apply the identity $I$ to $B$ and our measurement is $M_{AB} = M_A \otimes I_B \equiv M \otimes I$ [34]. The expectation value of this observable is

$$\langle M_{AB} \rangle = \langle \psi | M \otimes I | \psi \rangle = (\alpha^* \langle 00 | + \beta^* \langle 11 |) [M \otimes I] (\alpha | 00 \rangle + \beta | 11 \rangle)$$ \hspace{1cm} (2.5)$$

Expanding this out gives

$$\langle M_{AB} \rangle = \langle M | I \rangle = \langle M \rangle = |\alpha|^2 \langle 0 | M | 0 \rangle + |\beta|^2 \langle 1 | M | 1 \rangle$$ \hspace{1cm} (2.6)$$

where we’ve used $\langle i | i \rangle = \delta_{ij}$. Notice that this is exactly what we’d get if we followed the following protocol.

1. Prepare $A$ in a pure state such that with probability $|\alpha|^2$ we have $|\psi\rangle_A = |0\rangle$
   and with probability $|\beta|^2$ we have $|\psi\rangle_A = |1\rangle$

2. Measure $M$

3. Repeat

So while we cannot describe $A$ with any “pure” state, we can describe $A$ as a “mixed” state which is a mixture or ensemble of the pure state $|0\rangle$ with probability $p_0 = |\alpha|^2$ and $|1\rangle$ with probability $p_1 = |\beta|^2$. One may argue that we don’t know if it’s really the case that $A$ is a mixture of pure states, but no experiment can distinguish the two cases so that argument is better had in the philosophy department.

In general we can describe a mixed state as an ensemble of states with associated probabilities i.e. $\{|i\rangle : p_i\}$. So for this example we could describe $A$ with the ensemble $\{|0\rangle : |\alpha|^2, |1\rangle : |\beta|^2\}$. This ensemble notation is a very clumsy way of dealing with a mixed state and it would be really painful to try to actually do computations with it. There is a much cleaner way of representing mixed states, and it uses the density
operator or, when given a basis, the density matrix \( \rho \) to represent the state. To define the density matrix, first note that (2.6) can be rewritten in the following way (recall \( \text{Tr} \{ A \} = \sum_i \langle i | A | i \rangle \))

\[
\langle M \rangle = |\alpha|^2 \langle 0 | M | 0 \rangle + |\beta|^2 \langle 1 | M | 1 \rangle = \text{Tr} \left\{ M \left( |\alpha|^2 |0\rangle\langle 0 | + |\beta|^2 |1\rangle\langle 1 | \right) \right\}
\]

(2.7)

We denote

\[
\rho_A = |\alpha|^2 |0\rangle\langle 0 | + |\beta|^2 |1\rangle\langle 1 | = p_0 |0\rangle\langle 0 | + p_1 |1\rangle\langle 1 | = \begin{pmatrix} p_0 & 0 \\ 0 & p_1 \end{pmatrix} \rightarrow \langle M \rangle = \text{Tr} \{ M \rho_A \}
\]

(2.8)

the density matrix of \( A \). This object contains all of the information we have about \( A \). In general, an ensemble of states \( \{ |i \rangle : p_i \} \) can be written as the density operator

\[
\rho = \sum_i p_i |i\rangle\langle i |
\]

A few remarks are in order. Firstly, knowing the density matrix of each subsystem is insufficient to reconstruct the state of the full system. Information about the entanglement between subsystems is lost. Next, it is important to note that a mixed state is fundamentally different from a superposition of the states in the ensemble. In a superposition we have a relative phase between each state in the sum whereas here we have no information about the relative phases (or better yet, such information does not exist). A superposition of pure states is itself a pure state - a mixed state is different.

It is not too difficult to generalize the above to discussion to the case where \( A \) and \( B \) are general Hilbert spaces instead of just 2-level systems. Then for \( \mathcal{H}_A \) having orthonormal basis \( \{ |i \rangle \} \) and \( \mathcal{H}_B \) having orthonormal basis \( \{ |j \rangle \} \) the composite system \( \mathcal{H}_{AB} \) has orthonormal basis \( \{ |i \rangle \otimes |j \rangle \} \equiv \{ |ij \rangle \} \). A general state for the composite system is then

\[
|\psi\rangle = \sum_{i,j} \alpha_{ij} |ij \rangle \quad \text{with} \quad \sum_{i,j} |\alpha_{ij}|^2 = 1
\]

(2.9)
To get the density matrix of $H_A$, we take the partial trace over $H_B$. This can loosely be thought of as averaging over all the possible configurations of $H_B$ to just leave information about $H_A$. Formally

$$\rho_A = \text{Tr}_B \{ \rho_{AB} \} = \text{Tr}_B \{ |\psi\rangle\langle\psi| \} = \text{Tr}_B \left\{ \sum_{i,j,i',j'} \alpha_{ij} \alpha_{i'j'}^* |i'j'\rangle\langle ij| \right\} = \sum_{i,j,i',j,k} \alpha_{ij} \alpha_{i'j'}^* B(k | i'j' \rangle \langle ij| k) = \sum_{k,i,i'} \alpha_{ik} \alpha_{i'k}^* |i'\rangle\langle i| = \sum_{i,j} p_{ij} |i\rangle\langle j| \quad \text{(2.10)}$$

where $p_{ij} = \sum_{k} \alpha_{ik} \alpha_{ik}^*$. Clearly $\rho_A = \rho_A^\dagger$ by (2.11) so $\rho_A$ is Hermitian and so it can be diagonalized by a suitable choice of basis. This implies that w.l.o.g. we can rewrite (2.11) taking $i = j$ and we find

$$\rho_A = \sum_i p_{ii} |i\rangle\langle i| \equiv \sum_i p_i |i\rangle\langle i| \quad \text{(2.12)}$$

Where $p_i = \sum_k \alpha_{ik} \alpha_{ik}^* = \sum_k |\alpha_{ik}|^2 > 0$. From this form a few things are apparent. $\rho_A$ is positive semi-definite and $\text{Tr} \rho_A = 1$. Furthermore if $\rho_A$ describes a pure state then $\rho_A = \rho_A^2$ or to put it another way, the sum contains a single term or one of the $p_i = 1$ and the rest are 0. Note that in this case, the density operator is just a projector that projects onto said pure state. For a mixed state the density operator is a weighted sum of projectors onto the different states in the ensemble.

One thing to be aware of here is that performing an operation on a density matrix requires performing said operation on both sides of $\rho$. This is simple to see but easy to forget. If want to perform some operation, $\hat{O}$, on a pure state, $|\psi\rangle$, we simply have $|\psi'\rangle = \hat{O} |\psi\rangle$. If we construct the density matrix for $|\psi\rangle$ we have $\rho = |\psi\rangle\langle\psi|$. So under the action of $\hat{O}$, $\rho' = |\psi'\rangle\langle\psi'| = \hat{O} |\psi\rangle\langle\psi| \hat{O}^\dagger = \hat{O} \rho \hat{O}^\dagger$. 


2.3.1 Spin 1/2 Example

To explicitly see this difference, consider a spin-1/2 particle with basis states being the eigenvectors of $\sigma_z = \{|\uparrow\rangle, |\downarrow\rangle\}$. Take $|\psi\rangle = 1/\sqrt{2}(|\uparrow\rangle + |\downarrow\rangle)$ which is an equal superposition of $|\uparrow\rangle$ and $|\downarrow\rangle$. A mixed state with an equally weighted ensemble of $|\uparrow\rangle$ and $|\downarrow\rangle$ is

$$\rho_m = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) = \frac{1}{2}I. \quad (2.13)$$

Contrast this with the density matrix for the pure state $|\psi\rangle$

$$\rho_\psi = |\psi\rangle\langle\psi| = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|) \quad (2.14)$$

In both these cases we have $\langle\sigma_z\rangle = 0$ i.e. we have a 50/50 chance of up or down. However, consider $\langle\sigma_x\rangle$. The pure state $|\psi\rangle$ is the $+1$ eigenstate of $\sigma_x$ and so $\langle\sigma_x\rangle_\psi = 1$ as we can confirm

$$\langle\sigma_x\rangle_\psi = \text{Tr} \{\sigma_x \rho_\psi\} = \text{Tr} \{\rho_\psi\} = 1 \quad (2.15)$$

while

$$\langle\sigma_x\rangle_\rho = \text{Tr} \{\sigma_x \rho\} = \frac{1}{2} \text{Tr} \{\sigma_x I\} = 0 \quad (2.16)$$

This emphasizes that mixed states are fundamentally different from superpositions.

2.4 Density Operator Evolution

As we saw previously, in a closed quantum system, a pure state evolves according to the Schrödinger equation (Eq. 2.1), which can easily be extended to mixed states and density operators. Consider the density matrix with eigenstates indexed by $k$ : $\rho(t) = \sum_k p_k |\psi_k(t)\rangle\langle\psi_k(t)|$. Its time evolution follows directly from the Schrödinger equation.

$$\dot{\rho}(t) = \frac{\partial \rho(t)}{\partial t} = \sum_k p_k \left[ |\psi_k(t)\rangle \frac{\partial \langle\psi_k(t)|}{\partial t} + \frac{\partial |\psi_k(t)\rangle}{\partial t} \langle\psi_k(t)| \right] \quad (2.17)$$
Substituting in $\frac{\partial}{\partial t} |\psi(t)\rangle = -iH(t) |\psi(t)\rangle$ and $\frac{\partial}{\partial t} \langle \psi(t) | = iH(t) \langle \psi(t) |$ from the Schrödinger equation we get

$$\dot{\rho}(t) = \sum_k p_k |\psi_k(t)\rangle\langle \psi_k(t) | iH(t) - iH(t) \sum_k p_k |\psi_k(t)\rangle\langle \psi_k(t) | = (2.18)$$

$$i [\rho(t) H(t) - H(t) \rho(t)] = [i[\rho(t), H(t)]] (2.19)$$

Where $[A, B] \equiv AB - BA$ is the commutator. This equation, known as the Liouville-Von Neumann equation[35], describes the coherent evolution of the density matrix of a closed system. In terms of the time evolution operator, $U(t)$, defined by $|\psi(t)\rangle = U(t) |\psi(0)\rangle$ we have

$$\rho(t) = |\psi(t)\rangle\langle \psi(t) | = U(t) |\psi(0)\rangle\langle \psi(0) | U^\dagger(t) = U(t) \rho(0) U^\dagger(t) (2.20)$$

However, under the influence of an external environment (i.e. an open system) a quantum system will evolve decoherently. This decoherent evolution is non-unitary in general and cannot be described by the above formalism. For example, measurement is an example of non-unitary operation due to a system interacting with its environment. It is nonetheless always possible to recast an open system as an extended closed system by considering the system of interest, together with the environment as a single larger system which obeys unitary evolution. So in developing the formalism behind open quantum systems, a natural starting place is to consider system we wish to study together with its environment as one large closed system.

2.5 Kraus Operators

Motivation for this section comes in part from the contents in Refs. [34, 36]. Let the system be in Hilbert space $\mathcal{H}_S$ and the environment be in $\mathcal{H}_E$ so that the joint system is in $\mathcal{H}_{SE} = \mathcal{H}_S \otimes \mathcal{H}_E$ Assume that the environment and the system were unentangled
at some time in the past (e.g. before they started interacting) and denote this time \( t = 0 \). Then their combined density matrix may be written \( \rho(0) = \rho_S(0) \otimes \rho_E(0) \) to save space, drop the 0s i.e. \( \rho(0) \equiv \rho = \rho_S \otimes \rho_E \). For simplicity and w.l.o.g. assume the environment was in a pure state at time 0 and denote this state \( |0\rangle \) such that \( \rho_E \equiv |0\rangle \langle 0| \). Note that this loses no generality because a mixed state can be purified to a pure state by enlarging its state space[34]. Denote the time evolution operator for the joint system as \( U(t) \) so that \( \rho(t) = U(t)(\rho_S \otimes |0\rangle \langle 0|)U^\dagger(t) \). To isolate the system we take the partial trace over the environment, just as we did to define the density matrix above.

\[
\rho_S(t) = \mathrm{Tr}_E(\rho(t)) = \sum_i \langle i | U(t)(\rho_S \otimes |0\rangle \langle 0|)U^\dagger(t) | i \rangle = \sum_i \langle i | U(t) | 0 \rangle \langle 0 | U^\dagger(t) | i \rangle
\]

(2.21)

Where \( \{ |i\rangle \} \) is an orthonormal basis for the environment. Note that \( K_i(t) = \{ \langle i | U(t) | 0 \rangle \} \) are operators acting on \( \mathcal{H}_S \), not scalars, since \( U(t) \) acts on both \( \mathcal{H}_E \) and \( \mathcal{H}_S \) while \( \{ |i\rangle \} \) and \( |0\rangle \) are states in \( \mathcal{H}_E \) only. We call these operators the **Kraus operators** and they evolve the system forward in time.

\[
\rho_S(t + \Delta t) = \sum_i K_i(\Delta t)\rho_S(t)K_i^\dagger(\Delta t) \quad \text{with} \quad \sum_i K_i^\dagger K_i = 1
\]

(2.22)

Kraus operators are a completely general way to deal with quantum dynamics. In the case where there is only one Kraus operator, \( K_0 \neq 0, K_{i \neq 0} = 0 \), then by their completeness relation \( (\sum_i K_i^\dagger K_i = 1) \) we see that the system evolves in a unitary fashion. Furthermore since \( K_0(t) = \langle 0 | U(t) | 0 \rangle \) we see that the environment remains forever in its initial state so the system and the environment don’t interact. This means that \( K_0(t) = U(t) \) and (2.22) reduces to (2.20).

Conversely, when there are multiple non-zero Kraus operators, none of them may be unitary by the same completeness relation. This means that we now have dynamics for \( S \) that do not follow the unitary prescription of the Schrödinger equation. What
we have instead is a “map” or “channel” that when applied to $\rho_S$ evolves it forward in time by $\Delta t$ i.e. $\rho_S \mapsto \sum_i K_i(\Delta t)\rho_S K_i^\dagger(\Delta t)$ in much the same way the standard time evolution operator works: $|\psi\rangle \mapsto U(\Delta t)|\psi\rangle$. It is clear from the derivation that this Kraus map will always transform a proper density matrix into a proper density matrix. This means that it is a map which is: trace preserving, Hermiticity preserving, completely positive, and linear.

It is often unfeasible to actually analyze the full $U$ due to the shear size of, and/or lack of knowledge about, the environment. But if we are not interested in the environment itself, then it is sufficient to model the environment as a simpler system as long as the resulting $K_i$ are the same. In other words, we don’t care about the microscopic details of the environment - we only care about its influence on the system. This means that we can model the evolution of a system under the influence of a complicated environment using a simplified environmental model. This is sweeping a lot of difficulty under the rug as finding such an accurate model environment is not a simple task and almost always introduces approximations into the problem.

In fact, since the Kraus operators describe the dynamics of our open quantum systems exactly and generally, and since we know that the dynamics of quantum systems are in general very difficult to solve, this correctly suggests that the process of find the Kraus operators for a given system/environment pair is a difficult problem. Indeed finding the Kraus operators is tantamount to solving the system in full. For most systems this is not feasible. A variety of approximations can be introduced to get approximate solutions to such systems. An example will be given below where we make the approximation that the environment “forgets” what’s happened to it after each time interval $\Delta t$. We’ll see later on that it’s actually very common to use this approximation and take the limit $\Delta t \to 0$. This is the Markovian approximation.
2.5.1 Excited Atom Example

For concreteness let’s take our system of interest to be a single atom which may be in its ground state $|0\rangle_A$ or its first excited state $|1\rangle_A$. We neglect the unitary dynamics and focus solely on the dissipative dynamics (i.e. we take the Hamiltonian $H = 0$). This atom is in some environment with which it may trade energy. We don’t know the specifics of the environment but we’ll stipulate that, over a small time interval $\Delta t$, the environment can absorb a photon from the atom or the atom can absorb a photon from the environment. We’ll neglect higher order processes e.g. the atom absorbs then emits a photon in a single time step; this is a good approximation for small $\Delta t$/small rate of system-environment interactions. We’ll also assume the environment goes back to its original state after each time step $\Delta t$; this is a good approximation for large environments. The possible processes are then as follows

1. The atom is initially in $|0\rangle_A$, after some time $\Delta t$ it will
   
   (a) Interact with the environment and be excited to $|1\rangle_A$ with probability $p_e$
   
   (b) Not interact with the environment remain in $|0\rangle_A$ with probability $1 - p_e$

2. The atom is initially in $|1\rangle_A$, after some time $\Delta t$ it will

   (a) Interact with the environment and decay to $|0\rangle_A$ with probability $p_d$

   (b) Not interact with the environment remain in $|1\rangle_A$ with probability $1 - p_d$

So no matter how complicated the “true” environment may be, we can model these possibilities with a two qubit (i.e. has only 4 states) environment.

$$
|01\rangle_E |0\rangle_A \xmapsto{U} \sqrt{p_e} |00\rangle_E |1\rangle_A + \sqrt{1 - p_e} |01\rangle_E |0\rangle_A
$$

$$
|01\rangle_E |1\rangle_A \xmapsto{U} \sqrt{p_d} |11\rangle_E |0\rangle_A + \sqrt{1 - p_d} |01\rangle_E |1\rangle_A
$$

(2.23)
It should be obvious that the probabilities are time-dependent, since the longer we wait the higher chance of an interaction. For this reason, it is often desirable to work with *rates* instead of probabilities. For small $\Delta t$ we have $p \approx \gamma \Delta t$ where $\gamma$ is the interaction rate. Another way to think of this is that $\gamma$ is a measure of how strongly coupled the system and the environment are. Weak coupling $\rightarrow$ small $\gamma \rightarrow$ infrequent interactions, and vice versa for strong coupling. This lets us find the Kraus operators according to (2.22)

$$K_0(\Delta t) = \langle 01|U|01 \rangle = \begin{pmatrix} \sqrt{1-\gamma_e \Delta t} & 0 \\ 0 & \sqrt{1-\gamma_d \Delta t} \end{pmatrix}$$

$$K_1(\Delta t) = \langle 00|U|01 \rangle = \begin{pmatrix} 0 & 0 \\ \sqrt{\gamma_e \Delta t} & 0 \end{pmatrix}$$

$$K_2(\Delta t) = \langle 11|U|01 \rangle = \begin{pmatrix} 0 & \sqrt{\gamma_d \Delta t} \\ 0 & 0 \end{pmatrix}$$

The interpretation of the Kraus operators is now obvious. $K_0$ describes the evolution when no transition occurs, which can be seen from its diagonal form. $K_1$ describes the excitation of the ground state and $K_2$ describes the decay of the excited state.

We begin with an arbitrary density matrix for the system

$$\rho(0) = \begin{pmatrix} \rho_{00} & \rho_{10} \\ \rho^*_{10} & 1 - \rho_{00} \end{pmatrix}$$

(2.25)

then iterate (2.24) to see how the system behaves.

$$\rho(\Delta t) = \begin{pmatrix} \rho_{00} \left(1 - \gamma_d \Delta t - \gamma_e \Delta t \right) + \gamma_d \Delta t & \rho_{10} \sqrt{(1 - \gamma_d \Delta t)(1 - \gamma_e \Delta t)} \\ \rho^*_{10} \sqrt{(1 - \gamma_d \Delta t)(1 - \gamma_e \Delta t)} & 1 - \rho_{00} \left(1 - \gamma_d \Delta t - \gamma_e \Delta t - \gamma_d \Delta t \right) \end{pmatrix}$$

(2.26)

We can immediately see that the trace is trivially 1. It’s not hard to convince yourself that as long as $\rho(0)$ was a valid density matrix and $p_i = \gamma_i \Delta t$ are valid probabilities
(0 \leq p_i \leq 1) then \( \rho(\Delta t) \) is also still a valid density matrix (unit trace, Hermitian) - as it must be by the properties of Kraus maps.

We are now left with a recurrence relation for each element of the density matrix. The off-diagonal ones are trivial and just decay like \([(1 - \gamma_d \Delta t)(1 - \gamma_e \Delta t)]^{t/2\Delta t} \). The on-diagonals reduce to a single equation since we know the trace must be 1. So we are left to solve \( \rho_{00}(t + \Delta t) = \rho_{00}(t)(1 - \gamma_d \Delta t - \gamma_e \Delta t) + \gamma_d \Delta t \) which gives

\[
\rho_{00}(t) = \frac{((\rho_{00} - 1)\gamma_d + \rho_{00}\gamma_e) (1 - \Delta t (\gamma_d + \gamma_e))^{t/\Delta t} + \gamma_d}{\gamma_d + \gamma_e} \tag{2.27}
\]

This can be simplified by defining \( \Gamma = \gamma_d + \gamma_e, \Gamma_i = \gamma_i/\Gamma \) and substituting \( \rho_{11} = 1 - \rho_{00} \) which gives

\[
\rho_{00}(t) = \Gamma_d + (1 - \Gamma \Delta t)^{t/\Delta t} (\rho_{00} - \Gamma_d) \quad \text{and} \quad \rho_{11}(t) = \Gamma_e + (1 - \Gamma \Delta t)^{t/\Delta t} (\rho_{11} - \Gamma_e) \tag{2.28}
\]

In the limit \( \Delta t \to 0 \) we have

\[
\rho(t) = \begin{pmatrix}
\Gamma_d + e^{-\Gamma t} (\rho_{00} - \Gamma_d) & e^{-\Gamma t/2} \rho_{10} \\
e^{-\Gamma t/2} \rho_{10}^* & \Gamma_e + e^{-\Gamma t} (\rho_{11} - \Gamma_e)
\end{pmatrix} \tag{2.29}
\]

And in the limit \( t \to \infty \) we have

\[
\rho(t \gg 1) = \begin{pmatrix}
\Gamma_d & 0 \\
0 & \Gamma_e
\end{pmatrix} = \frac{1}{\gamma_d + \gamma_e} \begin{pmatrix}
\gamma_d & 0 \\
0 & \gamma_e
\end{pmatrix} \tag{2.30}
\]

Which is exactly what we would expect; an equilibrium is established between the decay and excitation rates. In an infinitesimal time-step \( dt \), the ground state population loses \( \gamma_e \gamma_d / (\gamma_d + \gamma_e) \) to excitations but gains \( \gamma_d \gamma_e / (\gamma_d + \gamma_e) \) from decays. Since these two are equal, this must be the steady state.

### 2.6 Master Equation

It is often convenient to work with the evolution of a system in terms of a differential equation, like we had with the Liouville-Von Neumann equation (2.19). So it is natural
to ask if such a description of decoherent evolution is possible. It turns out that the
answer is that it is not always possible, but that it is possible for a wide variety of
situations\[37\]. The technical conditions for when a given linear map (read Kraus map)
may be expressed by a differential equation are beyond the scope of this thesis but
are discussed in detail in Andersson’s paper\[37\]. We call such a differential equation
a master equation.

The general master equation is the so called Nakajima-Zwanzig Equation which
encodes information about the past in a “memory kernel”. Here we will restrict our
discussion to the simple yet widely useful case of Markovian dynamics. Markovian
dynamics are local in time so that \( \rho(t + dt) \) is completely determined by \( \rho(t) \). This
implies that the environment has no memory i.e. the evolution of the system is inde-
pendent of what has happened to the environment in the past. This is rarely truly
the case for any real physical system because we’d expect that any information trans-
ferred from the system to the environment can be transferred back, at a later time,
from the environment to the system. However, it is an accurate approximation to
reality when the timescale of the memory is much smaller than the timescale of the
dynamics in which we’re interested\[36\].

Under the Markovian approximation the master equation will take a special form
known as the Lindblad Equation which features the Lindbladian superoperator \( \mathcal{L}[\rho] \) as
the generator of infinitesimal time evolution in much the same way the Hamiltonian
operator is the generator of infinitesimal coherent time evolution in the Schrödinger
equation. Compare (for the time independent case)

- Lindblad Equation \( \dot{\rho} = \mathcal{L}[\rho] \rightarrow \rho(t) = e^{\mathcal{L}t}[\rho(0)] \)
- Schrödinger Equation \( \dot{\psi} = -iH \psi \rightarrow |\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle \)
To find an expression for $\mathcal{L}$ we begin with the Kraus representation for infinitesimal $dt$

$$\rho(t + dt) = \sum_i K_i(dt)\rho(t)K_i^\dagger(dt) = \rho(t) + dt\dot{\rho}(t) = \rho + dt\dot{\rho} \quad (2.31)$$

Recall the definition of the Kraus operators $K_i(t) = \langle i| U(t) |0 \rangle$ which describes a transition from state $|0\rangle$ to $|i\rangle$. So for $K_0(dt)$ we have no transition which can happen by either 1) transitioning to any $|i\rangle$ and back or 2) coherently evolving by $U(dt) = e^{-iHdt} \approx 1 - iHdt$. So we may write $K_0 = \mathbb{1} - iHdt + D$ where $D \propto \sum_{i>0} K_i K_i^\dagger$.

For $K_i(dt)$ we may write $K_i = \sqrt{dt}L_i$. This can be motivated by considering the form of $K_0$, (2.31), and/or the completeness relation for the $K_i$'s. Or alternatively by considering the following. Each $K_i(\Delta t)$ describes a transition of the system, induced by the environment, occurring with probability $p_i$ over a time $\Delta t$. Since we are in the Markovian limit, the $p_i$'s must be time independent. Together this implies that $p_i \propto \Delta t \rightarrow K_i \rho K_i^\dagger \propto dt \rightarrow K_i \propto \sqrt{dt}$. From here we use the completeness relation to get the constant of proportionality in $D$.

$$\mathbb{1} = \sum_i K_i K_i^\dagger = (\mathbb{1} - iHdt + D)(\mathbb{1} + iHdt + D) + \sum_{i>0} K_i K_i^\dagger = \mathbb{1} + 2D + \sum_{i>0} K_i K_i^\dagger + O(dt^2) \quad (2.32)$$

Dropping higher order terms in $dt$ and inserting the definition $K_i = \sqrt{dt}L_i$ we find

$$D = -\frac{dt}{2} \sum_{i>0} L_i L_i^\dagger \quad (2.33)$$

Plugging this back into (2.31) and dropping higher order terms, we see

$$dt\dot{\rho} = i\rho[H] + \{\rho, D\} + \sum_{i>0} K_i \rho K_i^\dagger + O(dt^2) \quad (2.34)$$

Where $\{\cdot, \cdot\}$ is the anti-commutator. Plugging in for $D$ and $K_i$ gives

$$\dot{\rho} = \mathcal{L}[\rho] = i[H] + \sum_i \left( L_i \rho L_i^\dagger - \frac{1}{2} \{\rho, L_i^\dagger L_i\} \right) \quad (2.35)$$
The difficulty of finding the Kraus operators has now been transferred to finding the Lindblad operators \( \{ L_i \} \) (as well as solving the differential equation). However, as generators of infinitesimal time evolution (instead of generating the full time evolution) they are usually simpler and less numerous than the Kraus operators. From the two boxed expressions above for \( K_0/K_i \), finding the Lindblad operators gives us approximate Kraus operators accurate to order \( O(dt^2) \). These operators may be found from considering the microscopics of the system/environment under study from the Kraus operators directly or they may be selected a priori and used to investigate the system they describe.

2.6.1 Excited Atom Example Revisited

Let’s revisit the example we solved using the Kraus operators above. We may immediately use the definitions for the Lindblad operators above to get

\[
L_1 = \frac{K_1(dt)}{\sqrt{dt}} = \frac{1}{\sqrt{dt}} \begin{pmatrix} 0 & 0 \\ \sqrt{\gamma_e dt} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ \sqrt{\gamma_e} & 0 \end{pmatrix} \quad \text{and} \quad L_2 = \begin{pmatrix} 0 & \sqrt{\gamma_d} \\ 0 & 0 \end{pmatrix} \tag{2.36}
\]

Combined with the fact that we are taking the Hamiltonian to be 0 for this particular example, we get our Lindblad equation as (invoking unit trace and Hermiticity)

\[
\begin{pmatrix} \dot{\rho}_{00} & \dot{\rho}_{01} \\ \dot{\rho}_{10} & \dot{\rho}_{11} \end{pmatrix} = \begin{pmatrix} \gamma_d - (\gamma_e + \gamma_d)\rho_{00} & -\frac{1}{2}(\gamma_d + \gamma_e)\rho_{10} \\ -\frac{1}{2}(\gamma_d + \gamma_e)\rho_{10}^{\ast} & 1 - \gamma_d + (\gamma_e + \gamma_d)\rho_{00} \end{pmatrix} \tag{2.37}
\]

Which we see is exactly what we’d get from (2.26) by taking \( \dot{\rho} = \lim_{\Delta t \to 0} \frac{\rho(\Delta t) - \rho(0)}{\Delta t} \).

Solving this differential equation, again using \( \Gamma = \gamma_d + \gamma_e, \Gamma_i = \gamma_i/\Gamma \) and substituting \( \rho_{11} = 1 - \rho_{00} \) gives

\[
\rho(t) = \begin{pmatrix} \Gamma_d + e^{-\Gamma t}(\rho_{00} - \Gamma_d) & e^{-\Gamma t/2}\rho_{10} \\ e^{-\Gamma t/2}\rho_{10}^{\ast} & \Gamma_e + e^{-\Gamma t}(\rho_{11} - \Gamma_e) \end{pmatrix} \rightarrow \rho(t \gg 1) = \begin{pmatrix} \Gamma_d & 0 \\ 0 & \Gamma_e \end{pmatrix} \tag{2.38}
\]

Which exactly matches (2.29) and (2.30)
This chapter is intended as a practical guide for those who wish to run algorithms on NISQ devices and in particular IBM’s devices. In order to successfully run protocols on noisy intermediate scale quantum (NISQ) devices a bit of finesse is required. This involves being aware of the types of errors which can occur, techniques to mitigate such errors, and which types and levels of error can be tolerated.

3.1 Errors in NISQ Devices

Current quantum devices are made of qubits which are subject to a variety of errors and use control mechanisms which implement imperfect gates. Together these errors severely limit the scope and scale of computations which can be run on currently available devices. Qubits are subject to uncontrollable physical processes arising from interactions with their local environment and/or with neighboring qubits. Additionally, the control mechanisms to implement gates have imperfections causing errors which compound as the computation is carried out.

In this section, we will describe the most common sources of errors encountered when running on actual quantum hardware. In the next section, we will discuss some techniques and approaches to help mitigate these errors to increase the chances of successfully executing a quantum computation on NISQ hardware. It is widely believed that eventually quantum computers will be fault tolerant, due to error correction[38],
hopefully rendering this chapter moot. However, fault tolerant quantum computation appears not to be on the near horizon, necessitating the effective use of NISQ hardware.

3.1.1 Superconducting Qubits

All of IBM’s devices use superconducting qubits. Superconducting qubits are essentially a quantum harmonic oscillator (QHO), built from a superconducting LC circuit. The state $|0\rangle$ is then simply the ground state of the QHO and the $|1\rangle$ state is the first excited state. However, recall that the QHO has an infinite ladder of equally spaced energy states. This equal spacing is unacceptable for building qubits, since we need to be able to drive the $|0\rangle \leftrightarrow |1\rangle$ transition without driving $|1\rangle \leftrightarrow |2\rangle$, $|2\rangle \leftrightarrow |3\rangle$, ...etc. This is accomplished by replacing the linear inductor in the LC circuit with a Josephson-junction[39]. This non-linear, dissipationless circuit element adds anharmonicity to the "harmonic" oscillator such that individual transitions become addressable. A superconducting qubit with a Josephson-junction is referred to as a transmon qubit.

Gates are implemented by hitting the transmon with microwave pulses. The specifics of how this is implemented goes beyond the scope of this thesis and more details can be found in Refs. [39, 40]. There is one detail I would like to draw attention to since it is important for understanding and avoiding error sources. The effective Hamiltonian of an isolated transmon is[39]

$$\hat{H} = \frac{\omega}{2} Z \quad \text{with} \quad \frac{\omega}{2\pi} \sim 5\text{GHz.}$$

This means the qubit is constantly precessing about the $\hat{z}$ axis of the Bloch sphere with frequency $\omega$. I.e. after a time $t$, $|\psi\rangle = a|0\rangle + b|1\rangle$ becomes $|\psi\rangle = a|0\rangle + e^{i\omega t/2} b|1\rangle$. Actual driving pulses must account for this extra phase and the software generating
the pulses subtracts the calculated phase. This means that IBM can implement $R_z(\theta)$ gates entirely in software, simply by adjusting the phase of the next pulse. It also means that if the frequency of the qubit drifts or is miscalibrated, then pulses will have the wrong phases on them - leading to errors which may become significant for long circuits. Other commons sources of errors are as follows.

3.1.2 Amplitude Damping

Amplitude damping is a single-qubit error which arises from energy exchange between the qubit and its environment which drives $|0\rangle \leftrightarrow |1\rangle$ transitions. Because $|1\rangle$ is the excited state, it emits energy into its surroundings when relaxing into the $|0\rangle$ states. Conversely, because $|0\rangle$ is the ground state, it absorbs energy from the environment to transition to $|1\rangle$. These interactions arise due to stochastic charge noise or quasiparticle tunneling[39]. Typical temperatures inside an IBM quantum device is on the order of 10mK ($\sim 1 \mu eV$). Combined with the fact that the level splitting between $|0\rangle$ and $|1\rangle$ is on the order of 30GHz ($\sim 20 \mu eV$) we expect, and indeed observe, that excitations from $|0\rangle$ to $|1\rangle$ are exponentially suppressed and only relaxation from $|1\rangle$ losing its energy to the cold environment need to be considered. Thus the amplitude damping channel “damps" the amplitude of the $|1\rangle$ state, relaxing the system toward $|0\rangle$.

The Kraus operators for the amplitude damping channel $E_x$, in terms of the decay rate $\Gamma_1$, on a single qubit are:

$$K^x_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{e^{-\Gamma_1 t}} \end{pmatrix} = \left( \frac{I+Z}{2} + \sqrt{e^{-\Gamma_1 t}} \frac{I-Z}{2} \right)$$

$$K^x_1 = \begin{pmatrix} 0 & \sqrt{1-e^{-\Gamma_1 t}} \\ \sqrt{1-e^{-\Gamma_1 t}} & 0 \end{pmatrix} = \sqrt{1-e^{-\Gamma_1 t}} \left( \frac{X+iY}{2} \right).$$

(3.2)
Applying these to a generic density matrix $\rho$ gives

$$\rho = \begin{pmatrix} a & b \\ b^* & 1-a \end{pmatrix} \mapsto E_x(\rho) = \begin{pmatrix} a + (1-a) \left(1-e^{-\Gamma_1 t}\right) & be^{-\Gamma_1 t/2} \\ b^* e^{-\Gamma_1 t/2} & (1-a)e^{-\Gamma_1 t} \end{pmatrix}$$

and we see the amplitude of $|1\rangle\langle 1|$ term is damped by $e^{-\Gamma_1 t}$. We also see the off-diagonal terms decay at half the rate of the damping. This off-diagonal term is a *dephasing* term, which will be discussed in more detail in the following subsection.

Most quantum providers report amplitude damping in terms of a timescale $T_1 = 1/\Gamma_1$. For example, IBM’s $T_1$ times are typically on the order of $100\mu s$. This is compared to an average single-qubit gate time of $\sim 30\, ns$, $cX$ time of $\sim 100\, ns$, and reset gate time of $\sim 3\mu s$ [41].

### 3.1.3 Dephasing

Pure dephasing is a single-qubit error that arises from couplings between the transmon and its surroundings which cause fluctuations in the precession frequency. This damps the coherence terms in the density matrix, i.e. damps the phase information in a superposition leaving a diagonal density matrix in the computational basis. Note that dephasing does not involve energy transfer between the qubit and the environment, as such it is sometimes possible to reverse the dephasing and undo the error - this will be discussed in the next section. Sources of pure dephasing include magnetic flux noise and quasi-particle tunneling[39].

The dephasing channel on a single qubit, $E_z$, is given by the Kraus operators

$$K_0^z = \sqrt{1-p_z} I \quad K_1^z = \sqrt{p_z} Z$$

which applies a $Z$ gate with probability $p_z$. We can also talk about dephasing in terms of rates instead of probabilities. A pure dephasing rate of $\Gamma_p$ transforms a
generic density matrix $\rho$ as

$$\rho = \begin{pmatrix} a & b \\ b^* & 1 - a \end{pmatrix} \mapsto \mathcal{E}_z(\rho) = \begin{pmatrix} a & b e^{-\Gamma_p t} \\ b^* e^{-\Gamma_p t} & (1 - a) \end{pmatrix}$$ (3.5)

As mentioned above, amplitude damping itself induces dephasing on a qubit. Taken together, amplitude damping at a rate $\Gamma_1$ with pure dephasing at a rate of $\Gamma_p$ results in total dephasing at a rate of $\Gamma_2 = \Gamma_p + \Gamma_1/2$ often indicated by the timescale $T_2 = 1/\Gamma_2$.

### 3.1.4 Measurement Error

The measurement process for transmon qubits is non-trivial and involves components which are beyond the scope of this thesis, details can be found in Ref. [39]. The important takeaway is that there is some probability, call it $p_0$, that a qubit in the $|0\rangle$ state will be correctly measured to be $|0\rangle$ and some other probability, call it $p_1$, that a qubit in the $|1\rangle$ state is correctly measured to be $|1\rangle$. Of course this leaves probability $1 - p_0$ of misidentifying the $|0\rangle$ state and $1 - p_1$ of misidentifying the $|1\rangle$ state.

For a system of $n$ qubits there are $2^n$ computational basis states and thus $2^n (2^n - 1)$ independent probabilities to specify. That’s $2^n$ possible states for the qubit to be in, times $2^n$ possible bit-strings to be measured, minus $2^n$ since the probabilities of the outcomes must sum to 1 for each basis state. These probabilities are of the form $p(x|y)$ where $x$ and $y$ are bit strings of length $n$ e.g. $p(101|111)$ is the probability of measuring the state to be $|101\rangle$ given the state was actually $|111\rangle$. As an approximation, we may reduce this exponential number of probabilities to a linear one by assuming the measurement errors are independent. Under this assumption our example $p(101|111)$ would be given by $p_1(1|1) \cdot p_2(0|1) \cdot p_3(1|1)$.
Since such errors typically happen at the end of the computation (see subsection 3.1.5 for an exception) they are one of the easiest types of errors to correct, as detailed in section 3.2.

3.1.5 Gate Errors

In general, single-qubit gates are around three times shorter and an order of magnitude more accurate than two-qubit gates - and so we are usually most concerned with the performance of the two-qubit gates. In IBM’s hardware the only two-qubit gate is the cX gate. The actual errors arising during the application of a cX gate are complex. In the ideal case, the control qubit remains unperturbed while the target qubit is hit with an $X = R_x(\pi)$ gate iff the control was in the state $|1\rangle$. In actuality the control qubit may be perturbed by the application of the gate, the target qubit may be hit with an $R_x(\pi \pm \epsilon)$ for some small $\epsilon$ instead of $R_x(\pi)$. It maybe even be hit with some $R_{\hat{n}}(\pi \pm \epsilon)$ where $\hat{n}$ isn’t exactly $\hat{x}$ or even more complicated things might occur.

It is infeasible for a researcher who just wants to run quantum algorithms and get a sense of expected errors to try to build a sophisticated model of all of these potential specific error types. Luckily, for most applications, a simple depolarizing error model appears to be quite accurate. A depolarizing error channel is a single-parameter channel with the parameter being the probability of an error. All possible errors are considered with equal weight. Although it might seem that “all possible errors" is an unreasonable thing to try to enumerate, it’s actually very straightforward considering that the Pauli matrices form a basis for all 2 complex matrices. Therefore our depolarizing error channel, $\mathcal{E}_d^n(p_e)$, for an $n = 1, 2$-qubit gate with error probability $p$ is defined by the Kraus operators

$$\{K_i^1\} = \left\{ \sqrt{1-p_e}I, \sqrt{\frac{p_e}{3}}X, \sqrt{\frac{p_e}{3}}Y, \sqrt{\frac{p_e}{3}}Z \right\} \quad (3.6)$$
and
\[ \{ K_i^2 \} = \left\{ \sqrt{1-p_e} I, \sqrt{\frac{p_e}{15}} I X, \sqrt{\frac{p_e}{15}} I Y, \ldots, \sqrt{\frac{p_e}{15}} Z Z \right\}. \quad (3.7) \]

There is one more type of gate, distinct in character from the one- and two-qubit gates above, that needs to be addressed. The algorithms presented in this work center around the simulation of open quantum systems. As said above, these systems do not obey unitary dynamics and as such, are typically difficult to implement on quantum computers which implement unitary gates. However, some newer quantum computing technologies come with a mid-circuit reset gate, which sets a desired qubit to the \(|0\rangle\) state in the middle of a protocol. This operation is clearly non-unitary - it maps every state to \(|0\rangle\), so an inverse mapping is not possible. Having a non-unitary operation opens the possibility of efficiently implementing non-unitary dynamics on a quantum computer. The following is an excerpt from Appendix I.

In IBM’s hardware a reset gate is performed by measuring the state of a qubit and then applying an \(X\) gate if the qubit was measured to be in the \(|1\rangle\) state and leaving it in the \(|0\rangle\) state otherwise. However, even assuming a perfect \(X\) gate, measurement fidelity is imperfect and so we expect an imperfect reset gate. Call the probability of measuring \(m\), given the qubit is actually in \(|m\rangle\) to be \(p(m|m) \equiv p_m\). If the qubit is initially in state \(\rho\) with \(\langle 0 | \rho | 0 \rangle = a_0\), then we model the state of the qubit after one reset gate, \(\rho_1\), to be characterized by

\[ \langle 0 | \rho_1 | 0 \rangle = a_0 (p_0 - p_1) + p_1 \quad \text{and} \quad \langle 0 | \rho_1 | 1 \rangle = 0. \quad (3.8) \]

In IBM’s hardware we have \(p_0 \geq p_1\), so we can improve the fidelity of a reset operation by applying multiple reset gates in succession. Call the qubit state after \(r\) reset gates \(\rho_r\). Given the above model we expect the probability of a successful reset to be

\[ \langle 0 | \rho_r | 0 \rangle = a_0 \left( p_0 - p_1 \right)^r + p_1 \frac{(1 - (p_0 - p_1)^r)}{1 - p_0 + p_1}. \quad (3.9) \]
3.2 Techniques to Minimize Errors

It is important, before running on actual hardware, to try to get a sense of how one expects errors to influence the results. A good starting point is to run your circuits through Qiskit Aer’s native error models to get a sense of the expected fidelity. This is done by creating a new simulator object via

```python
from qiskit.providers.aer import AerSimulator
noisy_simulator = AerSimulator.from_backend(backend)
```

where `backend` is the backend object for the quantum computer whose noise model you wish to simulate (more details and example can be found in the Qiskit textbook[42], in the Qiskit tutorials, and in the Qiskit documentation[41]). This essentially pulls the values for $T_1$, $T_2$, $p_0$, and $p_1$ for each qubit as well as $p_e$ and $t_{gate}$ for each gate, then uses these values to apply depolarizing errors to the application of each gate using the reported values for $p_e$ followed by amplitude damping and dephasing channels using the reported values for $T_1$, $T_2$, and $t_{gate}$. At the end of the circuit reported values for $p_0$ and $p_1$ are used to simulate measurement errors.

While this is a good start to get an idea of the error you’re likely to see when running on an actual quantum device, I have found it is not sufficient in at least two cases. Firstly, when circuits are extremely long due to frequency calibration errors which are not included in the basic error model. Secondly, when the circuit contains reset gates due to the fact that, at the time of this writing, error rates for reset gates are also not included. One can build a more accurate error model in Qiskit by using one of the many `NoiseModels` available[41] to add custom errors to the basic model if necessary. Armed with this model you can supply custom values for the
error parameters to identify the dominant error sources which will guide the error mitigation effort.

3.2.1 Measurement Error Mitigation

One simple and almost always useful thing to do is correct for measurement errors. This protocol is available in Qiskit Ignis. It prepares and immediately measures each computational basis state giving a confusion matrix (shown in Eq. 3.10) with estimates of $p(x|y)$. Each row give the measured counts for a given basis state while each column gives the measured counts for each basis state from initializing in a given basis state. Inverting this matrix and applying it to a column vector of the raw results then gives the mitigated results.

As detailed in subsection 3.1.4, there are $O(4^n)$ independent probabilities for an $n$ qubit system. If you are measuring a handful of qubits it likely makes sense to deal with the entire confusion matrix for the most accurate results. However, for a larger number of qubits, inverting an exponentially large matrix becomes infeasible. In this case we can construct an approximate confusion matrix as the outer product of the confusion matrices for the individual qubits, which is efficiently invertible, $(A \otimes B) = A^{-1} \otimes B^{-1}$.

For example, let’s say I run a single qubit protocol with 5000 shots. When I prepare $|0\rangle$, I measure 0 on 4950 shots and 1 on the remaining 50. When I prepare $|1\rangle$, I measure 1 on 4800 shots and 1 on the remaining 200. This would be summarized in the confusion matrix $M$

$$M = \frac{1}{5000} \begin{pmatrix} 4950 & 200 \\ 50 & 4800 \end{pmatrix} = \begin{pmatrix} 0.99 & 0.04 \\ 0.01 & 0.96 \end{pmatrix}$$ (3.10)

I then run a quantum circuit and get 3500 shots as 0 and 1500 as 1 for my raw data, $C_r$. My error mitigated data, $C_m$, would be given by inverting $M$ and applying it to...
\[ C_r \text{ as} \]
\[ C_m = M^{-1}C_r = \frac{1}{95} \begin{pmatrix} 96 & -4 \\ -1 & 99 \end{pmatrix} \begin{pmatrix} 3500 \\ 1500 \end{pmatrix} \approx \begin{pmatrix} 3474 \\ 1526 \end{pmatrix} \quad (3.11) \]

3.2.2 Run on the Best Qubits

One of the most effective things one can do is to run one’s jobs on “good” qubits. Inside IBM’s machines not all qubits are created equal. One can use the error model as described above to try out simulating different qubits and backends to gather a list of promising candidate qubits. For larger jobs containing lots of circuits it is often best to run a few representative circuits on as many trial sets of qubits as is feasible. One then examines these results and selects the best set of qubits on which to run the full job. In my experience this is probably the single most important factor in the success of a job and it pays to find good qubits. Note that while the error model is a useful tool, it does not take into account more exotic sources of errors which can sometimes be significant. Therefore it is really worth it to actually try as many sets of qubits as resources will allow.

Luckily it appears good qubits remain good, and bad remain bad, somewhat reliably. This means that identification of good qubits doesn’t need to be done in full for each job. Becoming familiar with the best few sets on a given backend is enough - then just test those sets each time since unpredictable errors and failures can sometimes crop up unexpectedly. In a similar vein, parameters inside the quantum computer drift with time. As such, for sensitive circuits in particular, it can pay to monitor the calibration logs and attempt to run as soon as possible after a calibration happens.
3.2.3 Transpilation and Mapping

Another major way to improve the performance of circuits is to transpile circuits carefully. IBM’s quantum computers have a native set of gates, \( \{R_z(\theta), \sqrt{X}, cX\} \) at the time of this writing. However, when designing algorithms we rarely think in terms of this basis set. We can often do better than Qiskit’s native transpiler (programmatic transpilation is a provably hard problem). This can involve things like recasting the problem in an equivalent way from a high level perspective, exploiting symmetries, leveraging commuting terms, or even simple informed trial and error.

One very important consideration at this stage is that all of IBM’s devices have limited connectivity. This means that the backend can only implement a native \( cX \) gate between select pairs of qubits. If you put a \( cX \) gate between two unconnected qubits, the backend will implement that using SWAP gates.

\[
|q_1\rangle = |q_1\rangle |q_2\rangle |q_3\rangle
\]

\[
|q_2\rangle = |q_2\rangle |q_1\rangle |q_3\rangle
\]

**Figure 3.1: SWAP gate.** Left: Quantum circuit showing a \( cX \) between two unconnected in IBM’s backend. The backend adds SWAP gates to move the qubits next to each other. Right: action of a SWAP gate is to swap the state of two qubits.

These SWAP gates become very costly very quickly and can ruin the performance of a circuit if not handled properly. Care should be taken to ensure a set of qubits is chosen which matches, or at least most closely matches, the requirements of the circuit. Commuting terms can be rearranged to attempt to combine terms which need SWAP gates. It will not generally be possible to eliminate SWAPs from a circuit but, without any consideration, Qiskit can add a significant number of them, which is detrimental to the fidelity of the circuit.
4.1 Summary

Current and near term quantum computers (i.e. NISQ devices) are limited in their computational power in part due to qubit decoherence. Here we seek to leverage qubit decoherence as a free quantum resource for simulating the behavior of real world open quantum systems (quantum systems which interact with their surroundings). As a first step toward this goal, we simulate the dynamics of a spin chemistry system undergoing thermal relaxation on a quantum computer using only coherent simulation and qubit decoherence. Because qubits naturally undergo decoherence, we are able to add the relaxation into our simulations with no additional computational overhead. We choose two simple, real-world chemical systems with both analytic solutions and experimental results as a benchmark for, and proof of concept of our method. For comparison purposes we present three methods for implementing the thermal relaxation: one which explicitly applies the relaxation Kraus operators, one which combines results from two separate circuits in a classical post-processing step, and one which relies on leveraging the inherent decoherence of the qubits themselves. We implement these methods on quantum computers made available by IBM and find excellent agreement between our results, experimental data, and the theoretical predictions.
4.2 Introduction

One of the most promising applications of quantum computers is the ability to efficiently simulate quantum dynamics. Much attention has been given to the problem of simulating closed quantum systems (those evolving in time according to the Schrödinger equation) producing multiple efficient algorithms which are continually being improved and generalized [13, 43, 44, 45, 46, 47, 48, 49]. However, considerably less progress has been made on simulating open quantum systems, i.e. closed quantum systems interacting with their environment. This is despite their importance to physics, chemistry, and beyond - in particular the preparation and use of thermal states. This is due in part to the fact that open quantum systems are more general and complex than closed quantum systems, which are a special case of open quantum systems. Certain cases of open quantum systems, like preparing general low temperature thermal states, are provably hard even on a quantum computer [50].

Furthermore, quantum computers implement unitary operations on their qubits whilst open quantum systems undergo non-unitary dynamics which further adds to the challenge of simulating such systems.

Nevertheless, there are numerous proposals for how to simulate open quantum systems on quantum computers [51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66] of varying efficiency, complexity, feasibility, and scope. They all, however, make use of a gate based approach. In this work we propose a different approach, based on the fact that a quantum computer itself is an open quantum system. This “openness” manifests itself as decoherence channels, namely amplitude damping and dephasing, of the qubits. While this decoherence is typically a limiting factor in quantum simulations, here we proposed leveraging it as a quantum resource for implementing dissipative channels of interest at no additional cost. We use this approach to simu-
late the behavior of spin chemistry systems undergoing thermal relaxation as a proof of concept.

Spin chemistry\cite{67, 68, 69, 70} is a subfield of physics and chemistry that deals with magnetic and spin effects in chemical reactions, most prominently those involving the so-called Radical Pair Mechanism (RPM) \cite{68, 70, 71}, with many applications in quantum biology \cite{70, 72, 73, 74, 75}, solar energy conversion \cite{70, 76, 77}, and material science\cite{70, 78, 79, 80}. Since the behavior of spin-correlated radical pairs, the key intermediates in the RPM, parallels the behavior of entangled spin-qubit pairs \cite{70, 81, 82, 83}, spin chemistry problems can be easily mapped on a quantum device, thus making spin chemistry/RPM a promising new application of quantum simulation in the field of chemistry.

Among spin chemistry problems, we have identified a simple yet experimentally important model simulation problem - quantum beats in radiation-generated radical pairs\cite{84, 85, 86, 87}. In a typical experiment, a burst of ionizing radiation is sent through a solution, forming radical pairs in a spin-correlated singlet state, due to spin conservation in the ionization process. This state then evolves due to hyperfine couplings (HFC), unequal Larmor precession rates (caused by unequal g-factors) in the presence of a magnetic field, and paramagnetic relaxation\cite{84, 85, 86, 87, 88}. The radical pairs undergo spin-selective recombination reactions, resulting in a fluorescent product when recombining in the singlet state, but not when recombining in a triplet state. The dynamics of the spin state of the radical pairs, often called “quantum beats”, offers insights into the properties of the pairs’ constituent molecules, allowing for determination of e.g. g-factors and HFC constants.

The intensity of the observed fluorescence is approximately given by\cite{84, 88}

\[
I(t) = F(t) \left( \theta S(t) + \frac{1}{4}(1 - \theta) \right)
\]  

\(4.1\)
where $F(t)$ is the time-dependent radical pair recombination rate, $\theta$ is the experimentally determined fraction of recombination events occurring between RPs produced from the same precursor and $S(t)$ is the probability of a RP being in the singlet state, which generally depends on magnetic field strength $B$. The spin dynamics are extracted from the fluorescence profile using the time-resolved magnetic field effect (TR-MFE) method. This is done by taking a ratio of $I(t)$ at high-field and low-field to cancel $F(t)$, which has no $B$ dependence. A quantity, $Q$, subject to a high-field is denoted as $Q_B$ and subject to a low-field as $Q_0$. Using Eq. 4.1 we have for the TR MFE

$$M(t) = \frac{I_B(t)}{I_0(t)} = \frac{F(t)}{F(t)} \left( \frac{4\theta S_B(t) + (1 - \theta)}{4\theta S_0(t) + (1 - \theta)} \right). \quad (4.2)$$

In this paper we present two methods for computing various quantities of interest, subject to thermal relaxation, on currently available quantum computers. A quantity, $Q$, calculated for an isolated system is denoted as $\tilde{Q}$ when subject to thermal relaxation.

In section 4.3 we cover the relevant theory of spin chemistry and thermal relaxation, as well as introducing the two real world systems we use to test our algorithms. In section 4.4 we present our algorithms for simulating thermal relaxation in these systems and discuss their scope and scalability. In section 4.5 we present data taken from applying our algorithms to these systems on real quantum computers provided by IBMQ[89, 90].

4.3 Theory

4.3.1 Calculation of $S(t)$

We consider systems of radical pairs in non-viscous solutions with no exchange between the pair’s constitutes. Such systems are described by Hamiltonians of the
\[ H = \sum_{i=1}^{2} \mu_B g_i B + \sum_{j=1}^{N_i} a_{ij} I_{ij} \mathbf{S}_i. \] (4.3)

Here \( \mu_B \) is the Bohr magneton, \( \mathbf{S}_i \) \((g_i)\) is the spin \((g\text{-factor})\) of the unpaired electron in molecule \( i \), \( I_{ij} \) refers to the \( j^{\text{th}} \) nuclear spin in molecule \( i \), \( a_{ij} \) is the HFC constant between \( \mathbf{S}_i \) and \( I_{ij} \), and \( B \) is the magnetic field.

From this Hamiltonian, we seek an expression for \( S(t) \), the probability of a pair being in the singlet state at time \( t \), given it was initially created in the singlet state at time \( t = 0 \). Alternatively, \( S(t) \) may be thought of as the fraction of pairs, which were initially in the singlet state, found in the singlet state at time \( t \). While the initial electronic state of the pair preserves the spin multiplicity of its precursor[86], the initial nuclear state has no constraints. Therefore, following Brocklehurst[87], we take the initial nuclear state of a newly formed RP to be the maximally mixed state (i.e. all nuclear states are equally likely). This gives an initial state of

\[ \rho(0) = \frac{1}{N_I} |S\rangle\langle S| \otimes I_{N_I} \quad \text{with} \quad |S\rangle = \frac{|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle}{\sqrt{2}}. \] (4.4)

where \( I_n \) is the \( n \times n \) identity matrix and \( N_I \) is the size of the Hilbert space of the nuclear spins.

We then compute \( S(t) \) by evolving \( \rho(0) \) by time \( t \) under the \( H \) from Eq. 4.3, tracing out the nuclear degrees of freedom (DOF) and taking the expectation value of the resulting reduced electronic density matrix w.r.t. \( |S\rangle \)

\[ S(t) = \langle S| \text{Tr}_I \left\{ e^{-iHt} \rho(0) e^{iHt} \right\} |S\rangle. \] (4.5)

There is no analytic expression for Eq. 4.5 in general, although it is known for a variety of simple cases[84, 87, 93]. Evaluating Eq. 4.5 numerically is straightforward, however it becomes exponentially expensive in the number of nuclear degrees of freedom.
4.3.2 Thermal Relaxation

The main mechanisms of relaxation in these systems are generalized amplitude damping (i.e. longitudinal paramagnetic relaxation or $T_1$ decay) and dephasing (i.e. transverse paramagnetic relaxation or $T_2$ decay)[68, 84, 86, 87, 92, 94]. It can be shown that only the effective $T_1$ and $T_2$ for the pair are relevant to $\tilde{S}(t)$ so for simplicity we take $T_1$ and $T_2$ to be equal for both radicals. The following remains unchanged if $T_1$ and $T_2$ are different for each radical. In general, we have $T^{-1} = T^{-1}_a + T^{-1}_c$ [94] where $T$ is either $T_1$ or $T_2$ and $a, c$ stand for anion and cation respectively.

We derive an expression for the evolution of the singlet state probability, $\tilde{S}(t)$, subject to these decoherence channels, in terms of the singlet state probability for the isolated system, $S(t)$. In general, a proper description of the dynamics of a system undergoing both relaxation and coherent time evolution is very complicated because the relaxation channels and coherent time evolution do not commute. However, this is not always the case, as we demonstrate in this work for spin chemistry systems at room temperature.

A quantum channel, $\mathcal{E}$, can be characterized by its Kraus operators, $K_i$, and transforms a general density matrix, $\rho$, as[34]

$$\rho \mapsto \mathcal{E}(\rho) = \sum_i K_i \rho K_i^\dagger.$$

(4.6)

The Kraus operators for the generalized amplitude damping channel on a single qubit, $\mathcal{E}_x$, are[95]:

48
\[
K^x_0 = \sqrt{p_n} \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{p_x} \end{pmatrix} = \sqrt{p_n} \left( \frac{I+Z}{2} + \sqrt{p_x} \frac{I-Z}{2} \right)
\]
\[
K^x_1 = \sqrt{p_n} \begin{pmatrix} 0 & \sqrt{p_x} \\ 0 & 0 \end{pmatrix} = \sqrt{p_n}p_x \left( \frac{X+iY}{2} \right)
\]
\[
K^x_2 = \sqrt{p_n} \begin{pmatrix} \sqrt{p_x} & 0 \\ 0 & 1 \end{pmatrix} = \sqrt{p_n} \left( \frac{I-Z}{2} + \sqrt{p_x} \frac{I+Z}{2} \right)
\]
\[
K^x_3 = \sqrt{p_n} \begin{pmatrix} 0 & 0 \\ \sqrt{p_x} & 0 \end{pmatrix} = \sqrt{p_n}p_x \left( \frac{X-iY}{2} \right)
\]

Where \( p_n = (1 + e^{-1/T})^{-1} \) is the Fermi function which gives the equilibrium population of \(|\downarrow\rangle\) as a function of the temperature, \( T \). \( p_n \) can be viewed as a temperature parameter controlling the ratio of damping of \(|\uparrow\rangle\) and \(|\downarrow\rangle\). \( p_x \) is the damping parameter, and for any quantity \( \alpha \) we define \( \bar{\alpha} \equiv 1 - \alpha \). At zero temperature, \( T = 0 \rightarrow p_n = 1 \) we recover the standard amplitude damping channel. Only \(|\uparrow\rangle\) \( \mapsto \rightarrow |\downarrow\rangle\) occurs, with probability \( p_x \). At infinite temperature, \( T = \infty \rightarrow p_n = 1/2 \), both \(|\uparrow\rangle\) \( \mapsto \rightarrow |\downarrow\rangle\) and \(|\downarrow\rangle\) \( \mapsto \rightarrow |\uparrow\rangle\) occur with probability \( p_x/2 \).

The dephasing channel on a single qubit, \( \mathcal{E}_z \), is given by the Kraus operators

\[
K^z_0 = \sqrt{p_z}I \quad K^z_1 = \sqrt{p_z}Z
\]

which intuitively reads, "With probability \( p_z \) apply \( Z \) otherwise do nothing".

It is shown in Appendix A that the relaxation channels and coherent dynamics all mutually commute for the class of problem considered here. Define the composite relaxation channel on a single qubit, at temperature \( T \), as

\[
\mathcal{E}_1^T \equiv \mathcal{E}_x \circ \mathcal{E}_z = \mathcal{E}_z \circ \mathcal{E}_x
\]
where the Kraus operators of $\mathcal{E}_a \circ \mathcal{E}_b$ are given by the products of pairs of Kraus operators from each channel, i.e. $\{K^a_j \cdot K^b_i\}$. The relaxation channel on the 2-qubit electronic system is then

$$\mathcal{E}^T \equiv \mathcal{E}_1^T \otimes \mathcal{E}_1^T$$

(4.10)

where the Kraus operators of $\mathcal{E}_a \otimes \mathcal{E}_b$ are given by the tensor products of pairs of Kraus operators from each channel, i.e. $\{K^a_j \otimes K^b_i\}$.

Finally the unitary time evolution of the full system (electronic + nuclear), induces non-unitary time evolution in the electronic system alone. This non-unitary evolution is itself represented by a quantum channel, $\mathcal{E}_U$, whose details are given in Appendix A. An important property of $\mathcal{E}_U$ is that

$$\mathcal{E}^\infty (\mathcal{E}_U (\rho^*(t))) = \mathcal{E}_U (\mathcal{E}^\infty (\rho^*(t)))$$

(4.11)

where $\mathcal{E}^\infty$ is the infinite temperature relaxation channel (Eqs. 4.7,4.9,4.10) and $\rho^*(t)$ is the reduced density matrix of the electronic subsystem after time $t$ given by

$$\rho^*(t) = \text{Tr} \left\{ e^{-iHt} \rho(0) e^{iHt} \right\}.$$  

(4.12)

It is important to note that Eq. 4.11 does not hold at finite temperature or for generic $\rho$. Despite these limitations, this is useful because, to a very good approximation, room temperature is infinite temperature for spin chemistry systems. The energies associated with the Hamiltonian in Eq. 4.3 (even for large $B$) are orders of magnitude smaller than $k_B T$ at room temperature.

We are thus able to compute $\tilde{S}(t)$ by applying each of $\mathcal{E}^\infty$ and $\mathcal{E}_U$ only once. When Eq. 4.11 does not hold, more complicated methods are required, e.g. time ordered products or Trotterization. In our simplified case, to evolve the system forward by a time $t$, we must compute the correct values of $p_x$ (Eq. 4.7) and $p_z$ (Eq. 4.8) to use. We do this by applying $\mathcal{E}_1^0$ (Eq. 4.9) to a generic $\rho$ and equate it to the known iterative
infinitesimal result[34].

\[ E^0_1 (\rho) : \begin{cases} 
\rho_{\uparrow\uparrow} \mapsto \bar{p}_x \rho_{\uparrow\uparrow} = e^{-t/T_1} \rho_{\uparrow\uparrow} \\
\rho_{\uparrow\downarrow} \mapsto \sqrt{p_x} (1 - 2p_z) \rho_{\uparrow\downarrow} = e^{-t/T_2} \rho_{\uparrow\downarrow}
\end{cases} \]  

(4.13)

where \( \rho_{ab} \equiv \langle a | \rho | b \rangle \), which gives

\[ p_x = 1 - e^{-t/T_1} \quad \text{and} \quad p_z = \frac{1}{2} \left( 1 - e^{-t/\left( \frac{T_2}{2} - \frac{1}{T_1} \right)} \right). \]  

(4.14)

Finally, \( \tilde{S}(t) \) is computed as

\[ \langle S | E^\infty (E_U (\rho^*(0))) | S \rangle = \langle S | E^\infty (\rho^*(t)) | S \rangle = \frac{1}{4} \left( 1 + e^{-t/T_1} + e^{-t/T_2} (4S(t) - 2) \right) \]  

(4.15)

which agrees with Ref. [84]. Although this result is already known, the algorithm given in the Sec. 4.4.1 relies on the fact that \( E^\infty \) and \( E_U \) commute in our case. To the best of our knowledge, this has not previously been shown. This expression, together with independent experimental results, will be used to benchmark the performance of our algorithms.

4.4 ALGORITHMS

We present two approaches for simulating the dynamics of these types of spin systems undergoing thermal relaxation on a quantum computer, and discuss the advantages and disadvantages of each. Both methods require implementing time evolution under the action of the Hamiltonian in Eq. 4.3. A wide variety of algorithms already exist for this step[43, 45, 47, 48]. The novel part in the approaches is the implementation of thermal relaxation.

Firstly, we explicitly simulate the generalized amplitude damping (Eq. 4.7) and dephasing channels (Eq. 4.8). This has the advantage of being highly controllable
since we are able to implement decoherence with any parameters we wish. However, it has the disadvantage of requiring a larger and deeper circuit which makes it less reliable, and scalable on NISQ devices.

Secondly, we leverage the decoherence of the qubits themselves to model the decoherence of the real spin system. This has the advantage that it requires no additional gates or qubits, so the circuit remains small and simple and should scale well to larger systems. However, it has the disadvantage that we are not in control of the decoherence parameters. A further complication is that the protocol requires waiting for the qubits to relax, which can amplify errors due to miscalibration. An in-depth discussion follows.

4.4.1 Explicit Decay, Kraus Method

We can implement the Kraus operators given in Eq. 4.7 and 4.8 using the quantum circuit shown in Fig. 4.1, following the approaches given in [2, 96]. The five gates operating only on the bottom three qubits implement the generalized amplitude damping channel, $E_x$, while the two gates involving the top qubit implement the dephasing channel, $E_z$.

It is easy to make sense of this circuit by thinking of the standard amplitude damping channel as: “If the qubit is in $|\uparrow\rangle$, apply an $X$ gate with probability $p_x$.”, the temperature correction part (added to give the generalized amplitude damping channel) as: “with probability $p_n$ apply $X$ to the amplitude damping control line, i.e. damp $|\downarrow\rangle$ instead of $|\uparrow\rangle$,” and similarly, the dephasing channel as: “With probability $p_z$ apply a $Z$ gate.”

The circuit in Fig. 4.1 can be optimized greatly. Both the “Temp” and “Dephase” parts of the circuit in Fig. 4.1 can be thought of as probabilistically implementing a
gate (X and Z respectively). This means the rotation gate and controlled operation can replaced by a probabilistic gate as follows.

1) We can run the circuit with and without each gate (X or Z), with the gate operating where the target of the (now deleted) controlled operation was, then taking a weighted average over the results. The weights should be the probabilities of the (now deleted) rotation gate leaving the ancilla in $|\uparrow\rangle$, i.e. $w_{XZ} = \bar{p}_n p_z$, $w_Z = p_n p_z$, $w_X = \bar{p}_n \bar{p}_z$, $w_I = p_n \bar{p}_z$. Since the number of possible combinations grows exponentially as more qubits are added, this approach will not scale well. However, it is easy to implement using currently available quantum software and the systems under consideration here only have decoherence on the two electrons - making this our method of choice in this work.

2) Alternatively, we can run the circuit with an $R_x(\theta_n)$ and $R_z(\theta_z)$, with the gate operating where the target of the (now deleted) controlled operation was, where $\theta_i$ is
drawn from a normal distribution of mean 0 and variance \( \log \left( (1 - 2p_i)^{-2} \right) \) for each shot. This has the advantage that it avoids the need to compute exponentially many weights, but with the disadvantage that each shot needs a different circuit. This may or may not be an issue with future quantum compilers.

More simplifications are possible by exploiting symmetries. \( \mathcal{E}_\infty, \mathcal{E}_U \) and \(|S\rangle\) are all invariant under the transformations \(|ab\rangle \mapsto |ba\rangle\) and \(|\uparrow\rangle \leftrightarrow |\downarrow\rangle\). Because of these symmetries, it is always the case that the populations of the parallel spin states are equal, i.e. \( \rho_{\uparrow\uparrow} = \rho_{\downarrow\downarrow} \) and the same holds for anti-parallel states i.e. \( \rho_{\uparrow\downarrow} = \rho_{\downarrow\uparrow} \). Here \( \rho \) is the state of the electronic subsystem and \( \rho_i \equiv \langle i | \rho | i \rangle \). We are only interested in \( \langle S | \rho | S \rangle \), which depends on \( \rho_0 \) and the coherence term \( \rho_c \equiv \langle \uparrow \downarrow | \rho | \downarrow \uparrow \rangle \) alone.

Dephasing either qubit with \( p_z = \frac{1}{2} \left( 1 - e^{-t/\tau} \right) \) (Eq. 4.14) has no effect on the populations and decays \( \rho_c \) by \( e^{-t/\tau} \). Dephasing both with the same \( p_z \) has the same effect except decays \( \rho_c \) by \( e^{-2t/\tau} \). We may therefore achieve the desired \( \tilde{S}(t) \) by dephasing either one of the two qubits at twice the rate.

A similar but less straightforward simplification occurs for amplitude damping. Using \( p_x = 1 - e^{-t/\tau} \) from Eq. 4.14 and \( p_n = 1/2 \) for infinite temperature we find that performing amplitude damping on either qubit decays \( \rho_c \) by \( e^{-t/(2\tau)} \). Amplitude damping also affects the populations and is not symmetric.

Amplitude damping on the first qubit gives transitions between \( \rho_{\uparrow\uparrow} \leftrightarrow \rho_{\downarrow\downarrow} \) and \( \rho_{\downarrow\downarrow} \leftrightarrow \rho_{\uparrow\downarrow} \) while amplitude damping on the second gives \( \rho_{\uparrow\uparrow} \leftrightarrow \rho_{\uparrow\downarrow} \) and \( \rho_{\downarrow\downarrow} \leftrightarrow \rho_{\downarrow\uparrow} \). Because \( \rho_{\uparrow\uparrow} = \rho_{\downarrow\downarrow} \) and \( \rho_{\uparrow\downarrow} = \rho_{\downarrow\uparrow} \) double flips leave the system unchanged. Also because of this symmetry, we see that flipping the first or second qubit actually yields the same transformation on the system. And because double flips leave the system unchanged, applying amplitude damping on both the qubits gives the same \( \tilde{S}(t) \) as applying amplitude damping on one of the qubits at twice the rate (i.e. halving \( T_{1,2} \)).
One final simplification that can be made is to replace the infinite temperature amplitude damping channel with the zero temperature channel. This breaks the symmetry between $|\uparrow\rangle$ and $|\downarrow\rangle$ but preserves the final $\tilde{S}(t)$. Without loss of generality, apply the channel on the first qubit. The infinite temperature channel induces the following transitions in the populations $\rho_{\uparrow\uparrow} \leftrightarrow \rho_{\downarrow\uparrow}$ and $\rho_{\downarrow\downarrow} \leftrightarrow \rho_{\uparrow\downarrow}$. By replacing it with the zero temperature channel, these transitions become unidirectional as $|\downarrow\rangle \rightarrow |\uparrow\rangle$ is forbidden, $\rho_{\uparrow\uparrow} \rightarrow \rho_{\downarrow\uparrow}$ and $\rho_{\uparrow\downarrow} \rightarrow \rho_{\downarrow\downarrow}$. Nevertheless, the final answer is unchanged because $\tilde{S}(t)$ depends only on the sum $\rho_{\uparrow\downarrow} + \rho_{\downarrow\uparrow}$. The zero temperature map on the first qubit overpopulates $\rho_{\downarrow\uparrow}$, but underpopulates $\rho_{\uparrow\downarrow}$ by exactly the same amount, leaving the sum unchanged. The temperature does not affect the coherences.

The equivalence of $\tilde{S}(t)$ by applying the infinite temperature channel to both qubits and by applying the zero temperature channel (at twice the rate) to a single qubit is easily verified using Eqs. 4.6, 4.7, and 4.8.

To summarize, naively we would need to apply the full circuit shown in Fig. 4.1 to both of the qubits representing the electronic subsystem. However, we can optimize this circuit to give the same $\tilde{S}(t)$ by

- Applying the circuit on either qubit with twice the decay, i.e. halving $T_{1,2}$
- Replace the infinite temperature channel with the zero temperature one, i.e. delete the "Temp" part of the circuit.
- Implement the "Dephase" part probabilistically by
  - Running two circuits with "Temp" replaced by $I$ or and $Z$ and combining the results in a post-processing step.
  - Replacing "Temp" with an $R_z(\theta)$ gate where $\theta$ is drawn from the appropriate normal distributions each shot.
Putting this all together, we get the circuit shown in Fig. 4.2.

Figure 4.2: Kraus method circuit. Circuit to simulate the dynamics of a spin system subject to thermal relaxation using the Kraus method. $\phi = 2\sin^{-1}\sqrt{p_x}$ and $(Z)$ indicates that the shots are to be split between implementing the circuit including the $Z$ gate and omitting the $Z$ gate. Results are then combined as a weighted average with weights $w_z = p_z$, $w_{\bar{z}} = \bar{p}_z$. The final $cX$ and $H$ gates transform from the Bell basis and map $|S\rangle \leftrightarrow |\uparrow\uparrow\rangle$ for measurement.

4.4.2 Leveraging Inherent Qubit Noise

An entirely different approach to simulating the thermal relaxation of a system is to try to take advantage of the inherent thermal relaxation of the qubits in the quantum computer. At the most basic level, the protocol is to simply run the simulation and rely on the qubits’ natural decoherence behavior to implement the dissipative channels for free. This approach is appealing since simulating dissipative channels will become increasingly expensive in time and space as system sizes grow. It is also an interesting application of NISQ devices, whose noise often hinders quantum simulation. Here we hope to turn that around and use the noise as an integral part of the simulation. Such a protocol will be most beneficial for NISQ devices when gate errors are sufficiently low and qubit decoherence is the limiting factor in a simulation.
Despite the apparent simplicity, there are a variety of challenges inherent to such an approach. One immediate challenge that arises is that the qubits are an effective zero-temperature system while the spin chemistry systems are effectively infinite temperature. Furthermore, a more practical issue is that during the long time-scales for this protocol systematic errors tend to be amplified. Specifically, the errors from effective $Z \otimes I$ and $I \otimes Z$ terms arising due to qubit frequency miscalibration[97] were particularly problematic in our simulations.

The qubits in IBMQ’s machines are always precessing under the action of the Hamiltonian term $\Omega \sigma_z/2[41]$. I.e. a qubit in state $|\psi\rangle$ at $t = 0$ will evolve to $e^{-i\Omega \sigma_z t/2} |\psi\rangle = R_z(\Omega) |\psi\rangle$ after time $t$. This precession is corrected for in software, but miscalibrations of $\Omega$ will result in imperfect corrections. If the true frequency is $\Omega$ but the backend is calibrated to $\omega = \Omega - \Delta \omega$, then after a time $t$ the corrected state will be $R_z(\Delta \omega t) |\psi\rangle$ instead of $|\psi\rangle$.

Because $\Delta \omega t$ tends to be small for $t$ values associated with typical circuits, this error tends to be negligible. However, our circuits run to long enough times where this becomes a significant error. We can mitigate this error by introducing $X$ gates (aka echo pulses) into our circuit, which has the effect of flipping the sign of the phase, so further phase accumulation will cancel instead of compound[98, 99]. It is easy to verify that using an even number of echo pulses, $n$, at $(k + 1/2)t/n$, $k \in \{0, 1, \ldots, n-1\}$ corrects this error

$$R_z(\frac{\Delta \omega t}{2n}) \cdot \prod_{k=1}^{n} X R_z(\frac{\Delta \omega t}{n}) \cdot R_z(\frac{\Delta \omega t}{2n}) = I$$

Additionally, these $X$ gates also have an effect on the decay characteristics of the state. As the qubits are at $T \approx 0$ they are always decaying toward $|\downarrow\rangle$. The $X$ gates flip $|\downarrow\rangle \leftrightarrow |\uparrow\rangle$ so the amplitude damping proceeds “in reverse" while the dephasing is unaffected. One would expect this to be a crude approximation to the infinite
temperature amplitude damping where a qubit is decaying toward an equal mixed state of $|\downarrow\rangle$ and $|\uparrow\rangle$. Indeed as $n \to \infty$ we recover the exact $\mathcal{E}^\infty$. Denote the probability of measuring $|S\rangle$ after running the protocol using $n$ (even) echo gates as $S^e(t)$. Then we find (by symbolic matrix products in Mathematica)

$$\tilde{S}(t) = S^e(t) - \left( \frac{e^{-\frac{t}{T_1}} - 1}{\cosh \left( \frac{t}{2nT_1} \right)} \right)^2$$

(4.16)

and $S^e(t)$ converges to $\tilde{S}(t)$ for all $t$ as $n$ increases. However, increasing $n$ also incurs errors due to imperfect $X$ gates. In this work, we find using $n = 4$ gives good results and the corresponding circuit is shown in Fig. 4.3.

\[\begin{array}{c}
|I\rangle \\
U\left(\frac{t}{8}\right) \\
\begin{array}{c}
X \\
X \\
X \\
X
\end{array} \\
U\left(\frac{t}{4}\right) \\
\begin{array}{c}
X \\
X \\
X \\
X
\end{array} \\
U\left(\frac{t}{4}\right) \\
\begin{array}{c}
X \\
X \\
X \\
X
\end{array} \\
U\left(\frac{t}{8}\right) \\
\end{array}\]

\[\begin{array}{c}
|S\rangle \\
\end{array}\]

\[\begin{array}{c}
\text{H} \\
\text{...}
\end{array}\]

**Figure 4.3: Inherent method circuit.** Circuit to simulate the dynamics of a spin system subject to thermal relaxation using the Inherent method where $U(t) = e^{-iHt}$. The final $cX$ and $H$ gates transform from the Bell basis and map $|S\rangle \mapsto |\uparrow\uparrow\rangle$ for measurement.

Another potential issue is that the $T_1$ and $T_2$ of the qubits may be significantly longer than typical simulation times. Typically the timescales for decoherence in superconducting qubits are 10s of microseconds[41] and potentially much longer for other technology, like trapped ions[100].

This issue can be overcome by slowing the execution of the circuit. This can potentially be done by, for example, pulse stretching[101], using large numbers of small Trotter steps and/or adding wait cycles into the circuit. Pulse stretching is especially appealing because it is continuously applying $\mathcal{E}_U$ while $\mathcal{E}^0$ is naturally occurring,
overcoming the issue associated with the fact that $[\mathcal{E}_U, \mathcal{E}_0] \neq 0$. It also uses fewer gates than applying a large number of small trotter steps. Adding in wait cycles between trotter steps is the easiest to implement but also incurs the largest error due to $[\mathcal{E}_U, \mathcal{E}_0] \neq 0$. Additionally, the ratio $T_1/T_2$ may be quite different between the radical pair and the qubits. One can always use the Kraus method above to implement dephasing to lower $T_2$ as far as desired. We show another general approach in the following subsection that can be used to fix the decoherence parameter mismatch between qubits and radical pairs.

4.4.3 Combining Time Evolution and Decoherence

We have devised a method to calculate the effect of the decoherence channels by separately applying the decoherence and the time evolution, then combining the results in a classical post-processing step to recover the full dissipative dynamics. This has the advantage that it can be used to produce the dynamics for a desired $T_1$ and $T_2$ that does not match the $T_1$ and $T_2$ of the qubits used. We do this as follows:

Step 1) Implement the time evolution with no decoherence, i.e. use the circuit in Fig. 4.2 without the decoherence part. Let the measured populations of $\{|S\rangle, |T_0\rangle, |T_\pm\rangle\}$ for this step be $\{S, T_0, T_\pm\}$ respectively, where $|S\rangle = \frac{1}{\sqrt{2}} (|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle)$ is the singlet state, $|T_0\rangle = \frac{1}{\sqrt{2}} (|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle)$ is the triplet state with $m_s = 0$ and $|T_+\rangle = |\uparrow\uparrow\rangle, |T_-\rangle = |\downarrow\downarrow\rangle$ are the triplet states with $m_s \neq 0$.

Step 2) In parallel, apply decoherence to the singlet state with no coherent time evolution, i.e. use circuit in Fig. 4.2 with $t = 0$ or Fig. 4.3 with $U(t)$ replaced by identity gates. Let the measured populations of $\{|S\rangle, |T_0\rangle, |T_\pm\rangle\}$ for this step be
\{S', T'_0, T'_\pm\} \text{ respectively.}

Step 3) Combine the results from steps 1 and 2 to recover the thermally relaxed dynamics, \( \tilde{S} \)

\[
\tilde{S} = SS' + T_0T'_0 + T_+T'_+ + T_-T'_-
\]  

(4.17)

Because of the symmetry in \( E_{\infty} \), the probability of \(|S\rangle \mapsto |T\rangle\), where \(|T\rangle\) is any triplet state, is equal to the probability \(|T\rangle \mapsto |S\rangle\). In this way we can view \( \{S, T_0, T_\pm\} \) as the undamped populations and \( \{S', T'_0, T'_\pm\} \) as the probability of those states transitioning to \(|S\rangle\).

This method can be used to add decoherence to a simulation implemented without decoherence. Additionally, this method can be used to “undo” any decoherence occurring during a simulation, which is often unavoidable on NISQ devices. Given simulation results subject to \( T_1 \) and \( T_2 \) decay i.e. \( \{\tilde{S}, \tilde{T}_0, \tilde{T}_\pm\} \) and \( \{S', T'_0, T'_\pm\} \), this provides a procedure to recover the undamped dynamics. This can be done by using Eq. 4.17 together with

\[
\tilde{T}_0 = T_0S' + ST'_0 + T_+T'_+ + T_-T'_-
\]

\[
\tilde{T}_\pm = T_+ + T'_+ - 4T_+T'_+
\]

(4.18)

to solve for the undamped populations \( \{S, T_0, T_\pm\} \).

Furthermore, the ability of this method to both apply and “undo” decoherence allows for more flexible decoherence protocols. In particular when using the inherent method, if the qubits have a \( T_1/T_2 \) value which is different from that of the radical pairs, the decoherence dynamics of the qubits will not mimic that of the system. In this situation, we can apply the procedure twice to fix these issues and recover the desired decay dynamics of the radical pair system. The idea is to first “undo” the decoherence from the qubits and then apply the desired decoherence.
To do this, we perform the time evolution with decoherence using the inherent method yielding \( \{ \tilde{S}, \tilde{T}_0, \tilde{T}_\pm \} \). We also perform the decoherence using the inherent method without time evolution, giving us \( \{ S', T'_0, T'_\pm \} \). Next, we decohere the singlet state using the Kraus method (circuit in Fig. 4.2 without the time evolution), inputting the desired \( T_1 \) and \( T_2 \) parameters, giving \( \{ S'', T''_0, T''_\pm \} \). We then use \( \{ \tilde{S}, \tilde{T}_0, \tilde{T}_\pm \} \) and \( \{ S', T'_0, T'_\pm \} \) to recover \( \{ S, T_0, T_\pm \} \) via Eqs. 4.17, 4.18 and then apply Eq. 4.17 with these values and \( \{ S'', T''_0, T''_\pm \} \) to produce the correct \( \tilde{S}(t) \) with the radical pair and qubits having arbitrary \( T_1 \) and \( T_2 \) values. In certain situation, e.g. \( T_1 \to \infty \) as outlined in the next section, this protocol may simplify.

4.5 Applications

In this section we benchmark our methods by using them to simulate two different radical pair systems that have been previously studied in spin chemistry experiments. The first pair consists of a perdeuterated para-terphenyl radical anion (PTP) and a perdeuterated diphenyl sulphide radical cation (DPS) and the second pair consists of a 2,2,6,6-tetramethylpiperidine radical cation (TMP) and PTP. The chemical structures of these species are shown in Fig. 4.4.

![Chemical structures of DPS, TMP and PTP](image)

**Figure 4.4: Chemical structures of DPS, TMP and PTP.** These are used in the remainder of the paper.
4.5.1 Quantum Beats in Diphenyl Sulfide-d$_{10}^+$ (DPS) / Para-Terphenyl-d$_{10}^-$ (PTP)

We begin with an application to a very simple system, the radical pair perdeuterated diphenyl sulfide$^+$ (DPS) and perdeuterated para-terphenyl$^-$ (PTP) in a dilute alkane solution. In this system, hyperfine couplings observed in the experiment are largely negligible due to the much smaller magnetic moment of deuteron, and due to fast ion-molecule electron exchange among the diphenyl sulfide molecules in solution[94]. However, while largely negligible, the large number of small hyperfine couplings can be approximated semi-classically by treating the effects of these couplings as a Gaussian dephasing term[102]. In this case, the expression Eq. 4.15 for $\tilde{S}(t)$ becomes[94]:

$$\tilde{S}(t) = \frac{1}{4} \left( 1 + e^{-t/T_1} + e^{-t/T_2 - \sigma^2 t^2} (4S(t) - 2) \right) \quad (4.19)$$

Where[102] $\sigma = \sqrt{\frac{1}{3} \sum_n a_n^2 I_n(I_n + 1)}$ is the second moment of the Gaussian distribution of the hyperfine components. This is interesting to note, because superconducting qubits are also potentially subject to such broadband dephasing processes from things like flux noise, charge noise and critical-current noise[39]. Indeed we did observe Gaussian type dephasing noise in some of our runs, but until these noise sources are more predictable and well documented, it will be difficult to leverage this noise as a resource.

If we neglect the HFC in PTP, we can directly simulate the Hamiltonian time evolution on currently available devices - due to the simple form the Hamiltonian takes:

$$H = \mu_B \mathbf{B} \cdot (g_1 \mathbf{S}_1 + g_2 \mathbf{S}_2) \propto g_1 S_1^z + g_2 S_2^z. \quad (4.20)$$
where \( g_1 = 2.0028, \ g_2 = 2.0082, \ B = B\hat{z} \) and \( B = 17\text{mT} \) for low-field and \( 960\text{mT} \) for high-field [94]. Note that this simple Hamiltonian gives

\[
U(t) = e^{-iHt} = R_z(\omega_1 t) \otimes R_z(\omega_2 t)
\]

where \( \omega_i \) is proportional to \( g_i \). In this case, with no hyperfine couplings present in both radicals, singlet-triplet (\( |S\rangle \leftrightarrow |T_0\rangle \)) oscillations in external magnetic field result from the difference in Larmor precession rates of the two electron spins caused by difference in their g-factors with no transitions to \( |T_{\pm}\rangle \). The singlet state population in this case is described by the expression [84]

\[
S_B(t) = \cos^2 \left( \frac{\omega_1 - \omega_2}{2} t \right)
\]

(4.21)

Since the Hamiltonian is composed of only \( S^z \) operators, it’s easy to see that \( [E_U, E^0] = 0 \). This allows us to do all of the time evolution in one step and then the decoherence in the next. For this system, we employ the inherent method (Sec. 4.4.2). For this simple case, the time evolution is accomplished with \( R_z \) gates and the decoherence step is just the echo pulses with pauses in between. We implement the pauses in IBMQ by using identity gates, which act as wait cycles. We choose the number of identity gates to use as

\[
N = \frac{t}{T_{qu} T_{rp} t_{id}}
\]

(4.22)

where \( t \) is the simulated time, \( T_{qu} \) is the average of \( T_1 \) and \( T_2 \) over both qubits, \( T_{rp} \) is the decay time of the radical pairs and \( t_{id} \) is the duration of the identity gate. \( T_{qu} \) and \( t_{id} \) are provided by the backend in Qiskit. The circuit implementing this protocol is shown in Fig. 4.5.

As a proof of concept of the Inherent method (Sec. 4.4.2), we begin by simulating the circuit shown in Fig. 4.5, with thermal noise added to the qubits using Qiskit.
Figure 4.5: Inherent method with echo pulses circuit. Circuit to simulate the dynamics and thermal relaxation of the DPS/PTP radical pair. $I$ is the identity gate, $N$ is given by 4.22 and $\omega_i \propto g_i$. $\tilde{S}(t)$ is given as the probability of measuring $|↑↑⟩$. This circuit uses four echo pulses ($XX$ gates) to mitigate errors from frequency miscalibration and to approximate the infinite temperature dynamics. The deviation from the true infinite temperature dynamics is given in Eq. 4.16. Over the time range simulated, the maximum deviation between the theoretical $\tilde{S}(t)$ and the ideal result of this circuit is less than $3 \times 10^{-5}$.

AER’s “thermal relaxation error” noise model. Qiskit takes as input the qubits temperature $(0)$, time, $T_1$ and $T_2$ and then simulates the circuit assuming the qubits thermally relax following amplitude damping and dephasing. Additionally, we generate the semi-classical broadband dephasing noise ($\sigma$ from Eq. 4.19) by modifying Qiskit AER’s “thermal relaxation error” module to assess the effect of neglecting the HFC in PTP. Note that one can easily implement this semi-classical dephasing on a quantum computer using the Kraus method outlined in Sec. 4.4.1 at essentially no computational cost. We run both circuits at 5,000 shots, which matches our runs on the actual quantum computers.

These results are shown in Fig. 4.6a and are in excellent agreement with both theory and experiment. We find that for PTP, the semi-classical hyperfine coupling approximation gives a correction much smaller than the other sources of uncertainty (e.g. experimental uncertainty in $T_1/T_2$ values[94]) and so we will neglect it moving forward.
(a) Results for $\tilde{M}(t)$ from Qiskit AER with thermal high- and low-fields, from the combining the data in Fig. relaxation, both including and quantum computer compared 4.6b as per Eq. 4.2 compared not including HFC, compared to theory (without HFC). with theory (without HFC) with theory and experimental $\tilde{S}_0(t)$ has a SD of 0.010 and and experimental data. $\tilde{M}(t)$ data. Both with and without $\tilde{S}_B(t)$ has a SD of 0.025 com- has a SD of 0.027 compared to pared to theory.

(b) Results for $\tilde{S}(t)$, for both theory QC $\tilde{S}_B(t)$: Theory QC $\tilde{S}_0(t)$: Theory QC

(c) Results for $\tilde{M}(t)$ from combining the data in Fig. 4.6b as per Eq. 4.2 compared with theory (without HFC) and experimental data. $\tilde{M}(t)$ has a SD of 0.027 compared to theory.

Figure 4.6: TR MFE data for the DPS/PTP radical pair. Data for the TR MFE ($\tilde{M}(t)$) and $\tilde{S}(t)$ at high- and low-fields from running the Inherent method for the DPS/PTP radical pair (circuit in Fig. 4.5) vs. theoretical calculations and experimental data. Runs were conducted by simulating our circuit in Qiskit AER with thermal noise as well as on IBM’s Toronto quantum computer, both using 5,000 shots. For runs including the HFC of PTP we take $T_1 = T_2 = 60$ns and take $T_1 = T_2 = 50$ns for runs without HFC. $\tilde{M}(t)$ is constructed from $\tilde{S}(t)$ as per Eq. 4.2 with $\theta = 0.425[94, 103]$
Having confirmed the validity of neglecting the HFC in PTP, we proceed to run the circuit shown in Fig. 4.5 on IBMQ’s Toronto quantum computer for both high- and low-field. These results are shown in Fig. 4.6b and show excellent agreement with the theory. We do note that our high-field run appears to have been subjected to some broadband dephasing noise, which becomes apparent at long times, in addition to the expected dephasing and amplitude damping.

The data from Fig. 4.6b is then combined to calculate $\tilde{M}(t)$ as per Eq. 4.2, using $\theta = 0.425[94]$. The result is shown in Fig. 4.6c alongside the experimental results[94] as well as our theoretical calculation. The simulation data are in excellent agreement with both the experimental and theory data, aside from the minor effects of broadband dephasing at long times.

4.5.2 Quantum Beats in 2,2,6,6-Tetramethylpiperidine$^+$/Para-Terphenyl-$d_{14}^-$

Now looking at another system, we consider the radical pair 2,2,6,6-tetramethylpiperidine$^+$ (TMP) and para-terphenyl-$d_{14}^-$ (PTP). As before, this radical pair can be formed by the passage of a burst of radiation through the solution of the two compounds, resulting in ionization of solvent molecules and subsequent capture of electrons by PTP molecules and holes by TMP molecules.

TMP is a radical cation, and its unpaired electron spin is localized on the nitrogen atom. There are two magnetic nuclei interacting with the electron spin, nitrogen with a nuclear moment of $1$, and amine hydrogen with a nuclear moment of $\frac{1}{2}$.

In the PTP radical anion the unpaired electron spin density is delocalized, and hyperfine couplings are very small due to small magnetic moments of the deuterium nuclei and are neglected in this treatment, as justified in Sec. 4.5.1. However, the

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HFC in TMP cannot be neglected because the electron density is localized and the couplings are much stronger.

The Hamiltonian describing this system is

\[ H = \mu_B B \cdot (g_1 S_1 + g_2 S_2) + a_H I_H \cdot S_1 + a_N I_N \cdot S_1 \]  

(4.23)

Here \( S_1 \) and \( S_2 \) refer to the electron spins in TMP and PTP respectively, \( I_i \) refers to the nuclear spin of species \( i \) and \( B \) is the magnetic field. This is similar to the DPS/PTP Hamiltonian (Eq. 4.20), with the addition of hyperfine couplings to the nitrogen and hydrogen nuclei on the TMP (last two terms in the Hamiltonian). The hydrogen and nitrogen HFC constants determined experimentally are \( a_H = -1.87 \text{mT} \), and \( a_N = 1.8 \text{mT} \) [88].

One large difference between the TMP and DPS radical pair with PTP is that the \( T_1 \) decay time is dependent on the magnetic field for TMP/PTP. In particular, we have \( T_1 = T_2 \) for the low-field but \( T_1 \gg T_2 \) for the high field. Therefore, to use the inherent method for high field we will need to do some classical post-processing on the data, as detailed in section 4.4.3. This will be described in more detail below.

Simulating the coherent time evolution under this Hamiltonian is no longer trivial like for DPS/PTP. As of this writing, simulating this system out to times of interest is beyond the capabilities of current quantum computers. Because using the quantum computer to simulate \( S(t) \) directly is not yet feasible, we demonstrate our protocols by classically precomputing \( S(t) \), as described in 4.3.1, and encoding it onto a pair of qubits.

Fig. 4.7a shows the classical precomputation of \( S(t) \), as computed by Eq. 4.5 for \( B = 0 \) and \( B = 0.1 \text{T} \), the values used in the experiment.

These are then combined as per Eq. 4.2 to yield \( M(t) \), shown in Fig. 4.7b. Encoding \( S(t) \) onto the qubits is simple and is accomplished with the circuit shown in Fig. 4.8.
(a) Plot of $S(t)$ for $B = 0$ and large $B = 0.1T$ corresponding to the fields used in the experiment.

(b) Plot of theoretical prediction for $M(t)$ without any thermal relaxation.

Figure 4.7: $M(t)$ and $S(t)$ without thermal relaxation.

Figure 4.8: Circuit for dynamics without relaxation. Raw circuit returning $S(t)$, the probability of the TMP/PTP radical pair being in a singlet state at time $t$, as the probability of measuring $|↑↑⟩$. Note that $S(t)$ is explicitly encoded in $\theta_t = 2 \cos^{-1}\left(\sqrt{S(t)}\right)$. 

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With $S(t)$ encoded on the qubits, we may directly apply the Kraus method. Note that although this encoding of $S(t)$ onto the qubits does not reproduce the correct electronic state in full (since this encoding does not induce transitions to $|T_{\pm}\rangle$), the resulting $\tilde{S}(t)$ is the same. For this situation, we use the circuits in Fig. 4.9 to implement the Kraus method for low- and high-field dynamics.

(a) Circuit for $B = 0$. Both amplitude damping and dephasing must be considered. $\theta_t = 2 \cos^{-1} \left( \sqrt{S_0(t)} \right)$, $\phi = 2 \cos^{-1} (e^{-t/(2\tau)})$ and $w_z = \frac{1}{2} \left( 1 - e^{-t/(2\tau)} \right)$

(b) Circuit for large $B$. Only dephasing needs to be considered. $\theta_t = 2 \cos^{-1} \left( \sqrt{S_B(t)} \right)$ and $w_z = \frac{1}{2} \left( 1 - e^{-t/T_2} \right)$

Figure 4.9: Inherent method circuits to simulate the thermal relaxation. Circuits to simulate the thermal relaxation of our system. The singlet state corresponds to measuring $|\uparrow\uparrow\rangle$. $(Z)$ indicates that the shots are to be split between implementing the circuit including the $Z$ gate and omitting the $Z$ gate. Results are then combined as $S = w_z P^{Z}_{\uparrow\uparrow} + (1 - w_z) P^{\text{no } Z}_{\uparrow\uparrow}$

The results of running these circuits on an actual quantum computer (IBMQ Toronto at 5,000 shots) are shown in Fig. 4.12. In general, they agree well with the theory and experimental data across the entire range of simulated time.

Because $T_1 \gg T_2$ for the high-field case, an implementation of the Inherent method must use an additional “correction” circuit (shown in Fig. 4.10) as outlined in section 4.4.3.
Figure 4.10: Correction circuit without coherent time evolution. “Correction” circuit to decohere the initial state without coherent evolution (Sec. 4.4.3) for use with Inherent method (Sec. 4.4.2). $I_n$ means apply $n$ identity gates.

However, since our encoding of $S(t)$ onto the qubits doesn’t induce transitions to $|T\pm\rangle$, this greatly simplifies the procedure to correct $T_1$. Because $|T\pm\rangle$ can only be populated by $T_1$ decay, and we wish to simulate $T_1 \to \infty$, we can simply take our $T_1 = T_2$ result and add the population of $|T\pm\rangle$ from the correction circuit. This in effect “repopulates” the singlet state with any probability that leaked into $|T-\rangle$ from the $T_1$ decay. In general such a simplification is not possible.

Figure 4.11: Inherent method circuit with identity gates. Circuit to implement the dynamics and thermal relaxation using the inherent method. $I_n$ means apply $n$ identity gates.

Denote the probability of measuring the singlet state (i.e. $|\uparrow\uparrow\rangle$) from the circuit shown in Figs. 4.11 as $P(S)$ and the probability of measuring $|T_-\rangle$ (i.e. $2|\downarrow\downarrow\rangle$) from the correction circuit shown in Fig. 4.10 as $P(T)$. Then we have $\tilde{S}(t) = P(S) + P(T)$. Both $P(S)$ and $\tilde{S}(t)$ are shown in Fig. 4.12b. While this is a nice simplification for our case, it will not work when doing true Hamiltonian simulation and the more involved method described in section 4.4.3 must be used.
The results from running the circuits which are shown in Figs. 4.10 (Simulation) and 4.11 (Correction) are shown in Figs. 4.12a and 4.12b. The final results for the TR-MFE obtained by classically combining the low- and high-field results are shown in Fig. 4.12c. For this system we used a combination of all three methods, and find excellent agreement with theory. The Kraus method gives a SD of 0.012 and the Inherent method + correction circuit gives a SD of 0.0077 compared to theory. Our results compare well with the experimental data.

(a) Results for $\tilde{S}_0(t)$ from the Kraus method and Inherent method compared with theory. $\tilde{S}_0(t)$ Kraus, $\tilde{S}_0(t)$ compared with theory. $\tilde{S}_B(t)$ Inherent method gives a SD of 0.031, Kraus, $\tilde{S}_B(t) : T_1 = \infty$ of 0.012, 0.0077 respectively compared to theory. The discrepancy between theory and experiment for $t \lesssim 12$ ns is due to additional non-magnetosensitive fluorescence arising from the excitation of solvent molecules[88].

Figure 4.12: Data for the TR MFE and singlet probability for both the Kraus and Inherent methods for the TMP/PTP radical pair vs. theoretical calculations and experimental data. Data for the TR MFE ($\tilde{M}(t)$) and $\tilde{S}(t)$ at high- and low-fields from running both the Kraus and Inherent + Correction Circuit methods for the TMP/PTP radical pair (circuits in Figs. 4.9, 4.11, 4.10) vs. theoretical calculations and experimental data. Runs for the Kraus method were conducted on IBM’s Almaden quantum computer, the other circuits were conducted on IBM’s Toronto quantum computer, all runs used 5,000 shots. $\tilde{M}(t)$ is constructed from $\tilde{S}(t)$ as per Eq. 4.2 with $\theta = 0.108$. The results are highly accurate for both methods, which is not terribly surprising given the simplicity of these circuits due to bypassing the Hamiltonian simulation step.
4.6 Conclusion

We have shown that thermal relaxation may be added to a spin chemistry simulation effectively on a quantum computer, with minimal added resources. This can be done by explicitly simulating the thermal relaxation Kraus operators (Sec. 4.4.1), by leveraging the inherent thermal relaxation of the qubits themselves (Sec. 4.4.2), or by separately 1) running the simulation without thermal relaxation and 2) running the simulation without coherent dynamics (using either previous method to implement the relaxation) and combining the results in a classical post-processing step (Sec. 4.4.3).

The Kraus method provides the most control over the thermal relaxation, allowing one to independently choose the relaxation parameters such as temperature, $T_1$ and $T_2$. However, this method is only suitable when the simulation can be performed in a time much shorter than the qubits’ natural decoherence time. Otherwise, the qubits’ natural decoherence will interfere with the artificial Kraus decoherence, leading to inaccurate results. This issue can be mitigated by using the correction circuit method outlined in Sec. 4.4.3. When the relaxation channels commute with the coherent dynamics, the Kraus method is likely to be the best choice. In this case the Kraus operators only need to be applied once and will therefore add minimally to the simulation cost.

On the other hand, when the relaxation channels and the coherent time evolution do not commute then the Kraus method may have an unacceptable cost. In this case the relaxation channels and coherent dynamics must be Trotterized and so the relaxation channels must be implemented at each step. This means a fresh register of ancilla and controlled operations at each step. On systems without mid-circuit reset of qubits, obtaining a fresh ancilla register for each step is prohibitively expensive in
terms of number of qubits and, if the device is sparsely connected, in terms of circuit depth as well. On systems with mid-circuit resets available, a fresh ancilla register may be obtained by resetting the old register. However, for current systems, resets are both the longest duration and lowest fidelity operations. It is therefore likely that the Kraus method may be sub-optimal when the relaxation channels and the coherent time evolution do not commute.

Alternatively, the inherent method suffers none of these problems, requiring neither additional gates nor additional qubits by utilizing the qubits natural decoherence to implement the relaxation channels. However, it is much more restrictive in its applicability since the relaxation parameters of the qubits are fixed. We have shown some examples of how to get around these constraints by invoking a correction circuit to map the natural qubit relaxation dynamics onto the relaxation dynamics of a system of interest.

Furthermore, we show how this correction circuit can be used to invert the relaxation of a simulation to recover the coherent dynamics as well as to add relaxation to the results of a purely coherent simulation. More study is needed to determine how widely applicable such methods are to simulations outside of those described by Hamiltonians of the form given in Eq. 4.3.

We demonstrate the effectiveness of these techniques on two simple, real-world systems of interest in spin chemistry. Due to the simplicity of the DPS/PTP radical pair system, we are able to implement the full Hamiltonian simulation. Using the Inherent method, we were able to reproduce the theoretical result for the TR MFE with a standard deviation of 0.027 (Fig. 4.6), despite the presence of broadband dephasing seen at longer times. This shows that such methods are an effective tool to model real world systems undergoing thermal relaxation that is usable on currently available quantum devices. Furthermore, these results are significantly less noisy than
the experimental data (SD 0.099), which suffers from a noise problem outlined in Appendix B.

We also demonstrate the effectiveness of these techniques for a more complicated system (the TMP/PTP radical pair) having two hyperfine coupling terms and a $B$-field dependent $T_1$ relaxation rate. Unfortunately, currently available quantum computers aren’t sufficiently robust enough to implement Hamiltonian simulation of this system - largely due to CNOT error rates. As quantum computers continue to improve gate fidelity, we hope in the near future this will be possible. In order to work around this, we classically precompute $S(t)$, encode this onto a pair of qubits and use our protocols to recover $\tilde{S}(t)$. This classical precomputation step is exponentially hard in the size of the nuclear degrees of freedom, making it desirable to develop optimal methods for Hamiltonian time evolution on a quantum computer.

The results for TMP/PTP using both the Kraus and inherent + correction circuit method are shown in Fig. 4.12. We find excellent agreement with theory, with both of our datasets again being less noisy than the experimental data. When directly simulating time evolution becomes reliable on NISQ devices, the encouraging results here suggest our methods could provide fast, easy and cheap ways to do primary investigations into spin chemistry problems to direct or supplement experiments. Because these methods do not suffer from the experimental noise problem outlined in Appendix B, they may also provide a way to probe experimentally inaccessible regimes.

Further research is needed to explore the applicability of the three methods presented here to Hamiltonians other than those of the form in Eq. 4.3. It is likely that these methods will be applicable to many systems relaxing in an effectively infinite temperature environment. More research is also needed to determine how these ideas can be extended to implement quantum channels other than amplitude damping and dephasing. We have shown how the application of echo pulses during
the decoherence step transforms the zero-temperature amplitude damping channel to
the infinite-temperature amplitude damping channel. We believe that applying other
sequences of unitaries during the decoherence will yield different quantum channels.
More study is needed to investigate how to construct desired channels in this fashion,
the efficiency of their construction and the scope of channels that can be constructed.
Chapter 5

Driven-Dissipative Quantum Mechanics on a Lattice: Simulating a Fermionic Reservoir on a Quantum Computer

5.1 Summary

The driven-dissipative many-body problem remains one of the most challenging unsolved problems in quantum mechanics. The advent of quantum computers may provide a unique platform for efficiently simulating such driven-dissipative systems. But there are many choices for how one can engineer the reservoir. One can simply employ ancilla qubits to act as a reservoir and then digitally simulate them via algorithmic cooling. A more attractive approach, which allows one to simulate an infinite reservoir, is to integrate out the bath degrees of freedom and describe the driven-dissipative system via a master equation, that can also be simulated on a quantum computer. In this work, we consider the particular case of non-interacting electrons on a lattice driven by an electric field and coupled to a fermionic thermostat.

Then, we provide two different quantum circuits: the first one reconstructs the full dynamics of the system using Trotter steps, while the second one dissipatively prepares the final non-equilibrium steady state in a single step. We run both circuits on the IBM quantum experience. For circuit (i), we achieved up to 5 Trotter steps. When partial resets become available on quantum computers, we expect that the maximum
simulation time can be significantly increased. The methods developed here sug-
gest generalizations that can be applied to simulating interacting driven-dissipative
systems.

5.2 Introduction

Dissipation is ubiquitous in nature and often a many-body system of interest is cou-
pled to other degrees of freedom that play the role of an external reservoir (such
as electrons and phonons in solid-state physics). The understanding of dissipative
many-body quantum systems represents a long standing problem that traces back to
the seminal works by Caldeira and Leggett [104, 105, 106], and has experienced a
renewed interest in the last decade. In fact, dissipation has been theoretically pro-
posed as a resource for quantum computation [107, 108, 109, 110] and experimentally
it has been demonstrated that an open quantum system can employ dissipation for
quantum state preparation [96, 111, 112]. Our interest, however, is motivated by the
advent of recent pump-probe experiments (see Refs. citepump-probe-review,pump-
probe-review2 for recent reviews), where systems can be easily driven out of equilib-
rium and then probed at different time delays to determine how they relax. Condensed
matter systems always have electrons coupled to a phonon reservoir. Hence, we are
ultimately interested in the possibility of eventually using quantum computers to
simulate driven-dissipative (and strongly interacting) systems of fermions coupled to
bosons.

In addition to removing energy from a system, dissipation can also be the source of
the phenomena one wants to study. For example, in the case of lattice electrons driven
by an electric field, an isolated noninteracting system displays Bloch oscillations[113,
114], leading to an alternating current due to Bragg reflection at the Brillouin zone
boundaries. Conversely, when interactions are turned on, dynamical mean field theory (DMFT) \cite{115} predicts that Bloch oscillations are damped as the system heats to an infinite temperature steady state where the current ultimately vanishes \cite{116}. When dissipation with the environment is taken into account, both noninteracting\cite{117} and interacting \cite{118, 119} systems stabilize a DC current in the steady state, that depends nontrivially on the interactions and the electric field intensities. Of course, this is exactly what any real system also does, as we know from Ohm’s law. Properly treating the dissipation is critical to being able to understand physical phenomena like Ohm’s law.

The difficulty in addressing strongly correlated systems in a nonperturbative way remains an obstacle for the classical simulation of driven-dissipative systems, even for model systems like the Hubbard model. However, simulations of quantum many-body models have been successfully performed using cold atom quantum simulators \cite{120}. Such simulations are analog simulations, meaning that a physical system (e.g. cold atoms), set under specific physical conditions (e.g. placed in an optical lattice), can reproduce the dynamics of another physical system of interest (e.g. electrons in solids). Other quantum simulators include trapped ions, which intrinsically simulate the transverse-field Ising model with tunable long-range interactions \cite{121, 122}, or the Dicke model \cite{123}. One can view these quantum simulators as essentially just being well-controlled experiments, which does allow one to learn new things about these complex systems. Nevertheless, there is great interest in transitioning toward digital quantum computation, following the progression from analog to digital classical computation.

Some progress has already been made in this realm, although the fact that current hardware is noisy (so-called noisy intermediate-scale quantum computers or NISQ machines), makes it quite difficult to perform time evolution accurately. For
example, some simplifications for the Heisenberg model on small clusters allowed the
time-evolution to be simulated without needing to Trotterize the evolution oper-
tors [124, 125]. In addition, there exist robust algorithms for time-evolving quantum
computers when fault-tolerant quantum computing becomes available [51]. An alter-
native approach to exact time evolution is to evolve systems variationally[126], which
is likely to also be a robust approach for NISQ-era machines.

There is a fair amount of work that has been completed already on how to simulate
open quantum systems on quantum computers. Ref. citeBarreiro2011 showed how to
prepare entangled states by simulating a master equation with a digital quantum
circuit, whose dissipative nonunitary “gates” were obtained by resetting ancilla qubits
that had been suitably entangled with the system qubits. For most systems of interest,
the size of the bath is much larger than that of the system, often taken to be infinite.
In these cases, if one could simulate a master equation, it would be more convenient
than digitally implementing the unitary dynamics of the system plus a finite bath
(so-called algorithmic cooling[127]). This is because a direct representation of the
bath requires far too many qubits, or accuracy is sacrificed to reduce the bath to
a reasonable size. However, the master equation approach integrates out the bath’s
degrees-of-freedom and replaces them with operations that act only on the system.
This makes it possible, in principle, to accurately simulate interactions with arbitrarily
large baths without requiring arbitrarily large resources.

However, when dealing with master equations, approximations are usually nec-
essary. One common choice is to use the Redfield Master Equation (RME) which is
obtained by making the Born-Markov approximation. This places some constraints
on the applicability of the method. Furthermore, it is not always possible to simulate
the RME on a quantum computer. This is because the RME is not guaranteed to
generate a quantum dynamical semigroup [128], and further approximations may be needed.

In the first part of our paper, we discuss these approximations thoroughly for the case of an exactly solvable model and compare our results to the exact solution [117]. In particular, we consider a tight-binding model of fermions with periodic boundary conditions (PBC) driven by an electric field and interacting with an external (fermionic) reservoir.

In the second part of the paper, we show how to engineer quantum circuits that reproduce the dynamics of this dissipative system. In particular, we devise two schemes:

(i) We simulate the dynamics of the Trotterized system directly on a quantum machine computer;

(ii) We show how to dissipatively prepare the long-time non-equilibrium steady state (NESS) in a single step.

For (ii) we need to know in advance the state that we want to prepare. For this simple system we can do this analytically, but in general we could also determine it from using (i). This is useful to reduce the number of quantum gates needed to prepare the steady state allowing us to perform quantum operations on the NESS. We implemented two quantum circuits, corresponding to schemes (i) and (ii), using IBMQ and obtain good results. For scheme (i), we could only run a few Trotter steps because IBMQ (and most current quantum computers) does not have the capability to reset ancilla qubits while leaving the others undisturbed. This forces us to use SWAP operations and extra qubits to accomplish a reset. Better results are expected once partial reset gates become available.
In this work we provide some important ideas that will hopefully help in the effort to devise quantum algorithms for simulating more complicated and realistic driven-dissipative systems, which we discuss further in the conclusion. We hope this work will provide a stepping stone toward tackling the simulation of more common solid-state systems (e.g. electrons interacting with a phonon bath). Because the problem of studying driven-dissipative systems is simultaneously important and challenging, we feel that our exposition of a concrete approach to a simple system will be useful for both considering more complex scenarios as well as gaining a general understanding of the complex phenomena that driven-dissipative quantum systems may exhibit.

In Sec. 5.3, we first derive the RME of our model and, using an additional approximation, derive a master equation in Lindblad form which is more suitable for simulation on a quantum computer. We compare these approximations with the exact solution and between each other. In Sec. 5.4, we explicitly derive the Kraus maps for the two different schemes (i) and (ii). In Sec. 5.5, we construct the quantum circuits for solving the dynamics of the system (i), and for the state preparation of the NESS (ii). Finally, we show data obtained directly from an IBM quantum computer. In Sec. 5.6, we summarize the main achievements of our work.

5.3 The Model

The open system that we consider is given by noninteracting lattice fermions on a one-dimensional chain with nearest-neighbor hopping in the presence of an electric field. The effect of the electric field is taken into account by introducing a complex Peierls phase \( \varphi(t) = \Omega t \) (given by \( \Omega = eEa \)) to the hopping integral \( \gamma \); we use \( \gamma \) for the hopping instead of the more common \( t \), so as to not confuse the hopping
Figure 5.1: Schematic representation of a one-dimensional tight-binding model. Electrons hop between nearest-neighbor sites under the effect of an electric field. Each lattice site is coupled to an infinite fermionic bath in thermal equilibrium that exchanges energy and fermions with the chain.

term with time. The system Hamiltonian then reads:

$$\hat{H} = -\gamma \sum_i e^{i\varphi(t)} d_i^\dagger d_{i+1}^\dagger + \text{h. c.} \quad (5.1)$$

Every site of the chain is coupled to an independent infinite fermionic bath, whose Hamiltonian is $$\hat{H}_b = \sum_{i\alpha} \omega_{\alpha} c_{i\alpha}^\dagger c_{i\alpha}$$, through a bilinear hybridization term that is given by:

$$\hat{V} = -g \sum_{i\alpha} d_i c_{i\alpha} + \text{h. c.} \quad (5.2)$$

Here $$g$$ is the bare interaction strength, and $$\alpha$$ is an index that runs over all the internal degrees of freedom of the bath, which are taken to be infinite. In Fig. 5.1, we
schematically represent the linear chain coupled to the reservoir. The entire Hamiltonian of the system plus the bath is given by $\hat{H}_{\text{tot}} = \hat{H} + \hat{H}_b + \hat{V}$ and can be recast in a block diagonal form by expressing the fields in the Fourier basis, that is

$$d_k = \frac{1}{\sqrt{N}} \sum_n d_n e^{-ikn}, \quad c_{k\alpha} = \frac{1}{\sqrt{N}} \sum_n c_{n\alpha} e^{-ikn}$$

and their Hermitian conjugates. In this basis, the Hamiltonian decomposes into a sum of Hamiltonians for each momenta. In Ref. citeHan2012, the dynamics of the electrons in the chain ($d$ fermions) are exactly solved by determining the nonequilibrium Green’s function on the Keldysh contour; the problem can be solved exactly because it is quadratic in the fermion operators.

In this section, we will introduce the master equation (ME) that defines the model that we will simulate on the quantum computer. In particular, we will derive the RME and subsequently a Lindbladian Master Equation (LME), which is easier to translate on a quantum circuit, showing what approximations we have to perform to obtain it. In passing, we also compare the expected theoretical results with those of Ref. citeHan2012, to show in which regimes our scheme significantly deviates from the physics that we want to simulate.

5.3.1 The Master Equation

The master equation governs the dynamics of the system’s reduced density matrix $\dot{\rho} = \text{Tr}_b \dot{\rho}_{\text{tot}}$, where $\text{Tr}_b$ indicates the partial trace over the bath subspace. Within the Born approximation[130], the density matrix of the whole system is given by $\dot{\rho}_{\text{tot}} = \dot{\rho} \otimes \dot{\rho}_b(0)$, and we choose $\dot{\rho}_b(0) = \exp\left(-\beta \hat{H}_b\right)/Z_b$, where $\beta$ is the inverse temperature of the bath. The 0 argument on the bath density matrix denotes the initial start of the system at time $t = 0$.

Given the block diagonal form of the full Hamiltonian (system plus bath), the system’s reduced density matrix factorizes as a tensor product in momentum space, i.e. $\dot{\rho} = \bigotimes_k \dot{\rho}^{(k)}$, meaning that we can define a $k$-dependent master equation for
each $2 \times 2$ $k$-dependent density matrix $\hat{\rho}_k$. The master equation for each momentum subblock is:

\begin{align}
\partial_t \hat{\rho}_k &= \text{Re} a_k(t) \left[ 2d_k \hat{\rho}_k d_k - \left\{ d_k d_k, \hat{\rho}_k \right\} \right] \\
&\quad + \text{Re} A_k(t) \left[ 2d_k \hat{\rho}_k d_k - \left\{ d_k d_k, \hat{\rho}_k \right\} \right], \quad (5.3)
\end{align}

where:

\begin{align}
a_k(t) &= g^2 \exp \left[-if_k(t) \int_{-\infty}^{0} dt_1 C_p(-t_1) \exp \left[i f_k(t + t_1) \right] \right] , \\
A_k(t) &= g^2 \exp \left[i f_k(t) \int_{-\infty}^{0} dt_1 C_h(-t_1) \exp \left[-i f_k(t + t_1) \right] \right]. \quad (5.4)
\end{align}

with $f_k(t) = \sin(k + \Omega t)/\Omega$, and where $C_p(t)$ and $C_h(t)$ are respectively the greater and lesser Green function of the bath fermions (see App. C for their definition and a derivation of these equations). In our case, we choose to attach an infinite bath to every site (see Fig.5.1) that is at half-filling. In this, situation $C_p(t) = C_h(t)$. Given the simple form of the bath Hamiltonian, the correlation function is $k$-independent and can be calculated analytically. In particular, in the limit of an infinite bandwidth with a flat density of states $[N(\epsilon) \equiv \sum_\alpha \delta(\epsilon - \omega_\alpha) \sim N(0)]$ (see Appendix C, for further discussions about this limit), we find that:

\begin{align}
C_p(t) &= \pi N(0) \left[ \delta(t) - \frac{i}{\beta} \text{PV cosech} \left( \frac{\pi t}{\beta} \right) \right]. \quad (5.5)
\end{align}

Here, PV denotes the principal value.

The coefficients that appear in Eq. (5.4) are not always positive. This is made apparent by expanding the coefficients in terms of Bessel functions, as we show in App. C. The loss of positivity can complicate our ultimate goal, i.e. to write a quantum circuit that simulates the driven-dissipative dynamics. In order to obtain a master
equation that preserves positivity, we have to perform some additional approximations. In particular, we consider the following expansion:

\[ f_k(t + t_1) \sim f_k(t) + \epsilon_k(t)t_1, \]  

(5.6)

in Eq.(5.4), which yields the following approximate coefficients:

\[ \text{Re}a_k(t) \sim \Gamma n_F[\epsilon_k(t)] \]
\[ \text{Re}A_k(t) \sim \Gamma n_F[-\epsilon_k(t)]. \]  

(5.7)

The expansion that we consider is valid as long as the \( t_1 \) in the integral in Eq. (5.4) can be considered small, i.e. the time scale set by the correlation function of the bath, roughly \( \tau_b = \beta/\pi \), is small compared to the period of Bloch oscillations \( \tau_b \ll 2\pi/\Omega \) and the inverse of the bandwidth \( \tau_b \ll 1/\gamma \). In this regard, we can consider the expansion in Eq. (5.6) as perturbative in \( \Omega \) and it is reminiscent of a recent approximation scheme to derive a Markovian time-dependent ME [131]. Eq.(5.6) We shall refer to Eq. (5.3), with the coefficients given in Eq. (5.4), as the RME; it is the LME when the coefficients are given in Eq. (5.7).

5.3.2 Comparison of the RME, LME and Exact Solution

From Eq. (5.3), we can obtain a differential equation for the momentum distribution function \( n_k(t) = \text{Tr} \left( \hat{\rho}_k(t) d_k d_k^\dagger \right) \), which can be immediately integrated to yield its solution. This is given by

\[ \dot{n}_k = -2\Gamma n_k + 2\text{Re}a_k(t). \]  

(5.8)

In Fig. (5.2), we show the time evolution of the momentum distribution function evaluated at \( \Omega/\gamma = 0.2, \Gamma/\gamma = 0.1 \), and \( (ka) = \pi/2 + 0.1 \). As one might expect for a driven-dissipative system, the system initially has transient behavior, which then
Figure 5.2: Momentum distribution function $n_k(t)$ as a function of time. Here $k = \pi/2 + 0.1$, $\Gamma/\gamma = 0.1$, and $\Omega/\gamma = 0.2$. We observe, that after an initial transient behavior, the occupation number reaches steady oscillations. We compare our results obtained by integrating the RME and LME, with the exact calculation\cite{117} of $n_k(t)$. See App. C for technical details.
evolves into steady oscillations at long times. The oscillatory behavior arises from the
time-dependence of $a_k(t)$ [see Eq. (D.4)]. In Fig. 5.2, we also plot the result obtained
through the master-equation formalism. Comparing with the exact solution provided
in Ref. citeHan2012, we see excellent quantitative agreement, especially for long times.

To understand the oscillating behavior at long times, we compute the occupation
number as a function of the gauge-invariant wavevector $k_m = k + \Omega t$. Fig. (5.3), shows
$n(k_m)$ [from Eq. (D.6)], where we replaced $k_m$ with $k + \Omega t$, as done in Ref. citeHan2012,
for different values of the driving field $\Omega$ at $\Gamma/\gamma = 0.1$. The momentum distribution
shifts toward the driving field direction when $\Omega$ is increased, as expected since the
electric field drives electrons in the direction of the field. When the field is large,
the momentum distribution function loses its original shape and becomes sinusoidal
with a smaller width (this is probably due to a tendency toward a Wannier-Stark
ladder[132], but with broadening due to the dissipation). We compare our results
with the exact solution and find excellent quantitative agreement between the RME
and the exact solution for all values of the field strength. The LME predictions deviate
from the exact solution when $\Omega$ is sufficiently large, as expected given the perturbative
nature of the expansion in Eq. (5.6) that we used to set the LME. We observe that
for large field values the $n(k_m)$ profile obtained with the LME is shifted by a phase
compared to the exact solution and its shape tends to a triangular wave rather than
a sinusoidal. However, the amplitude and mean value of the oscillations appear to
agree with the exact solution also for large $\Omega$.

The total current of the system in the steady state is given by the formula
$J = (2\pi)^{-1} \int dk_m v_{km} n_{km}$, where the band velocity is defined as $v_k = \partial_k \epsilon_k$,
with the bandstructure given by $\epsilon_k = -2\gamma \cos k$. For generic times the current is a time-
dependent function, however the long-time behavior of $J(t)$ is a constant in time. It
is evident that in order to obtain a finite current, $n_{km}$ must not be symmetric with
Figure 5.3: Momentum distribution function in the long time limit. Momentum distribution function $n(k_m)$ as a function of the gauge-invariant wavevector $k_m = k + \Omega t$ in the long time limit. Here we take different values of $\Omega$ and $\Gamma/\gamma = 0.1$. We compare the RME (red dashed line) and the LME (black solid line) results with the exact solution (blue thin line) given in Ref. citeHan2012. See App. C for technical details.
respect to the origin (not an even function), and we have already shown that a finite electric field tends to distort the momentum-distribution function towards the field direction [see Fig. 5.3]. In App. C, we give the analytic expressions for the current in the long-time limit for both the RME and the LME, here we will limit ourselves to show and comment on the results.

The dc current as a function of the electric field is shown in Fig. 5.4. For small enough values of $\Omega$, the current grows linearly with the electric field, illustrating the expected Ohm’s law-behavior in the linear-response regime. When the field intensity increases and becomes comparable to the dissipation rate $\Gamma$, a Bloch electron has enough life time to reach the Brillouin zone boundary. In this regime, Bloch oscillations effects become important and the dc current first reaches a maximum at $\Omega \sim 2 \Gamma$. When $\Omega$ is further increased, the period of the oscillations is very high so that Bloch electrons reach the BZ boundaries and are reflected back multiple times, decreasing the expectation value of the current, that averages to zero in the limit $\Omega \to \infty$.

We compare our result with the exact one calculated in Ref. citeHan2012. The agreement is excellent for small values of $\Gamma$ for both the RME and LME results. Note that when the coupling with the bath is increased, the master-equation prediction starts to deviate from the exact result. However, as shown in Fig. 5.4 for $\Gamma/\gamma = 0.2$, there is a region of intermediate values of $\Gamma$ where the RME reproduces all the qualitative features of the exact solution; it just has some quantitative mismatch. This disagreement is largest for intermediate values of $\Omega$. When the dissipation rate is increased further the RME stops to be a reliable approximation, as we can see in Fig. 5.4 for $\Gamma/\gamma = 0.5$, where also in this case the disagreement is maximal for intermediate values of $\Omega$. Instead, in the asymptotic limit when $\Omega \to \infty$, the RME seems to give good results also for large values of $\Gamma$. It is worthwhile to note that the LME predictions are in an excellent quantitative agreement with the exact solution.
Figure 5.4: DC current in the long-time limit as a function of the driving field. Here we take different values of the coupling with the bath $\Gamma$. Our results from the RME (red dashed lines) and LME (black solid line) are compared with the exact curves of the current (blue thin lines) calculated in Ref. [117]. See App. C for technical details.
for a broad range of $\Omega$ and $\Gamma$. This is surprising given that the LME was obtained in the limit of both $\Gamma, \Omega \ll \gamma$. We note that only in the asymptotic limit do we start to appreciate a mismatch between the exact solution and the LME, which is enhanced by increasing $\Gamma$. This might be a peculiarity of our model and further investigations are needed to establish if the LME yields good results in the strongly driven regime when on-site Coulomb repulsion between electrons is taken into account. However, this would go beyond the aim of our paper and we postpone it to future study.

5.4 The Kraus Maps

Because we are interested in the possibility of simulating dissipative dynamics on a quantum computer, we now explore some of the details behind how one would do this. We devise two schemes:

(i) The dynamics of the system is solved directly by the quantum computer using Trotter steps;

(ii) We show how to dissipatively prepare the long-time NESS in one step.

To create a better connection with quantum computation, it is useful to express the time evolution of the density matrix in terms of the operator-sum representation:

\[ \rho(t) = \sum_i K_i(t) \rho(t_0) K_i^\dagger(t), \quad (5.9) \]

where $\rho(t)$ is the system density matrix at time $t$, $\rho(t_0)$ is set by the initial condition, and $K_i$ are the Kraus operators that satisfy the following sum rule:

\[ \sum_i K_i^\dagger K_i = 1. \quad (5.10) \]

In our case, the set of $K_i$ depends on the master equation we started with and on the particular scheme that we want to adopt: (i) or (ii).
5.4.1 The Trotterised Map

In general, determining the map in Eq. (5.9) is tantamount to finding the exact solution of the problem, which would be very challenging especially for large enough systems. Instead, it is possible to construct an infinitesimal map that evolves a state from an initial time $t$ to a final state at time $t + dt$, when the master equation is in Lindblad form [133]. In fact in this case, the Kraus map is given by $K_1 = 1 - iHdt - \frac{1}{2} \sum_{i>1} L_i^\dagger L_i dt$, and $K_{i>1} = \sqrt{dt}L_i$, where $L_i$ are the Lindbladians, and $\sum_{i=1}^4 K_i^\dagger K_i = 1 + O(dt^2)$.

In analogy with algorithms for closed systems [134], where the dynamics of a quantum state are obtained in an approximate fashion using Trotter steps, we can construct a semi-positive trace preserving map, that satisfies exactly the sum rule in Eq. (5.10), and that reconstructs approximately the state at time $t + \Delta t$ from the state at time $t$, performing the following mapping:

$$\rho(t) \mapsto \rho(t + \Delta t) = \sum_i K_i(t)\rho(t)K_i^\dagger(t), \quad (5.11)$$

where $\Delta t$ is finite and:

$$K_1 = \exp (iH(t)\Delta t) \sqrt{1 - \sum_i L_i^\dagger(t)L_i(t)\Delta t}$$

$$K_i = \sqrt{\Delta t}L_i(t) \quad \text{when } i > 1. \quad (5.12)$$

We note that the map defined by Eqs. (5.11,5.12) recovers the infinitesimal map when expanded to first order in $\Delta t$, i.e. $K_1 \sim 1 - iH(t)\Delta t - \frac{1}{2} \sum_i L_i^\dagger L_i \Delta t$, and when the dissipation rates go to zero, it gives back the time evolution of the isolated system, i.e. $K_1 = \exp(iH\Delta t)$ and $K_{i>1} = 0$. We note further that such a construction is generic and can be applied to any system when the Hamiltonian and the Lindbladians are specified.
Let us now consider as an example our system of non-interacting electrons in an electric field. In this case, we might be tempted to define as Lindbladians the following operators \( \sqrt{2} \text{Re} a_k(t) d_k \) and \( \sqrt{2} \text{Re} A_k(t) d_k \). However, this would not correspond to a trace preserving map, when \( \text{Re} a_k(t) \) or \( \text{Re} A_k(t) \) become negative. Therefore, this scheme is suitable for simulating only the LME where the time-dependent coefficients are defined in Eq. (5.7).

Under these assumptions, the Trotterised Kraus map becomes:

\[
K_1 = \sqrt{1 - 2 \Gamma n_F [-\epsilon_k(t)]} \Delta t P_1 + \sqrt{1 - 2 \Gamma n_F [\epsilon_k(t)]} \Delta t P_0
\]
\[
K_2 = \sqrt{2 \Gamma n_F [-\epsilon_k(t)]} \Delta t XP_1
\]
\[
K_3 = \sqrt{2 \Gamma n_F [\epsilon_k(t)]} \Delta t XP_0,
\]

(5.13)

where we defined \( P_0 = d_k d_k^\dagger \), \( P_1 = d_k^\dagger d_k \) and \( X = d_k^\dagger + d_k \). We note that Eq. (5.13) gives a constraint to the maximum allowed time step, which is given by \( \Delta t < 1/2\Gamma \).

5.4.2 The Integrated Map

In this section, we determine the integrated Kraus map for our system of non-interacting electrons. We closely follow the work by Andersson et al. [135].

We first express the density matrix at time \( t \) \( \rho_k(t) \) from Eq. (5.3) as a map from its initial value \( \rho_k(0) \) via

\[
\rho_k(t) = \phi_t(\rho_k(0)) = \sum_{a=0}^{3} \sum_{b=0}^{3} S_{ab}(t) \sigma_a \rho_k(0) \sigma_b,
\]

(5.14)

where \( \sigma_0 = 1_{2 \times 2}/\sqrt{2} \), \( \sigma_1 = \sigma^x/\sqrt{2} \), \( \sigma_2 = \sigma^y/\sqrt{2} \), \( \sigma_3 = \sigma^z/\sqrt{2} \), with \( \sigma^a = \{x, y, z\} \) being the standard \( 2 \times 2 \) Pauli matrices and where \( S_{ab}(t) \) is the so-called Choi matrix (which is a Hermitian and time-dependent \( 4 \times 4 \) matrix) expressed in the Pauli basis (the time evolution of the density matrix is a positive trace-preserving map). \( \phi_t \) and \( S_{ab} \) generally have a \( k \) dependence which we have omitted for readability. Note that we
are working in a specific fixed momentum subspace, so the density matrix here is a
$2 \times 2$ matrix and the Choi matrix is a $4 \times 4$ matrix; the indices in the summations run
over only four values. We can rewrite this map in a diagonalized form in the following
way:

$$\phi_t(\rho_k(0)) = \sum_{i=1}^{4} K_i(t) \rho_k(0) K_i^\dagger(t),$$

(5.15)

where $K_i(t) = \sqrt{\lambda_i} \sum_{a=0}^{3} X(i)_a \sigma_a$ are the Kraus operators with $\lambda_i$ and $X(i)$ being the
eigenvalues and eigenvectors of the Choi matrix (the Kraus operators are effectively
square-roots of the Choi matrix). Note that the Kraus operators are expressed as
operators in a two-dimensional space, given by the Pauli matrices.

We can obtain the Choi matrix directly from the master equation by realizing that
the equation of motion can be re-expressed as $\partial_t \rho_k(t) = \Lambda_t(\rho_k)$, where $\Lambda_t$ is a linear
map such that $\Lambda_t(\rho_k)$ is Hermitian and traceless. Using this form, it can be shown
that[135]

$$S_{ab}(t) = \sum_{r=0}^{3} \sum_{s=0}^{3} F_{sr}(t) \text{Tr} [\sigma_r \sigma_a \sigma_s \sigma_b],$$

(5.16)

where $F_{rs} = \text{Tr}(\sigma_r \phi_t(\sigma_s))$ is a matrix representation of the linear map $\phi_t$. In App. E,
we give more details on the analytical derivation of the linear map $\phi_t$. This matrix
is related through a differential equation to the matrix representation of $\Lambda_t$ in the
following way: $\dot{F}(t) = L(t) \cdot F(t)$, where "." indicates the matrix product, with initial
condition $F(0) = \mathbb{1}_{4 \times 4}$ and with $L_{rs} = \text{Tr}(\sigma_r \Lambda_t(\sigma_s))$.

In general, finding the Choi matrix is tantamount to finding an exact solution of
the problem, so it can be quite complex. But, for the noninteracting system that we
consider here, the procedure is greatly streamlined. Indeed, an analytic solution is
possible, as we now show. For long enough times, the Kraus operators become

\begin{align}
K_1 &= \sqrt{1 - n_k(t)} P_0 \\
K_2 &= \sqrt{n_k(t)} P_1 \\
K_3 &= \sqrt{n_k(t)} X P_0 \\
K_4 &= \sqrt{1 - n_k(t)} X P_1
\end{align}

(5.17)

where \( n_k(t) \) is defined in Eq. (D.6), and we generically focus on taking the long-time limit. Note how we need to know the final momentum distribution in order to determine these Kraus operators, again indicating that determining them is equivalent to completely solving the system. Given fermionic statistics, namely that \( 0 \leq n_k(t) \leq 1 \), these long-time Kraus operators satisfy the normalization condition \( \sum_i K_i^\dagger K_i = 1_{2 \times 2} \). When the Kraus map is applied to a generic initial state \( \rho_k(0) \), it returns the following time-dependent mixed state:

\[
\rho_k(t) = \phi_t(\rho_k(0)) = [1 - n_k(t)] |0\rangle\langle 0| + n_k(t) |1\rangle\langle 1|
\]

(5.18)

which depends only on the population of electrons with momentum \( k \). We call it the steady-state density matrix or \( \rho_{ss} \).

### 5.5 Quantum Circuits

#### 5.5.1 Quantum Simulation of Driven-Dissipative Dynamics

Now we discuss how one can simulate the action of the Kraus map given in Eq. (5.13) by using a quantum circuit. The circuit implementing a single Trotter step must perform the mapping written in Eq. (5.11).

This is not a unitary map (because we are simulating dissipation), so ancilla qubits must be employed to purify the channel into a unitary operation. Such a unitary operator is guaranteed to exist by Stinespring’s dilation theorem[34].

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We may interpret this Kraus map as performing the following: If the system is in state $|0\rangle$, apply $X$ with probability $k_1 \equiv 2\Gamma n_F[\epsilon_k(t)]\Delta t$ and apply the identity $I$ with probability $1 - k_1$. If the system is in state $|1\rangle$, apply $X$ with probability $k_2 \equiv 2\Gamma n_F[-\epsilon_k(t)]\Delta t$ and apply $I$ with probability $1 - k_2$.

One way of doing this is as shown in Fig. 5.5. Here we have defined $\theta_t = 2 \arcsin(\sqrt{k_1})$ and $\phi_t = 2 \arcsin(\sqrt{k_2})$. We begin by rotating the ancilla qubit by $\theta_t$, then if the system is in $|0\rangle$, we do nothing, and if the system is in $|1\rangle$, we undo the rotation of $\theta_t$ and rotate by $\phi_t$. This leaves the ancilla in $|1\rangle$ with probability $P(1|0) = \sin^2 \theta_t/2 = k_1$ and $P(1|1) = \sin^2 \phi_t/2 = k_2$, as desired. Finally, we flip the system qubit if the ancilla is $|1\rangle$. This accomplishes the operation described above.

$|0\rangle \xrightarrow{R_x(\theta_t)} R_x(\phi_t - \theta_t) |0\rangle$

Figure 5.5: Circuit fragment inducing correct transitions in the system. The $|0\rangle$ gate indicates a selective reset of that qubit to the $|0\rangle$ state. $\theta_t = 2 \arcsin(\sqrt{k_1})$ and $\phi_t = 2 \arcsin(\sqrt{k_2})$. This will give the correct diagonal terms in the resulting density matrix.

However this is not sufficient to implement the proper Kraus map. The form of the Kraus Map arises from taking the partial trace over the ancillary degrees of freedom of the system+ancilla density matrix, after evolving with the joint time evolution operator. Calling the initial state of the ancilla $|a_0\rangle\langle a_0|$ and choosing $\{|a_i\rangle\}$ as the basis for the ancilla, this gives

$$\rho(t) = \sum_i \langle a_i| U(t) |a_0\rangle \rho(0) \langle a_0| U^\dagger(t) |a_i\rangle .$$

(5.19)

This means that to get the proper system density matrix after tracing over the ancilla, the circuit must induce the desired transitions, $\{K_i(t)\}$, on the system qubit as well.
\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
Initial State & Final State \\
\hline
$|0\rangle|a_0\rangle$ & $\sqrt{k_1} |1\rangle|a_1\rangle + \sqrt{1-k_1} |0\rangle|a_0\rangle$ \\
$|1\rangle|a_0\rangle$ & $\sqrt{k_2} |0\rangle|a_2\rangle + \sqrt{1-k_2} |1\rangle|a_0\rangle$ \\
\hline
\end{tabular}
\caption{Action of Trotterized Kraus map.}
\end{table}

\{\langle a_i\rangle\} are any three orthogonal states in the ancilla register, $k_1 = 2\Gamma n_F[-\epsilon_k(t)]\Delta t$, and $k_2 = 2\Gamma n_F[\epsilon_k(t)]\Delta t$.

as map $|a_0\rangle \mapsto |a_i\rangle$ in the ancilla register for the corresponding $K_i$. That is, we seek a circuit implementing a unitary $U$ that accomplishes the mapping given in Table 5.1.

The circuit shown in Fig. 5.5 implements a $U$ which results in $|a_1\rangle = |a_2\rangle$; this gives incorrect off-diagonal terms in the density matrix. This is not an issue for this study, since our quantity of interest, $n_k(t)$, is given solely by the diagonal terms, whose evolution is not influenced by the off-diagonals. Furthermore, the steady-state density matrices produced by the circuit from Fig. 5.5 as well as from Eq. 5.13 are identical, being purely diagonal because our eigenstates are computational basis states. However, if one wishes to access the proper transient states—the circuit given in Fig. 5.6 implements a Trotter step of the Kraus map in Eq. 5.13 exactly. We verify the equivalence of the circuits and Kraus maps by recasting both in terms of matrix operations and directly comparing their action on a generic $\rho$. 

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Figure 5.6: Circuit implementing a single Trotter step of the Kraus map. This map is given in Eq. 5.13. The $|0\rangle$ gate indicates a selective reset of that qubit to the $|0\rangle$ state. In addition, we have $\theta_t = 2\arcsin\sqrt{2\Gamma n_F[\epsilon_k(t)]\Delta t}$ and $\phi_t = 2\arcsin\sqrt{2\Gamma n_F[-\epsilon_k(t)]\Delta t}$. For the initial state $\rho_i = \rho(t)$, the final state of that same qubit is $\rho(t + \Delta t)$.

Fig. 5.7 shows the result for $n_k(t)$ obtained by numerically solving the Lindblad master equation from Eq. (5.3) using the coefficients in Eq. (5.7), plotted against $n_k(t)$ as obtained by classically iterating either circuit given in Figs. 5.5,5.6 (both circuits give identical results). Being a classical simulation of the circuit, the discrepancies between the two curves shown in Fig. 5.7 arise only from using a finite $\Delta t$. Indeed the two curves converge as $\Delta t \to 0$. Ideally we would like to use a very small $\Delta t$ and take a large number of steps to avoid the error associated with finite $\Delta t$, however this is not possible on current hardware as discussed below.

We ran the circuits shown in Figs. 5.5 and 5.6 on IBMQ’s quantum hardware[41]. The resulting output was corrected by the “pseudo-inverse" method as outlined in Qiskit’s “Measurement Error Mitigation" tutorial and implemented in Qiskit Ignis[41]. The data from the circuit in Fig. 5.5 is in good agreement overall with the predicted behavior at early times, beginning to deviate for $t > 4\Delta t$. The data from the circuit in Fig. 5.6 is expectedly worse at all times, and begins to show significant deviations for $t > 3\Delta t$.

As can be seen from Fig. 5.7, many Trotter steps must be run in order to reach the steady state. This is problematic since, at the time of this writing, most quantum
hardware, including IBMQ, do not support selective reset of qubits. This means that each additional Trotter step requires swapping in additional fresh qubits in lieu of an actual reset. Given the limited connectivity of these devices, fidelity drops off quickly as more and more distant qubits are required to be swapped into position near the system qubit. Ultimately selective reset capabilities will be required to implement such protocols on near-term devices with limited connectivity and qubits. The results of these runs are shown in Fig. 5.8 and the computational cost of each step is given in Table 5.2.

\[
\lim_{\Delta t \to 0} n_k(t) = \frac{8 \pi}{30 \Omega} \frac{t}{\Delta t}
\]

Figure 5.7: Comparison of numerically solving the Lindblad master equation versus using a finite Trotter step size. The Lindblad master equation is from Eq. (5.3) using the coefficients in Eq. (5.7). We have used \( \Gamma = 0.1, \Omega = 0.2, \beta = 5, \Delta t = 8\pi/30\Omega, k = 7\pi/8 \) and \( \rho(0) = |1\rangle \langle 1| \)
Figure 5.8: Result from iteratively running the circuits on IBMQ’s Singapore machine. The circuits are shown in Figs. 5.5 and 5.6 (orange and green respectively). We have used $\Gamma = 0.1$, $\Omega = 0.2$, $\beta = 5$, $\Delta t = 8\pi/30\Omega$, $k = 7\pi/8$ and $\rho(0) = |1\rangle\langle 1|$. The idealized results, from Fig. 5.7, are included in blue for reference. Note that the time axis runs only out to 5 units here because we can only implement a small number of Trotter steps.

Table 5.2: Quantum resources for running circuits.

<table>
<thead>
<tr>
<th>Trotter Step</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>q.b. = qubits</td>
<td>$R_x$</td>
<td>$cX$</td>
<td>q.b.</td>
<td>$R_x$</td>
<td>$cX$</td>
</tr>
<tr>
<td>Fig. 5.5 Circuit</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Fig. 5.6 Circuit</td>
<td>7</td>
<td>7</td>
<td>3</td>
<td>14</td>
<td>20</td>
</tr>
</tbody>
</table>

| Trotter Step | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 | 72 | 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 | 86 | 87 | 88 | 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 |
5.5.2 Dissipative Quantum State Preparation of the Non-Equilibrium Steady State

Due to the lack of selective reset capabilities, it is generally not possible to run our protocol far enough out in time to reach and investigate the steady-state dynamics of our system. Note that for Eq. 5.13 to represent a physical map, we must have $\Delta t \leq 1/(2\Gamma)$, so we cannot take arbitrarily large steps even if we were willing to accept the associated error. Therefore we present a quantum circuit implementing the integrated Kraus map given in Eq. 5.17. Given any initial state, pure or mixed, this circuit prepares the desired steady state in a single step and thus circumvents the need to employ partial reset gates. The obvious drawbacks here are that the steady state must be known in advance and one cannot access the transient dynamics.

Following the procedure given in the preceding section, we seek a circuit implementing a unitary $U$ that accomplishes the mapping given in Table 5.3. This is very similar to the map above with two key differences.

First, we have four distinct ancillary states, which allows us to replace the two $cR_x(\pm\pi)$ gates in the circuit in Fig. 5.6 with a single $cX$ gate. This is because in the Trotterized map, we need that an application of $I$ on the system, for both possible system states, maps the ancilla to the same state; the integrated map, however, requires that $I$ applied on the system in $|0\rangle$ and $I$ applied to the system in $|1\rangle$ leaves the ancilla in distinct states, which is precisely what a $cX$ does.

Second, we have $k_1 = 1 - k_2 \equiv n_k(t)$. This means $\theta_t = \pi - \phi_t$ and this symmetry allows us to convert the $R_x(\theta_t)$ and $cR_x(\phi_t - \theta_t)$ into $R_y(\theta_t)$ and $cX$. Because of this, we can simplify the circuit in Fig. 5.6 giving the circuit in Fig. 5.9. We again verify the equivalence of the circuit and Kraus map by recasting both in terms of matrix operations and directly comparing their action on a generic $\rho$. A similar circuit to
Table 5.3: Action of integrated Kraus map.

<table>
<thead>
<tr>
<th>Initial State</th>
<th>Final State</th>
</tr>
</thead>
<tbody>
<tr>
<td>$</td>
<td>0\rangle</td>
</tr>
<tr>
<td>$</td>
<td>1\rangle</td>
</tr>
</tbody>
</table>

$\{|a_i\}\}$ are any four orthogonal states in the ancilla register, and $n_k(t)$ is given in Eq. (D.6).

that one shown in Fig. (5.9) has been run on an IBM Quantum Experience platform to reproduce topological thermal states [136].

We ran the circuit shown in Fig. 5.9 on IBM’s Boeblingen quantum computer [90] for 3 different initial conditions using 3 different angles (three different $n_k$ values) for a total of 9 different circuits. We also performed quantum state tomography on the resulting density matrix, which requires measurements in the $X$, $Y$ and $Z$ bases for each circuit, for a total of 27 different runs. The circuits were optimized by hand in Qiskit [41] to maximize the fidelity of the process by choosing the ideal set of qubits. The $R_y(\theta)$ gate is implemented as $U_3(\theta, -\pi/2, \pi/2)$. The connectivity of the chip allowed for an implementation without any SWAP operations. As was done above, the resulting output was corrected by Qiskit Ignis’ “pseudo-inverse” method [41]. The data is in good agreement overall with the predicted behavior, having an average fidelity of over 99.6% across the 9 runs with a minimum fidelity of 99.1%.

The results in Fig. 5.10 show the components of the $2 \times 2$ density matrix in the standard tomography format. We plot only the amplitudes of the matrix elements, because the off-diagonal elements of the exact result vanish (hence the measured phase of those elements varies widely due to noise, and represents unimportant, but
distracting, errors). The label on the left hand side indicates the state that the system was initialized in (\( \rho_0 = |\psi_0\rangle\langle\psi_0| \)) for a particular run.

Figure 5.9: Final version of the circuit implementing the integrated Kraus map. The map is given in Eq. 5.17, which was run on IBM’s Boeblingen quantum computer[90]. Here we have \( \theta_t = 2 \arcsin \sqrt{n_k(t)} \)
Figure 5.10: Quantum state tomography of the simplified Kraus map circuit. This is implemented on the IBM Boeblingen machine. The amplitudes of the four density matrix elements are plotted for three different target final states, indicated by the value of $n_k$ (top label)—for a given $k$ value, the precise value for $n_k$ is determined from Eq. D.5—here, we chose three representative values to test. The circuit is designed to work for arbitrary initial states $\rho_0$. In this work, we tested three initial states, given by: $|\psi_0\rangle = |0\rangle$, $|\psi_1\rangle = H |0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$, $|\psi_2\rangle = R_x(\pi/4) |0\rangle$. The measured density matrices agree well with the exact results from the simulator (extrapolated to an infinite number of shots) given in the top row, having an average fidelity of over 99.6%.
While this result is a simple implementation of a driven-dissipative system on a quantum computer, it does show that one can run such hybrid classical-quantum simulations even on quantum computers that have no selective reset capability. As selective resets become more widely available, more complex circuits for these types of problems will become possible (and, of course, will be needed to work on more complex systems).

5.6 Conclusions and Discussions

We are interested in the question of how to most efficiently simulate driven-dissipative systems on a quantum computer. While the work presented here does not solve that problem, it provides some important results that will help us along this path. In particular, we have considered a system of non-interacting electrons in a lattice driven out of equilibrium by an electric field and coupled to a bath, whose dynamics is governed by the ME in Eq.(5.3).

We investigated how one can simulate this master equation on a quantum computer with a hybrid classical-quantum algorithm. We did not focus on the general result, which is known to be a hard problem, but instead looked at the simplest concrete example which can be simulated now on NISQ machines—the case of a single qubit system. We did this two ways. First with a Trotterized Kraus map that can examine the transient dynamics and does not require knowledge of the NESS a priori. However, for this we need to reset the ancilla register every Trotter step. Due to the lack of native reset capabilities this protocol is prohibitively expensive on current devices. To mitigate this we use large Trotter steps, which introduce an error, and still cannot evolve all the way to the steady state. Due to the prohibitive cost of simulating the dynamics with current hardware, we introduced a second circuit
that reproduces the quantum operation encoded in the long-time limit of the Kraus map. This then produces the steady-state dynamics of the driven-dissipative system. The simplified circuit requires only three qubits and three controlled gates. Both of these circuits were run on IBMQ’s machines[90]. The data are generally in excellent agreement with the exact results.

One question that we need to discuss is how scalable is such an approach? In this work, the noninteracting nature of the problem allowed for the Kraus map to be found in an integrated form. In the more realistic scenario where the system has on-site Coulomb repulsion between electrons, the situation becomes much more complicated. Finding an analytic form for the Kraus map is no longer possible and so a Trotterized form must be found. Implementing such a map requires either a fresh ancilla register for each Trotter step or the ability to reset the ancilla register without affecting the system. Furthermore, given the many-body nature of the interacting system, each Trotter step is likely to become cumbersome, making the simulation much more challenging. Our Trotterized scheme (i) could be applied to a more complicated multi-qubit system where the jump operators connect different computational basis states. However, most interesting systems are not described by such simple jump operators, and constructing an approximation or extension of our method for handling a many-body interacting problem goes beyond the scope of our current work.

Devising approximate methods to find and implement the Kraus map related to a master equation will be important in order to simulate an interacting driven-dissipative system on currently available (or near term) quantum machines. We plan to tackle this problem in future work.
Chapter 6

Demonstrating Robust Simulation of Driven-Dissipative Problems on Near-Term Quantum Computers

6.1 Summary

Quantum computers are poised to revolutionize the simulation of quantum-mechanical systems in physics and chemistry. Current simulations are limited by uncorrected noise, gate errors, and decoherence. We show that algorithms for solving the driven-dissipative many-body problem, among the hardest problems in quantum mechanics, are inherently robust against errors by executing circuits containing thousands of entangling gates. We simulate 1000 steps of time evolution for driven electrons subject to dissipation on an infinite lattice and compute their steady-state current. We also prepare the thermal state of the atomic limit of the Hubbard model. These two algorithmic primitives are the basic building blocks of many general condensed-matter-physics systems, opening the door to tackling classically intractable problems on quantum computers before error correction is available. One of the grand challenges in science is to understand the behavior of driven-dissipative quantum systems. While the general formalism for the nonequilibrium problem was introduced in the 1960s, it is only recently that conventional computers have begun to be able to solve some of these problems; a long-time nonequilibrium many-body quantum solver does not exist for conventional computers. In this work, we show that quantum computers
with reset gates, even noisy intermediate-scale quantum (NISQ) computers, have the potential to solve these problems in the near future.

6.2 Introduction

The nonequilibrium many-body problem is a frontier of research in many different disciplines: (i) in condensed-matter physics, pump-probe experiments drive a system into nonequilibrium and watch how it evolves [137]; (ii) in chemistry, driving and dissipation play important roles in photochemistry [138] and in cavity-enhanced reactions [139]; (iii) in nuclear and high-energy physics, collisions of heavy nuclei induce nonequilibrium dynamics [140]; and many more. A prototypical example found in condensed matter physics is a pump-probe experiment. In such an experiment, an ultrashort high-energy pump pulse excites the crystal to a high-energy state that is far from equilibrium, and the system is then probed with different time delays afterwards to determine what state was created, and how that state relaxes. In some cases, the system is driven to new (meta)stable nonequilibrium phases that cannot be produced any other way. Within the many-body problem, the two simplest types of dissipative dynamics are (i) dynamics that dissipate to a steady thermal state and (ii) driven dynamics in response to a constant external field. We discuss both cases in this work.

While many quantum algorithms are known for the simulation of closed quantum systems, fewer studies have considered the simulation of open quantum systems despite their rich and interesting behavior[141]. Current approaches include using inherent qubit decoherence[1, 142, 143], direct simulation of an environment[26, 144, 145], implementing Kraus maps / Lindblad operators[52, 56, 146, 147, 148], variational techniques[149, 150], and more [151, 152]. Since Barreiro et al. first demonstrated their
open-system quantum simulator[153], current early-stage dissipative simulations of quantum systems in the areas of quantum chemistry and physics [1, 56, 151, 154] have been completed.

While fault-tolerant quantum computers will be robust for many types of algorithms[155], current hardware has too many errors to be able to carry out long-time coherent quantum evolution[156]. The time evolution for driven-dissipative systems is intrinsically error mitigating[157, 158] and it can be carried out to much longer times than coherent time evolution. With the advent of reset gates being available on quantum computers, this opens up a new realm of computation, where NISQ devices can be focused on solving this important and difficult quantum problem.

The time evolution of a system driven out of equilibrium by an external field that dissipates energy (through the coupling with a reservoir) is not unitary; it is described by a completely positive trace preserving map (also known as a Kraus map)[141]. The density matrix of the system at time \( t + \Delta t \), \( \rho(t + \Delta t) \), can be constructed from \( \rho(t) \) via a (time-dependent) Kraus map in the following way:

\[
\rho(t + \Delta t) = \sum_i K_i(t) \rho(t) K_i^\dagger(t),
\]

where the Kraus operators \( K_i(t) \) satisfy the sum rule \( \sum_i K_i^\dagger(t)K_i(t) = \mathbb{I} \). Since Kraus maps are nonunitary, they are difficult to directly apply on quantum computers via universal (reversible) gates. Instead, we implement dissipative dynamics via irreversible processes using selective resets during the computation. When driving toward a time-periodic “steady” state, the target goal at each time step changes with time, but because the Kraus map at each time step maps all inputs towards a single output, errors in one step tend to be mitigated in subsequent steps. This makes the time evolution for dissipative dynamics inherently robust to errors and well suited for NISQ devices, as discussed further in the supplemental information.
Because of this inherent stability and because these problems are challenging to solve on conventional computers, the driven-dissipative problem may be the best application for near-term quantum computing. In this work, we illustrate how dissipative quantum simulation can be performed on IBM’s quantum computers by considering two problems: the driven-dissipative Hubbard model in its noninteracting and atomic limits.

### 6.3 Non-Interacting Limit

First, we examine the non-interacting limit of the driven-dissipative Hubbard model, i.e. electrons freely moving on an infinite one-dimensional lattice via nearest-neighbor hopping (used as our energy unit), with semi-infinite electronic thermal reservoirs (taken in the wide-band limit) attached to each lattice site. A DC electric field of strength $E$ is applied by employing a linearly varying Peierls phase in the lattice hopping and summarized by $\Omega = eEa$, with $e$ the electric charge and $a$ the lattice spacing (we set $\hbar$ and $c$ to one). Each reservoir is coupled via a lattice-reservoir hopping term to the system at each lattice site; all properties of this coupling are summarized in a parameter $\Gamma$ given by the square of the lattice-reservoir hopping multiplied by the density of states of each reservoir. The infinite system is diagonalized by Fourier transforming to momentum space. In this fashion, the dynamics of the infinite lattice is addressed by solving many independent one-qubit systems, each of which depends on the specific value of the crystalline momentum $k$; in the steady state, we construct the results for all momenta from the results for any single momentum by invoking gauge invariance, as described in Suppl. G. The time and momentum
dependent Kraus operators (for the time step of duration \( \Delta t \)) are given by:

\[
K_0 = d_k^\dagger d_k \sqrt{1 - 2 \Gamma n_F[-\epsilon_k(t)] \Delta t} e^{-i \epsilon_k(t) \Delta t} + d_k^\dagger d_k \sqrt{1 - 2 \Gamma n_F[\epsilon_k(t)] \Delta t}
\]

\[
K_1 = \sqrt{2 \Gamma \Delta t n_F[\epsilon_k(t)]} d_k^\dagger
\]

\[
K_2 = \sqrt{2 \Gamma \Delta t n_F[-\epsilon_k(t)]} d_k,
\]

where \( d_k^\dagger \) is the creation operator of a lattice electron with momentum \( k \); \( \epsilon_k(t) \) is the time-dependent dispersion relation, and \( n_F(x) = 1/(1 + e^{\beta x}) \) is the Fermi-Dirac distribution at the temperature of the reservoirs (here set to \( \beta = \frac{1}{k_B T} = 5 \)).

From the Kraus map given in Eq. 6.2 the quantum circuit can be constructed [2] and appears in Fig. 6.1(d). The \( |0\rangle \) gate in the circuit is a reset operation which ideally sets the qubit to the \( |0\rangle \) state. However, this operation is not perfect on current hardware and the reset fidelity can be improved by applying it to a qubit multiple times in succession (at the cost of additional amplitude damping on the remaining qubits). We run our circuit using one to four reset gates per Trotter step to extrapolate away some of these errors. Details are given in supplement I.

Figure 6.1(a) plots the results of running the circuit shown in 6.1(d) with a single reset gate per Trotter step. The first 300 steps were run on one set of qubits and the remaining 700 on a second set. These runs are robust both with respect to the qubits run on and with respect to the total time of the run. The circuit for the 1000\(^{th}\) step required 2000 CNOT gates and yet the data show no sign of a decaying signal. Note that the transients have died off after about 30 Trotter steps. In panel (b), the raw data with one to four resets is shown for up to 400 Trotter steps. After processing the data via extrapolating to the zero-reset-time limit and then correcting the result by shifting and stretching as described in the supplement J, one can see that the post-processed data (c) agrees with the exact results to high precision. This simulation clearly shows the stability of driven-dissipative circuits on near-term quantum
**Figure 6.1: Electron density vs. time.** (a) 1000 steps of time evolution on ibmq_mumbai using one reset gate per Trotter step. Reported data has been corrected for measurement errors. Different shades of blue represent different sets of qubits while the solid black line is the ideal result of running the circuit. (b) 400 steps of time evolution on ibmq_boeblingen using one to four reset gates per Trotter step. Reported data has been corrected for measurement errors. (c) Left panel shows a zoom in on one period of the data shown in (b). Middle panel shows one period of data obtained by averaging together all periods of steady-state data (step > 30). Right panel shows post-processed averaged data as described in supplement J. (d) Quantum circuit for one Trotter step of time evolution. Here, $\theta_i = 2 \sin^{-1} \sqrt{\frac{2 \Gamma \Delta t}{e^{\varepsilon_i} + 1}}$ and $\phi_i = 2 \sin^{-1} \sqrt{\frac{2 \Gamma \Delta t}{e^{-\varepsilon_i} + 1}}$ where $\varepsilon_i = -2 \cos(k + \Omega_i \Delta t)$ is the dispersion relation at step $i$ (at time $t = i \Delta t$).

computers, producing accurate time evolution far longer than is currently possible with coherent dynamics of electrons[156].

Figure 6.2 shows the steady-state average DC current response of our system to an applied electric field calculated from electron density data as described in supplement G. The data are post-processed in the same manner as in Fig. 6.1 and described in supplement J, which is also compared against the ideal circuit and theoretical results from Lindblad techniques, as described in Ref. [2]. As shown in the inset of Fig. 6.2, the transient region extends to longer times as the electric field is increased,
requiring the simulation to run further in time. Hence, the calculation requires a trade-off between Trotter error (large time step size) and convergence error (steady state not yet reached).

![Figure 6.2: DC current versus electric field strength.](image)

Comparison of the DC response at a given field strength as computed (supplement G) using: (i) the Lindblad master equation (black circles), (ii) the ideal circuit (red squares), and (iii) the measured data from ibmq_boeblingen (blue triangles). All circuits for the current were run for 50 Trotter steps each due to total quantum computer time available, leading to a trade-off between Trotter error and convergence error. $\Delta t$ was chosen empirically such that $\Delta t/\tau$ is linear in $\Omega$. Convergence to the steady-state current is shown in the inset with the solid dots representing $t_{\text{max}}$ for that run.

To minimize the total error, we choose $\Delta t$ empirically with $\Delta t/\tau \approx 0.022 + 0.031 \Omega$ (here, $\tau = 2\pi/\Omega$). At large driving fields it is clear that we have not yet reached the steady state and oscillations in the DC current data are observed even in the ideal case. At small driving field $\Delta t = O(1/\Omega)$ and we incur large Trotter errors. Despite
these limitations, the quantum computer results match the theoretical results fairly accurately across the entire range of simulated field strengths.

6.4 Atomic Limit

The second problem we simulate is the atomic limit of the driven-dissipative Hubbard model in an external magnetic field, $B$. This is a strongly correlated electron problem, which can be simulated with four qubits. The energy cost of double occupancy is given by $U$ and the magnetic field shifts the energy levels of the single-spin states up or down with an energy splitting given by $B$, measured in units of the Bohr magneton.

We build our dissipative circuit by using Kraus operators that induce transitions between computational basis states, which are the energy eigenstates. These transitions are implemented by mapping the system state to an ancilla register and rotating the system qubits controlled on the ancilla [2, 159] (shown in Fig. 6.3(a)); the approach uses just the transitions that correspond to a cycle through the states (depicted in Fig. 6.3(b)). Details are given in supplement H. This circuit is iterated $n$ times to simulate $n$ Trotter steps of time evolution; here we use up to $n = 19$. 
Figure 6.3: Dissipative Hubbard model in the atomic limit. (a) Circuit for a single Trotter step of time evolution. The rotation angles $\Theta$ are given in terms of transition probabilities $\gamma$, which are derived from the detailed balance condition as depicted in (b) and described in supplement H. $\Theta_{i,j} = 2 \sin^{-1}(\sqrt{\gamma_{i,j}})$ and $\gamma_{i,j} \propto e^{\beta \varepsilon_i}$, where $\varepsilon_i$ is the energy of state $|i\rangle$. (c)–(f) Results showing the populations of each of the four possible occupation states versus Trotter step for the ideal case (red squares), measurement-error mitigated data from ibmq_mumbai (blue circles), and the theoretical thermal population (dashed black line). (g)–(i) Full tomography of the density matrix at selected time steps.

Figure 6.3 shows the transient evolution of the Hubbard atom from the vacuum state (with no electrons) to a thermal state with filling $n \approx 0.83$ at a temperature
$T = U/2$ in an external magnetic field $B = U/4$ using one reset per Trotter step. These data are only post-processed for measurement-error corrections. The transient data lie close to the ideal circuit, but show deviations due to intrinsic errors in the hardware implementation. Nevertheless, the steady state is reproduced accurately for the four different populations of the thermal state (c-f) and for the thermal density matrix (g-i). This further exemplifies the robustness of these types of algorithms to noise and how errors in early time steps are largely corrected in subsequent steps.

6.5 CONCLUSION

This work is a strong demonstration of the capabilities of near-term quantum hardware. It also leverages the newly developed capabilities of mid-circuit measurements and reset gates. These novel features are critical for building error-corrected, fault-tolerant quantum computers[38]; as we have shown, they are also essential for pushing the limits of NISQ computers. This convergence will drive further advances that can accelerate the development of fault-tolerant quantum computers.

These successful demonstrations of two algorithmic primitives show that one can directly and robustly simulate the driven-dissipative Hubbard model on near-term quantum computers in both the noninteracting and atomic limits. This lays the groundwork to simulate the general driven-dissipative many-body problem on a quantum computer. Future research that builds on this foundation, aimed at properly combining these two algorithmic primitives to dissipate energy for arbitrary interactions, will solve the general problem and enable quantum computers to simulate important real-world cases, such as pump-probe experiments, quark-gluon plasmas, and cavity-enhanced chemistry.
In this thesis we have explored multiple ways in which near terms quantum computers, i.e. NISQ devices, can be used to simulate the dynamics of open quantum systems. In particular, we have shown how the intrinsic decoherence channels of the imperfect qubits can be harnessed to simulate open quantum systems since the qubits themselves interact with their environment [1]. This makes the qubits themselves de facto open quantum systems, circumventing the need to add ancilla qubits to achieve non-unitary time evolution. This is a promising research direction and more work is needed to classify the types of quantum channels which are implementable using unitary gates in conjunction with the intrinsic noisy channels of the qubits. It is conceivable that a wide variety of interesting and useful quantum channels can be implemented in this fashion with negligible overhead, in which case such techniques would prove incredibly powerful for the simulation of open quantum systems on NISQ devices. However, the extent of the channels which can be simulated in this fashion remains an open research question.

Furthermore, our work with the non-interacting, driven-dissipative Hubbard model [2, 3] gives a concrete demonstration of the robustness of algorithms for simulating open quantum systems on NISQ devices. In particular we simulate 1,000 time-steps of Trotterized time evolution, at least an order of magnitude further than has been done to date, on a digital quantum computer. Additionally we simulate a
strongly interacting model showing that this phenomenon is not limited to single-qubit or non-interacting cases. Our strongly interacting simulation clearly shows the ability of such algorithms to recover from errors incurred at early times. This is in stark contrast to typical Hamiltonian simulations, in which errors compound making long time data unreliable. We show the recovery from significant errors incurred at early times, reproducing with high fidelity and subsequently stabilizing an entangled, many-body, thermal state on a pair of qubits seemingly indefinitely.

Furthermore, the algorithm for the non-interacting, driven-dissipative Hubbard model and the algorithm for the atomic limit of the driven-dissipative Hubbard model span the two subroutines involved in the simulation of a wide variety of condensed-matter physics models. The non-interacting algorithmic primitive simulates particle hopping i.e. the kinetic energy term of lattice models. Meanwhile, the algorithmic primitive for the atomic limit simulates local interactions i.e. the potential energy terms of lattice models. Unfortunately, it turns out that a sequential application of these two algorithmic primitives, in the same spirit as Trotterization, does not effectively reproduce the correct driven-dissipative dynamics of systems having both hopping and scattering. This is in part due to the fact that the dissipators for the limiting cases are not general. Rather, they were derived incorporating the Hamiltonians of the limiting cases of our model. This means our Kraus map effectively represents interaction with a thermal reservoir only when applied to a system with the same spectrum as the Hamiltonian used to derive the Kraus operators. Because the Hamiltonian of the general system is a non-trivial linear combination of the non-interacting and atomic limit Hamiltonians, it has a fundamentally different spectrum compared to each limiting case spectra.

More research is needed to find an efficient way to combine these algorithmic primitives to correctly reproduce the dynamics of more general many-body, driven-
dissipative, lattice models. If this can be accomplished, it would allow for the efficient simulation of some of the most challenging and interesting problems in condensed matter physics. This would represent a promising new pathway to reach for quantum advantage.
Appendix A

Commutation of Time Evolution and Decoherence Channels

It is fairly simple to show that the generalized amplitude damping, $\mathcal{E}_x$, and dephasing, $\mathcal{E}_z$, channels commute. That is, $\mathcal{E}_x(\mathcal{E}_z(\rho)) = \mathcal{E}_z(\mathcal{E}_x(\rho))$. A sufficient (but not necessary) condition for two quantum channels to commute is that all of the Kraus operators from the two channels satisfy $K^1_iK^2_j = e^{i\phi}K^2_jK^1_i$. This follows directly from Eq. 4.6 because all of the phases simply cancel, $K\rho K^\dagger = (e^{i\phi}K)\rho(e^{i\phi}K)^\dagger$.

It is easy to see then that $\mathcal{E}_x$ and $\mathcal{E}_z$ commute because $K^x_iK^z_j = \pm K^z_jK^x_i$ which follows directly from anti-commutation relations of the Paulis and the form of the Kraus operators in Eqs. 4.7 and 4.8. Let $\mathcal{E}(\cdot) \equiv \mathcal{E}_x(\mathcal{E}_z(\cdot))$.

It is less obvious that coherent time evolution and $\mathcal{E}$ commute, largely because it is untrue. However, we show that at laboratory temperatures the time evolution of only the electronic DOFs commutes with $\mathcal{E}$. Denote $\mathcal{E}$ operating at infinite temperature to be $\mathcal{E}^\infty$.

We argue as follows, by tracing out the nuclear subsystem we are formally treating it as a finite bath interacting with the electronic subsystem. The interaction can be read off of Eq. 4.3 and is given by

$$\sum_{i,j} a_{ij} I_{ij} \cdot S_i = \sum_{i,j} \frac{a_{ij}}{2} \left( I_{ij}^+ S_i^- + I_{ij}^- S_i^+ + 2I_{ij}^z S_i^z \right).$$

(A.1)

The two terms involving $S^\pm$ can be thought of as performing amplitude damping. Because the initial nuclear state is the maximally mixed state, i.e. the infinite temperature state, this interaction applies infinite temperature amplitude damping.
term involving \( S^z \) performs the phase damping channel. As such, the interaction between the electronic and nuclear subsystems performs \( \mathcal{E}^\infty \) on the electronic subsystem. Since \( \mathcal{E}^\infty \) trivially commutes with itself, it is not surprising that the coherent time evolution and decoherence channel commute as well. We now make the argument more precise, although a rigorous proof is beyond the scope of this work.

The action of coherent time evolution, from an initial time \( t = 0 \) to \( t \), on the electronic subsystem only is itself represented by a quantum channel, \( \mathcal{E}_U \). The Kraus operators for \( \mathcal{E}_U \) are given by

\[
K_{ij}^U = \sqrt{P(|I_i\rangle)} \langle I_i | e^{-iHt} | I_j \rangle
\]

such that

\[
\rho_U = \mathcal{E}_U(\rho(0)) = \sum_i \langle I_i | e^{-iHt} \rho(0) e^{iHt} | I_i \rangle
\]

where the sum traces out the nuclear DOF and

\[
\langle I_i | \hat{A} | I_i \rangle = \sum_{j,k} \langle I_i, e_j | \hat{A} | I_i, e_k \rangle | e_k \rangle \langle e_j |.
\]

Here \( |I_i\rangle \) (\( |e_i\rangle \)) is the \( i \)th basis state for the nuclear (electronic) subsystem, \( P(|I_i\rangle) \) is the probability of being in that nuclear state at \( t = 0 \) and \( \rho_U \) is the state of the electronic subsystem at time \( t \). For our case the initial nuclear state is the maximally mixed state, \( P(|I_i\rangle) = P = 1/N_I \). From here, a few observations may be made. For simplicity we take \( \rho(0) = |S\rangle \langle S| \) moving forward, although the argument holds for any initial state of the form \( \rho(0) = e^{-i\alpha H} |S\rangle \langle S| e^{i\alpha H} \).

Transitions from the singlet state \( |S\rangle \) to either triplet state with \( m_s \neq 0 \) (\( |T_+\rangle = |\uparrow\uparrow\rangle, |T_-\rangle = |\downarrow\downarrow\rangle \)) occur from the terms containing an \( S_i^\pm \) in Eq. A.1. These terms come with a corresponding, distinct transition in the nuclear state from \( I_i^\pm \). Furthermore, due to symmetry in the Hamiltonian, and therefore in Eq. A.1, the probability of transition to \( |T_+\rangle \) is equal to \( |T_-\rangle \). Due to spin conservation, a nuclear
state corresponding the electronic state being in either $|T_\pm\rangle$, cannot correspond to any other electronic state. From Eqs. A.3 and A.4 then, we see $\rho_U$ has a term of $a(|T_+\rangle\langle T_+| + |T_-\rangle\langle T_-|)$ and no other terms involving $|T_\pm\rangle$.

Likewise, transitions from $|S\rangle$ to $|T_0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ mediated by nuclear interactions will contribute a term of $b|T_0\rangle\langle T_0|$. Finally, evolution that leaves the nuclear state unchanged, i.e. evolution mediated by $B$, coherently rotates between $|S\rangle$ and $|T_0\rangle$. This contributes a term to $\rho_U$ of the form $c(R_z(\phi) \otimes R_z(\varphi)) |S\rangle\langle S| (R_z(-\phi) \otimes R_z(-\varphi))$. Explicitly writing this out gives

$$\rho_U = \begin{pmatrix}
|\uparrow\uparrow\rangle & |\downarrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\downarrow\rangle \\
|\uparrow\uparrow\rangle & a & 0 & 0 & 0 \\
|\downarrow\uparrow\rangle & 0 & b + c & b - ce^{-i\theta} & 0 \\
|\uparrow\downarrow\rangle & 0 & b - ce^{i\theta} & b + c & 0 \\
|\downarrow\downarrow\rangle & 0 & 0 & 0 & a
\end{pmatrix} \tag{A.5}$$

where normalization implies $a = \frac{1}{2} - b - c$ and we’ve defined $\theta = \phi - \varphi$. It is much more straightforward to show that $\rho_D = \mathcal{E}^\infty(\rho(0)) =

$$\frac{1}{4} \begin{pmatrix}
1 - \bar{p}_z^2 & 0 & 0 & 0 \\
0 & \bar{p}_x^2 + 1 & -2\bar{p}_x P_z^2 & 0 \\
0 & -2\bar{p}_x P_z^2 & \bar{p}_x^2 + 1 & 0 \\
0 & 0 & 0 & 1 - \bar{p}_x^2
\end{pmatrix} \tag{A.6}$$

where $P_z = 1 - 2p_z$. If we then modify this slightly by adding an $R_z(\phi/2)$ gate to act on one of the qubits before acting with $\mathcal{E}^\infty$, we get the same result as in Eq. A.6 but with $P_z \mapsto e^{i\phi}P_z$. A lone $R_z(\phi/2)$ itself defines a quantum channel, $\mathcal{E}^z(\rho) = R_z(\phi/2)\rho R_z^*(\phi/2)$.

It is now explicitly obvious that this new $\mathcal{E}^\infty\mathcal{E}^z$ map implements the same transformation as $\mathcal{E}_U$, i.e. $\mathcal{E}_U(\rho(0)) = \mathcal{E}^\infty(\mathcal{E}^z(\rho(0)))$. By the same logic that showed $\mathcal{E}_x$ and
\( \mathcal{E}_z \) commute, it is easy to see that \( \mathcal{E}_z \) and \( \mathcal{E} \) commute. Furthermore, since \( \mathcal{E} \) commutes with itself, we conclude that \( \mathcal{E}^\infty \) and \( \mathcal{E}_U \) must themselves commute. Note that for \( T \neq \infty \) or for a different Hamiltonian, e.g. one that contains direct interactions between the two species, the above no longer holds.
Appendix B

Noise in Experimental Data

The TR MFE is calculated as per Eq. 4.2 in order to cancel \( F(t) \) from 4.1. This is sound as \( F(t) \) has no \( B \) dependence, however \( F(t) \) is a rapidly decaying function representing lifetime distribution of the radical pairs. So relative noise in the experiment grows for long times as \( F(t) \) damps the signal while the noise stays approximately constant.

More technically, \( F(t) \) for radical pairs is well approximated by\[84, 160\]

\[
F(t) \approx Ae^{-t/t_1} + B \left(1 + \frac{t}{t_2}\right)^{-\alpha}
\]

(B.1)

with best fit parameters \( A = 3.12 \times 10^6, B = 2.21 \times 10^5, t_1 = 3.47\text{ns}, t_2 = 123\text{ns}, \alpha = 6.11 \) for TMP/PTP as determined by non-linear regression. And \( A = 1.317 \times 10^6, B = 6.658 \times 10^5, t_1 = 2.1432\text{ns}, t_2 = 5.1549\text{ns}, \alpha = 1.223 \) for DPS/PTP[160, 161].

We assumed that the PMT detector is a primary source of noise in the experimental data. We approximated the PMT noise with white noise following a normal distribution and applied it to both the high-field and low-field theoretical recombination fluorescence functions, \( I(t) \) (Eq. 4.1) constructed from Eqs B.1, 4.15. We then reconstruct the TR MFE (Eq. 4.2) using these noisy data. The result is shown in Fig. B.1b.

We find a normal distribution of \( \mu = 0 \) and \( \sigma = 75 \) reproduces the noise behavior from the experiment very well. Such errors are an inherent challenge to producing good experimental data out to long times. In this regard, performing a quantum simulation
Figure B.1: Comparisons of noise seen in experimental data vs. noise from assuming Gaussian background noise on the detectors in an otherwise ideal experiment. $\tilde{M}(t)$ is constructed by adding independent Gaussian noise to $\tilde{S}_0(t)$ and $\tilde{S}_B(t)$ at each time point. We see that such a simple model reproduces the data well and explains the main effect behind increasing noise in the TR MFE vs. time.

opens the potential to investigate the behavior of such systems in finer detail and to longer times than is possible in experiments - once Hamiltonian simulation becomes feasible on these machines.
Appendix C

Derivation of the Master Equation

For completeness, we show the derivation of the master equation as it appears in Eq. (5.3). The total Hamiltonian of the system is given by $\hat{H}_{tot}^{(k)} = \hat{H}^{(k)} + \hat{H}_b^{(k)} + \hat{V}^{(k)}$, where:

\begin{align*}
\hat{H}^{(k)} &= -2\gamma \cos (k + \Omega t) d_k d_k, \quad \text{(C.1)} \\
\hat{H}_b^{(k)} &= \sum_{\alpha} \omega_\alpha c^\dagger_{\alpha k} c_{\alpha k}, \quad \text{(C.2)} \\
\hat{V}^{(k)} &= -g \sum_{\alpha} d_k c_{\alpha k} + \text{h. c.} \quad \text{(C.3)}
\end{align*}

Therefore, in our case, we have a master equation for every $k$-point, but we will omit the $k$-subscript to simplify the notation.

For deriving the master equation, it is useful to work within the interaction picture, where the interaction in this case is given by the bilinear hybridization term $\hat{V}$. A generic operator $\hat{O}$ can be written in the interaction picture as $\hat{O}_I(t) \equiv \hat{U}_b^\dagger(t) \otimes \hat{U}(t) \hat{O}_b(t) \otimes \hat{U}_b(t)$, where $\hat{U}(t)$ and $\hat{U}_b(t)$ are respectively the time-evolution operators of the isolated system and the bath and they obey the following differential equations $i\partial_t \hat{U} = \hat{H}\hat{U}$, $i\partial_t \hat{U}_b = \hat{H}_b\hat{U}_b$, with initial condition $\hat{U}(0) = 1$, $\hat{U}_b(0) = 1$.

The Von-Neumann equation for the density matrix $\hat{\chi}_I(t)$ of the system plus bath (in the interaction picture) reads: $\partial_t \hat{\chi}_I(t) = i \left[ \hat{\chi}_I(t), \hat{V}_I(t) \right]$, and can be recast in an integral formulation as follows:

$$\hat{\chi}_I(t) = \hat{\chi}_I(0) + i \int_0^t dt' \left[ \hat{\chi}_I(t'), \hat{V}_I(t') \right]. \quad \text{(C.4)}$$
Substituting the last equation into the Von-Neumann equation in the differential form, one obtains:

$$\partial_t \hat{\chi}_I(t) = i[\hat{\chi}_I(0), \hat{V}_I(t)] - \int_0^t dt' \left[ [\hat{\chi}_I(t'), \hat{V}_I(t')], \hat{V}_I(t) \right].$$  \hspace{1cm} (C.5)

If the hybridization strength is small enough, we can neglect the correlations between the system and the bath. Furthermore, if the bath is a proper thermal reservoir, it is not affected very much by the dynamics of the system and its evolution as a function of time can be neglected. Under these circumstances we can assume the following form of the density matrix $\hat{\chi}_I(t) = \hat{\rho}_I(t) \otimes \hat{\rho}_b(0)$, also known as the Born approximation.

A further approximation that we consider consists in replacing the time dependence of $\hat{\rho}_I(t') \to \hat{\rho}_I(t)$ in the integral in Eq. (C.5) and sending the lower extremum of the integral from zero to $-\infty$, which is known as the Markov approximation. In fact, following this prescription, we obtain a first-order differential equation for $\hat{\rho}(t)$ with constant coefficients at equilibrium.

After making all these assumptions, setting $\hat{\rho}_b(0) = e^{-\beta \hat{H}_b}$, and tracing out the bath degrees of freedom we obtain the master equation:

$$\partial_t \hat{\rho}_I(t) = -\text{Tr}_b \int_{-\infty}^t dt_1 \left[ \hat{V}_I(t), \left[ \hat{V}_I(t_1), \hat{\rho}_I(t) \otimes \hat{\rho}_b(0) \right] \right],$$  \hspace{1cm} (C.6)

where $\hat{\rho}_I(t) = \text{Tr}_b \hat{\chi}_I(t)$. The time evolved destruction operators of the bath are given by $c_\alpha(t) = \hat{U}_b(t) c_\alpha \hat{U}_b(t) = e^{-i\omega_\alpha t} c_\alpha$. Therefore the operator defined in Eq. (C.6) takes the following form in the interaction picture:

$$\hat{V}_I(t) = -g \sum_\alpha d_\alpha(t) c_\alpha e^{-i\omega_\alpha t} + c_\alpha^\dagger d(t) e^{i\omega_\alpha t},$$  \hspace{1cm} (C.7)

where $d(t) = \hat{U}_b^\dagger(t) \hat{d} U(t)$.

If we substitute Eq. (C.7) into Eq. (C.6), after some significant algebra, we obtain the master equation in the interaction picture:
\[
\partial_t \hat{\rho}_I(t) = g^2 \int_{-\infty}^t dt_1 C_p(t - t_1) \left[ -d(t) d(t_1) \hat{\rho}_I(t) + d(t_1) \hat{\rho}_I(t) d(t_1) \right] + \text{h. c.} \\
+ g^2 \int_{-\infty}^t dt_1 C_h(t - t_1) \left[ -d(t) d(t_1) \hat{\rho}_I(t) + d(t_1) \hat{\rho}_I(t) d(t_1) \right] + \text{h. c.} \tag{C.8}
\]

where \( C_p(t) = \text{Tr}_b \sum_\alpha \hat{\rho}_b c_{k\alpha}^\dagger(t) c_{k\alpha} \), \( C_h(t) = \text{Tr}_b \sum_\alpha \hat{\rho}_b c_{k\alpha}(t) c_{k\alpha}^\dagger \) are the correlation functions of the bath. We choose a half-filled bath, which implies that \( C_p(t) = C_h(t) \) due to particle-hole symmetry.

In order to solve the master equation, we have to specify the form of the correlation function of the bath. Given the simple form of the bath Hamiltonian in Eq. (C.2), the correlation function is \( k \)-independent and can be calculated analytically. In particular, in the limit of an infinite bandwidth with a flat density of states \( N(\epsilon) \equiv \sum_\alpha \delta(\epsilon - \omega_\alpha) \sim N(0) \), we find that

\[
C_p(t) = \pi N(0) \left[ \delta(t) - \frac{i}{\beta} \text{PV cosech} \left( \frac{\pi t}{\beta} \right) \right]. \tag{C.9}
\]

Here, PV denotes the principal value.

Let us discuss some peculiarities arising from considering a flat density of states. First, in this limit the correlation function does not depend on the chemical potential of the bath, that we can set to an arbitrary number since the beginning (zero in our case). Second, it leads to divergences when one wants to calculate observables of the bath as for instance the density. It would have been more formally correct to consider an half-filled normalized density of states as a Lorentzian or a uniform box of length \( W \), but this would also complicate our analytical calculations. Furthermore, this does not give appreciable deviations from what we have calculated in the limit of a flat DOS, in the case of a large bandwidth is considered, as we checked numerically.

So far, we used the interaction picture. For obtaining the master equation for the density matrix in the Schrödinger frame, we have to “erase” the time evolution on
the system operators, that is \( \hat{\rho}(t) = \hat{U}(t)\hat{\rho}(t)\hat{U}^\dagger(t) \) and if we do so in Eq. (C.8), we obtain the following equation:

\[
\partial_t \hat{\rho}(t) = -i[H, \hat{\rho}(t)]
- d \mathcal{D}^{(p)\dagger}(t) \hat{\rho}(t) + \mathcal{D}^{(p)\dagger}(t) \hat{\rho}(t) d + \text{h. c.}
- d^\dagger \mathcal{D}^{(h)}(t) \hat{\rho}(t) + \mathcal{D}^{(h)}(t) \hat{\rho}(t) d^\dagger + \text{h. c.},
\]

(C.10)

where we defined the following operators:

\[
\mathcal{D}^{(p)\dagger}(t) \equiv g^2 \int_{-\infty}^{t} dt_1 C_p(t - t_1) \mathcal{D}^\dagger(t, t_1),
\]

(C.11)

\[
\mathcal{D}^{(h)}(t) \equiv g^2 \int_{-\infty}^{t} dt_1 C_h(t - t_1) \mathcal{D}(t, t_1).
\]

(C.12)

Here \( \mathcal{D}^\dagger(t, t_1) \equiv \hat{U}(t)\hat{U}^\dagger(t_1) d \hat{U}(t_1)\hat{U}^\dagger(t) \). It is worthwhile to note that the two operators defined in Eqs. (C.11) and (C.12) are not conjugates of each other (because of the finite imaginary part in \( C_p/h \)).

Therefore, since we do not neglect the structure of the correlation functions of the bath, we have in principle to construct the new operators defined in Eqs. (C.11) and (C.12). If the Hamiltonian of the system does not depend explicitly on time, the operators in Eqs. (C.11) and (C.12) would not depend on time and a similar expression can be found as those found in the studies of transport in quantum dots[162, 163, 164, 165]. In our case, the time dependence of the Hamiltonian and a nontrivial structure of the correlation function [see Eq. (5.5)] yields time-dependent operators.

A further simplification comes from the one-body nature of our problem. From now on, we will introduce again the \( k \) subscript in our notation. In this case, the time-dependent annihilation operator can be written as \( d_k(t) = e^{-iF_k(t)}d \), where \( F_k(t) = -2\gamma [\sin(k + \Omega t) - \sin(k)] / \Omega \). Therefore
\[ D_k(t, t_1) = e^{-i[f_k(t_1) - f_k(t)]} d, \quad \text{(C.13)} \]

with \( f_k(t) = \sin(k + \Omega t)/\Omega \), and the RME reads:

\[
\partial_t \hat{\rho}_k = \text{Re} a_k(t) \left[ 2d_k \hat{\rho}_k d_k - \{ d_k d_k, \hat{\rho}_k \} \right]
+ \text{Re} A_k(t) \left[ 2d_k \hat{\rho}_k d_k - \{ d_k d_k, \hat{\rho}_k \} \right], \quad \text{(C.14)}
\]

where we introduced the time and momentum dependent coefficients:

\[
a_k(t) = g^2 \exp \left[ -i f_k(t) \right] \int_{-\infty}^{0} dt_1 C_p(-t_1) \exp \left[ i f_k(t + t_1) \right],
A_k(t) = g^2 \exp \left[ i f_k(t) \right] \int_{-\infty}^{0} dt_1 C_h(-t_1) \exp \left[ -i f_k(t + t_1) \right], \quad \text{(C.15)}
\]

and we used the fact that \( \text{Im}(a_k(t) - A_k(t)) = 0 \).
Appendix D

Analytic Expressions of $n(k_m)$ and $\langle J \rangle$ in the RME and LME

Our next step is to simplify the coefficients $a_k(t)$ and $A_k(t)$. Employing the standard Bessel function identity
\[
\exp[i f_k(t)] = \sum_{\ell=-\infty}^{+\infty} J_\ell \left( \frac{2\gamma}{\Omega} \right) \exp[-i\ell(k + \Omega t)],
\] (D.1)
allows us to re-express the coefficients in Eq. (5.4) as the following:

\[
a_k(t) = \Gamma \sum_{\ell} J_\ell \left( \frac{2\gamma}{\Omega} \right) J_{\ell'} \left( \frac{2\gamma}{\Omega} \right) F(\Omega \ell) e^{-i(\ell - \ell')(k + \Omega t)},
\]
\[
A_k(t) = \Gamma \sum_{\ell} J_\ell \left( \frac{2\gamma}{\Omega} \right) J_{\ell'} \left( \frac{2\gamma}{\Omega} \right) F(-\Omega \ell) e^{i(\ell - \ell')(k + \Omega t)}.
\] (D.2)

We choose $\Gamma = \pi g^2 N(0)$ and
\[
F(x) = n_F(-x) + \frac{i}{\pi} \Re \psi \left( \frac{1}{2} - i \frac{\beta x}{2\pi} \right),
\] (D.3)
with $\psi(z)$ being the digamma function.

From Eq. (5.3), we can obtain a differential equation for the momentum distribution function $n_k(t) = \text{Tr} \left( \hat{\rho}_k(t) d_k d_k \right)$, that reads:
\[
\dot{n}_k = -2\Gamma n_k + 2\Re a_k(t).
\] (D.4)

Since this is a first-order linear differential equation, it can be immediately integrated to yield its solution, which given by
\[
n_k(t) = e^{-2\Gamma(t-t_0)} n_k(t_0) + \int_{t_0}^{t} ds e^{-2\Gamma(t-s)} 2\Re a_k(s).
\] (D.5)
In the limit of $t_0 \to -\infty$, Eq. (D.5) becomes

$$n_k(t) = 2 \Gamma \text{Re} \sum_{\ell \ell'} \frac{J_\ell \left( \frac{2\gamma}{\Omega} \right) J_{\ell'} \left( \frac{2\gamma}{\Omega} \right) \mathcal{F}(\Omega \ell)}{2\Gamma - i(\ell - \ell')\Omega} e^{-i(\ell - \ell')(k + \Omega t)}.$$  \hspace{1cm} (D.6)

The equation for the current is given by $\langle J \rangle = (2\pi)^{-1} \int dk 2\gamma \sin(k + \Omega t)n_k(t)$ and in the limit of $t \to \infty$ we have:

$$\langle J \rangle = 4\gamma \Gamma \text{Re} \left[ \sum_{\ell} \frac{J_\ell \left( \frac{2\gamma}{\Omega} \right) J_{\ell+1} \left( \frac{2\gamma}{\Omega} \right) \mathcal{F}(\Omega \ell)}{\Omega - 2i\Gamma} \right] + 4\gamma \Gamma \text{Re} \left[ \sum_{\ell} \frac{J_\ell \left( \frac{2\gamma}{\Omega} \right) J_{\ell-1} \left( \frac{2\gamma}{\Omega} \right) \mathcal{F}(\Omega \ell)}{\Omega + 2i\Gamma} \right].$$  \hspace{1cm} (D.7)

In Figs. (5.2,5.3), where we evaluated the momentum distribution function as well as in Fig. (5.4) where we evaluated the current in the RME, we had to set a cut-off to the maximum index $\ell$ appearing in Eqs. (D.6) and (D.7). This value ranges from 20 in the case of strong-driving fields to 160 in the case of our smallest finite field that is $\Omega/\gamma = 0.05$. Now, we will derive the analytic expression for the momentum-distribution function obtained through the LME. In this case, we do not need to employ the Bessel function expansion and the integral in Eq. (D.5) can be calculated directly. In fact, the coefficient $a_k(t) \sim \Gamma n_F \{c_k(t)\}$ and if we define $k_m = k + \Omega t$, we can rewrite Eq. (D.5) as:

$$n(k_m) \sim \frac{2\Gamma}{\Omega} \int_{-k_m}^{0} dx e^{-i\frac{2\gamma}{\Omega}(x+k_m)} n_F[-2\gamma \cos(x)] + \frac{2\Gamma}{\Omega} \sum_{n=0}^{\infty} \int_{2\pi n}^{2\pi(n+1)} dx e^{-i\frac{2\gamma}{\Omega}(x+k_m)} n_F[-2\gamma \cos(x)].$$  \hspace{1cm} (D.8)

In the limit of $T \to 0$, the integrals in Eq. (D.8) can be calculated straightforwardly and for $k_m \in [0, 2\pi]$ we obtain:

$$n(k_m) \sim e^{-i\frac{2\pi}{\Omega}k_m} \left[ \mathcal{I}(k_m) - \frac{1}{2}\text{sech} \left( \frac{\Gamma}{\Omega} \right) \right],$$  \hspace{1cm} (D.9)
where:

\[ I(x) = \begin{cases} 
  e^{2 \Gamma x} & x < \frac{\pi}{2} \\
  e^{3 \Gamma x} & \frac{\pi}{2} \leq x \leq \frac{3\pi}{2} \\
  e^{\Gamma x} - e^{3\pi \Gamma x} + e^{2\pi \Gamma x} & \frac{3\pi}{2} < x \leq 2\pi.
\end{cases} \quad (D.10) \]

We note that the solutions of the LME depend solely on the ratio \( \Gamma/\Omega \), while the solutions of the RME do not have this property. This is due to the fact that the coefficients \( a_k(t) \) depend on \( \Omega \) in a non-trivial way, while in the case of the LME the \( a_k(t) \) depends on \( \Omega \) only through \( k_m \).

The expression of the current significantly simplifies as well if one calculates it from the LME. In fact, we can rewrite the equation of motion of the momentum distribution function as

\[ \frac{dn}{dk_m}(k_m) = 2\Gamma \Omega (n(k_m) + n_F(k_m)). \quad (D.11) \]

In order to obtain the current, we first multiply both sides of Eq. (D.11) times \( 2\gamma \sin(k_m) \) and integrate over \( k \) and then we multiply the same equation times \( 2\gamma \cos(k_m) \) and integrate again. In this way, we obtain the following set of equations:

\[
\begin{align*}
\langle \tilde{J} \rangle &= \frac{2\Gamma}{\Omega} \langle J \rangle \\
\langle J \rangle &= -\frac{2\Gamma}{\Omega} \langle \tilde{J} \rangle + \frac{4\gamma \Gamma}{\Omega} I,
\end{align*}
\]

where, \( \langle \tilde{J} \rangle = (2\pi)^{-1} \int dk_m 2\gamma \cos(k_m) n(k_m) \), \( I = (2\pi)^{-1} \int dk n_F(\epsilon_k) 2\gamma \cos(k) \). At zero temperature \( I = 2\gamma/\pi \) and the current obtained using the LME reads:

\[
\langle J \rangle \sim \frac{2\gamma}{\pi} \frac{2\Gamma/\Omega}{1 + (2\Gamma/\Omega)^2}.
\]

The same formula has been found in Ref. [117] using the Keldysh formalism in the limit \( \Omega \ll 1 \) and \( \Gamma \ll 1 \), which is consistent with the Born approximation and the expansion in Eq. (5.6) that we performed to obtain the LME.
Appendix E

Derivation of the Linear Map $\phi_t$

Here we explicitly solve for the linear map $\phi_t$ in its matrix representation $F_{rs} = \text{Tr}(\sigma_r \phi_t(\sigma_s))$, which is defined in Sec. 5.4.2, where $\sigma_0 = \mathbb{1}_{2 \times 2}/\sqrt{2}$, $\sigma_1 = \sigma^z/\sqrt{2}$, $\sigma_2 = \sigma^x/\sqrt{2}$, $\sigma_3 = \sigma^y/\sqrt{2}$. For this purpose, let us construct the matrix representation of the map $\Lambda_t(\rho) = \dot{\rho}$, which is defined as $L_{rs} = \text{Tr}_r \Lambda_t(\sigma_s)$. As a matter of fact, $L$ has a block diagonal form where the blocks are defined in the parallel subspace, spanned by $\mathbb{1}_{2 \times 2}$ and $\sigma^z$ and the transverse subspace, spanned by $\sigma^x$ and $\sigma^y$. The matrix representation of $\Lambda_t$ in the two different channels reads:

$$L_\parallel = -2 \begin{pmatrix} 0 & 0 \\ \text{Re}[\alpha_k(t) - A_k(t)] & \Gamma \end{pmatrix}, \quad (E.1)$$

$$L_\perp = -\Gamma \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (E.2)$$

where we used the fact that $\text{Re}[\alpha_k(t) + A_k(t)] = \Gamma$. We note that these two properties are satisfied in the infinite flat bandwidth limit, and they would not hold for a non-trivial choice of the bath electrons DOS. Therefore, the dynamics of the two channels is totally decoupled. We further note, that $F_\perp$ vanishes when $t \to \infty$. Hence, the information about the steady state is fully contained in the parallel channel, whose time evolution is given by $\partial_t F_\parallel = L_\parallel F_\parallel$, with the initial condition $F_\parallel(0) = \mathbb{1}_{2 \times 2}$ and its solution reads:

$$F_\parallel = \begin{pmatrix} 1 & 0 \\ \Phi(t) & e^{-2\Gamma t} \end{pmatrix}, \quad (E.3)$$
where

\[ \Phi(t) = -2\text{Re} \int_0^t dt_1 [a_k(t_1) - A_k(t_1)] e^{2\Gamma(t_1 - t)}. \]  

(E.4)

Using the fact that \( \text{Re} [a_k(t) - A_k(t)] = \text{Re} [a_k(t) - A^*_k(t)] = 2\text{Re}[a_k(t)] - 2\Gamma \), substituting this into the last equation, for long enough time we have

\[ \Phi(t) = -4\text{Re} \int_{-\infty}^t dt_1 a_k(t_1) e^{2\Gamma(t_1 - t)} + 1 = -2n_k(t) + 1, \]  

(E.5)

where we substituted \( t_0 = 0 \to -\infty \) and used Eq. (D.5).

With this information, we are now able to calculate the Choi matrix \( S_{ab} = \sum_{r=0}^3 \sum_{s=0}^3 F_{sr} \text{Tr} [\sigma_r \sigma_a \sigma_s \sigma_b] \), whose orthogonal decomposition yields the Kraus operators defined in Eq. (5.17).
All data were taken using quantum computers made available by IBM, either ibmq_mumbai (Fig. 6.1(a) and Fig. 6.3) or ibmq_boeblingen (Fig. 6.1(b,c) and Fig. 6.2). ibmq_boeblingen is a 20-qubit quantum device and ibmq_mumbai is 27-qubit device. The reported error rates were used to select sets (≈5-10) of candidate qubits on which a limited number of Trotter steps were run. Results from these were then used to select the final qubits on which the full job(s) would be run. Raw shot counts were processed using Qiskit Ignis'[41] built in measurement error mitigation protocol. This prepares and immediately measures each computational basis state giving a confusion matrix, which is inverted and applied to the raw shot counts to yield the mitigated shot counts.

This work pushed current near-term quantum computers to their limits. This created some unique issues when trying to run these extremely deep circuits. We encountered buffer overflow errors after running a large number of our larger circuits indicating we had overflowed the device’s capacity to record more measurement data. This is why we limited our DC current data to 50 Trotter steps per unique set of parameter values. We avoided this limit when taking data for Fig. 6.1(b) by breaking our jobs into smaller chunks, but this meant long queue times, which would have been prohibitive to get the data in Fig. 6.2. The data in Fig. 6.1(a) were obtained through exclusive access to ibmq_mumbai, which allowed us to break our circuits into individual jobs without worrying about queue times. Nevertheless, we still overflowed
the buffer around step 300, forcing us to change to a new pair of qubits with a fresh buffer. Finally, we began to exceed the limits of the system generating the driving microwave pulses at around 1000 Trotter steps, which is why this is the upper limit for Fig. 6.1(a).

For the full tomography results in Fig. 6.3, we made use of the “state tomography circuits” and “StateTomographyFitter” functions built into Qiskit Ignis. The “state tomography circuits” creates a list of $3^n$ circuits which carries out the desired quantum circuit and then measures in the $X$, $Y$, and $Z$ bases. These results are then fed into the “StateTomographyFitter.fit” function in order to reconstruct the full quantum state.
The open quantum system examined in the first part of the paper is given by non-interacting fermions on a one-dimensional lattice with nearest-neighbor hopping and driven out of equilibrium by an electric field. The effect of the field is taken into account by introducing a complex Peierls phase $\varphi(t) = \Omega t$ (given by $\Omega = eEa$) to the hopping amplitude $\gamma_h$. The system Hamiltonian then reads:

$$\hat{H} = -\gamma_h \sum_i e^{i\varphi(t)} d_i^\dagger d_{i+1} + \text{h. c.} \quad (G.1)$$

We let the system interact with a thermostat by coupling every lattice site to an independent fermionic bath, whose Hamiltonian is $\hat{H}_b = \sum_{ia} \omega_\alpha c_{ia}^\dagger c_{ia}$, through a hopping term that is given by:

$$\hat{V} = -g \sum_{ia} \left( d_i^\dagger c_{ia} + c_{ia}^\dagger d_i \right) \quad (G.2)$$

Here $g$ is the bare hybridization amplitude, and $\alpha$ is an index that runs over all the internal degrees of freedom of the bath, which are taken to be infinite. The total Hamiltonian of the system plus the bath is given by $\hat{H}_{tot} = \hat{H} + \hat{H}_b + \hat{V}$ and can be block diagonalized by expanding the fields in their Fourier components; that is, $d_k = \frac{1}{\sqrt{N}} \sum_n d_n e^{-ikn}$, $c_{ka} = \frac{1}{\sqrt{N}} \sum_n c_{na} e^{-ikn}$. In this basis, the Hamiltonian decomposes into a sum of Hamiltonians for each momenta, $\hat{H}_{tot} = \sum_k \hat{H}_{tot}^{(k)}$, with $\hat{H}_{tot}^{(k)} = \hat{H}^{(k)} + \hat{H}_b^{(k)} + \hat{V}^{(k)}$ and where
\[ \hat{H}^{(k)}(t) = -2\gamma_h \cos(k + \Omega t) d_k^\dagger d_k, \quad (G.3) \]
\[ \hat{H}_b^{(k)} = \sum_\alpha \omega_\alpha c^\dagger_{k\alpha} c_{k\alpha}, \quad (G.4) \]
\[ \hat{J}^{(k)} = -g \sum_\alpha d_k^\dagger c_{k\alpha} + \text{h. c.} \quad (G.5) \]

The Lindblad master equation of the density matrix for a given \( k \)-point then becomes

\[
\partial_t \rho_k = -i[\hat{H}_k(t), \rho_k] + \sum_{\ell=\{1,2\}} L_\ell \rho_k L^\dagger_\ell - \{\rho_k, L^\dagger_\ell L_\ell\}, \quad (G.6)
\]

where the Lindblad operators are \( L_1 = \sqrt{\Gamma} n_F(\epsilon_k(t))d_k \) and \( L_2 = \sqrt{\Gamma} n_F(-\epsilon_k(t))d_k^\dagger \), with \( \Gamma = g^2 N(0) \) and \( N(0) \) being the bath DOS evaluated at the Fermi level (see Ref.\([2]\) for further details on the formal derivation).

The driven electric current is found from

\[
J = \frac{\gamma_h}{\pi} \int dk \sin(k + \Omega t) n_k(t), \quad (G.7)
\]

where \( n_k(t) = \text{Tr} \left[ \rho_k(t) d_k^\dagger d_k \right] \). By multiplying Eq. G.6 times \( d_k^\dagger d_k \) and computing the trace of both sides of the equation, we obtain the following differential equation for the momentum distribution function \( \dot{n}_k = -2\Gamma(n_k(t) - n_F(\epsilon_k(t))) \). Solving yields

\[
n_k(t) = n_k(0)e^{-2\Gamma t} + 2\Gamma \int_0^t ds e^{-2\Gamma(t-s)} n_F[\epsilon(k + \Omega s)] \quad (G.8)
\]

Next introduce the gauge-invariant wave vector \( k_m = k + \Omega t \) into the integral

\[
n_k(t) = n_k(0)e^{-2\Gamma t} + 2\Gamma \int_0^t ds e^{-2\Gamma(t-s)} n_F[\epsilon(k_m + \Omega(s - t))] \quad (G.9)
\]

Then for \( t \to \infty \) at fixed \( k_m \), we can perform the change of coordinates \( y = k_m + \Omega(s - t) \) to yield the following formula for the momentum distribution function:
\[ n(k_m) = \frac{2\Gamma}{\Omega} \int_{-\infty}^{k_m} dy \ exp \left( \frac{2\Gamma}{\Omega} (y-k_m) \right) n_F[\epsilon(y)], \] (G.10)

which depends only on \( k_m \). This implies that for large enough time, we can reconstruct the full momentum distribution function by fixing the value of the crystalline momentum \( k \) and letting \( t \) run over one full Floquet period. In practice, we use the fact that the transients die off quickly to use the data averaged over one Floquet period to represent the long-time limit of the momentum distribution.
Appendix H

Atomic Hubbard Circuit

We describe how to dissipatively prepare the thermal state of the atomic limit of the Hubbard model on a pair of qubits. Our Hamiltonian is given by

\[ \mathcal{H} = U n_\uparrow n_\downarrow - \frac{\mu}{2} (n_\uparrow + n_\downarrow) - \frac{B}{2} (n_\uparrow - n_\downarrow) \]

where \( U \) is the on-site interaction strength, \( \mu \) is the chemical potential, \( B \) is the magnetic field in units of the Bohr magneton, and \( n_\alpha \) is the occupation number operator for state \( |\alpha\rangle \). Our desired mixed state is then \( \tilde{\rho} = e^{-\beta \mathcal{H}} / \text{Tr} e^{-\beta \mathcal{H}} \) where \( \beta \) is the inverse temperature of the thermal state.

We prepare this state by iteratively applying a dissipative map, \( \mathcal{E} \), to the qubits such that \( \tilde{\rho} \) is the unique fixed point of \( \mathcal{E} \). We define \( \mathcal{E} \) by a set of Kraus operators \( \{K_i\} \) such that

\[ \rho_{i+1} = \mathcal{E}(\rho_i) = \sum_s K_s \rho_i K_s^\dagger \quad \text{with} \quad \sum_s K_s^\dagger K_s = 1 \quad \text{and} \quad \mathcal{E}(\tilde{\rho}) = \tilde{\rho}. \]

Such a map may be realized by choosing Kraus operators which induce transitions between eigenstates of the Hamiltonian \( (|j\rangle \langle i|) \) with fixed transition probabilities \( (\gamma_{i,j}) \). These transition probabilities define a detailed-balanced condition,

\[ \sum_j \gamma_{i,j} \langle i | \rho | i \rangle = \sum_j \gamma_{i,j} \langle j | \rho | j \rangle, \]

i.e. the density transitioning out of each state is exactly balanced by the density transitioning in. When this condition is met, \( \rho \) is a fixed point of \( \mathcal{E} \). To reduce the
complexity of the final circuit, we take only a minimal set of these transitions that correspond to a cycle through the states as depicted in Fig. 6.3(b).

Solving Eq. H.3 reveals \( \gamma_{i,j} \) is proportional to the inverse Boltzmann factor for state \( i \), i.e. \( \gamma_{i,j} = N e^{\beta \varepsilon_i} \) where \( \varepsilon_i \) is the energy of state \( |i\rangle \) given by \( \mathcal{H}|i\rangle = \varepsilon_i |i\rangle \). \( N \) can be thought of as an effective time step or system/bath coupling strength. Because \( \mathcal{E} \) must satisfy the normalization condition given in Eq. H.2, we find \( 0 \leq \gamma_{i,j} \leq 1 \) which bounds the values \( N \) can take. To maximize convergence speed, we take \( N \) to be such that the largest \( \gamma_{i,j} \) is 1.

Armed with the Kraus operators, we can build a circuit that implements \( \mathcal{E} \) in a straightforward way. Note that the eigenstates of \( \mathcal{H} \) are the computational-basis states, so we can transition between states with single-qubit rotations. To do this, we first map the state of the system onto an ancilla register. Then we rotate the system qubits, controlled on the ancilla register, to implement the transitions. A transition probability of \( \gamma_{i,j} \) is achieved with rotation angle \( \theta_{i,j} = 2 \sin^{-1}(\sqrt{\gamma_{i,j}}) \). Finally the ancilla qubits are reset in preparation for the next step. This circuit is shown in Fig. 6.3(a) and yields Kraus operators of the form

\[
K_{i,j} = \sqrt{1 - \gamma_{i,j}} |i\rangle\langle i| - i \sqrt{\gamma_{i,j}} |j\rangle\langle i|,
\]

as desired.

Ultimately this circuit needs to be transpiled down into IBM’s native gates and conform to the qubit connectivity in a real device. This was done in part by hand and in part using the transpilation tools in Qiskit, the result of which is shown in Fig. H.1.
Figure H.1: Atomic Hubbard circuit transpiled into CNOT gates and single-qubit rotations suitable for nearest neighbor connectivity. The circuit to be transpiled is given in Fig. 6.3(a). We have adopted the shorthand $a = \Theta_{\uparrow\downarrow}/2$, $b = \Theta_{0\downarrow}/2$, $c = \Theta_{\downarrow\uparrow}/2$, $d = \Theta_{\uparrow0}/2$. We note that this circuit is the same as that shown in Fig. 6.3(a) up to a unitary on the ancilla register before resetting and an $R_z(\pm \pi/2)$ gate before the first Trotter step and after the last Trotter step on both system qubits. These differences leave the dissipative map $E$ unaffected with the initial $R_z(\pi/2)$ being absorbed into the initial state.
APPENDIX I

ERROR MODEL

The ideal curve for the steady state of the electron density, $n_k(t)$, is distorted by errors occurring in the quantum computer during the run. We can model this new distorted curve well by taking into account only two sources of error: 1) imperfect reset gates and 2) the $T_1$ decay of the system qubit.

We first discuss the reset gates. In IBM’s hardware, a reset gate is performed by measuring the state of a qubit and then applying an $X$ gate if the qubit was measured to be in the $|1\rangle$ state and leaving it in the $|0\rangle$ state otherwise. However, even assuming a perfect $X$ gate, measurement fidelity is imperfect and so we expect an imperfect reset gate. Call the probability of measuring $m$, given the qubit is actually in $|m\rangle$ to be $p(m|m) \equiv p_m$. If the qubit is initially in state $\rho$ with $\langle 0 | \rho | 0 \rangle = a_0$, then we model the state of the qubit after one reset gate, $\rho_1$, to be characterized by

$$\langle 0 | \rho_1 | 0 \rangle = a_0 (p_0 - p_1) + p_1 \quad \text{and} \quad \langle 0 | \rho_1 | 1 \rangle = 0. \quad (I.1)$$

In IBM’s hardware, we have $p_0 \geq p_1$, so we can improve the fidelity of a reset operation by applying multiple reset gates in succession. Call the qubit state after $r$ reset gates $\rho_r$. Given the above model, we expect the probability of a successful reset to be

$$\langle 0 | \rho_r | 0 \rangle = a_0 (p_0 - p_1)^r + \frac{p_1 (1 - (p_0 - p_1)^r)}{1 - p_0 + p_1}. \quad (I.2)$$

This simple model of reset infidelity appears sufficient to explain most of the observed results. We find $p_0 = 0.97$ and $p_1 = 0.91$ on average over all our runs.
Now, we discuss the $T_1$ decay. Because a reset gate is approximately an order of magnitude longer than the combined duration of the other operations in a single Trotter step, we assume all of amplitude damping of the system qubit occurs during the time it takes for the reset operation on the ancilla qubit. We can model the amplitude damping channel as performing the following map on a single qubit:

$$\rho \mapsto \sum_k M_k \rho M_k^\dagger \equiv \mathcal{E}_x(\rho)$$

where

$$M_k \in \{ \sqrt{1 - e^{-rT}} |0\rangle\langle 1|, |0\rangle\langle 0| + \sqrt{e^{-rT}} |1\rangle\langle 1| \}$$

are the Kraus operators for the amplitude damping channel, $T$ is the duration of a single reset gate in units of the $T_1$ time of the system qubit, and $r$ is the number of reset gates used in a reset operation. We find the average duration of a reset gate is approximately 6% of the system qubit $T_1$ time.

Putting these together with the circuit shown in Fig. 6.1(d) gives our error model. Call $\rho^S_s$ and $\rho^a_s$ the density matrix of the system and ancilla at Trotter step $s$ (or time $t = s\Delta t$), respectively. Because the error incurred during a single Trotter step propagates non-trivially to the next steps, we express our model below in terms of recursive formulae for the populations $n_s \equiv \langle 0| \rho^S_s |0\rangle$ and $a_s \equiv \langle 0| \rho^a_s |0\rangle$. We explicitly represent the unitary part of the circuit for step $s$ as a matrix $U_s$ so that applying the circuit to a generic two-qubit state $\rho$ gives $\rho \mapsto U_s \rho U_s^\dagger$. This yields

$$\rho_{s+1} = \rho^a_{s+1} \otimes \mathcal{E}_x \left( \text{Tr}_a \left[ U_s (\rho^a_s \otimes \rho^S_s) U_s^\dagger \right] \right),$$

which leads to the following coupled recurrence relations

$$n_{s+1} = 1 - e^{-rT} ((2a_s - 1) (2\Gamma \Delta t (n_s - n_F[\varepsilon_s]) - n_s) + a_s)$$

$$a_{s+1} = \frac{a_s + 2\Gamma \Delta t (2a_s - 1) ((n_s - 1) n_F[\varepsilon_s] - n_s n_F[-\varepsilon_s])}{(p_0 - p_1)^{r}} + \frac{p_1 (1 - (p_0 - p_1)^{r})}{1 - p_0 + p_1}.$$
Here \( \varepsilon_s \equiv -2\cos(k + \Omega s\Delta t) \) is the dispersion relation, \( n_F[x] \) is the Fermi-Dirac distribution, and the angles at step \( s \) are defined by

\[
\begin{align*}
\theta_s &= 2\sin^{-1}\sqrt{\frac{2\Gamma \Delta t}{e^{\beta \varepsilon_s} + 1}} \quad \text{and} \quad \phi_s = 2\sin^{-1}\sqrt{\frac{2\Gamma \Delta t}{e^{-\beta \varepsilon_s} + 1}} \\
\end{align*}
\] (I.6)

These recurrence relations can easily be solved numerically. We use an optimizer to find an average of \( T = 0.06T_1, \ p_0 = 0.97, \) and \( p_1 = 0.91, \) which best match our data. The same values for \( T, \ p_0, \) and \( p_1 \) are used for each \( r = 1, 2, 3, \) and 4 iterated reset gates per reset operation, since the parameters should be approximately constant for a given pair of qubits on a given quantum device. A comparison of the error model vs. ideal circuit vs. actual quantum computer data is shown in Fig. I.1.

**Figure I.1:** Comparison of the ideal circuit, our error model and the actual data from the quantum computer. Here we take \( r = 1, 2, 3, \) and 4 reset gates per Trotter step. The ideal circuit and quantum computer data are the same as shown in Fig. 6.1. The error model and data agree well overall and adequately explain the majority of the error observed.
This error model also gives insight into why our system, and dissipative systems in general, are robust against noise. Inspecting Eq. I.4 shows that \( n_{s+1} \) (the electron density at step \( s + 1 \)) depends on \( n_s \) as \( e^{-rT}(2a_s - 1)(2\Gamma \Delta t - 1)n_s \). Furthermore, we have \( 0 \leq e^{-rT}, 2a_s - 1 \leq 1, \) and \( 0 \leq 2\Gamma \Delta t - 1 < 1 \) when \( \Gamma > 0 \), i.e. when dissipation is non-zero. This tells us that the effect of an error at step \( s \) on the density at step \( s' > s \) is exponentially small in \( s' - s \). This further suggests that if we have a sufficiently small base error rate, the compounding effect of these errors are offset by the dissipation, and this is why our error model does not need to take into account other errors, such as gate errors.

We can get an intuitive sense for how this works if we make the assumption that \( a_s = a_0 \) for all \( s \), i.e. reset fidelity is independent of the qubit state. This is a good assumption when \( p_0 \approx p_1 \) or \( r \gg 1 \) since the reset fidelity depends on the qubit state through \( \langle 0 | \rho_a | 0 \rangle (p_0 - p_1) \). This then recasts Eq. I.4 as

\[
 n_{s+1} = 1 - e^{-rT} \left( (2a_0 - 1) (2\Gamma \Delta t (n_s - n_F[\varepsilon_s]) - n_s) + a_0 \right) \tag{I.7}
\]

for which Mathematica gives the analytic solution of the recurrence relation for \( n_s \), \( s \gg 1 \) as

\[
 \frac{1}{2} + \frac{1 - e^{-rT}}{2(1 - a_0 e^{-rT}(1 - 2\Gamma \Delta t))} - \frac{a_0}{e^{rT} \Gamma \Delta t} \sum_{t=0}^{s-1} \tanh \left( \frac{\beta \varepsilon_t}{2} \right) \left( \frac{a_0}{e^{rT}} (1 - 2\Gamma \Delta t) \right)^{s-t-1}. \tag{I.8}
\]

Plugging in \( a_0 = 1 \) and \( T = 0 \) recovers the error free solution

\[
 \frac{1}{2} - \Gamma \Delta t \sum_{t=0}^{s-1} \tanh \left( \frac{\beta \varepsilon_t}{2} \right) ((1 - 2\Gamma \Delta t))^{s-t-1}. \tag{I.9}
\]

These two solutions are qualitatively the same. They differ by a shift (second term in Eq I.8), a stretch of \( a_0 e^{-rT} \) and deformation in shape equivalent to using \( \Gamma' \) instead of \( \Gamma \), such that \( (1 - 2\Gamma' \Delta t) = a_0 e^{-rT}(1 - 2\Gamma \Delta t) \). This shows that the errors in the quantum hardware tend to perturb but not destroy the steady-state dynamics.
We anticipate this result to hold true for many dissipative algorithms—as we can consider the error channels occurring inside the quantum computer to supplement the dissipative channels we are explicitly simulating. As long as the error rates are low and/or our dissipation rate is high, we should expect to reach a nearly error-free steady state.
After the transients have died (about 30 Trotter steps for the data in Fig. 6.1), the population of the $|0\rangle$ state gives our raw data for $n_k(s\Delta t)$. We then correct this data for measurement errors using the built in tools in Qiskit Ignis\cite{41} to obtain the steady state data (e.g. data with green background in Fig. 6.1(b)). We then discard these first Trotter steps as transient data. The remaining data is (ideally) periodic according to Floquet theory with a period of $\tau = 2\pi/\Omega$, since our Hamiltonian is periodic with the same period (even though the field is DC, it drives periodic Bloch oscillations, making the system periodic). Because the step size $\Delta t$ is not always commensurate with the Floquet period, we use quadratic interpolation to generate a smooth curve, on a common time grid, and average together distinct periods to obtain an averaged curve for $n_k^{\text{ave}}(t)$ over a single period

$$n_k^{\text{ave}}(t) = \sum_{\ell=0}^{(t_{\text{max}}-t)/\tau} n_k(t + \ell\tau), \quad (J.1)$$

where $t$ lies on the common time grid. It is from this quantity that steady-state observables (e.g. DC current) can be calculated.

The constructed $n_k^{\text{ave}}(t)$ is distorted by errors occurring within the quantum computer, as detailed in supplement I. However, we can correct for the majority of this distortion. First, we know that $\int_0^\tau dt n_k(t) = 0.5$, which allows us to center the momentum distribution curve about its true midpoint (at $n_k = 0.5$). Second, we ran our circuits with $r = 1, 2, 3$, and 4 native reset gates per Trotter step. We would like to be able
to scale our results to an instantaneous application time for the resets, similar to Richardson extrapolation[101]. But, while the additional reset gates do boost the fidelity of the reset operation, they also add decoherence errors, because the gates are non-negligibly long compared to the $T_1$ time of the qubits, as described in supplement I. For this work, we find a negligible difference in reset fidelity between $r = 2, 3, 4$. This then allows us to extrapolate to $r = 0$, the limit of no $T_1$ decay.

As can be seen in supplement I, the functional dependence of $n_k(t)$ on $T_1$ errors is complex and so we opt for using a simple quadratic extrapolation. Doing this tends to be reasonably effective in improving the data. However, this does nothing to correct reset infidelity. Furthermore, when we have a limited number of periods of steady-state data, or when $\Omega$ is large and the curves are quite flat, noise from counting statistics and other random errors inside the quantum computer make the extrapolation less reliable. This is especially true when computing the DC response, which is quite sensitive to the shape of $n_k(t)$. To mitigate these issues, we correct the amplitude by computing the theoretical maximum of $n_k(t)$ at zero temperature and then use that as an approximate scale factor. Starting with our master equation in terms of our gauge-invariant wavevector, $k_m = k + \Omega t$, we have

$$\dot{n}(k_m) = 2\Gamma \left(1 + \frac{1}{1 + e^{2\beta \cos k_m}} - n(k_m)\right). \quad (J.2)$$

Taking the zero temperature limit, $\beta \rightarrow \infty$, gives

$$\dot{n}(k_m) = \Gamma \left(1 + \text{sgn}(\cos k_m) - n(k_m)\right) \rightarrow \begin{cases} \cos k_m < 0 & \dot{n} = -2\Gamma n \\ \cos k_m > 0 & \dot{n} = 2\Gamma(1 - n). \end{cases} \quad (J.3)$$

Since $0 \leq n \leq 1$, the derivative changes sign when $\cos k_m = 0$. But the solution for $n(k_m)$ actually ranges from a minimal value larger than 0 to a maximal value smaller
than 1. The differential equation can be immediately solved, and we find that

\[ n_{\text{max}} = \frac{1}{2} \left( 1 + \tanh \frac{\pi \Gamma}{\Omega} \right). \]  

We use this value to stretch the curves about 1/2 (their midpoint), which gives our final curve. Despite the distortions remaining after the extrapolation due to reset infidelity, uncorrected \( T_1 \) effects and other sources of error, we generally find excellent agreement between the ideal result and our final post-processed curve.


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