Driven-dissipative quantum mechanics on a lattice: Describing a fermionic reservoir with the master equation and simulating it on a quantum computer

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(Dated: December 19, 2019)

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 engineers 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. But how accurate is this for a fermionic bath? In this work, we use the exact solution for a noninteracting driven-dissipative system to benchmark the accuracy of this master-equation formalism. Such a master equation can be directly implemented on a quantum computer. The Kraus map required to do this enables us to create a quantum circuit that reproduces the dissipative dynamics. Because partial resets are not available in current quantum hardware, we simulate only the simplest example of such a Kraus map on an IBM machine, which can be simulated exactly without requiring any resets. The simulations are in excellent agreement with the exact results.

I. INTRODUCTION

Dissipation is ubiquitous in nature and often a many-body system of interest is coupled 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 Leggett1–3, and has experienced a renewed interest in the last decade. In fact, dissipation has been theoretically proposed as a resource for quantum computation4–7 and experimentally it has been demonstrated that an open quantum system can employ dissipation for quantum state preparation8–10. Our interest, however, is motivated by the advent of recent pump-probe experiments (see Refs. 11 and 12 for recent reviews), where systems can be easily driven out of equilibrium 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 oscillations13,14, 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)15 predicts that Bloch oscillations are damped as the system heats to an infinite temperature steady state where the current ultimately vanishes16. When dissipation with the environment is taken into account, both noninteracting17 and interacting18,19 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.

On the other hand, the difficulty to address 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. But simulations of quantum many-body models have been successfully performed using cold atom quantum simulators20. 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 interactions21,22, or the Dicke model23. 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, just as one moved from analog to digital computation when classical computers were being developed, there is great interest in doing the same transition for quantum computers.

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 operators\textsuperscript{24,25}. In addition, there exist robust algorithms for time-evolving quantum computers when fault-tolerant quantum computing becomes available\textsuperscript{26}. An alternative approach to exact time evolution is to evolve systems variationally\textsuperscript{27}, which is likely to 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. 8 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. In general, the direct simulation of a master equation is more convenient than digitally implementing the unitary dynamics of the system plus a finite bath (so-called algorithmic cooling\textsuperscript{28}). This is because the master-equation approach integrates out the degrees-of-freedom of the infinite bath and replaces them with operations that act directly on the system. Hence, a master-equation formalism is always performing an infinitely large computation.

However, when dealing with master equations, approximations are usually necessary. Two of the most common ones are the Born approximation and the Markov approximation\textsuperscript{29}. Unfortunately, we do not know \textit{a priori} how good these approximations actually are. In this work, we partially fill this gap by addressing an exactly solvable model using the master-equation approach and compare our results with its exact solution\textsuperscript{17}. In particular, we consider a tight-binding model of fermions driven by an electric field and interacting with an external (fermionic) bath. Due to the one-body character of the Hamiltonian of the bath, the reduced density matrix of the system factorizes in momentum space, allowing the master equation to be solved analytically.

We are interested in simulating fermionic, rather than bosonic baths, because such baths are easier to simulate on a quantum computer, and because they can exchange both energy and particles, they may equilibrate faster. But, of course, we cannot immediately translate the results of such an open system with the common solid-state system of electrons interacting with a phonon bath. Because the problem of studying driven-dissipative systems is so important, we feel looking into this type of problem will be a useful one to pursue to gain general understanding of the complex phenomena that driven-dissipative quantum systems have.

In Sec. II, we introduce the model and the master equation formalism that we use to solve the dynamics of the system. In Sec. III A, we show the results for the momentum distribution function of fermions as a function of time as well as the DC current of the system and compare our results with the exact solution. We also attempt to quantify the accuracy of the master equation by defining a suitable norm between our approximate solution and the exact one. In Sec. III B, we explicitly derive the Kraus map related to our master equation and in Sec. IV we construct a quantum circuit that reproduces this quantum operation. Finally, we show some data obtained directly from a quantum machine. In Sec. V we summarize the main achievements of our work.

II. MODEL AND METHODS

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\textsuperscript{30} \( \varphi(t) = \Omega t \) (given by \( \Omega = eEA \)) to the hopping integral \( \gamma i \); we use \( \gamma \) instead of \( t \), so as to not confuse the hopping term with time. The system Hamiltonian then reads:

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

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

\begin{equation}
\hat{V} = -g \sum_{i,a} d_i^\dagger c_{ia} + \text{h. c.}
\end{equation}

Here \( g \) is the bare interaction strength, and \( a \) is an index that runs over all the internal degrees of freedom of the bath, which are taken to be infinite. In Fig. 1, we schematically represent the linear chain coupled to the reservoir. The entire Hamiltonian of the system plus the bath is given by \( \hat{H}_{tot} = \hat{H} + \hat{H}_b + \hat{V} \) and can be recast in a block diagonal form by expressing the fields in the Fourier basis, that is \( d_k = \frac{1}{\sqrt{N}} \sum_n d_n e^{-ikn} \), \( c_{ko} = \frac{1}{\sqrt{N}} \sum_n c_{na} e^{-ikn} \) and their Hermitian conjugates. In this basis, the Hamiltonian decomposes into a sum of Hamiltonians

![FIG. 1. Schematic representation of a one-dimensional tight-binding model, where 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.](image-url)
for each momenta. We have $\hat{H}_{tot} = \sum_k \hat{H}^{(k)}$, where $\hat{H}^{(k)} = \hat{H}^{(k)}_0 + \hat{V}^{(k)}$ and
\[
\hat{H}^{(k)} = -2\gamma \cos (k + \Omega t) \hat{d}_k^{\dagger}\hat{d}_k, \tag{3}
\]
\[
\hat{H}^{(k)}_0 = \sum_\alpha \omega_\alpha \hat{c}_\alpha^{\dagger}\hat{c}_\alpha, \tag{4}
\]
\[
\hat{V}^{(k)} = -g \sum_\alpha \hat{d}_k^{\dagger}\hat{c}_\alpha + \text{h.c.}. \tag{5}
\]

In Ref. 17, 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 work, we address the problem using the master-equation formalism and compare our results with the exact solution in order to determine how accurate the master equation is.

The master equation governs the dynamics of the system’s reduced density matrix $\hat{\rho} = \text{Tr}_b \rho_{tot}$, where $\text{Tr}_b$ indicates the partial trace over the bath subspace. Within the Born approximation, the density matrix of the whole system is given by $\hat{\rho} = \hat{\rho}^{(k)} \otimes \hat{\rho}_b^{(0)}$, 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. $\hat{\rho} = \bigotimes_k \hat{\rho}^{(k)}$, 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
\[
\partial_t \hat{\rho}_k = -i[\hat{H}^{(k)}, \hat{\rho}_k] + \left[ a_k(t) \left( -\hat{d}_k^{\dagger}\hat{d}_k \hat{\rho}_k + \hat{d}_k^{\dagger}\hat{d}_k \hat{\rho}_k \right) + \text{h.c.} \right] + \left[ A_k(t) \left( -\hat{d}_k^{\dagger}\hat{d}_k \hat{\rho}_k + \hat{d}_k^{\dagger}\hat{d}_k \hat{\rho}_k \right) + \text{h.c.} \right], \tag{6}
\]
where we introduced the time and momentum dependent coefficients:
\[
a_k(t) = g^2 \exp \left[ -i f_k(t) \right] \int_{-\infty}^{0} \text{d}t_1 C_p(-t_1) \exp \left[ -i f_k(t_1 + t_1) \right],
\]
\[
A_k(t) = g^2 \exp \left[ i f_k(t) \right] \int_{-\infty}^{0} \text{d}t_1 C_h(-t_1) \exp \left[ i f_k(t_1 + t_1) \right], \tag{7}
\]
with
\[
f_k(t) = -2\gamma \sin (k + \Omega t) / \Omega, \tag{8}
\]
\[
C_p(t) = \text{Tr}_b \left( \sum_\alpha \hat{\rho}_b \hat{c}_\alpha^{\dagger}(t) \hat{c}_\alpha(t) \right), \tag{9}
\]
and
\[
C_h(t) = \text{Tr}_b \left( \sum_\alpha \hat{\rho}_b \hat{c}_\alpha^{\dagger}(t) \hat{c}_\alpha(t) \right) \tag{10}
\]
being the bath lesser and greater Green functions, respectively. We choose a half-filled bath, which implies that $C_p(t) = C_h(t)$ due to particle-hole symmetry. This function of time is called the correlation function of the bath. A detailed derivation of Eqs. (6) and (7) is given in App. A.

In order to solve Eq. (6), we have to specify the form of the correlation function of the bath. Given the simple form of the bath Hamiltonian in Eq. (4), 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
\[
C_p(t) = \pi N(0) \left[ \delta(t) - \frac{i}{\beta} \text{PV cosech} \left( \frac{\pi t}{\beta} \right) \right]. \tag{11}
\]
Here, PV denotes the principal value. In many cases, the correlation function of the bath is approximated by a delta function times a constant. In fact, in the case of noninteracting fermions, the real part of the correlation function is a delta function, however there is also an imaginary part that decays exponentially as $\exp(-\pi |t|/\beta)$ for $|t| \gg 1$. We stress the importance of the imaginary part of the correlation function in Eq. (11), first because it is where the information about the temperature of the bath is encoded and second because if we kept only the real part of $C_p(t)$ in Eq. (11), the coefficients defined in Eq. (7) would not depend on time. We will see later on, that if the coefficients did not depend on time, then we will have qualitative differences between the dynamics predicted by the master equation and the exact solution.

Our next step is to simplify the coefficients $a_k(t)$ and $A_k(t)$. Employing the standard Bessel function identity
\[
\exp[i f_k(t)] = \sum_{\ell=-\infty}^{+\infty} J_\ell \left( \frac{2\gamma}{\Omega} \right) \exp[-i \ell(k + \Omega t)], \tag{12}
\]
allows us to re-express the coefficients in Eq. (7) as the following:
\[
a_k(t) = \Gamma \sum_{\ell \ell'} J_\ell \left( \frac{2\gamma}{\Omega} \right) J_{\ell'} \left( \frac{2\gamma}{\Omega} \right) \mathcal{F}(\Omega t) e^{-i(\ell - \ell')(k + \Omega t)},
\]
\[
A_k(t) = \Gamma \sum_{\ell \ell'} J_\ell \left( \frac{2\gamma}{\Omega} \right) J_{\ell'} \left( \frac{2\gamma}{\Omega} \right) \mathcal{F}(-\Omega t) e^{i(\ell - \ell')(k + \Omega t)}. \tag{13}
\]
We chose $\Gamma = \pi g^2 N(0)$ and
\[
\mathcal{F}(\Omega t) = n_F(-\Omega t) + \frac{i}{\pi} \left[ \text{Re} \psi \left( \frac{1}{2} - i \frac{\beta \Omega t}{2\pi} \right) + \gamma_{EM} \right], \tag{14}
\]
with $\psi(z)$ being the digamma function and $\gamma_{EM}$ the Euler-Mascheroni constant.

Of course, all of these expressions depend on temperature as we expect they should. To be concrete in the remainder of this work, we fix the temperature of the bath to be $\beta = 10 \gamma^{-1}$ for all our calculations.
III. RESULTS

A. Non-Equilibrium Dynamics

From Eq. (6), we can obtain a differential equation for the momentum distribution function \( n_k(t) \) = Tr \( \hat{\rho}_k(t) d_k \hat{d}_k \), that reads:

\[
\dot{n}_k = -2\Gamma n_k + 2 \text{Re} a_k(t). \tag{15}
\]

Since this is a first-order linear differential equation, it can be immediately integrated to yield its solution, which given by

\[
n_k(t) = e^{-2\Gamma(t-t_0)}n_k(t_0) + \int_{t_0}^{t} ds e^{-2\Gamma(t-s)} 2 \text{Re} a_k(s) \tag{16}
\]

In Fig. (2), we show the time evolution of the momentum distribution function evaluated at \( \Omega/\gamma = 0.5 \), \( \Gamma/\gamma = 0.1 \), and at \( (k a) = \pi/2 + 0.1 \). As one might expect for a driven-dissipative system, the system initially has transient behavior, which then evolves into steady oscillations at long times. The oscillatory behavior arises from the time-dependence of \( a_k(t) \) [see Eq. (15)]; this time-dependence would vanish if we approximated the correlation function of the bath [given in Eq. (11)] with just a delta function, neglecting its exponentially vanishing tails. In Fig. 2, we also plot the result obtained through the master equation formalism. Comparing with the exact solution provided in Ref. 17, we see excellent quantitative agreement, especially for long times.

In the limit of \( t_0 \to -\infty \), Eq. (16) becomes

\[
n_k(t) = 2\Gamma \text{Re} \sum_{\ell \ell'} J_{\ell} \left( \frac{2\pi}{\gamma} \right) J_{\ell'} \left( \frac{2\pi}{\gamma} \right) F(\Omega \ell) e^{-i(\ell-\ell')(k+\Omega t)} \tag{17}
\]

To understand the oscillating behavior at long times, we compute the occupation number as a function of the gauge-invariant wavevector \( k_m = k + \Omega t \) in the long time limit, for different values of \( \Omega \) and for \( \Gamma/\gamma = 0.1 \). We compare our results (red line) with the exact solution (blue line) given in Ref. 17. Note the excellent quantitative agreement. Note also that it continues to work well even for large electric fields (large \( \Omega/\gamma \)).
becomes

$$\langle J \rangle = 4\gamma \Gamma \text{Re} \sum_{\ell} \frac{J_\ell (2\gamma / \Omega) J_{\ell+1} (2\gamma / \Omega) F(\Omega \ell)}{\Omega - 2i\Gamma} + 4\gamma \Gamma \text{Re} \sum_{\ell} \frac{J_\ell (2\gamma / \Omega) J_{\ell-1} (2\gamma / \Omega) F(\Omega \ell)}{\Omega + 2i\Gamma}. \quad (18)$$

The dc current as a function of the electric field is shown in Fig. (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, Bloch oscillations become important and the dc current decreases. We compare our result with the exact result calculated in Ref. 17. The agreement is excellent for small values of $\Gamma$. Note that when the coupling with the bath is increased, the master-equation results start to deviate from the exact result. However, as shown in Fig. 4 for $\Gamma/\gamma = 0.2$, there is a region of intermediate values of $\Gamma$ where the master equation reproduces all the qualitative features of the exact solution; it just has some quantitative mismatch. This disagreement is largest for intermediate values of $\Omega$.

We quantify the mismatch between the exact solution and the master-equation predictions by defining a norm between the exact momentum-distribution function and the approximate (master-equation) one. We define a “norm” via

$$||\Delta n|| = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_m \left| n(k_m) - n_{ex}(k_m) \right|. \quad (19)$$

In Fig. (5), we illustrate a false-color plot of the “norm” $||\Delta n||$ as functions of the electric field and the coupling strength. We have good quantitative agreement when $||\Delta n|| < 0.1$. When $0.1 < ||\Delta n|| < 0.2$, we see larger quantitative discrepancy, but the qualitative features of the exact curves are still captured by the master equation. For larger values of the norm, we have both quantitative and qualitative deviations.

Ref. 17. The range of $\Gamma$, for good agreement, shrinks almost linearly with $\Omega$. This is expected, because the master equation is necessarily perturbative in the coupling strength (due to the Born approximation). Hence, we only expect the master equation to be accurate when $\Gamma \ll \Omega$ and $\Gamma \ll \gamma$. Nevertheless, as shown in Fig. 5, we see that $||\Delta n||$ indicates good accuracy for a much wider range:
it holds when $\Gamma$ is of the same order of magnitude of $\Omega$ (up to $\Gamma \approx \Omega/2$). It also holds well for intermediate values of $\Omega$. For larger values of $\Omega$, the norm appears to oscillate around a finite value and does not vary significantly, suggesting that in this regime, there could be a finite threshold of the coupling for the applicability of the master equation.

**B. Kraus Map**

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. The basic strategy is to determine the so-called Kraus map (see below), which can be implemented in a Trotterized form, if the quantum hardware has the capability of partial resets, or in an integrated form for special cases, such as the noninteracting limit studied here.

The relationship between a Kraus map and its associated master equation, such as the one in Eq. (6), is well known. It is determined by studying the formal time evolution of a density matrix described by the given master equation. We can then think of this as a quantum map of one density matrix onto another as a function of time—this essentially defines the so-called Kraus map.

The details for how to do this follow next.

We first express the density matrix at time $t$ [$\rho_k(t)$ from Eq. (6)] as a map from its initial value $\rho_k(0)$ via

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

where $\sigma_0 = 1_{2 \times 2} / 2^{1/2}$, $\sigma_1 = \sigma^x / 2^{1/2}$, $\sigma_2 = \sigma^y / 2^{1/2}$, $\sigma_3 = \sigma^z / 2^{1/2}$, with $\sigma^{\alpha} = (x,y,z)$ 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’ve 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:

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

where $K_i(t) = \sqrt{\lambda_i} \sum_{a=0}^{3} X(i)_a \sigma_a$ are the Kraus operators with $\lambda_i$ and $X(i)_a$ 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 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

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

where $F_{rs} = \text{Tr}(\sigma_r \phi_t(\sigma_s))$ is a matrix representation 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: $F = LF$, with initial condition $F(0) = I_{4 \times 4}$ 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 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

$$K_1 = \sqrt{1 - n_k(t)} |0\rangle \langle 0|, K_2 = \sqrt{n_k(t)} |1\rangle \langle 1|,$$

$$K_3 = \sqrt{n_k(t)} |1\rangle \langle 0|, K_4 = \sqrt{1 - n_k(t)} |0\rangle \langle 1|$$

where $n_k(t)$ is defined in Eq. (17), 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 $0 < n_k(t) < 1$, 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:

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

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

**IV. QUANTUM CIRCUIT**

Now we discuss how one can simulate the action of the Kraus map given in Eq. (23) by using a quantum circuit. We imagine that the system has been prepared in some arbitrary initial state $\rho_0$. The desired circuit then needs to map all possible input states to the correct final state given in Eq. (24).

This means constructing a circuit such that it transforms an initial state $\rho(0) \mapsto \rho_{ss} = \sum_i K_i \rho(0) K_i^\dagger$. This is not a unitary operation so ancilla qubits must be utilized to purify the channel into a unitary operation. Such a
unitary operator is guaranteed to exist by Stinespring’s dilation theorem.

The form of the Kraus Map arises from taking the partial trace over the environmental degrees of freedom of the system+environment density matrix, after evolving with the joint time evolution operator. Calling the initial state of the environment \(|E_0\rangle \langle E_0|\) and choosing \({|E_i\rangle}\) as the basis for the environment this gives

\[
\rho = \sum_i \frac{|E_i\rangle \langle E_i| U^\dagger}{K_i} \rho(0) \frac{|E_0\rangle \langle E_0| U}{K_i^\dagger} \langle E_i|,
\]

(25)

So for the transition which \(K_1\) induces in the system, \(U\) must both induce the transition in the system qubit as well as the map \(|E_0\rangle \mapsto |E_i\rangle\) in the ancilla register. We seek a circuit which implements a \(U\) meeting these criteria. Such a \(U\) is not unique, corresponding to the fact that the Kraus operators are not unique. Sending \(K_1 \mapsto \sum_j W_{i j} K_j\) leaves the Kraus map unaffected for any unitary \(W\), and is equivalent to choosing a different basis for the environment. Our approach in designing the circuit is similar to the procedure given in Ref. 8, but in this case, it does not require a dissipative partial reset operation.

Note that the Kraus operators may be recast [using \(n \equiv n_k(t)\)] as

\[
\begin{align*}
K_1 &= \sqrt{1-nIP_0} \\
K_2 &= \sqrt{nIP_1} \\
K_3 &= \sqrt{nXP_0} \\
K_4 &= \sqrt{1-nXP_1}
\end{align*}
\]

(26)

Where \(P_i = |i⟩⟨i|\) is the projector onto \(|i⟩\). We may then interpret the Kraus map as performing the following: If the system is in state \(|0⟩\), apply \(I\) with probability \(1 - n\) and apply \(X\) with probability \(n\). If the system is in state \(|1⟩\), apply \(I\) with probability \(n\) and apply \(X\) with probability \(1 - n\). For example, the \(K_3\) operator flips \(|0⟩\langle 0| \mapsto |1⟩⟨1|\) with probability \(n\)

\[
K_3 \rho(0) K_3^\dagger = nXP_0 \rho(0) P_0 X = n\rho_{00}(0) P_1
\]

These operations are implemented by a controlled \(R_x\) (\(cR_x\)) gate. \(R_x(\theta)\) flips a qubit (applies \(X\)) with probability \(\sin^2(\theta/2)\) and does nothing (applies \(I\)) with probability \(\cos^2(\theta/2) = 1 - \sin^2(\theta/2) = \sin^2((\pi - \theta)/2)\). This tells us that \(\theta = 2 \arcsin(\sqrt{n})\). The projection is accomplished by (anti-)controlling the operation on a suitably initialized ancilla.

We must ensure that the application of \(K_1\) also induces \(|E_0\rangle \mapsto |E_i\rangle\) in the ancilla register. \(K_1\) and \(K_3\) are implemented by a single anti-controlled rotation, which means the ancilla qubit is in the same state for both. We proceed similarly for the controlled rotation implementing \(K_2\) and \(K_4\). We add a \(cX\) gate controlled on the system qubit, targeting a second ancilla qubit to distinguish \(K_{1/3}\) from \(K_{2/4}\) (i.e. \(I\) vs \(X\)). This results in Fig. 6 with \(R_y\) swapped in for \(R_x\), as explained below. To simplify things further, we note that replacing \(X\) with \(Y\) in \(K_3\) and \(K_4\) just multiples each by either \(\pm i\). These factors will cancel when evaluating \(K_i \rho(0) K_i^\dagger\) and thus we are free to replace \(R_x\) with \(R_y\) in the circuit. This will be advantageous when economizing the circuit because \(R_x(\pi - \theta) = -Y R_y(\theta) Z\) which leads a \(cY\) gate, which is not native in IBM’s hardware. However \(R_y(\pi - \theta) = X R_y(\theta) Z\) leads to the natural \(cX\) gate. Putting this all together results in the circuit shown in Fig. 6.

FIG. 6. Quantum circuit modeling the action of the Kraus map related to the dissipative dynamics of the master equation of Eq. (6) where \(\theta = 2 \arcsin(\sqrt{n_k(t)})\). For any initial state \(\rho(0)\), the circuit will return the desired steady state \(\rho(t)\).

This circuit may be further economized by exploiting complementary controlled and anti-controlled rotations. Specifically we make use of the following to simplify Fig. 6 to Fig. 7:

1. \(R_y(\pi - \theta) = X R_y(\theta) Z\)
2. \(c(AB) = cA cB\)
3. \(c(-Z) = acZ\) with control and target swapped
4. \(cU\) commutes with \(acV\)
5. \(cU acU = I \otimes U\)

FIG. 7. Economized version of the circuit depicted in Fig. 6 utilizing \(R_y(\pi - \theta) = X R_y(\theta) Z\). Note the initial \(cZ\) may be deleted since the circuit works for any initial state, i.e. we can “absorb” the \(Z\) into the initial state). This results in the final form of the circuit, given in Fig. 8, which we implement on IBM’s Boeblingen quantum computer.
We verify that this circuit produces the correct results by direct matrix multiplication. We use the convention that qubit 1 is the top line and qubit 3 is the bottom (system) line. Defining $cX^j_i$ be the operation which applies $cX$ controlled on $i$, targeting $j$ and the identity on all other qubits, we find that our circuit is given by

$$U = (cX^3_1) \cdot (cX^3_3) \cdot [I \otimes I \otimes R_y(\theta)] \cdot (cX^2_3).$$

This gives the final density matrix of the joint system+ancilla registers as

$$\rho_3 = U \left[ |00\rangle \langle 00| \otimes \begin{pmatrix} a & b \\ b^* & 1-a \end{pmatrix} \right] U^\dagger,$$

where $\rho(0) = \begin{pmatrix} a & b \\ b^* & 1-a \end{pmatrix}$ is a generic input state. Taking the partial trace of $\rho_3$ over the ancilla returns the reduced density matrix of the system, $\rho(t)$. Recalling $\theta = 2 \arcsin \left( \sqrt{n_k(t)} \right) \rightarrow \sin(\theta/2)^2 = n_k(t)$, we find (see App. B)

$$\text{Tr}_{\text{anc}} \rho_3 = \rho(t) = \begin{pmatrix} 1 - n_k(t) & 0 \\ 0 & n_k(t) \end{pmatrix}$$

for any incident $a$ and $b$, as claimed.

We ran the circuit shown in Fig. 7 on IBM’s Boeblingen quantum computer 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 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. The resulting output was corrected by the “pseudo-inverse” method as outlined in Qiskit’s “Measurement Error Mitigation” tutorial and implemented in Qiskit Ignis. 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. 7 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.

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).

V. 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 addressed the question of how accurate is the master equation in describing the coupling of a system to a bath? To do this, we examined a noninteracting system of fermions in a lattice that is driven out of equilibrium by an electric field and exchanges energy and particles with a fermionic reservoir at each lattice site. Such a system can be solved exactly. We also employed the master equation formalism to solve this problem and benchmarked its accuracy against the exact results. Despite the perturbative nature of the master equation, we find remarkably good agreement with the exact solution in nearly all regimes (including the regime of intermediate coupling of the system to the bath).

Next, 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, 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 by determining the Kraus map associated with the given master equation and then constructing a 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 was run on the IBM Boeblingen machine. The data are 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 many-body interactions, 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. For these reasons, devising approximate methods to find and implement the Kraus map related to a master equation will be important, in order to fully simulate an interacting driven-dissipative system on currently available (or near term) quantum machines.
VI. ACKNOWLEDGMENTS

This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Division of Materials Sciences and Engineering under Grant No. de-sc0019469. J. K. F. was also supported by the McDevitt bequest at Georgetown. B. R. was also supported by the National Science Foundation under Award DMR-1747426 (QISE-NET). We acknowledge the use of IBM Q for this work. The views expressed are those of the authors and do not reflect the official policy or position of IBM or the IBM Q team.

Appendix A: Derivation of the master equation

For completeness, we show the derivation of the master equation as it appears in Eq. (6). The total Hamiltonian of the system is given by $\hat{H}_{tot} = \hat{H}(k) + \hat{H}(b) + \hat{V}(k)$, as defined in Eqs. (3), (4) and (5). 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 $\hat{O}(t) = \hat{U}_b(t) \otimes \hat{U}_I(t) \hat{O} \hat{U}_I(t) \otimes \hat{U}_b(t)$, 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 $\hat{\chi}(t)$ of the system plus bath (in the interaction picture) reads: $\partial_t \hat{\chi}(t) = i \left[ \hat{\chi}(t), \hat{V}(t) \right]$, and can be recast in an integral formulation as follows:

$$\hat{\chi}(t) = \hat{\chi}(0) + \int_0^t dt' \left[ \hat{\chi}(t'), \hat{V}(t') \right].$$

(A1)

Substituting the last equation into the Von-Neumann equation in the differential form, one obtains:

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

(A2)

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

(A3)

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

$$\hat{\rho}(t) = \hat{\rho}(0) + g^2 \int_{-\infty}^t dt_1 C_p(t-t_1) \left[ -d(t) d(t_1) \hat{\rho}(t) + d^\dagger(t_1) \hat{\rho}(t_1) d(t_1) \right] + \text{h. c.},$$

(A4)

$$\partial_t \hat{\rho}(t) = g^2 \int_{-\infty}^t dt_1 C_p(t-t_1) \left[ -d(t) d(t_1) \hat{\rho}(t) + d^\dagger(t_1) \hat{\rho}(t_1) d(t_1) \right] + \text{h. c.},$$

(A5)

where $C_p(t) = \text{Tr}_b \sum_\alpha \hat{\rho}_b c^\dagger_{\alpha \alpha}(t) c_{\alpha \alpha}(t)$, $C_h(t) = \text{Tr}_b \sum_\alpha \hat{\rho}_b c_{\alpha \alpha}(t) c^\dagger_{\alpha \alpha}(t)$ are the correlation functions of the bath.
At is point, it is common to take the following additional approximation: $C_{P/h}(t) \sim \gamma_{P/h}(t)$. This would yield the master equation directly in the Lindblad form with time-independent coefficients. We do not adopt such a prescription in this work, because the time-independent Lindblad form does not produce the known oscillating steady state obtained in the exact solution.

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. (A5), we obtain the following equation:

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

where we defined the following operators:

$$\mathcal{D}^{(p)}(t) \equiv g^2 \int_{-\infty}^{t} dt_1 \mathcal{C}_{P}(t-t_1)\mathcal{D}^\dagger(t, t_1), \quad \text{(A7)}$$
$$\mathcal{D}^{(h)}(t) \equiv g^2 \int_{-\infty}^{t} dt_1 \mathcal{C}_{h}(t-t_1)\mathcal{D}^\dagger(t, t_1). \quad \text{(A8)}$$

Here $\mathcal{D}^\dagger(t, t_1) \equiv \hat{U}(t)\hat{U}^\dagger(t_1) \, d\hat{U}(t)\hat{U}^\dagger(t)$. It is worthwhile to note that the two operators defined in Eqs. (A7) and (A8) are not conjugates of each other (because of the finite imaginary part in $\mathcal{C}_{P/h}$).

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. (A7) and (A8). If the Hamiltonian of the system does not depend explicitly on time, the operators in Eqs. (A7) and (A8) would not depend on time and a similar expression can be found in the studies of transport in quantum dots $^{36-39}$. In our case, the time dependence of the Hamiltonian and a nontrivial structure of the correlation function [see Eq. (11)] yields time-dependent operators.

A further simplification comes from the one-body nature of our problem. In this case, the time-dependent annihilation operator can be written as $\hat{d}(t) = \hat{e}^{-i\hat{F}(t)\hat{d}}$, where $\hat{F}(t) = -2\gamma \sin(k + \Omega t) - \sin(k)/\Omega$. Therefore

$$\mathcal{D}(t, t_1) = \hat{e}^{-i\hat{F}(t_1)\hat{d}} \hat{d} \quad \text{(A9)}$$
and the operators in Eqs. (A7) and (A8) reduce to

$$\mathcal{D}^{(p)}(t) = a(t) \hat{d}^\dagger$$
$$\mathcal{D}^{(h)}(t) = A(t) \hat{d}^\dagger,$$

with the time-dependent coefficients defined in Eq. (7). After substituting the last two equations into Eq. (A6), we obtain the master equation presented in the main text in Eq. (6).

**Appendix B: Matrix Representations**

These matrices are represented using the standard computational basis, indexed as $|\text{ancilla}_{\text{top}}\rangle \otimes |\text{ancilla}_{\text{bottom}}\rangle \otimes |\text{system}\rangle$.

$$U = \begin{pmatrix}
\cos \left( \frac{\theta}{2} \right) & 0 & 0 & -\sin \left( \frac{\theta}{2} \right) & 0 & 0 & 0 & 0 \\
0 & \cos \left( \frac{\theta}{2} \right) & \sin \left( \frac{\theta}{2} \right) & 0 & 0 & 0 & 0 & 0 \\
0 & \cos \left( \frac{\theta}{2} \right) & \sin \left( \frac{\theta}{2} \right) & 0 & 0 & 0 & 0 & 0 \\
\sin \left( \frac{\theta}{2} \right) & 0 & 0 & \cos \left( \frac{\theta}{2} \right) & 0 & 0 & 0 & 0 \\
0 & \sin \left( \frac{\theta}{2} \right) & \cos \left( \frac{\theta}{2} \right) & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix} \quad \text{(B1)}$$

$$\hat{\rho}_3 = \begin{pmatrix}
 a \cos^2 \left( \frac{\theta}{2} \right) & 0 & b \cos^2 \left( \frac{\theta}{2} \right) & 0 & \frac{1}{2} a \sin(\theta) & 0 & \frac{1}{2} b \sin(\theta) \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
b^* \cos^2 \left( \frac{\theta}{2} \right) & 0 & (1-a) \cos^2 \left( \frac{\theta}{2} \right) & 0 & \frac{1}{2} b^* \sin(\theta) & 0 & \frac{1}{2} (1-a) \sin(\theta) \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} a \sin(\theta) & 0 & \frac{1}{2} b \sin(\theta) & 0 & a \sin^2 \left( \frac{\theta}{2} \right) & 0 & b \sin^2 \left( \frac{\theta}{2} \right) \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} b^* \sin(\theta) & 0 & \frac{1}{2} (1-a) \sin(\theta) & 0 & b^* \sin^2 \left( \frac{\theta}{2} \right) & 0 & (1-a) \sin^2 \left( \frac{\theta}{2} \right) \\
\end{pmatrix} \quad \text{(B2)}$$
To perform the partial trace, we partition $\rho$ into $2 \times 2$ submatrices and then sum the submatrices on the diagonal. The penultimate step uses our definition $\theta = 2 \arcsin \left( \sqrt{n_k(t)} \right)$.

$$\text{Tr}_{\text{anc}} \rho_3 = \left( a \cos^2 \left( \frac{\theta}{2} \right) \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \right) + \left( 1 - a \right) \cos^2 \left( \frac{\theta}{2} \right) \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} + \left( \begin{pmatrix} 0 & 0 \\ 0 & a \sin^2 \left( \frac{\theta}{2} \right) \end{pmatrix} \right) = \left( \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \right) = \rho(t). \quad (B3)$$

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