Simulation of open quantum system dynamics based on the generalized quantum master equation on quantum computing devices

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Abstract

The simulation of open quantum system dynamics, namely the reduced dynamics of a quantum system coupled to a quantum bath, is the cornerstone of quantum rate theory, optical response theory and decoherence science, which are central concepts in modern physics and chemistry. The generalized quantum master equation (GQME) formalism provides a universal framework for simulating the dynamics of open quantum systems. Using this framework allows one to derive a formally exact equation of motion, \textit{i.e.}, the GQME, for the reduced density matrix that describes the state of a system coupled to a bath, without employing commonly made restrictive assumptions such as weak system-bath coupling and Markovity. Within this GQME, the effect of the bath on the time evolution of the system’s reduced density matrix is fully captured by a memory kernel superoperator. In this work we develop a general-purpose GQME-based

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quantum algorithm for simulating open quantum system dynamics. Starting out from the memory kernel as the input, we solve the GQME for the system’s non-unitary time evolution superoperator. We then use dilation techniques to convert the non-unitary time evolution superoperator into a unitary time evolution superoperator in an extended Hilbert space, which can be implemented on quantum circuits. The GQME-based quantum algorithm is demonstrated with the spin-boson benchmark model, including implementations on the IBM QASM quantum simulator and IBM quantum computers.

1 Introduction

Real-life quantum systems are rarely perfectly isolated, which makes it necessary to account for the effect of their surrounding, or bath, on the system’s dynamics. Furthermore, many important phenomena, such as rates of a wide range of chemical and physical processes, lifetimes of excited states, spectral diffusion, and line-broadening, either rely on or are driven by interactions between the system of interest and its surrounding. The simulation of open quantum system dynamics, namely the reduced dynamics of a system coupled to a bath, is therefore central to many science and engineering disciplines, including physical chemistry, molecular physics, condensed-phase physics, nanoscience, molecular electronics, quantum optics, nonequilibrium statistical mechanics, spectroscopy and quantum information science [1–30]. Open quantum system dynamics therefore serves as a unifying platform that brings together different disciplines and bridge the gap between theory and experiment. Notable examples include electronic energy and charge transfer and dephasing, vibrational relaxation and dephasing, nonadiabatic dynamics, photochemistry, and a variety of other light-induced physical and chemical processes [22,23,28,31–49].

Although numerous quantum algorithms have been developed for calculating electronic structure [50–53] and simulating quantum dynamics of closed quantum systems [54–57], relatively few studies have targeted simulating open quantum system dynamics [58–63]. Furthermore, the majority of those previous studies were based on Lindblad-type quantum master equations (QMEs), which are guaranteed by construction to satisfy complete positivity and conservation of probability, but also assume Markovity, which, strictly speaking, is only valid in the weak system-bath coupling limit or the singular bath limit [9]. It is therefore highly desirable to develop quantum algorithms for simulating open quantum system dynamics based on a less-restrictive equation of motion (EoM).

In this paper, we propose such a quantum algorithm based on the generalized quantum master equation (GQME), which corresponds to the formally exact EoM for an open quantum system.

A major challenge facing the quantum simulation of open quantum system dynamics is the fact that the time evolution operators are non-unitary whereas quantum gates are unitary. To this end, we have previously developed a quantum algorithm for open quantum dynamics based on the Sz.-Nagy unitary dilation theorem, which converts non-unitary operators into unitary operators in
an extended Hilbert space. This algorithm was originally applied to simulating a Markovian two-level model on the IBM quantum computer [64]. Later, the same method was applied to simulating a non-Markovian two-level model (Jaynes-Cummings model) on the IBM quantum computer [65]. In a recent work, the same quantum algorithm was generalized to also work with the Lindblad QME and applied to simulate the dynamics of the Fenna-Matthews-Olson complex, which includes five quantum levels and seven elementary physical processes [66]. Thus far, this quantum algorithm has been used to simulate the dynamics of open quantum systems described by the operator sum representation or Lindblad-type QMEs.

Figure 1: A comparison of the workflows for simulating the dynamics of a closed quantum system governed by the quantum Liouville equation vs. an open quantum system governed by the GQME. 1. The EoM is established; 2. the time evolution superoperator is generated from the EoM; 3. A unitary dilation is required in order to convert the GQME-based non-unitary time evolution superoperator into a unitary superoperator in an extended Hilbert space; 4. Translation of the unitary matrix into a quantum gate sequence.

However, these approaches are not entirely general: the Lindblad QME used in Ref. [66] has several restrictive approximations including Markovian dynamics and the ensemble of Lindbladian trajectories method in Ref. [65] while capable of describing non-Markovian dynamics, involves user selection of ad-hoc system-bath parameters, therefore limiting the range of applications. Furthermore, while the operator sum representation of open quantum system dynamics is general, it requires knowledge of the Kraus operators, which to the best of our knowledge are only known in closed form for systems whose dynamics can be described by Lindblad-type QMEs.

Extending the range of quantum simulation of open quantum systems therefore calls for describing the dynamics by a less restrictive theoretical framework. The GQME formalism introduced by Nakajima [67] and Zwanzig [68] represents
such a general framework since the GQME it leads to corresponds to the formally exact EoM of the open quantum system, as opposed to the Lindblad-type QMEs which correspond to approximate EoMs of the open quantum system.

A comparison of the workflows for simulating the dynamics of a closed quantum system governed by the quantum Liouville equation vs. an open quantum system governed by the GQME is shown in Fig. 1. The derivation of the GQME involves projecting out the bath degrees of freedom (DOF) to obtain the EoM of the system’s reduced density matrix. Within this EoM, which is referred to as the GQME, the memory kernel superoperator, $K(\tau)$, fully accounts for the impact of the bath on the system’s dynamics. Thus, the GQME replaces the Liouville equation as the formally exact EoM of the system when we transition from a closed quantum system to an open quantum system, with the memory kernel playing a similar role in the open system to that of the Hamiltonian or Liouvillian in the closed system.

In this work, we develop a GQME-based quantum algorithm for simulating the dynamics of an open quantum system. Firstly, we provide a route from the memory kernel to the non-unitary time evolution superoperator that describes the dynamics generated by the GQME for that memory kernel. Then the Sz.-Nagy unitary dilation theorem is used to convert the GQME-based non-unitary time evolution superoperator into a unitary superoperator in an extended Hilbert space. Given this dilated and now unitary time evolution superoperator and the initial state of the system, we can evolve the dynamics for any open quantum system on quantum computers. Given the fact that the GQME is the exact EoM of the open quantum system, this quantum algorithm greatly extends the range of possible systems that can be simulated on a quantum computer, including complex non-Markovian photosynthetic and photovoltaic systems [28, 69], molecular electronics [48], linear and nonlinear spectroscopy [70], systems with inter-system crossing [71], and conical intersections [72]. Thus, this GQME-based quantum algorithm provides an essentially universal protocol for simulating open quantum system dynamics on quantum computing platforms. Given a powerful enough quantum computer, this algorithm opens the door for simulating open quantum system dynamics of large and complex molecular systems, which are currently beyond the reach of classical computers.

2 Results

2.1 The GQME-based time evolution superoperator

In this sub-section, we describe the first step in the workflow outlined in Fig. 1, namely obtaining the time evolution superoperator of an open quantum system starting from its formally exact EoM in GQME form.

For the sake of concreteness, we will focus on molecular systems with an
overall Hamiltonian of the following commonly encountered form

\[ \hat{H} = \sum_{j=1}^{N_e} \hat{H}_j |j\rangle \langle j| + \sum_{j,k=1 \atop k \neq j}^{N_e} \hat{V}_{jk} |j\rangle \langle k| \]  

(1)

and an overall system initial state of the following commonly used single-product form

\[ \hat{\rho}(0) = \hat{\rho}_n(0) \otimes \hat{\sigma}(0). \]  

(2)

It should be noted that the GQME approach is not limited to this form of Hamiltonian and initial state and that the choice to focus on them is solely motivated by clarity of presentation. The system and bath in this case correspond to the electronic and nuclear DOF, respectively. In Eqs. (1) and (2), \( \hat{H}_j = \hat{P}^2/2 + V_j \left( \hat{R}_j \right) \) is the nuclear Hamiltonian when the system is in the diabatic electronic state \( |j\rangle \), with the index \( j \) running over the \( N_e \) electronic states; \( \hat{R} = \left( \hat{R}_1, ..., \hat{R}_{N_n} \right) \) and \( \hat{P} = \left( \hat{P}_1, ..., \hat{P}_{N_n} \right) \) are the mass-weighted position and momentum operators of the \( N_n \gg 1 \) nuclear DOF, respectively; \( \{ \hat{V}_{jk} | j \neq k \} \) are the coupling terms between electronic states (which can be either nuclear operators or constants); and \( \hat{\rho}_n(0) \) and \( \hat{\sigma}(0) \) are the reduced density operators that describe the initial states of the nuclear (bath) and electronic (system) DOF, respectively. Throughout this paper, boldfaced variables, e.g., \( A \), indicate vector quantities; a hat over a variable, e.g., \( \hat{B} \), indicates an operator quantity; and calligraphic font, e.g., \( L \), indicates a superoperator.

Using projection operator techniques, one can then derive the following formally exact EoM, or GQME, for the reduced electronic density operator, \( \hat{\sigma}(t) \) [27–30]:

\[ \frac{d}{dt} \hat{\sigma}(t) = -\frac{i}{\hbar} \langle L \rangle_n^0 \hat{\sigma}(t) - \int_0^t d\tau \, K(\tau) \hat{\sigma}(t - \tau) . \]  

(3)

The open quantum system dynamics of the reduced electronic density matrix described by this GQME is generated by the two terms on the R.H.S. of Eq. (3).

The first term is given in terms of the projected overall system Liouvillian \( \langle L \rangle_n^0 \equiv \text{Tr}_n \{ \hat{\rho}_n(0) L \} \) [where \( L(\cdot) = [\hat{H}, \cdot] \) is the overall system Liouvillian and \( \text{Tr}_n \{ \cdot \} \) is the trace over the nuclear (bath) Hilbert space], which is represented by a \( N^2_e \times N^2_e \) time-independent matrix. The second term is given in terms of the memory kernel \( K(\tau) \), which is represented by a \( N^2_e \times N^2_e \) time-dependent matrix. Further details about the GQME approach, including the derivations of Eq. (3), and the explicit form of the memory kernel are provided in Sec. 4.

For the purpose of this paper, it is more convenient to rewrite the GQME in Eq. (3) in terms of the system’s time evolution superoperator, \( \mathcal{G}(t) \), which is defined by:

\[ \hat{\sigma}(t) = \mathcal{G}(t) \hat{\sigma}(0) . \]  

(4)
Substituting Eq. (4) into Eq. (3) and noting that the GQME should be satisfied for an arbitrary choice of $\hat{\sigma}(0)$, it is straightforward to show that $G(t)$ satisfies the same GQME as $\hat{\sigma}(t)$:

$$\frac{d}{dt} G(t) = -\frac{i}{\hbar} \langle L \rangle 0_n G(t) - \int_0^t d\tau \ K(\tau) G(t - \tau) .$$

(5)

Thus, given the projected Liouvillian and memory kernels $[\langle L \rangle 0_n$ and $K(\tau)$, respectively], $G(t)$ can be obtained by solving Eq. (5).

2.2 The GQME-based quantum algorithm for simulating open quantum system dynamics

In this sub-section, we describe the next step in the workflow outlined in Fig. 1, namely using the Sz.-Nagy’s unitary dilation procedure [73] to convert the non-unitary quantum open system time evolution superoperator $G(t)$ [see Eqs. (4) and (5)] into a unitary time evolution superoperator in an extended Hilbert space.

We start out by calculating the operator norm of $G(t)$ to determine if it is a contraction. For $G(t)$ to be a contraction, the operator norm of $G(t)$ needs to be less than or equal to 1, i.e., $\|G(t)\|_O = \sup \frac{\|G(t)v\|}{|v|} \leq 1$. In the case where the original $G(t)$ is not a contraction, we introduce a normalization factor $n_c = \|G(t)\|_O$ in order to define a contraction form of $G(t)$, namely $G'(t) = G(t)/n_c$.

In the next step, we apply a 1-dilation procedure to $G'(t)$ to obtain a unitary $U_{G'}(t)$ in an extended Hilbert space of double the dimension of the original system Hilbert space:

$$U_{G'}(t) = \left( \begin{array}{cc} G'(t) & D_{G'}(t) \\ D_{G'}(t)^\dagger & -G'^\dagger(t) \end{array} \right) .$$

(6)

Here, $D_{G'}(t) = \sqrt{I - G'(t) G'(t)}$ and $D_{G'}(t)^\dagger = \sqrt{I - G'(t)^\dagger G'^\dagger(t)}$, where $D_{G'}(t)$ is the so-called defect superoperator of $G'(t)$. The 1-dilation procedure generates a unitary superoperator $U_{G'}(t)$ that operates in the extended Hilbert space and replicates the effect of the contraction form of the original time evolution superoperator, $G'(t)$, when the input and output vectors are both restricted to the original smaller Hilbert space.

In the original system Hilbert space, the system reduced density operator $\hat{\sigma}(t)$ is represented by an $N_e \times N_e$ matrix:

$$\hat{\sigma}(t) \doteq \begin{pmatrix} \sigma_{11}(t) & \cdots & \sigma_{1N_e}(t) \\ \vdots & \ddots & \vdots \\ \sigma_{N_e1}(t) & \cdots & \sigma_{N_eN_e}(t) \end{pmatrix} .$$

(7)

Alternatively, the same system reduced density operator can also be represented by an $N_e^2$-dimensional vector in Liouville space:

$$\tilde{\sigma}(t) \doteq (\sigma_{11}(t), ..., \sigma_{1N_e}(t), \sigma_{21}(t), ..., \sigma_{2N_e}(t), ..., \sigma_{N_e1}(t), ..., \sigma_{N_eN_e}(t))^T .$$

(8)
Since the GQME formalism is given in terms of superoperators, it is convenient to work in Liouville space, which we will do from this point on. We also define the norm of the vector representing $\hat{\sigma}(t)$ in Liouville space as the Frobenius norm:

$$\|\sigma(t)\|_F = \sqrt{\sum_{ij} |\sigma_{ij}|^2}$$

and divide $\hat{\sigma}(t)$ by $\|\sigma(t)\|_F$ to normalize $\hat{\sigma}(t)$.[64]

Given the dilated unitary operator $U_G'(t)$ and the initial quantum input state $\hat{\sigma}(0)$, operating with the non-unitary $G'(t)$ on $\hat{\sigma}(0)$ has now been converted into a unitary transformation as follows:

$$G'(t)\hat{\sigma}(0) \xrightarrow{\text{unitary dilation}} U_G'(t) (\hat{\sigma}(0)^T, 0, \cdots, 0)^T.$$  \hfill (9)

The 0s in the input vector on the R.H.S. are added to match the dimension of the input vector with that of $U_G'(t)$. The unitary process can then be simulated on a quantum circuit with unitary quantum gates. The electronic populations, $\{\sigma_{jj}(t) \equiv \langle j | \hat{\sigma}(t) | j \rangle | j = 1, \ldots, N_e \}$ can be retrieved by taking the square roots of the probability of measuring each basis state $P_j(t) = |\sigma'_{jj}(t)|^2$ and multiplying by the $n_c$ factor.

Finally, we perform a complexity analysis of the quantum algorithm. Given that $G(t)$ in its most general form is represented by an matrix of $N^4_e$ non-zero elements, the defect superoperators $D_G'(t)$ as well as $-G'(t)$ as shown in Eq. [6] all have $N^4_e$ non-zero elements. Generally speaking, the number of the two-level unitaries necessary to decompose a unitary gate is comparable to the number of non-zero elements in the lower-triangular part of the gate[74,75]. Therefore, the gate complexity to simulate this specific $U_G'(t)$ is $O(N^4_e)$. If the two-level unitaries are further decomposed into 1-qubit and 2-qubit elementary gates commonly used to design conventional quantum circuits, they need to be transformed to the Gray code sequences and some multi-control gate sequences, adding another factor of complexity logarithmic in $N^2_e$, and the total complexity becomes $O(N^4_e \log^2 N^2_e)$.[74]. This means that the maximum total complexity of a GQME-based simulation of an open quantum system dynamics is comparable to classical methods[64]. However, as demonstrated in previous simulations of certain dynamical models, our quantum algorithm can take advantage of the case when the $G(t)$ is a sparse matrix, and thus the gate complexity scaling for $G(t)$ can be reduced to $O(\log^2 N^2_e)$ instead of $O(N^4_e)$[64,66].

2.3 A demonstrative application to the spin-boson model

In this sub-section, we demonstrate the applicability of the quantum algorithm outlined in the previous sections on the spin-boson benchmark model. This model has a wide range of applicability to chemical and physical systems, including electron, proton, energy, and charge transfer processes; polaron formation and dynamics in condensed phase environments; vibrational relaxation, impurity relaxation in solids, and spin-lattice relaxation; and dissipation effects in qubits in quantum computing[22,23,76,77]. It should also be noted that quantum-mechanically exact memory kernels can be calculated for this model[78,80].
Table 1: Spin-boson model and simulation parameters.

<table>
<thead>
<tr>
<th>Model #</th>
<th>(\epsilon)</th>
<th>(\Gamma)</th>
<th>(\beta)</th>
<th>(\xi)</th>
<th>(\omega_c)</th>
<th>(\omega_{\text{max}})</th>
<th>(N_n)</th>
<th>(\Delta t)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0 (\Gamma)</td>
<td>1.0 (\Gamma)^{-1}</td>
<td>0.1</td>
<td>1.0 (\Gamma)</td>
<td>5 (\Gamma)</td>
<td>60</td>
<td>1.50083 (\times 10^{-3}) (\Gamma)^{-1}</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1.0 (\Gamma)</td>
<td>1.0 (\Gamma)^{-1}</td>
<td>0.1</td>
<td>0.1</td>
<td>2.0 (\Gamma)</td>
<td>100</td>
<td>60</td>
<td>1.50083 (\times 10^{-3}) (\Gamma)^{-1}</td>
</tr>
<tr>
<td>3</td>
<td>1.0 (\Gamma)</td>
<td>1.0 (\Gamma)^{-1}</td>
<td>0.4</td>
<td>2.0 (\Gamma)</td>
<td>60</td>
<td>1.50083 (\times 10^{-3}) (\Gamma)^{-1}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.0 (\Gamma)</td>
<td>1.0 (\Gamma)^{-1}</td>
<td>0.2</td>
<td>2.5 (\Gamma)</td>
<td>60</td>
<td>1.50083 (\times 10^{-3}) (\Gamma)^{-1}</td>
<td></td>
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</tr>
</tbody>
</table>

The spin-boson Hamiltonian has the form of Eq. (1) with \(N_e = 2\) and \(\{\hat{H}_j, \hat{V}_{jk}\}\) given by:

\[
\hat{H}_0 \equiv \hat{H}_D = \epsilon \sum_{k=1}^{N_n} \frac{\hat{P}_k^2}{2} + \frac{1}{2}\omega_k^2 \hat{R}_k^2 - c_k \hat{R}_k,
\]
\[
\hat{H}_1 \equiv \hat{H}_A = -\epsilon \sum_{k=1}^{N_n} \frac{\hat{P}_k^2}{2} + \frac{1}{2}\omega_k^2 \hat{R}_k^2 + c_k \hat{R}_k,
\]
\[
\hat{V}_{01} \equiv \hat{V}_{DA} = \hat{V}_{10} \equiv \hat{V}_{AD} = \Gamma.
\]

Here, the two electronic states are designated as the donor and acceptor (\(|D\rangle\) and \(|A\rangle\), respectively), \(2\epsilon\) is the shift in equilibrium energy between the donor (\(D\)) and acceptor (\(A\)) states, and \(\Gamma\) is a positive constant describing the electronic coupling between the donor and acceptor states. Since \(\Gamma\) is a constant, this system is assumed to satisfy the Condon approximation.

The results shown below were obtained for the case where the nuclear modes’ frequencies and coupling coefficients \(\{\omega_k, c_k\}\) are sampled from an Ohmic spectral density with exponential cutoff:

\[
J(\omega) = \frac{\pi}{2} \sum_{k=1}^{N_n} \frac{c_k^2}{\omega_k}\delta(\omega - \omega_k) \quad \text{as} \quad N_n \to \infty \quad \frac{\pi \hbar}{2} \xi \omega e^{-\omega/\omega_c}.
\]

Here, \(\xi\) is the Kondo parameter and \(\omega_c\) is the cutoff frequency. The reader is referred to Appendix C of Ref. 27 for a description of the procedure used to obtain a discrete set of \(N_n\) nuclear mode frequencies \(\{\omega_k\}\) and coupling coefficients \(\{c_k\}\) from the spectral density in Eq. (11).

The initial state is assumed to be of the form of Eq. (2), with the initial electronic (system) reduced density operator given by \(\hat{\sigma}(0) = |D\rangle\langle D|\) and the initial nuclear (bath) reduced density operator given by

\[
\hat{\rho}_n(0) = \frac{e^{-\beta(\hat{H}_D + \hat{H}_A)/2}}{\text{Tr}_n\{e^{-\beta(\hat{H}_D + \hat{H}_A)/2}\}}.
\]

Calculations were carried out for four different sets of parameter values (see Table 1). Models 1 and 2 correspond to systems with an energy bias between
the donor and acceptor states ($\epsilon \neq 0$) and differ in their cutoff frequencies, with model 2 having a higher cutoff frequency. Model 3 corresponds to a biased system with the same parameters as model 2 except for a larger Kondo parameter. Model 4 corresponds to a symmetric system with zero energy bias between the donor and acceptor states ($\epsilon = 0$). The results reported in this paper were obtained with a time step of $\Delta t = 1.50083 \times 10^{-3} \Gamma^{-1}$ for models 1-3 and a time step of $\Delta t = 4.50249 \times 10^{-3} \Gamma^{-1}$ for model 4.

Starting with the quantum-mechanically exact memory kernels (adopted from Ref. [80]), the time evolution superoperator for the electronic reduced density matrix $\mathcal{G}(\tau)$ was generated for the four models given in Table 1 by solving the corresponding GQME, Eq. (5). Details on the method used to obtain $\mathcal{G}(\tau)$ are given in Sec. 4.

The GQME-based quantum algorithm for simulating the electronic dynamics within the spin-boson model was implemented on the IBM quantum platforms via the Qiskit package [81]. The quantum implementation involved the translation at each time step of $\mathcal{G}^{\prime}(t)$ into $\mathcal{U} \mathcal{G}^{\prime}(t)$, followed by the construction of a quantum circuit based on $\mathcal{U} \mathcal{G}^{\prime}(t)$, and lastly the use of the quantum circuit to simulate the time evolution of the reduced electronic density matrix. To build the circuit, we dilate the $4 \times 4$ $\mathcal{G}^{\prime}(t)$ into a unitary $8 \times 8 \mathcal{U} \mathcal{G}^{\prime}(t)$ using a 1-dilation procedure [see Eq. (6)]. The unitary $\mathcal{U} \mathcal{G}^{\prime}(t)$ is then transpiled into a 3-qubit quantum circuit composed of three elementary quantum gates: $R_Z$, $\sqrt{X}$, and $CX$. Examples of $\mathcal{U} \mathcal{G}^{\prime}(t)$ and details of the elementary quantum gates and circuits are shown in the supplementary information (SI). The initial electronic state is set to $(1, 0, 0, 0, 0, 0, 0, 0)^T$, where the last four 0s are the extra dimensions from the dilation procedure. The QASM simulator and the real quantum devices initialize the input state $(1, 0, 0, 0, 0, 0, 0, 0)^T$ and apply the unitary operation $\mathcal{U} \mathcal{G}^{\prime}(t)$ to the input state followed by projection measurements to retrieve the probability distribution of all the 8 basis states. Each circuit runs 2000 shots and the resulting probabilities $P_{000}(t)$ of measuring the state $|000\rangle$ and $P_{011}(t)$ of measuring $|011\rangle$ correspond to the diagonal elements of the modified density matrix $|\sigma_{00}^{(t)}|^{2}$ and $|\sigma_{11}^{(t)}|^{2}$.

To retrieve the populations of the donor state $\sigma_{00}(t)$ and acceptor state $\sigma_{11}(t)$ we have

$$\sigma_{00}(t) = \sqrt{P_{000}(t)} \times n_c$$

and

$$\sigma_{11}(t) = \sqrt{P_{011}(t)} \times n_c . \tag{13}$$

In what follows, we report results in terms of the difference between the donor and acceptor populations, $\sigma_z(t) = \sigma_{00}(t) - \sigma_{11}(t)$.

The comparison between the exact results obtained by solving the GQME on a classical computer and results obtained by performing the quantum algorithm on the QASM simulator is shown in Fig. 2. The QASM simulator results are in excellent agreement with the exact results for all four models under consideration. The small amplitude oscillations of the QASM-based results around the exact results can be traced back to the inherent uncertainty associated with projection measurements. These results validate the GQME-based quantum algorithm and demonstrate its ability to reproduce results obtained via the GQME-based classical algorithm.
Figure 2: The spin-boson model simulated by the GQME-based quantum algorithm as implemented on the IBM QASM quantum simulator, showing the electronic population difference between the donor state and acceptor state $\sigma_z(t) = \sigma_{DD}(t) - \sigma_{AA}(t)$ as a function of time for (a) model 1, (b) model 2, (c) model 3, and (d) model 4 as given in Table 1, with units scaled to the electronic coupling, $\Gamma$. Each figure shows the comparison between the GQME-generated exact results represented by the black curves and the QASM-simulated results represented by the yellow dots. The time step for both the exact and simulated results is $\Delta t = 1.50083 \times 10^{-3} \Gamma^{-1}$ for models 1-3 and $\Delta t = 4.50249 \times 10^{-3} \Gamma^{-1}$ for model 4. Each model is simulated for 4000 time steps. The number of projection measurements applied by the QASM simulator to simulate a single time step is 2000 shots.

To test the performance of the quantum algorithm on real quantum devices, we also performed the simulations on the quantum computers provided by IBM Quantum (IBM Q). The simulations were performed for models 3 and 4 on ibmq_quito and ibmq_lima, respectively. Both devices are equipped with 5 qubits that have the same qubit connectivity and use IBM’s Falcon r4T processor with the same architecture. In each simulation of a given model, three qubits were used and 10 repeated experiments were performed. In a single experiment, 40 time steps are chosen at an equal spacing out of the 4000 time steps used in the QASM simulations, i.e., the time step in each experiment is 100 times greater than the time step used in the QASM simulations as listed in Table 1. The average CX gate error and readout error are $(1.191 \times 10^{-2}, 5.194 \times 10^{-2})$ for
Figure 3: The spin-boson model simulated by the GQME quantum algorithm as implemented on the IBM quantum computers **ibmq quito** and **ibmq lima**, showing the electronic population difference between the donor state and acceptor state $\sigma_z(t) = \sigma_{DD}(t) - \sigma_{AA}(t)$ as a function of time for (a) model 3 and (b) model 4 as given in Table 1 with units scaled to the electronic coupling, $\Gamma$. Each figure shows the comparison between the GQME-based results represented by the black curves and quantum-computer-simulated results represented by the red dots with error bars. The time step for the real machine simulation is $\Delta t = 0.150083 \Gamma^{-1}$ for model 3 and $\Delta t = 0.450249 \Gamma^{-1}$ for model 4. The experiments of both models take 40 evenly-spaced time steps out of the 4000 time steps used in the QASM simulator runs and the error bars represent the standard derivations of the 10 separate runs on the **ibmq quito** and **ibmq lima** for models 3 and 4. The number of projection measurements applied by both the devices to simulate a single time step is 2000 shots.

the **ibmq quito** and $(1.032 \times 10^{-2}, 2.834 \times 10^{-2})$ for the **ibmq lima** as of the time of the experiments. The quantum circuits are the same in both the QASM simulations and the real machine simulations. The transpiled quantum gate
counts for each of the $U_G(t)$ superoperators are 153 $R_Z$ gates, 98 $\sqrt{X}$ gates, and 41 $CX$ gates. The transpiling process is done internally by the Qiskit package and examples of the quantum circuits can be found in the SI.

The comparison between the GQME-generated exact results and real machine simulations is given in Fig. 3. In the figure, the red dots are the average of the 10 experiments and the error bars represent standard derivations of the 10 experiments. The simulations with the IBM Q quantum computers are seen to be in qualitative agreement with the exact results, which demonstrate that the GQME-based quantum algorithm can capture the essential features of the dynamics even with the noise and errors within real quantum devices.

3 Discussion

The GQME-based quantum algorithm proposed herein substantially expands the range of open quantum systems that can be simulated on a quantum computer. We demonstrated the applicability and versatility of the algorithm with the implementations on the IBM QASM quantum simulator and IBM quantum computers.

The results obtained via the QASM simulator were found to be highly accurate, with the error that is inherently associated with the quantum projection measurements giving rise to very slight deviations from the exact results. The results obtained by implementing the simulation on the IBM Q quantum computers were also found to be in reasonable qualitative agreement with the exact results, although clearly the noise and errors inherent to the NISQ era quantum machines negatively affected the accuracy [82]. For model 3, the results obtained on the IBM quantum computer capture the general dynamical trends [see Fig. 3(a)]. The fact that the quantum result vanishes asymptotically rather than relaxes to the actual non-zero equilibrium value is likely due to decoherence caused by the gate errors. It should be noted that the quantity plotted is the donor-acceptor population difference. Thus, the gate errors and system noise cause the computational basis states to be more uniformly populated, so that the difference between them is diminished. Indeed, the agreement with the exact results is better for model 4, which is symmetrical and therefore corresponds to zero population difference at equilibrium [see Fig. 3(b)].

There are several future directions of research that have the potential to improve the performance of the quantum algorithm on the NISQ quantum machines. One direction is to optimize the quantum circuit design and reduce the circuit depth. In general, the shallower the circuit depth (in terms of the number of elementary gates), the less the overall error in simulations on real quantum devices. To this end, there have been many proposals for possible ways to optimize the decomposition of unitary operations into elementary gate sequences [83–86]. One particularly interesting idea is to reduce the circuit depth by adding additional qubits [87], which may be applicable to the current model, as we have only used 3 qubits out of the 5 currently available on freely accessible IBM quantum computers. Another method to mitigate the errors on
the IBM machine is dynamical decoupling (DD) \cite{88-92}. This method employs pulses to suppress the system’s coupling with the environment. Some recent implementations of DD on IBM machines improve the fidelity of the overall performance \cite{93-95}. Yet another direction is to implement the circuit on high-dimensional qudit systems. Quantum computers based on three-dimensional circuit quantum electrodynamics (3D cQED) microwave cavities are particularly promising, as they feature unique quantum error correction schemes \cite{96-98} and longer coherence times \cite{99,100} than standard superconducting quantum computers. Bosonic quantum computing algorithms have also been recently shown to significantly reduce the number of quantum gates required for the calculation of the Franck-Condon factors \cite{101} and dynamics of rhodopsin near conical intersections \cite{102}. Lossless 3D cQED systems have not yet been employed to simulate open quantum system dynamics. An adaptation of the algorithm presented here to bosonic quantum computing could therefore provide another way to efficiently simulate open quantum system dynamics and demonstrate how qudit-based quantum architectures can reduce the computational cost and enhance the accuracy of quantum simulations.

4 Methods

The GQME formalism provides a general framework for deriving the exact EoM for any quantity of interest. The derivation begins with the Nakajima-Zwanzig equation \cite{67,68}, which describes the dynamics of a projected state $\mathcal{P}\hat{\rho}(t)$, where $\mathcal{P}$ is a projection superoperator and $\hat{\rho}(t)$ is the density operator of the overall system:

$$\frac{d}{dt} \mathcal{P} \hat{\rho}(t) = -\frac{i}{\hbar} \mathcal{L} \mathcal{P} \hat{\rho}(t) - \frac{1}{\hbar^2} \int_0^t d\tau \mathcal{P} \mathcal{L} e^{-iQ \mathcal{L} \tau/\hbar} Q \mathcal{L} \mathcal{P} \hat{\rho}(t-\tau)$$

(14)

$$-\frac{i}{\hbar} \mathcal{P} \mathcal{L} e^{-iQ \mathcal{L} t/\hbar} Q \hat{\rho}(0).$$

Here, $\mathcal{L}$ is the overall system-bath Liouvillian and $Q = 1 - \mathcal{P}$ is the complimentary projection superoperator to $\mathcal{P}$. Importantly, the only requirements are that $\mathcal{L}$ is Hermitian and $\mathcal{P}$ satisfies $\mathcal{P}^2 = \mathcal{P}$. Otherwise, there is complete flexibility in the choice of $\mathcal{L}$ and $\mathcal{P}$, with each choice leading to a different GQME for a different quantity of interest \cite{30}.

Following Ref. \cite{27} we focus an overall system-bath Hamiltonian of the form of Eq. (1) and the following choice of projection operator which gives rise to the GQME for the system reduced density matrix, $\hat{\sigma}(t)$:

$$\mathcal{P}(\hat{A}) = \hat{\rho}_n(0) \otimes \text{Tr}_n \{ \hat{A} \}.$$  

(15)

Plugging Eq. (15) into Eq. (14) and tracing over the nuclear (bath) Hilbert space leads to the GQME in Eq. (3). The memory kernel in Eq. (3) is given by

$$\mathcal{K}(\tau) = \frac{1}{\hbar^2} \text{Tr}_n \left\{ \mathcal{L} e^{-iQ \mathcal{L} \tau/\hbar} Q \mathcal{L} \hat{\rho}_n(0) \right\},$$

(16)
and can be obtained by solving the following Volterra equation \([27]\):

\[
\mathcal{K}(\tau) = i\dot{F}(\tau) - \frac{1}{\hbar} F(\tau) (\mathcal{L})_n^0 + i \int_0^\tau d\tau' F(\tau - \tau') \mathcal{K}(\tau').
\] (17)

Here, \(F(\tau)\) and \(\dot{F}(\tau)\) are the so-called projection-free inputs (PFIs), which are given by

\[
F(\tau) = \frac{1}{\hbar} \text{Tr}_n \left\{ L e^{-i L \tau / \hbar} \hat{\rho}_n(0) \right\},
\]

\[
\dot{F}(\tau) = -\frac{i}{\hbar^2} \text{Tr}_n \left\{ L e^{-i L \tau / \hbar} L \hat{\rho}_n(0) \right\}.
\] (18)

The memory kernels for the spin-boson model used in this paper were adopted from Ref. [80], where they were obtained from quantum-mechanically exact PFIs calculated via the tensor-train thermo-field dynamics (TT-TFD) method.

The derivation of Eq. (5) begins with the definition of the time evolution operator, Eq. (4). Plugging Eq. (4) in Eq. (3), we obtain:

\[
\frac{d}{dt} \bar{G}(t)\hat{\sigma}(0) = -\frac{i}{\hbar} (\mathcal{L})_n^0 \bar{G}(t)\hat{\sigma}(0) - \int_0^t d\tau \mathcal{K}(\tau) \bar{G}(t - \tau)\hat{\sigma}(0).
\] (19)

Then, by eliminating \(\hat{\sigma}(0)\) on both sides, we reach Eq. (5), which was then solved for \(\bar{G}(t)\) numerically via a Runge–Kutta fourth-order (RK4) algorithm \([28]\).

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A Supplementary Information

A.1 Quantum circuit examples

In this section, we include further details concerning the quantum algorithm, including the dilation process, circuit transpiling, QASM simulations, and simulations running on the IBM quantum computers ibmq quito and ibmq lima. The normalized time evolution operator of the electronic reduced density operator \( G'(t) = G(t)/n_c \) (where \( G(t) \) is generated from the GQME formalism) is dilated into a unitary operator \( U_G'(t) \). We start with \( G_3 \), which corresponds to the \( G(t) \) of the 1500th time step from model 3, and \( G_4 \), which corresponds to the \( G(t) \) of the 1500th time step from model 4. The matrix of \( G_3 \) and \( G_4 \) are, respectively:

\[
G_3 = \begin{pmatrix}
0.38 - 3.76 \times 10^{-10} & 0.04 + 2.90 \times 10^{-2} & 0.04 - 2.90 \times 10^{-2} & 0.06 - 1.88 \times 10^{-10} \\
-0.13 + 7.04 \times 10^{-2} & 0.28 - 2.63 \times 10^{-2} & 0.02 + 2.37 \times 10^{-2} & -0.15 - 3.06 \times 10^{-2} \\
-0.13 - 7.04 \times 10^{-2} & 0.02 - 2.37 \times 10^{-2} & 0.28 + 2.63 \times 10^{-2} & -0.15 + 3.06 \times 10^{-2} \\
0.62 + 3.77 \times 10^{-10} & -0.04 - 2.90 \times 10^{-2} & -0.04 + 2.90 \times 10^{-2} & 0.94 - 1.87 \times 10^{-10}
\end{pmatrix}, \tag{A.1}
\]

and

\[
G_4 = \begin{pmatrix}
0.54 + 4.7 \times 10^{-11} & -1.7 \times 10^{-6} + 5.7 \times 10^{-7} & -1.6 \times 10^{-6} - 5.6 \times 10^{-7} & 0.46 + 7.1 \times 10^{-11} \\
-0.46 + 5.7 \times 10^{-2} & 3.6 \times 10^{-2} + 6.1 \times 10^{-3} & -1.6 \times 10^{-2} - 5.7 \times 10^{-3} & -0.46 - 5.7 \times 10^{-2} \\
-0.46 - 5.7 \times 10^{-2} & -1.6 \times 10^{-2} + 5.7 \times 10^{-3} & 3.7 \times 10^{-2} - 6.1 \times 10^{-3} & -0.46 + 5.7 \times 10^{-2} \\
0.54 - 4.7 \times 10^{-11} & 1.6 \times 10^{-6} - 5.6 \times 10^{-7} & 1.6 \times 10^{-6} + 5.6 \times 10^{-7} & 0.54 - 7.1 \times 10^{-11}
\end{pmatrix}. \tag{A.2}
\]

The normalization factors used for model 3 and model 4 are \( n_{c3} = 1.376 \) and \( n_{c4} = 1.376 \).

Following the 1-dilation process, the \( 4 \times 4 G'(t) \) [derived from corresponding \( G(t) \) divided by the \( n_c \) factor] is converted into a unitary \( 8 \times 8 U_G'(t) \). We show \( U_G3 \) and \( U_G4 \) in the form of heat maps in Fig. 4.

The unitary operation \( U_G'(t) \) is transpiled into a 3-qubit quantum circuit composed of three elementary quantum gates: \( R_Z \), \( \sqrt{X} \), and \( CX \), which have the matrix form:

\[
R_Z(\lambda) = \exp \left( -i \frac{\lambda}{2} Z \right) = \begin{pmatrix}
1 & 0 \\
0 & e^{i \frac{\lambda}{2}}
\end{pmatrix}, \tag{A.3}
\]

\[
\sqrt{X} = \frac{1}{2} \begin{pmatrix}
1 + i & 1 - i \\
1 - i & 1 + i
\end{pmatrix}, \tag{A.4}
\]

\[
CX \ q_0, q_1 = I \otimes |0\rangle \langle 0| + X \otimes |1\rangle \langle 1| = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 1 & 0 \otimes |0\rangle \\
0 & 1 \otimes |0\rangle
\end{pmatrix}. \tag{A.5}
\]

The full quantum circuits for \( U_{G3} \) and \( U_{G4} \) are shown in Fig. 5 and 7. The probability distribution of the projection measurement results of the two circuits are shown in Fig. 3. Both the QASM simulator results and the real machine simulated results are recorded.
A.2 Amplitude-damping model

In this section, we will show that the method of flattening the density matrix for dilation, which was outlined in the supplementary information in our previous publication [64], can be implemented on the quantum device for the simple amplitude damping model. The same method is verified by the implementation described in this and the following section. This verification allows us to confidently incorporate the general algorithm with GQME.

The general algorithm for open quantum system dynamics is applicable to the time-evolution of density matrices governed by Kraus operators [64]. The time-evolution representation for such open systems is given by \( \dot{\rho}(t) = \sum_k M_k(t)\dot{\rho}M_k^\dagger(t) \). For simplicity, the notation of time dependency is omitted hereafter for superoperators \( M \) and superoperators derived from it. In the first step, the density matrix is flattened to vector form: \( \dot{\rho} \rightarrow \mathbf{v}_\rho = \)
Figure 5: Probability distribution of the quantum state after the projection measurement applied to the circuit for $U_G^3$ and $U_G^4$ on the QASM and real quantum devices. The $|000\rangle$ state corresponds to the population squared of the donor state $\sigma_{DD}(t)$ and the $|100\rangle$ state corresponds to the population squared of the acceptor state $\sigma_{AA}(t)$. The last four states are ancilla states.

\[ (\rho_{11}, \ldots, \rho_{1n}, \rho_{21}, \ldots, \rho_{2n}, \ldots, \rho_{n1}, \ldots, \rho_{nn})^T. \]

We calculate the Frobenius norm of $v_\rho$ as $\|v_\rho\|_F = \sqrt{\sum_{ij} |\rho_{ij}|^2}$ and divide $v_\rho$ by $\|v_\rho\|_F$ to normalize $v_\rho$. Next, for every $k$, the $\mathcal{M}_k$ is transformed into $\tilde{\mathcal{M}}_k = \mathcal{M}_k \otimes I$; similarly, the $\mathcal{M}_k^\dagger$ is transformed into $\tilde{\mathcal{N}}_k = I \otimes \mathcal{M}_k$. The $\otimes$ stands for the Kronecker product and the bar over $\mathcal{M}_k$ indicates complex conjugation. The new equivalent form for the Kraus representation is:

\[ \mathcal{M}_k \hat{\rho} \mathcal{M}_k^\dagger \leftrightarrow \tilde{\mathcal{N}}_k \tilde{\mathcal{M}}_k v_\rho. \]
gates, we need two separate 2-dilations:
\[ \tilde{N}_k \tilde{M}_k v_\rho \xrightarrow{\text{unitary dilation}} U_{N_k} U_{M_k} (v_\rho^T, 0, ..., 0)^T. \]
\( A.7 \)

For \( M_k \) of dimension \( n \times n \), \( \tilde{M}_k \) and \( \tilde{N}_k \) are \( n^2 \times n^2 \) and consequently, the 2-dilations \( U_{M_k} \) and \( U_{N_k} \) are \( 3n^2 \times 3n^2 \). The \( U_{M_k} \) and \( U_{N_k} \) are fragmented into sequences of two-level unitary gates and tallied to compute the gate complexity. To realize \( \tilde{N}_k \tilde{M}_k v_\rho \), the total gate complexity is \( 3n^3 + n^2 \) for each \( k \). The classical complexity to realize \( \hat{M}_k \hat{\rho} \hat{M}_k^\dagger \) based on a naive algorithm is higher, though of same order as quantum algorithm, namely \( 4n^3 - 2n^2 \).

All the evolved density matrices in the circuit calculated at each timestep are obtained as the output vector \( v_k(t) = \tilde{N}_k \tilde{M}_k v_\rho \). The desired information to be collected from the density matrix is extracted by applying projection measurements on \( v_k(t) \) using an optical setup [103]. The detailed procedure for obtaining information located at both diagonal and off-diagonal elements of \( \hat{\rho}_k(t) \) from final \( v_k(t) \) is described in the supplementary information of Ref. [64].

### A.3 Simulation of the amplitude damping model with Kraus operators

We tested the theory mentioned in the previous section for spontaneous emission of a 2-level atom modeled by amplitude-channel damping. The corresponding Lindblad master equation is:
\[ \dot{\hat{\rho}}(t) = \gamma \left[ \sigma^+ \rho(t) \sigma^- - \frac{1}{2} \{ \sigma^- \sigma^+, \rho(t) \} \right], \]
where the spontaneous emission rate is \( \gamma = 1.52 \times 10^9 \text{ s}^{-1} \), and the \( \sigma^+ = |0\rangle \langle 1| \) and \( \sigma^- = (\sigma^+)^\dagger \) are Pauli raising and lowering operators, respectively. The density matrix \( \rho(t) \) in the Kraus representation is as follows:
\[
\begin{align*}
\hat{\rho}(t) &= M_0(t) \hat{\rho} M_0(t)^\dagger + M_1(t) \hat{\rho} M_1(t)^\dagger, \\
M_0(t) &= \frac{1 + \sqrt{1 - e^{-\gamma t}}}{2} \mathbb{I} + \frac{1 - \sqrt{1 - e^{-\gamma t}}}{2} \sigma_z = \left( \begin{array}{cc} 1 & 0 \\
0 & \sqrt{1 - e^{-\gamma t}} \end{array} \right), \\
M_1(t) &= \sqrt{1 - e^{-\gamma t}} \sigma^+ = \left( \begin{array}{cc} 0 & \sqrt{1 - e^{-\gamma t}} \\
0 & 0 \end{array} \right).
\end{align*}
\]
\( A.8 \)

For \( M_k \) of dimension \( 2 \times 2 \), \( \tilde{M}_k \), \( \tilde{N}_k \), and \( D_A \) are \( 4 \times 4 \) matrices, as given below in Eq. \( A.9 \). In this way, the 2-dilations \( U_{M_k} \) and \( U_{N_k} \) are \( 12 \times 12 \) following the \( k \)-dilation [64, [73]. Note that, though these superoperators are time dependent, only for simplicity we omitted the notation of time dependency. However, realization of the dilated matrices using quantum gate is of dimension of form \( 2^n \times 2^n \). We append the dilated matrix with an ancillary \( 12 \times 4 \) zero matrix on the right and \( 4 \times 12 \) at the bottom, and an \( 4 \times 4 \) identity matrix along the diagonal. The resulting dilated superoperator matrix is \( 16 \times 16 \), requiring 4 qubits for quantum implementation. Quantum implementation is accomplished with Qiskit as mentioned in the main text.
\[ \tilde{M}_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{e^{-\gamma t}} & 0 \\ 0 & 0 & 0 & \sqrt{e^{-\gamma t}} \end{pmatrix}, \quad \tilde{N}_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{e^{-\gamma t}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \sqrt{e^{-\gamma t}} \end{pmatrix}, \]
\[ \tilde{M}_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{1-e^{-\gamma t}} & 0 \\ 0 & 0 & 0 & \sqrt{1-e^{-\gamma t}} \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \tilde{N}_1 = \begin{pmatrix} 0 & 0 & \sqrt{1-e^{-\gamma t}} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{1-e^{-\gamma t}} \\ 0 & 0 & 0 & 0 \end{pmatrix}. \]

For an initial density \( \hat{\rho}(0) = \frac{1}{4} \begin{pmatrix} 1 & 1 \\ 1 & 3 \end{pmatrix} \), we calculate the populations in the basis \( \{ |0\rangle, |1\rangle \} \) from \( t = 0 \) to \( t = 1000 \) ps with a time step of 10 ps. With \( \| \hat{\rho} \|_{HS} = \frac{\sqrt{3}}{2} \), the input state is:
\[ \mathbf{v}_0 = \frac{1}{\| \hat{\rho} \|_{HS}} \begin{pmatrix} \mathbf{v}_\rho^T, \circ, \circ, \circ, \circ, \circ, \circ, \circ, \circ, \circ, \circ, \circ, \circ, \circ, \circ \end{pmatrix}^T = \frac{1}{2\sqrt{3}} \begin{pmatrix} 1, 1, 1, 3, 0, ..., 0 \end{pmatrix}^T, \]
where \( m = 12 \) for the vector \( \mathbf{v}_\rho^T \) to be of length 16. After extracting the output \( \mathbf{v}_k(t) \), the ground state and excited state populations are obtained as the first and fourth entry of the vector, respectively. The Fig. 8 result manifests the consistency with the result in Ref. 64.

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Figure 6: Transpiled quantum circuit of the dilated $U_{G_{3}}$ matrix at 1500 time steps for model 3. Each horizontal black line denotes a qubit. The $\sqrt{X}$ gate (blue square) is the square root of $X$ gate; the $R_z$ gate (magenta square) is the rotation $Z$ gate. The two-qubit gates are the controlled-NOT gate, where the dot denotes the controlled qubit and $\bigoplus$ denotes the target qubit. The black gates at the end of the circuit denote the projection measurements. The number of required $R_z$, $\sqrt{X}$, and CNOT gates are 153, 98, and 41, respectively.
Figure 7: Transpiled quantum circuit of the dilated $U_{g_4}$ matrix at 1500 time steps for model 4. Each horizontal black line denotes a qubit. The $\sqrt{X}$ gate (blue square) is the square root of $X$ gate; the $R_z$ gate (magenta square) is the rotation $Z$ gate. The two-qubit gates are the controlled-NOT gate, where the dot denotes the controlled qubit and $\bigoplus$ denotes the target qubit. The black gates at the end of the circuit denote the projection measurements. The number of required $R_z$, $\sqrt{X}$, and CNOT gates are 153, 98, and 41, respectively.
Figure 8: Population of ground state and excited state for the amplitude-damping model obtained by the quantum implementation on the IBM Qiskit simulator.