A quantum algorithm for solving open quantum system dynamics on quantum computers using noise

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In this paper we present a quantum algorithm that uses noise as a resource. The goal of the quantum algorithm is the calculation of operator averages of an open quantum system evolving in time. Selected low-noise system qubits and noisy bath qubits represent the system and the bath of the open quantum system. All incoherent qubit noise can be mapped to bath spectral functions. The form of the spectral functions can be tuned digitally, allowing for the time evolution of a wide range of open-system models at finite temperature. We study the feasibility of this approach with a focus on the solution of the spin-boson model and assume intrinsic qubit noise that is dominated by damping and dephasing. We find that classes of open quantum systems exist where the algorithm performs very well, even with gate errors as high as 1%. In general the quantum algorithm performs best if the system-bath interactions can be decomposed into native gates.

I. INTRODUCTION

Quantum computers promise a substantial speedup for solving certain types of numerical tasks, in particular the simulation of large quantum systems [1]. However, due to large error rates and short coherence times of present quantum computers [2], only small examples have been demonstrated. For useful near-term applications, there is a need for current research to be focused on more efficiently exploiting noisy intermediate-scale quantum (NISQ) computers. In this paper we present a quantum algorithm which in fact utilizes typical noise in NISQ devices by incorporating it into the computation itself.

Models for open quantum systems [3, 4] (short, open-system models) have been developed for efficient modeling of a small number of degrees of freedom, the system, interacting with a large environment, the bath. Accordingly, the use of an open-system model is often called the system-bath approach. The idea is that certain dynamical or steady-state properties of the system can be the key to understanding the overall behavior of the full system-environment pair. The bath can be modeled with less accuracy, e.g., it can be linear or non-interacting. One widely studied example is the energy transfer in photosynthesis [5], where a finite number of local excitations (excitons, the system) have dissipative interaction with vibrational modes of the large molecule (the bath), enabling the energy transfer. The effect of the bath on the system is described by a bath spectral function, which is a continuous function of frequency. The time evolution of the reduced density matrix of the system strongly depends on the form of the spectral function [6]. A system coupled to a bath with a smooth spectral function can be described by the well-known Lindblad master equation.

A quantum algorithm that time evolves an open-system model on a quantum computer must implement non-unitary gates in some way. These can be realized by introducing couplings to external qubits and performing additional measurements [7–15]. Most such approaches directly consider an open-system model that can be described by a Lindblad master equation. A time evolution under a Lindblad master equation can be implemented on a quantum computer using the same Trotterization approach known for closed quantum systems: the system is coupled to the external qubits at each Trotter step, which are measured and thus create non-unitary quantum operations. A technical challenge here is the reset of the external qubits after each Trotter step. Without access to a quantum feedback control, one solution is to implement the reset gates by utilizing intrinsic damping [8, 12, 16]. Other approaches to calculate Lindblad time-evolution on a quantum computer include the quantum imaginary time algorithm [17, 18]. Here the density matrix is represented by a pure state of qubits and the effect of non-unitary processes is calculated from operator expectation values.

However, the most efficient way to implement non-unitary gates on NISQ computers is to utilize intrinsic noise [10, 13, 19, 20]. By doing so, noise is no longer an impediment, but is rather a key component of the computation itself. Indeed, while quantum computers performing a Trotter time-evolution might involve many different gate operations, it is possible to derive a description of a noisy quantum computer in the form of an effective Lindblad master equation [21]. This effective Lindbladian description plays a central role in the quantum algorithm we present in this paper.

A limitation of noise-utilizing quantum algorithms has been that most previous work falls in the category of smooth spectral functions. Here, we present a new approach that supports a wide range of structured spectral functions. This opens the possibility to study significantly wider range of open quantum systems, e.g., systems at finite temperature.

In this paper, we describe how to establish a mapping between an open-system model and the effective Lindblad description of a noisy quantum computer. In this mapping, selected system qubits and bath qubits represent the system and the bath of the open quantum system. Significant variations in qubit coherence times may
appear in state-of-the-art quantum computers [22]. It is also typically possible during calibration to make some qubits better at the expense of others. For example, for the good qubits we can avoid problems like frequency crowding. In our work, we use this to our advantage, in particular, by using the lower quality qubits for mimicking the noise of a model bath. Even though the bath qubit time evolution is governed by the effective Lindblad master equation, corresponding to a smooth spectral function as seen by the bath qubits, it is the spectral function as seen by the system that can be made strongly structured and digitally tunable. We find that the mapping to arbitrary open-system models performs best when there is large asymmetry between the system- and the bath-qubit decoherence rates. However, for some specific classes of open system models, we find the especially interesting result that an arbitrary system-qubit noise may be included.

The performance of the proposed quantum algorithm is studied through numerical simulation on conventional computers. In particular, we study the quality of the results of the algorithm for a spin coupled to a bosonic resonance mode as well as to a bosonic ohmic bath. Here, we realize a mapping between the open-system model and the effective Lindbladian in the case of noiseless system-qubits. We also show the example of an electron-transport model by representing it through a generalized spin-boson model. Here, we map also the system-qubit noise to the model spectral function. Our central finding is that the quantum algorithm performs best if the system-bath interactions can be decomposed into native gates, such as the variable Mølmer-Sørensen (MS) gate or the variable iSWAP gate, i.e., XX or XX + YY Ising interactions. The restriction to native gates can, however, be lifted for some open-system models.

The paper is structured as follows. In Sec. II, we introduce the concrete open system model whose noise-utilizing quantum algorithm will be studied later. In Sec. III, we present the protocol of the bath mapping, i.e., the mapping between an open-system model and a noisy-algorithm model. In Sec. IV, we show three practical examples of solving open-system dynamics using the quantum algorithm. The examples were implemented using numerical simulations on conventional computers. The conclusions and discussion are given in Sec. V. Many important details of our approach are left to be presented in the Appendix. In Appendix A, we generalize the approach to cover also multi-spin systems. In Appendix B, we introduce the noisy-algorithm model, which describes a noisy quantum computer performing Trotterized time evolution. In Appendix C, we discuss key principles of a quantum circuit optimization, which is needed for a successful mapping between an open-system model and a noisy-algorithm model. In Appendix D, we quantify the main errors sources in our approach. Finally, in Appendix E, we show how to map a fermionic open-system model to a generalized spin-boson model.

II. OPEN-SYSTEM MODEL

While the plethora of physical phenomenon encountered in nature naturally correspond to a wide range of potential open system models, we focus here on one concrete model of a specific form. In particular, in its most general form, the open-system Hamiltonian we consider can be written

\[ \hat{H}_0 = \hat{H}_S + \hat{H}_B + \hat{H}_C, \]  

where \( \hat{H}_S \) is the Hamiltonian of the system, \( \hat{H}_B \) of the bath, and \( \hat{H}_C \) describes their coupling.

In this work, we explicitly consider problems that can be represented as a two-state system interacting with a bosonic bath [6], i.e., the spin-boson model,

\[
\begin{align*}
\hat{H}_S &= \frac{\hbar \Delta}{2} \hat{\sigma}_z, \\
\hat{H}_B &= \sum_k \hbar \omega_k \hat{b}_k \hat{b}_k^\dagger, \\
\hat{H}_C &= \hat{\sigma}_z \sum_k v_k \left( \hat{b}_k + \hat{b}_k^\dagger \right).
\end{align*}
\]

The model system consists of a single spin which has an energy-level splitting \( \hbar \Delta \). The model bath consists of bosonic modes \( k \) with natural frequencies \( \omega_k \). The boson creation and annihilation operators satisfy \( [\hat{b}_k, \hat{b}_k^\dagger] = \delta_{kl} \). The coupling between the system and bath is here chosen to be transverse [23] and occurs via linear bath operators

\[ \hat{X} = \sum_k v_k (\hat{b}_k + \hat{b}_k^\dagger). \]

In this open-system model the couplings \( v_k \) are real numbers (possible phases were absorbed in the definition of bosonic operators). A generalization to the multi-spin case is presented in Appendix A.

The effect of the bath on the system is fully determined by a bath spectral function. This also plays a central role in the bath mapping presented in this paper. The spectral function is defined as

\[ S(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \hat{X}(t)\hat{X}(0) \rangle_0, \]  

where the index 0 refers to an average according to a free evolution of the bath. In thermal equilibrium we have

\[ S(\omega) = 2\pi \sum_k \frac{v_k^2 |\delta(\omega - \omega_k)|}{1 - \exp(-\frac{\omega_k}{k_B T})} \text{sign}(\omega). \]  

The spectral function is characterized by two essential properties: the temperature \( T \), as well as its overall functional form. The temperature controls the symmetry between the positive (photon absorption by the bath) and negative (photon emission by the bath) frequencies. The
functional form of the spectral function is important in the sense that it is not a constant, i.e., it does not correspond to white noise. In particular, this implies that the bath has a memory, i.e., it is non-Markovian.

The wide applicability of the spin-boson theory is based on the fact that the bath described by $\hat{H}_B$ does not necessarily need to consist microscopically of bosonic modes, but need only be effectively Gaussian. For example, if the coupling with a bath is mediated by some operator $\hat{F}$ which is quadratic in fermion operators, then this coupling operator can be replaced by a linear bosonic operator $\hat{X}$ of a bosonic model bath, if the statistics of $\hat{F}$ are (to a good approximation) Gaussian and the spectral functions match. This example is discussed more detailed in Appendix E.

III. BATH MAPPING

At the center of our approach is the mapping between an open-system model and a noisy-algorithm model. The noisy-algorithm model describes a quantum computer performing Trotterized time evolution [21]. In the mapping, the open-system model is coarse grained to a spin model with Hamiltonian $\hat{H}$ and additional spin broadening. On the quantum computer, the spins are represented by qubits and a Trotterized time evolution corresponding to $\hat{H}$ is being performed. The combined effect of unitary gates and non-unitary qubit noise is described by the effective Lindbladian $\mathcal{L}_{\text{eff}}$. The form of this Lindbladian depends on the chosen gate decomposition. The form can be optimized by following certain decomposition strategies (Appendix C). The spin broadenings and the broadening described by $\mathcal{L}_{\text{eff}}$ are set equal by a correct choice of the Trotter time step $\tau$. This bath-mapping protocol is visualized in Fig. 1. The full self-consistent procedure has three main parts and is described in more detail below.

A. Coarse graining the spectral function

In the first part, we reduce the (infinite) number of bath modes to $n$ auxiliary boson modes with broadenings $\kappa_i$. Practically, in this step, we fit the target spectral function by $n$ Lorentz functions (Lorentzians). The broadenings can be interpret as a coupling between the auxiliary modes and an external smooth environment. In the fitting, the relative sizes of $\kappa_i$ are fixed so that they correspond to broadenings as implied by the noisy-algorithm model $\mathcal{L}_{\text{eff}}$ (Sec. III C).

1. Coarse-graining scheme I: only the bath modes couple to the environment

In this commonly applied coarse-graining scheme, the target spectral function, Eq. (7), is fitted by

$$S(\omega) = \sum_{i=1}^{n} \frac{v_i^2 \kappa_i}{(\kappa_i/2)^2 + (\omega - \omega_i)^2},$$

where $\kappa_i = \kappa$, or to have relative variations as given by $\mathcal{L}_{\text{eff}}$. Note that the fitting values for frequencies $\hbar \omega_i$ are allowed to be also negative.

The couplings and frequencies obtained in the fitting establish the coarse-grained Hamiltonian

$$\hat{H} = \hat{H}_S + \hat{\sigma}_x \sum_{i=1}^{n} \frac{v_i}{2} (\hat{b}_i + \hat{b}_i^\dagger) + \sum_{i=1}^{n} \hbar \omega_i \hat{b}_i^\dagger \hat{b}_i,$$

and the mode broadenings correspond to damping in the Lindblad master equation

$$\dot{\hat{\rho}} = \frac{i}{\hbar} [\hat{\rho}, \hat{H}] + \sum_{i=1}^{n} \kappa_i \left( \hat{b}_i \hat{b}_i^\dagger \hat{\rho} - \frac{1}{2} \{ \hat{b}_i^\dagger \hat{b}_i, \hat{\rho} \} \right),$$

where $\hat{\rho}$ is the density matrix of the spin and the auxiliary boson modes. This master-equation is equivalent with a spin-boson model and spectral function (8).

Similar coarse graining approaches have been applied earlier, for example, in the context of Lindbladian description of non-Markovian baths [24–29] and analog quantum simulation [23, 30–32]. This approach is also closely related to the approach of hierarchical equations of motion [33–35].

2. Coarse-graining scheme II: the noisy system qubit

The fitting process can also account for decoherence of a qubit representing the spin. The decoherence of this system qubit contributes via a background rate in the spectral function. Here, we instead optimize the spectral function

$$S(\omega) = \sum_{i=1}^{n} \frac{v_i^2 \kappa_i}{(\kappa_i/2)^2 + (\omega - \omega_i)^2} + 4\hbar^2 \kappa_{\text{system}},$$

where the ratio between the system noise and the bath broadening is fixed to certain constant ratio,

$$r = \frac{n \kappa_{\text{system}}}{\sum_{i=1}^{n} \kappa_i}.$$

This ratio is defined by the hardware properties and the used algorithm. For example, if the system and bath
FIG. 1: Mapping between an open-system model and the noisy-algorithm model. As described in the main text, the open-system model $\hat{H}_0$ is coarse grained to an auxiliary-spin model $\hat{H}$ and additional spin broadening. A quantum algorithm time evolves the qubits describing the spins according to $\hat{H}$. The combined effect of unitary gates and non-unitary qubit noise is described by the effective Lindbladian $L_{\text{eff}}$, including effective noise. The auxiliary-spin broadening and the broadening described by $L_{\text{eff}}$ are set equal by a correct choice of the Trotter time step.

$qubits$ will have equal decoherence rates, we will most probably have $r = 1$ or $r = 1/2$ (the latter if a system-qubit noise symmetrization algorithm is applied, see Appendix C).

This spectral function corresponds to a time-evolution described by the master equation

$$\dot{\rho} = \frac{i}{\hbar}[\rho, \hat{H}] + \sum_{i=1}^{n} \kappa_i \left( \hat{b}_i \rho \hat{b}_i^\dagger - \frac{1}{2} \left\{ \hat{b}_i^\dagger \hat{b}_i, \rho \right\} \right) + \kappa_{\text{system}} (\hat{\sigma}_x \rho \hat{\sigma}_x - \rho) .$$

The difference is the term proportional to $\kappa_{\text{system}}$. We see that the system operator is here $\hat{\sigma}_x$. This means that this coarse-graining scheme is exact when the system-qubit noise operator is $\hat{\sigma}_x$. Note that by redefining the spin-boson model coupling to be longitudinal, the system-qubit noise operator would be $\sigma_z$, corresponding dephasing. An exact mapping in the case of all qubits being subject to damping is demonstrated in Sec. IV C. The fitting in these two different schemes is illustrated in Fig. 2.

B. Representing auxiliary bosons by auxiliary spins

In the second part, we represent auxiliary boson modes by auxiliary spins. Common "digital" encodings [36] cannot be applied, since they do not map damping of an arbitrary auxiliary spin to single-boson annihilation, which is the key correspondence in our algorithm. Instead, we replace bosonic energy operators $\hat{b}_i^\dagger \hat{b}_i$ by spin operators $\hat{\sigma}_i^z / 2$ and bosonic coupling operators $\hat{b}_i + \hat{b}_i^\dagger$ by spin operators $\hat{\sigma}_i^x$. The spectral function, Eq. (8) or (11), keeps its form, with the summation performed now over the corresponding auxiliary-spin parameters. There is no strict rule how the auxiliary-boson and auxiliary-spin parameters should be exactly related. Two possible approaches are discussed below.

Perhaps the clearest approach is to represent each auxiliary boson mode $i$ by $N_i$ identical spins. This allows to keep the spectral function unchanged with a clear control of the bath Gaussianity (through varying $N_i$). This approach can be applied if the bath qubits have similar
FIG. 3: Principles of two different approaches for representing auxiliary-bosons by auxiliary spins (and later finally by bath qubits). (a) The coarse-grained spin-boson model includes a spin coupled to one auxiliary boson mode. The auxiliary boson mode is chosen to be represented by $N = 2$ identical auxiliary spins. The new couplings are down-scaled by a factor $\frac{1}{\sqrt{N}}$ in order to keep the total spectral weight unchanged. We also demand $\kappa = \gamma^*$, where the effective spin broadening is a sum of damping and dephasing rates, $\gamma^* = \gamma + 2\Gamma$. This mapping approach can be applied if the bath qubits representing the auxiliary spins have uniform decoherence rates. (b) An approach that can be applied when the bath qubits have significantly different decoherence rates. Here one imposes one-to-one correspondence between the boson modes and the auxiliary spins. For auxiliary spins the spectral-peak broadening can be theoretically not only due to damping rate $\gamma$ but also partly due to dephasing rate $\Gamma$,

$$\kappa = \gamma^*, \quad (17)$$

where the total spin broadening is defined as

$$\gamma^* \equiv \gamma + 2\Gamma. \quad (18)$$

The corresponding master equation has the form (assuming identical damping and dephasing rates)

$$\dot{\rho} = \frac{i}{\hbar}[\rho, \hat{H}] + \sum_{i=1}^{n} \sum_{j=1}^{N_i} \gamma \left( \hat{\sigma}_+^{i,j} \hat{\rho} \hat{\sigma}_-^{i,j} - \frac{1}{2} \left\{ \hat{\sigma}_+^{i,j} \hat{\sigma}_-^{i,j}, \rho \right\} \right) + \sum_{i=1}^{n} \sum_{j=1}^{N_i} \frac{\Gamma}{2} \left( \hat{\sigma}_z^{i,j} \hat{\rho} \hat{\sigma}_z^{i,j} - \rho \right), \quad (19)$$

This property is important since it allows for connecting an open-system model to a quantum computer with bath-qubit damping as well as dephasing.

It should be noted that broadening due to dephasing alone does not lead to Gaussian equilibrium statistics: a finite damping rate $\gamma$ is needed. This is because bath time-correlations that describe non-bosonic statistics decay according to $\gamma/2$ instead of $\gamma/2 + \Gamma$. A slow decay of non-Gaussian elements can however always be compensated by an increase in the bath-spin number $N_i$. If differences in the bath-qubit decoherence rates are large, it may be better if one imposes one-to-one correspondence between the auxiliary-boson modes and the auxiliary spins, i.e., fixes $N_i = 1$. In the coarse graining, Sec. III A, one accounts for the relative variations of the mode broadenings as implied by the noise given by $\mathcal{L}_{\text{eff}}$. The Gaussianity can be improved by letting the spectral peaks overlap. These two different approaches are visualized in Fig. 3.
C. Matching auxiliary-spin broadening to effective noise of $\mathcal{L}_{\text{eff}}$

In this third part of the bath-mapping protocol, we match the auxiliary-spin broadening to the effective qubit noise given by $\mathcal{L}_{\text{eff}}$. This step should be done self-consistently with the coarse graining, Sec. III A, since variations in the effective noise of different bath qubits must appear as corresponding variations in the auxiliary mode broadenings $\kappa_i$.

Central here is the noisy-algorithm model [21] (Appendix B), which represents the effect of the noise during Trotterized time-evolution in the form of an effective Lindbladian $\mathcal{L}_{\text{eff}}$.

\[
\dot{\rho} = \mathcal{L}_{\text{eff}}[\rho] \equiv \frac{i}{\hbar} [\rho, \hat{H}] + \sum_{ij} R_{ij} \left( \hat{A}_i \hat{\rho} \hat{A}_j^\dagger - \frac{1}{2} \{ \hat{A}_j^\dagger \hat{A}_i, \hat{\rho} \} \right),
\]

where $\dot{\rho}$ is now identified as the density matrix of the system and auxiliary spins. The form of the rate matrix $R$ is determined not only by the physical noise but also by the circuit decomposition. The operators $\hat{A}_i$ can be multi-qubit Pauli operators. Importantly, the operator form and the rates are not dependent on the parameters of the Hamiltonian $\hat{H}$, such as the couplings $\kappa_i$ or frequencies $\omega_i$. From this it follows that the demanded self-consistency with coarse graining does not lead to a self-consistency loop, but rather to a single fixation of correct relative values of broadenings $\kappa_i$ used in Sec. III A.

In this paper we assume that the physical as well as the effective noise is dominated by qubit (or auxiliary spin) damping and dephasing. Such physical qubit noise is typical for superconducting architectures [37]. The form of the effective noise may stay the same (as the form of the physical noise) by optimal choice of gate decompositions, which is discussed more detailed in Appendix C. Ultimately, the assumption of similar noise models can be verified by numerical studies, as is done in Sec. IV.

The noisy-algorithm model gives the effective auxiliary spin damping and dephasing rates [21]

\[
\gamma_i = \frac{D t_G \tilde{\gamma}_i}{\tau}, \quad \Gamma_i = \frac{D t_G \tilde{\Gamma}_i}{\tau}.
\]

Here $\tau$ is the Trotter time step, $D$ the circuit depth, $t_G$ the physical time needed to perform one gate (assumed here to be a constant), and $\tilde{\gamma}_i$ and $\tilde{\Gamma}_i$ the physical damping and dephasing rates of the qubit representing the auxiliary spin $i$. We also assume (without losing generality) that the errors are similar for every gate and that they act also on idling qubits. In the following, we also assume that all bath qubits have the same damping and dephasing rates. The contribution from finite system qubit noise is analogous.

Eqs. (21-22) with Eqs. (17-18) let us to identify the correct Trotter time step to be used in the quantum algorithm,

\[
\tau = \frac{D \epsilon}{\kappa}.
\]

Here we have defined the gate error

\[
\epsilon \equiv t_G (\bar{\gamma} + 2 \bar{\Gamma}).
\]

In terms of qubit decay and pure dephasing times, $T_1 = 1/\bar{\gamma}$ and $T_2^* = 1/\bar{\Gamma}$, the gate error is defined equivalently

\[
\epsilon = t_G \left( \frac{1}{T_1} + \frac{2}{T_2^*} \right).
\]

Since the size of all terms of the normalized Hamiltonian $\hat{H}/\kappa$ are known, Eq. (23) indeed fixes the angles of $\exp (-i\hat{H}\tau)$, i.e., the angles of the unitary gates in the Trotterization of the time-evolution operator over simulation time $t = m \tau$.

IV. EXAMPLES

In this section we present examples of solving open-system dynamics using the quantum algorithm. We solve dynamics for three different open system models and study the quality by comparing to exact or approximate solutions derived in literature. We also study the use of different gate decompositions and give estimates for the corresponding upper limits of the gate errors needed to time-evolve the models on quantum computers with the same accuracy. The shown numerical results for the Trotterized time evolution with noise were obtained using qoqo [38] with QuEST [39] as the simulator backend.

In Sec. IV A, we study the relaxation dynamics of a spin ultra-strongly coupled to a resonator mode with broadening. In Sec. IV B, we study a spin coupled to an ohmic bath. In these examples we assume an access to a quantum computer with a noiseless system qubit. In Sec. IV C, we study the steady state and relaxation dynamics of strongly interacting electrons hopping between an island and leads. In this example the system qubit is allowed to be noisy, too.

A. Spin ultra-strongly coupled to a resonance mode with broadening

Here we study the case of a bath with a resonance frequency. We assume a Lorentzian spectral function, which can be coarse grained exactly by single auxiliary boson mode. The coarse-grained open-system model has the Hamiltonian

\[
\hat{H} = \frac{\hbar \Delta}{2} \hat{\sigma}_z + \frac{v}{2} \hat{\sigma}_z (\hat{b} + \hat{b}^\dagger) + \hbar \omega_0 \hat{b}^\dagger \hat{b}.
\]
We consider the case of ultra-strong coupling, \( v = \omega_0 \sim \Delta \), and \( \kappa = v/2 \), which leads to clear non-Markovian dynamics.

In the mapping, the auxiliary boson mode is replaced by \( N \) identical auxiliary spins, see Sec. III. On the quantum computer, the auxiliary spins are represented by bath qubits with identical damping and dephasing rates, \( \gamma \) and \( \Gamma \). We also set \( \tilde{\gamma} = 2\Gamma \), or equivalently \( \tilde{T}_1 = T_2^* / 2 \).

The time evolution is realized by a Trotter expansion of the time-evolution operator \( \exp \left( -iH\tau \right)^m \), with total simulated time \( t = m\tau \). The Trotter time step \( \tau \) is given by Eq. (23). Its size is proportional to the circuit depth \( D \) and the gate error \( \epsilon \).

In Fig. 4, we show the time evolution of the expectation value \( \langle \hat{\sigma}_x(t) \rangle \) when the system-spin is set initially to \( +1 \) eigenstate of \( \hat{\sigma}_x \) and when the bath is initially at equilibrium. In Fig. 4(a), we compare the solutions obtained when using different number of bath qubits \( N \) (or equivalently auxiliary spins) to the numerically exact solution of the bosonic open-system model. The time evolution on the quantum computer is done using variable MS two-qubit gates and we consider the spin-splitting \( \Delta = 0.9\omega_0 \). We find that the difference to the correct solution decreases with increasing \( N \). This demonstrates that the mapping between the auxiliary boson mode and the bath qubits works: the spectral functions match for all bath-qubit numbers \( N \), but the bath becomes (to a good approximation) Gaussian only after multiple qubits are used to represent the boson mode. The exact number depends on the parameters of the Hamiltonian: for weak-coupling \( N = 1 \) would be adequate. The Trotter step used here for all \( N \) is \( v\tau = 0.18 \) which corresponds for \( N = 8 \) and \( D = 1 + N \) to a gate error of 1%, as defined in Eqs. (24-25). We keep the Trotter step constant for all \( N \) in order to have changes only from the bath Gaussianity error (not from the Trotter error). For \( N = 2 \) the gate error used in the simulation is then as high as 3%.

The variable MS two-qubit gate is a native gate of the XX-interaction. The XX-interaction is needed for a time evolution according to the Hamiltonian (16). Native gates keep the physical and effective noise models equivalent [21] and thereby for the variable MS decomposition the effective noise of \( \mathcal{L}_{\text{eff}} \) is also bath-qubit damping and dephasing. In Fig. 4(b), we study the use of non-native gate decompositions. We show results for two CNOT-decompositions with restricting us to the case of \( N = 8 \) bath qubits. The optimal decomposition with CNOT (Appendix C) consists here of a CNOT, a small-angle X-rotation, and another CNOT. There are two versions of this circuit: either the bath qubits being the control qubits (CNOT-B) or the system qubit being the control qubit (CNOT-S). The results differ since the CNOT operation as well as the noise properties are asymmetric with exchanging the system and the bath.

In Fig. 4(b), we find only a small difference between the CNOT-B and the correct open-system model result. The variable MS decomposition result is not plotted since it is practically indistinguishable from the CNOT-B result on the shown scale. This is a rather unexpected result. It can indeed be derived analytically that differences in the noise models appear only when individual bath qubits become strongly populated, which is not the case here since \( N \gg 1 \). This remains true also for control-Z decompositions. The derivation of the effective noisy algorithm model is given in Appendix B.
In the case of CNOT-S, we however find a noticeable difference, which implies significant changes in $L_{\text{eff}}$. It can be shown that it has here the approximate form

$$\dot{\rho} = L_{\text{eff}}[\rho] = \frac{i}{\hbar}[\rho, \hat{H}] + \sum_{j=1}^{N} \gamma \left( \hat{a}^{\dagger} \hat{a} \rho - \frac{1}{2} \left\{ \hat{a}^{\dagger} \rho \hat{a}, \rho \right\} \right) + \sum_{j=1}^{N} \Gamma \left( \hat{a} \rho \hat{a} - \rho \right) + \frac{\tilde{\Gamma}}{2} \left( \hat{a} \rho \hat{a} - \rho \right).$$

The last term on the right-hand side is additional and describes system-qubit dephasing with rate $\tilde{\Gamma}$. This emerges even though the physical system-qubit is noiseless. In Fig. 4(b), we do comparison also to an open-system model, where the physical bath component is added as an additional coupling term $H_{B} = \hat{a} \sum_{j=1}^{N} v_{j} (\hat{a}^{\dagger} + \hat{a}) / 2$, where operators $\hat{a}$ describe an additional bosonic bath. Equivalently, it adds another (independent) spectral function to the open-system model with a constant value $S_{a}(\omega) = 2\hbar^{2} \tilde{\Gamma}$. We find that the differences in the quantum-algorithm results indeed map to such alternation in the original spin-boson problem. We have then recovered the open-system model the quantum computer is effectively simulating. This result is general: changes in the noisy algorithm model can be always interpret as changes in the actually time-evolved open-system model [21].

In Fig. 4(c), we show a Fourier analysis of the time-evolution dynamics. Here we use a spin-splitting $\Delta = \omega_{0}$ and a variable MS decomposition. The correct result, i.e. the open-system model result, shows a splitting of a resonance, located originally at $\omega_{0}$, to frequencies $\omega_{0} \pm \nu / 2$. This is reproduced very well by the quantum algorithm with the bath-qubit number $N = 8$ and Trotter step $\nu \tau = 0.18$. We also show the result for a very large Trotter step, $\nu \tau = 1.0$ and the bath-qubit number $N = 8$, corresponding to gate error $\epsilon = 5.6\%$. We find somewhat unexpectedly that this result is clearly closer to the correct result than the one with a small bath-qubit number and a small Trotter step, $N = 1$, $\nu \tau = 0.18$, corresponding to gate error 4.5%. This result is specific for the case of ultra-strong coupling where the overall bath population can be large. A general error tradeoff in the quantum algorithm is discussed more in Appendix D.

**B. Spin coupled to an ohmic bath**

The case of an ohmic bath emerges in many areas of physics and is perhaps the most well-known showcase of the spin-boson model. It highlights how the system-bath dynamics can drastically change with the interaction strength. The interaction is characterized by the so-called the Kondo parameter $\alpha$ as well as the temperature. In a rough overall picture [6], for $\alpha \ll 1$ and at low temperatures the excited system shows damped oscillations, whereas for higher $\alpha$ the dynamics transform from strong damping to incoherent relaxation. For $\alpha > 1$ the system relaxes with a very small rate (temperature $T > 0$) or not at all ($T = 0$). Below, we study how well this transition is reproduced when time-evolving the dynamics using the presented quantum algorithm.

Following [40], we consider an ohmic spectral function of the form,

$$S(\omega) = \frac{4 \pi \hbar^{2} \alpha \omega}{1 - \exp \left( -\frac{\omega}{\tilde{\Gamma}} \right)},$$

and a cutoff function $\exp (-|\nu| / \omega_{c})$. We choose $\hbar \omega_{c} T / \Delta = 1.5$ and $\omega_{c} / \Delta = 10$, where $\Delta$ is the spin splitting. The coarse graining is done by eight auxiliary boson-modes with a constriction to identical broadenings $\kappa_{i} = \kappa$. The result is shown in Fig. 6. The varying of $\alpha$ is done by changing the couplings $v_{i}$ accordingly, $v_{i} \propto \sqrt{\alpha}$. Each of the auxiliary boson modes is represented by one auxiliary spin. When time evolving on the quantum computer, we assume the corresponding bath qubits are subjected to damping.

The quantum algorithm for the ohmic bath is of the same form as for the resonant bath considered in Sec. IV A. The difference is that for the ohmic case the auxiliary spin parameters are not identical. However, the conclusion made for the use of different gate decompositions are valid here as well.

In Fig. 5, we show the time evolution of $\langle \hat{\sigma}_{x}(t) \rangle$ when the system-spin is set initially to the $+1$ eigenstate of $\hat{\sigma}_{x}$ and when the bath is initially at equilibrium. We show the resulting dissipative dynamics for weak, intermediate, and strong coupling limits, corresponding to $\alpha = 0.02, 0.1, 1.0$. We compare the quantum algorithm results to the so-called NIBA (non-interacting blip approximation) calculation of the spin dynamics [6, 40]. We perform this calculation for the original ohmic spectral function as well as for the coarse-grained spectral function. Since a noticeable difference appeared only for strong couplings, the latter result is shown only for $\alpha = 1.0$. The quantum algorithm uses the variable MS decomposition. We find that the celebrated transition, from a weak-to-strong damping and finally to a slow decay, is reproduced well by the quantum algorithm. We find a good agreement with the NIBA even though each of the auxiliary boson modes is represented by only one auxiliary spin. A difference to the NIBA emerges only for large $\alpha$. This difference is due to a combination of imperfect fitting (see the result for the NIBA with the coarse-grained bath) and elevated bath-qubit populations at low-frequencies. The accuracy of the quantum algorithm can be improved by using more auxiliary modes in the coarse graining.

The results are obtained with the Trotter step $\Delta \tau = 0.1$ and gate error $\epsilon = 0.3\%$. The need for a low gate error is due to reduced individual broadenings of the bath modes (the fitting value for $\kappa = 0.25 \Delta$) and the wide spread of relevant frequencies when $\alpha = 1$. However, good quality results can be obtained for the cases $\alpha = 0.02$ and $\alpha = 0.1$ also with significantly higher gate.
errors, since here the width of the relevant bath frequencies, for a fixed $\Delta$, is much narrower.

C. Electronic transport

In this example we time evolve open system dynamics according to a generalized spin-boson model that can describe electronic transport across metallic islands or quantum dots. This model is also interesting since it allows for mapping system-qubit damping to the coarse-grained spectral function exactly. The Hamiltonian $H_0 = H_s + H_B + H_C$ has the form

$$
\begin{align*}
\hat{H}_S &= \frac{\hbar \Delta_z}{2} \hat{\sigma}_z \\
\hat{H}_B &= \sum_k \hbar \omega_k \hat{a}_k^\dagger \hat{a}_k + \sum_k \hbar \omega_k \hat{b}_k^\dagger \hat{b}_k \\
\hat{H}_C &= \hat{\sigma}_x \sum_k \frac{\nu_k}{2} \left( \hat{a}_k + \hat{a}_k^\dagger \right) + \hat{\sigma}_y \sum_k \frac{\nu_k}{2} \left( \hat{b}_k + \hat{b}_k^\dagger \right).
\end{align*}
$$

The model bath has two sets of bosonic modes, described by the bosonic operators $\hat{a}$ and $\hat{b}$, coupled to the system via operators $\hat{\sigma}_x$ and $\hat{\sigma}_y$. The spectral functions of individual components are defined similarly as before, Eq. (7), and are here identical, $S_a(\omega) = S_b(\omega) \equiv S(\omega)$. An example of an open quantum system that can be modeled with this Hamiltonian is a single-electron transistor [41]. For strongly interacting electrons only two island-charge states are relevant and the island charge reduces to a two-state system. The gate voltage of the transistor translates into the energy-level splitting $\Delta$ and the average island charge into the average excitation number $\langle \hat{\sigma}_+ \hat{\sigma}_- \rangle$. The source-drain bias is assumed to be here zero. The derivation of this Hamiltonian and the corresponding spectral function is presented in Appendix E.

We consider now a spectral function $S(\omega)$ that is ohmic at low frequencies and has resonances at $\omega_0$ and $2\omega_0$ (Appendix E). The spectral function satisfies the detailed balance $S(-\omega)/S(\omega) = \exp(-\hbar \omega/k_B T)$ with the temperature $k_B T = 0.3 \hbar \omega_0$. In Fig. 7(a), we show the result of coarse graining this spectral function by two auxiliary boson modes. Each auxiliary boson mode is represented by
(a) Coarse-graining scheme I

(b) Steady-state island charge

(c) Spectrum of $\langle \sigma_x(t) \rangle$

(d) Coarse-graining scheme II

(e) Steady-state island charge

(f) Spectrum of $\langle \sigma_y(t) \rangle$

FIG. 7: The steady-state and open-system dynamics of a single-electron transistor solved using the quantum algorithm and a comparison to a numerical solution obtained by a method presented in Ref. [41] (referred as OSM). We vary the gate voltage and set the source-drain bias to zero. The quantum algorithm is done with variable MS gate decomposition assuming $\varepsilon = 1\%$ gate error. (a) The coarse graining of the resonant spectral function by two auxiliary boson modes assuming identical mode broadenings $\kappa$. (b) A comparison between the solutions for the steady-state island charge. We calculate the OSM solution for the original spectral function as well as for the coarse-grained spectral function. A difference appears at high gate voltages due to an increased effective temperature of the coarse-grained bath at high energies. (c) A Fourier transformation of the charge relaxation dynamics when initially setting the island charge to +1 eigenstate of $\hat{\sigma}_x$. A peak tripling with broadening appears in the vicinity of the bath resonances at $\omega_0$ and $2\omega_0$. (d) Coarse graining the spectral function in the presence of system-qubit noise. (e) In the presence of the system-qubit noise, a difference to the original open-system model result appears at all gate voltages due to an increased effective temperature of the coarse-grained bath at all energies. The quantum algorithm result and the OSM result for the coarse-grained bath however stay similar. (f) With the system noise, an additional broadening appears in the spectral structure but the key characteristics remain similar to (c). The spectrum is normalized to the maximum of (c).

In Fig. 7(b), we show the obtained steady-state value for the island charge $\langle \hat{\sigma}_+ \hat{\sigma}_- \rangle$ as a function of the energy-level splitting $\Delta$ (gate voltage). The quantum algorithm solution corresponds to variable MS decomposition (Appendix E) with the Trotter step $\omega_0 \tau = 0.13$. The fitting value of the mode with is $\kappa = 0.7\omega_0$. The bath qubits are subjected to damping with a gate error of 1%. We do a comparison to an open-system model solution obtained by applying the numerical method developed in Ref. [41]. We again apply the reference method to the original spectral function as well as to the coarse-grained spectral function. The shown classical solution is the result in the limit $\alpha = 0$ and corresponds to the fermi function. We find a good agreement between the quantum algorithm result and the approximate open-system model solution. In particular, all different results (expect the classical one) are practically identical when the bias $\Delta/h$ is at the well-fitted spectral-function region. For larger $|\Delta/h|$, differences appear due to imperfect coarse graining. However, importantly, the results for the same spectral functions stay practically identical. The coarse-grained spectral function can be interpret to describe a non-equilibrium bath, with elevated temperature at higher energies.

In Fig. 7(c), we study the dynamical behavior of the island charge. We set the island charge initially to symmetric superposition, i.e., to +1 eigenstate of $\hat{\sigma}_x$, and the bath at equilibrium. We present the resulting behavior of the expectation value $\langle \hat{\sigma}_x(t) \rangle$ in the frequency space. We see that when being far from resonances $\Delta = \omega_0$ or $\Delta = 2\omega_0$, a narrow peak appears at frequency $\omega \approx \Delta$, describing coherent phase oscillations between the charge states with exponential decay of the coherence. Closer to the bath resonances, the peak shows strong broadening as...
well as splitting into a triplet. This implies a hybridization of the system and bath states in this region. We then find that even when the steady-state of the island charge, Fig. 7(b), shows a rather smooth behavior as a function of level-splitting $\Delta$, the underlying system-bath interaction can be strongly non-Markovian and can be revealed by non-equilibrium dynamics.

Next we redo the same computations but let the system qubit also be noisy: all qubits are subject to damping with the same rate. Using the approach introduced in Sec. III A 2, we account for the system noise on the level of the coarse graining as a background rate $\kappa_{\text{system}}$. At the same time, in the quantum algorithm, X-gates are introduced between the Trotter circuits in order to transform damping to a sum of X-noise and Y-noise, see Appendix C. This makes the correspondence between the system noise and a background in the spectral function exact. The circuit depth $D$ increases from $1 + 2n_q$ to $4 + 4n_q$, where $n_q$ is the total number of bath qubits. We insert $\kappa_{\text{system}} = \kappa/2$ to Eq. (11). The result of the fitting with this constriction is shown in Fig. 7(d). The obtained optimal mode broadening is here $\kappa = 0.55\omega_0$ and assuming again a gate error of 1%, the changes in the circuit depth and mode broadening need to be compensated by an increase in the Trotter step, Eq. (23), which becomes now $\omega_0\tau = 0.36$.

In Fig. 7(e), we show the steady-state value for the island charge. We see that a difference to the original open-system model solution emerges. However, most importantly, the results for the same spectral functions stay again almost identical. This confirms that the system-qubit noise can indeed be mapped to the spectral function of the open-system model. The new (coarse-grained) spectral function corresponds to a bath with elevated temperature. Furthermore, in Fig. 7(f), we find that the corresponding dynamical behavior still has the same key characteristics as the result obtained with the noiseless system qubit, Fig. 7(c). This highlights that dynamics of open quantum systems with a structured bath can be solved using the presented quantum algorithm also in the presence of strong system-qubit noise.

V. DISCUSSION

In this paper we have presented a new framework for noise-utilizing quantum simulations. The quantum algorithm developed here maps typical noise in NISQ computers to spectral function properties of open system models. At the center of this approach is the effective Lindbladian description of a Trotterized time-evolution performed on a noisy quantum computer [21].

The effective Lindbladian description, and thereby the form of the spectral function, depends on the circuit decomposition. In the examples we have considered, optimal circuit decompositions were based on native gates, such as the small-angle single-qubit rotations, variable MS two-qubit gates (XX interaction), or variable iSWAP two-qubit gates (XX + YY interaction). We also found that non-native gate decompositions can work as well, but may lead to alternations to the actually time-evolved open-system model. The examples considered also showed that the algorithm can perform very well even with gate errors as high as 1%. The performance improves with decreasing gate error. The central parameters used in the examples are summarized in Table I.

In the examples we considered single-spin systems. It should be emphasized that the quantum algorithm can be applied also to multi-spin systems, such as exciton-transport models [5]. Indeed, the algorithm is most efficient when time evolving a model with multiple system spins, due possibility to more efficient gate parallelization. More specifically, for a fixed number of bath modes, system spins can be added without additional cost (e.g., decrease in the needed gate error) when exploiting all-to-all connectivity or the system-bath SWAP algorithm presented in Appendix C.

The derivation of the quantum algorithm assumed an intrinsic qubit noise that can be described adequately using Lindbladian formalism. However, we note that the approach is also directly applicable to noise whose effect is rather of Bloch-Redfield form. Furthermore, the general principles of modifying the effective noise could also be applied to general non-Markovian noise. Utilization of non-Markovian noise in quantum computing has been addressed recently in Ref. [42].

The focus in this article was on utilizing intrinsic qubit noise. However, it is indeed also possible that one may implement the required non-unitary operations through the use of measurements [7–15]. The desired large difference in decoherence rates between the system and bath qubits could in fact be implemented more easily within such approach. One can, of course, consider algorithms which are based on combining both of these approaches. The bath qubits may also be replaced by resonators or phonon modes on hardware [23, 30–32], with engineered damping.

Finally, the quantum algorithm and conclusions presented in this paper are not restricted to simulating the spin-boson model, but are applicable also for more general open-system models.

Acknowledgments

This work was supported by the German Federal Ministry of Education and Research, through PhoQuant (13N16107), and QSolid (13N16155), and by the German Federal Ministry of Economic Affairs and Climate Action, through the PlanQK project (01MK20005H). This work was also supported by the European Union’s Horizon 2020 program number 899561, AVaQus.
Appendix A: Generalization to multi-spin systems

For simplicity, the main text considers only the case of one system spin. The presented algorithm can however be generalized to cover also multi-spin systems. An example of a multi-spin Hamiltonian is

$$\hat{H}_S = \sum_{i \in \text{system}} \frac{\hbar \Delta_i}{2} \hat{\sigma}_z^i + \frac{1}{2} \sum_{i < j \in \text{system}} \left( g_{ij} \hat{\sigma}_+^i \hat{\sigma}_-^j + g_{ji}^* \hat{\sigma}_-^i \hat{\sigma}_+^j \right)$$

$$\hat{H}_B = \sum_k \hbar \omega_k \hat{b}_k^\dagger \hat{b}_k$$

$$\hat{H}_C = \frac{1}{2} \sum_{i \in \text{system}} \sum_k \left( \hat{v}_k \hat{b}_k + \hat{v}_k^* \hat{b}_k^\dagger \right)$$

The couplings $g$ and $v$ may be complex numbers. This Hamiltonian is commonly used to describe exciton transport in the photosynthesis, where the system spins correspond to excitons and the bosonic modes to molecular vibrations.

The spectral function is defined analogously as for the single-spin system. The multi-dimensional spectral function is defined as

$$S_{ij}(\omega) = \int e^{i \omega t} \langle \hat{X}_i(t) \hat{X}_j(0) \rangle dt,$$

where

$$X_i = \sum_k (v_{ik} \hat{b}_k + v_{ik}^* \hat{b}_k^\dagger).$$

In thermal equilibrium,

$$S_{ij}(\omega) = \frac{2\pi}{1 - \exp \left(-\frac{\hbar \omega}{k_B T}\right)} \sum_k v_{ik} v_{jk}^* \delta(\omega - \omega_k), \quad \text{for } \omega > 0$$

$$S_{ij}(\omega) = \frac{2\pi}{\exp \left(-\frac{\hbar \omega}{k_B T}\right) - 1} \sum_k v_{ik} v_{jk}^* \delta(\omega + \omega_k), \quad \text{for } \omega < 0.$$

We see that cross-correlations ($i \neq j$) can appear if different spins couple to the same bath modes. We also have $S_{ij}(\omega) = S_{ji}^*(\omega)$.

The coarse graining is done similarly as for the single-spin system. The original bosonic bath is replaced by $n$ auxiliary boson modes. Each of these auxiliary modes has a central frequency $\omega_m$, coupling to the $i$th spin $v_{im}$, and broadening $\kappa_m$. The multi-dimensional spectral function that follows is

$$S_{ij}(\omega) = \sum_{m=1}^n v_{im} v_{jm}^* \frac{\kappa_m}{(\omega_m/2)^2 + (\omega - \omega_m)^2}.$$  

In the fitting we optimize, for example, the cost function

$$C = \sum_{i \leq j} \int_{\omega_{\text{min}}}^{\omega_{\text{max}}} d\omega \left| S_{ij}(\omega) - S_{ij}^{\text{target}}(\omega) \right|^2,$$

by seeking optimal values for $\omega_m$, $v_{im}$, and $\kappa_m$. The fitting problem includes $n$ frequencies, $n$ couplings, and $n$ broadenings, where $n_q$ is the number of system spins. Furthermore, the system-qubit noise can be included similarly as in the case of the single-spin system (Sec. III A 2). Here, a constant background rate is added to diagonal components of $S_{ij}(\omega)$, if assuming the system-qubit noise is uncorrelated. Possible differences in the system-qubit decoherence rates can be accounted for by generalizing the constant $r$ in Eq. (12) to a vector $r_i$, where the index $j$ refers to a system spin.

Appendix B: Noisy-algorithm model

Here we give a short description of our model of quantum computing with incoherent error. A more detailed derivation and validity analysis is given in Ref. [21].
1. Physical noise

For the following discussion, we assume that the time-propagation algorithm is based on a Trotter expansion over time \( t = m \tau \),

\[
e^{-iHt} = e^{-iHm\tau} = \left[e^{-iH \tau}\right]^m \approx \left[ \prod_j e^{-iH_j \tau} \right]^m. \tag{B1}
\]

Here the Hamiltonian \( H \) is divided into partial Hamiltonians,

\[
\hat{H} = \sum_j \hat{H}_j, \tag{B2}
\]

whose contributions to the time evolution are implemented using available unitary gates. For native (or natural) gates we have

\[
e^{-i\hat{H}_j \tau} = \hat{U}_j, \tag{B3}
\]

whereas other unitaries need to be decomposed like

\[
e^{-i\hat{H}_j \tau} = \Pi_k \hat{U}_{j,k}. \tag{B4}
\]

Here the elementary gates \( \hat{U}_{j,k} \) practically include large-angle operations, such as \( R_{\pi/2} \) or CNOT.

In our modeling, the physical noise is included as non-unitary operations after unitary gates,

\[
\hat{U} \to N\hat{U}. \tag{B5}
\]

On the right-hand side, the unitary gate is represented as a superoperator \( \hat{U} \) and the non-unitary noise as a Kraus operator \( N \). It is always possible to establish such description of an incoherent error, assuming it keeps qubits in their computational basis. In our modeling, also the identity gate is assumed to come with noise. In other words, the noise is acting also on idling qubits.

Assuming the effect of the noise per gate is weak, it is possible replace the Kraus superoperators by Lindbladians \( \mathcal{L}_j \) and physical gate times \( t_j \) such that

\[
\mathcal{N}_j \approx 1 + t_j \mathcal{L}_j, \tag{B6}
\]

where \( \mathcal{L}_j \) is a Lindblad operator describing the physical noise.

2. Effective noise

Physical noise can appear in a different form in the simulated system [21]. To understand how this "noise mapping" works, consider a simple example of decomposing some unitary to three elementary gates, \( \hat{V} = \hat{U}_3 \hat{U}_2 \hat{U}_1 \). Since unitary gates have also inverse gates, we can rewrite the noisy version of this circuit as

\[
\hat{U}_3 \hat{U}_2 \hat{U}_1 \to \mathcal{N}_3 \mathcal{N}_2 \mathcal{N}_1 \hat{U}_1 = \mathcal{N}_3 \mathcal{N}_2 \mathcal{N}_1 \hat{U}_3^{-1} \hat{U}_2 \hat{U}_1 = \mathcal{N} \hat{V}, \tag{B7}
\]

where \( \mathcal{N} = \mathcal{N}_3 \mathcal{N}_2 \mathcal{N}_1 \) and

\[
\mathcal{N}_1 = \hat{U}_3 \hat{U}_2 \hat{N}_1 \hat{U}_3^{-1} \approx 1 + t_3 \mathcal{L}_4 (1 + t_2 \mathcal{L}_3 (1 + t_1 \mathcal{L}_1)) \approx 1 + t_1 \mathcal{L}_1' + t_2 \mathcal{L}_2' + t_3 \mathcal{L}_3'. \tag{B8}
\]

Here, the operators in the individual Lindbladians \( \mathcal{L}_j \) are rotated by unitary gates \( \hat{U}_{j'} \) exactly in the same way as the noise superoperators were rotated by \( \hat{U}_{>1} \). The (noise part in) the effective Lindbladian then becomes

\[
\tau \mathcal{L}_{\text{eff}} = t_1 \mathcal{L}_1' + t_2 \mathcal{L}_2' + t_3 \mathcal{L}_3'. \tag{B9}
\]

This result can be generalized to arbitrary circuits [21].

The transformation of noise to other effective forms in a series of unitary gates has also been studied recently in Refs. [13, 43, 44]. The effect of quasistatic noise in digital quantum simulation has been studied in Ref. [45].

3. Central transformations

A simple but very relevant example of the used noise model is the transformation of damping noise under \( X \) gates,

\[
\begin{align*}
R_x(\pi) & \to \sqrt{\gamma} \sigma^- & R_x(\pi) \\
\rightarrow & \ - R_x(\pi) \ - \sqrt{\gamma} \sigma^- & \ - \ R_x(\pi) \ \ - \sqrt{\gamma} \sigma^- \\
= & \ - R_x(\pi) \ - R_x(\pi) \ - \sqrt{\gamma} \sigma^+ & \ - \sqrt{\gamma} \sigma^- 
\end{align*}
\]

where we have used that \( R_x(\pi) \hat{\sigma}^+ R_x(-\pi) = \hat{\sigma}^+ \). Here we have effectively transformed qubit damping to combination of damping and excitation.

Another central example is the case of native gates. A Trotter-step circuit of a noiseless system-qubit coupled to a noisy bath-qubit via XX-interaction is
where we have approximated that for the noise operator
\[ N' = XX(\tau v) \times N \times XX(-\tau v) \approx N , \]
which is true when \( \tau v \ll 1 \) and \( XX \) is a native gate.

4. Noise transformations in the examples

In the example of Sec. IV A, the CNOT decomposition with bath qubits as control qubits (labelled as CNOT-B) did not lead to large changes in the effective noise model. This can indeed be derived analytically by looking how the control-qubit \( i \) damping and dephasing operators transform under CNOT, see Table II.

- CNOT \( \hat{\sigma}_z \) CNOT = \( \hat{\sigma}_z \hat{\sigma}_z \) \( \hat{\sigma}_x \) \( \hat{\sigma}_x \) (B13)
- CNOT \( \hat{\sigma}_z \) CNOT = \( \hat{\sigma}_z \hat{\sigma}_z \) (B14)

Remember that a superscript \( i \) in a Pauli operator refers to a bath qubit (or the corresponding auxiliary spin). This tells us that physical bath-qubit damping gets translated into simultaneous bath-spin damping and system-spin flip, whereas dephasing keeps its form. This result means that the effective Lindbladian has the form

\[ \mathcal{L}_{\text{eff}}[\hat{\rho}] \approx \frac{i}{\hbar} [\hat{\rho}, \hat{H}] + (\gamma - \delta \gamma) \sum_i \mathcal{L}_{\sigma^+_i}[\hat{\rho}] + \frac{\Gamma}{2} \sum_i \mathcal{L}_{\sigma^-_i}[\hat{\rho}] \]

\[ + \delta \gamma \sum_i \mathcal{L}_{\sigma^+_i, \sigma^-_i}[\hat{\rho}] , \]

where we use a notation \( \mathcal{L}_A \) for a noise Lindbladian with only finite rate-matrix element \( R_{A,B} \). It turns out that the last term on the right-hand side of Eq. (B15) can be approximately factored to two uncorrelated contributions,

\[ \mathcal{L}_{\text{eff}}[\hat{\rho}] \approx \frac{i}{\hbar} [\hat{\rho}, \hat{H}] + (\gamma - \delta \gamma) \sum_i \mathcal{L}_{\sigma^+_i}[\hat{\rho}] + \frac{\Gamma}{2} \sum_i \mathcal{L}_{\sigma^-_i}[\hat{\rho}] \]

\[ + \delta \gamma \sum_i \mathcal{L}_{\sigma^+_i, \sigma^-_i}[\hat{\rho}] + \gamma_{\text{system}} \mathcal{L}_{\sigma^+_i}[\hat{\rho}] , \] (B16)

where

\[ \gamma_{\text{system}} = \delta \gamma \sum_i \langle \hat{\sigma}^+_i \hat{\sigma}^-_i \rangle . \] (B17)

We also get \( \gamma_{\text{system}} \ll \gamma, \Gamma \), following from that most of the time the individual bath qubits are at ground. It follows that \( \gamma_{\text{system}} \) can be neglected and we have

\[ \mathcal{L}_{\text{eff}}[\hat{\rho}] \approx \frac{i}{\hbar} [\hat{\rho}, \hat{H}] + \gamma \sum_i \mathcal{L}_{\sigma^+_i}[\hat{\rho}] + \frac{\Gamma}{2} \sum_i \mathcal{L}_{\sigma^-_i}[\hat{\rho}] , \] (B18)

This has the same form as the physical noise.

For CNOT-S, i.e., when the system qubit is the control qubit, the changes in the effective model are larger. This can be derived by looking at the target-qubit noise conversions, see Table II,

- CNOT \( \hat{\sigma}^+_i \) CNOT = \( \hat{P}_0 \hat{\sigma}^+_i + \hat{P}_1 \hat{\sigma}^-_i \) (B19)
- CNOT \( \hat{\sigma}^+_i \) CNOT = \( \hat{\sigma}^-_i \hat{\sigma}^+_i \) (B20)

where \( \hat{P}_0 = (1 + \hat{\sigma}_z)/2 \) and \( \hat{P}_0 = (1 - \hat{\sigma}_z)/2 \) are projection operators of the system qubit. The first equation implies that physical bath-qubit decay can also transform into effective bath-spin excitation. It can therefore be active even when the bath is empty. Furthermore, this correlated noise wants to project the system spin to one of its \( \hat{\sigma}_z \) eigenstates.

The effective Lindbladian becomes

\[ \mathcal{L}_{\text{eff}}[\hat{\rho}] \approx \frac{i}{\hbar} [\hat{\rho}, \hat{H}] + \gamma \sum_i \mathcal{L}_{\sigma^+_i}[\hat{\rho}] + \frac{\Gamma}{2} \sum_i \mathcal{L}_{\sigma^-_i}[\hat{\rho}] \]

\[ + \frac{\Gamma}{2} \mathcal{L}_{\sigma^+_i}[\hat{\rho}] , \] (B21)

where we have done noise factoring and neglected a contribution introducing bath excitation (this approximation was verified numerically). The size of \( \Gamma \) can also be solved numerically [21] and gives a noticeable system-spin dephasing.

The effective noise analysis of a control-Z decomposition (defined later in Appendix C) is essentially the same as made for the CNOT-B decomposition, see Table II. This means that the effective noise of a control-Z decomposition has the same form as the physical noise.
TABLE II: Effective noise for different incoming noise types and two-qubit gates. We consider physical noise operators $\hat{\sigma}_-, \hat{\sigma}_+, \hat{\sigma}_z$ under control-X (CNOT) and control-Z unitary transformations. Here $P_0 = (1 + \hat{\sigma}_z^{\text{control}})/2$ and $P_1 = (1 - \hat{\sigma}_z^{\text{control}})/2$ are control-qubit projection operators.

| Gate      | $\sigma_-^{\text{control}}$ | $\sigma_+^{\text{control}}$ | $\sigma_z^{\text{control}}$ | $\sigma_-^{\text{target}}$ | $\sigma_+^{\text{target}}$ | $\sigma_z^{\text{target}}$ |
|-----------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|
| CNOT      | $\sigma_-^{\text{target}}$ | $\sigma_+^{\text{target}}$ | $\sigma_z^{\text{target}}$ | $\sigma_-^{\text{target}} + P_1 \sigma_z^{\text{target}}$ | $\sigma_+^{\text{target}} + P_1 \sigma_z^{\text{target}}$ | $\sigma_z^{\text{target}}$ |
| Control-Z | $\sigma_+^{\text{target}}$ | $\sigma_-^{\text{target}}$ | $\sigma_z^{\text{target}}$ | $\sigma_+^{\text{target}}$ | $\sigma_-^{\text{target}}$ | $\sigma_z^{\text{target}}$ |

Appendix C: Quantum circuit optimization

We assume that the effective noise given by $L_{\text{eff}}$ is dominated by spin damping and spin dephasing. This is a common form of qubit noise in many NISQ devices, including superconducting quantum computers. We want to avoid transforming this physical noise to other (effective) forms in the Trotterized time evolution.

1. Avoiding large-angle bath-qubit rotations

Large-angle rotations of bath qubits may rotate the noise operators $\sigma_+$ and $\sigma_-^z$ to very different forms. Such rotations should then be avoided. We give below several examples of gate decompositions that follow this principle. One key approach is that if large-angle rotation cannot be avoided, we do them to low-noise system qubits.

Ideally we have an access to a native gate of some two-qubit interaction. In this paper we construct time-propagation according to XX-interaction between a system qubit and a bath qubit. Consider realizing this using a variable iSWAP two-qubit gate, which is a native gate of an excitation hop,

$$i\text{SW}(\tau v) = e^{-i(\hat{\sigma}_z^b \hat{\sigma}_b + \hat{\sigma}_z^s \hat{\sigma}_s)^2} \tau v/2.$$  \hspace{1cm} (C1)

Here ”s" refers to a system qubit and ”b" to a bath qubit. To obtain the full XX-interaction, we need to add the counter-rotating terms. We can create these terms by another variable iSWAP gate by surrounding it by X-gates of one qubit. To avoid rotations of the bath qubit, the X-gates are done to the system qubit,

$$R_{x,s}(\pi) i\text{SW}(\tau v) R_{x,s}(\pi) = e^{-i(\hat{\sigma}_z^b \hat{\sigma}_b^x + \hat{\sigma}_z^s \hat{\sigma}_s^x)^2} \tau v/2.$$ \hspace{1cm} (C2)

The full XX-interaction time-propagation during one Trotter time step $\tau$ is then generated by

$$R_z(\tau v) R_z(\pi) R_z(\pi) R_z(\tau v).$$

A variable Mølmer-Sørensen gate is a native gate of the XX-interaction,

$$MS(\tau v) = e^{-i\hat{\sigma}_z^s \hat{\sigma}_z^b \tau v/2}.$$ \hspace{1cm} (C3)

On the other hand, to obtain an excitation hop using the variable MS gate, we need to add this with YY-gate. The YY-gate can be created from an XX-gate with the help of Z-rotations,

$$R_{z,s}(-\frac{\pi}{2}) R_{z,b}(-\frac{\pi}{2}) MS(\tau v) R_{z,b}(\frac{\pi}{2}) R_{z,s}(\frac{\pi}{2}) = e^{-i\hat{\sigma}_z^b \hat{\sigma}_z^s \tau v/2}.$$ \hspace{1cm} (C4)

Note that this includes large-angle rotations of the bath qubit also. However, Z-rotations do not change the form of damping ($\hat{\sigma}^-$) or dephasing ($\hat{\sigma}^+$) operators (they just introduce a phase shift which cancels out in the Lindbladians). The excitation hop is then generated by

$$s \quad MS \quad R_{z,b}(\frac{\pi}{2}) \quad MS \quad R_{z,s}(\frac{\pi}{2}) \quad b$$

Here $MS = MS(\tau v/4)$.

Also non-native decompositions should follow this principle. Decompositions based on applying Hadamard-gates to all qubits should be avoided. Instead decompositions based on small-angle X-rotations should be used. Furthermore, in the case of CNOT decompositions, using the bath qubit as a control-qubit seems beneficial (which could be understood qualitatively as a result of that the bath qubit is then never "flipped"). A non-native decomposition of the XX-interaction following these principles is

$$s \quad R_y(\frac{\pi}{2}) \quad Z \quad R_z(\tau v) \quad Z \quad R_y(-\frac{\pi}{2}) \quad b$$

This is used in the CNOT-B decomposition of Sec. IV A. Another example of the XX-interaction is

$$s \quad R_y(\frac{\pi}{2}) \quad Z \quad R_z(\tau v) \quad Z \quad R_y(-\frac{\pi}{2}) \quad b$$
FIG. 8: A two-dimensional qubit architecture that is optimal for performing a Trotterized time evolution of a system-bath model. In total \( n_s \) system qubits locate between \( 2n_s \) bath qubits. The bath qubits can also refer to any other resonance modes in the device, whose interaction with the system qubits can be controlled digitally.

2. System-bath SWAP algorithm

In common open-system models the bath is non-interacting. For the presented quantum algorithm this means that a direct connectivity between the bath qubits is not desired. Rather a connectivity from the system to all bath qubits. If this system-to-all-bath connectivity is provided, a simple Trotter expansion of the time-propagation is adequate,

![Graphical representation of the system-bath interaction and SWAP process.](image)

On the other hand, if only nearest-neighbor interactions are possible, but the device has a two-dimensional architecture, an efficient SWAP-algorithm can be applied. Our proposed system-bath SWAP algorithm converts the time evolution into a sequence of nearest-neighbor interactions and SWAP processes. Here the quantum state(s) of the system spin(s) are moved in a system-qubit network, located between the bath qubits, see Fig. 8. The difference to the common SWAP algorithm [46] is that bath states are not swapped. Within this modification, one avoids doing large-angle rotations of the bath qubits. In the example shown in Fig. 9, the state of one system-spin is stored by two system qubits, one per time. The system spin interacts with four auxiliary spins, represented by the four bath qubits.

![Graphical representation of the system-bath interaction and SWAP process.](image)

is transformed into some physically sound form.

X-gates can be used to transform physical qubit-damping into effective spin-excitation. This is based on the transformation

\[ \hat{\sigma}_x \hat{\sigma}_x - \hat{\sigma}_x = \hat{\sigma}_+ . \]  

(C5)

In the simplest version of the noise symmetrization, we insert X-gates between (original) Trotter-steps, and do corresponding changes to the unitary gates (such as \( Y \rightarrow -Y \)). In the case of system-qubit damping symmetrization, we then have the new Trotter-step circuits

![Graphical representation of the system-bath interaction and SWAP process.](image)

where \( \tilde{U} = R_x(\pi)U R_x(\pi) \). Ideally the decomposition of \( U \) is similar as of \( \tilde{U} \), or even \( U = \tilde{U} \) (which would be
the case for an XX-interaction). This symmetrizes the effective Lindbladian $L_{\text{eff}}$ terms like
\[ \gamma \hat{\sigma}^- \hat{\rho} \hat{\sigma}^+ \rightarrow \frac{\gamma}{2} \hat{\sigma}^- \hat{\rho} \hat{\sigma}^+ + \frac{\gamma}{2} \hat{\sigma}^+ \hat{\rho} \hat{\sigma}^- . \]

Furthermore, since we see that damping has changed to a coupling to two independent baths, via operators $\hat{\sigma}_x$ and $\hat{\sigma}_y$. As demonstrated in Sec. IV C and discussed more in Appendix E, this can be mapped to a constant background of spectral functions in a certain interesting class of open system models.

The system-noise symmetrization can be generalized to all spin-directions, in which case the system-noise becomes equivalent to depolarization. This corresponds to coupling to three independent baths, via operators $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$.

Various noise symmetrization approaches have been studied recently experimentally in Refs. [10, 13].

Appendix D: Error sources and error tradeoff

Here we analyze three main error sources in the quantum algorithm and discuss how they are connected to each other. These are the Trotter error, the coarse-graining error, and the bath-Gaussianity error.

1. Trotter error

The time propagation is realized in time steps $\tau$. Unless all terms in the Trotter expansion commute, there is an error in the time propagation. To have a small Trotter error, one commonly demands
\[ v \tau \ll 1, \]

where $v$ is some effective frequency describing the non-commuting contributions. One should note that even though this relation would not be clearly valid, the Trotter error can still be small.

The accumulation of noise within one Trotter step is also "discrete", which implies that a similar error exists also in the effective noise model $L_{\text{eff}}$ [21]. Assuming that the noise terms commute with each other, or that the noise has a smaller or similar magnitude as the coherent terms, the condition for the corrections to the noise model being small is
\[ v \kappa \tau^2 \ll \kappa \tau, \]

This condition turns out to be equivalent with Eq. (D1).

In the mapping (see Sec. III), the time step $\tau$ becomes related to the circuit depth $D$, the mode broadening $\kappa$, and the gate error $\epsilon$, such that
\[ \kappa \tau = D \epsilon, \]

The condition for the Trotter error and the noise-model error being small can now be rewritten as
\[ D \epsilon \ll \frac{\kappa}{v}. \]

The main message here is that the Trotter error is expected to decrease with the gate error $\epsilon$. Moreover, for large $\epsilon$, one may be forced to reduce the circuit depth $D$, which is practically done by reducing the total bath-qubit number $n_q = \sum_{i=1}^{N} N_i$. Also notable is that a decrease in the broadening $\kappa$ makes the condition more strict. The role of the broadening $\kappa$ in the error analysis will be discussed more below.

2. Coarse-graining error and error correction

Unless the target spectral function is a Lorentzian, or a (finite) sum of Lorentzians, there is always an error in the coarse graining. This error can be characterized, for example, by the root mean-square error of the spectral-function fit.

Several recent works study errors originating in the imperfect spectral-function fitting, as well as their correction, in the context of classical numerical methods [25, 47, 48]. Particularly interesting for the noise-utilizing quantum algorithm is an error-correction approach based on calculating functional derivatives with respect to spectral-function changes [25]. For the quantum algorithm considered here, this would correspond to using a low-noise qubit as a narrow-peak perturbation in the spectral function, to implement a functional derivative. The leading-order correction is the derivative multiplied by the coarse-graining error [25].

3. Error tradeoff

There is a close tradeoff between the different error sources. The coarse graining is always done within some frequency window, for example, within a cutoff frequency $\omega_c$. In the simplest (but pretty good) estimate, the auxiliary boson modes are inserted at constant frequency intervals with broadenings
\[ \kappa \approx \frac{\omega_c}{n}, \]

We already note that an increase of $n$ decreases $\kappa$. The circuit depth also depends on $n$ and for the models considered in this paper it is approximately
\[ D \approx nN D_0 = n_q D_0, \]
where \( N \) is the number of qubits representing an auxiliary boson mode and for simplicity we assume that it is the same for every boson mode. Thereby the number of bath qubits \( n_q = nN \). The constant \( D_0 \) is defined by the simulation algorithm and the gate decomposition, see Table I.

Combining the above results with Eq. (D3), we obtain a seemingly fundamental relation

\[
\frac{\omega_c \tau}{\epsilon} \approx n^2 N D_0 . \tag{D7}
\]

On the left-hand side, the numerator \( \omega_c \tau \) is a measure of the gate error. The denominator \( \epsilon \) is a measure of the gate error. On the right-hand side, we have the number of Lorentzians used in the coarse graining \( n \) (defining the coarse-graining error) and the number of bath qubits per boson mode \( N \).

Eq. (D7) implies that reduction of gate error \( \epsilon \) lets us to increase \( n \), or lets us to increase \( N \), or lets us to reduce the Trotter error \( \omega_c \tau \), when keeping the other variables unchanged. In other words, the lower the gate error \( \epsilon \), the better the quantum algorithm can perform. Alternatively, the lower the gate error \( \epsilon \), the more difficult problems it can solve. We also observe that higher gate errors can be compensated by increased Trotter error. Also notable is that the number of auxiliary boson modes \( n \) is harder to increase than \( N \), since it appears as squared. This is since increasing \( n \) not only increases the circuit depth but also decreases \( \kappa \).

**Appendix E: Spin-boson model of electronic transport**

In this Appendix we show how to map a fermionic open-system model to a spin-boson model. The key steps are the assumption of Gaussian statistics of the bath coupling-operator and the matching of the bath spectral functions.

We consider a fermionic open quantum system described by the Hamiltonian (1) with

\[
H_S = \frac{\hbar \Delta}{2} \sigma_z , \tag{E1}
\]

\[
H_B = \sum_m \sum_k E_{km} \hat{c}_{km} \hat{c}_{km}^\dagger + \sum_m \sum_l E_{lm} \hat{d}_{lm} \hat{d}_{lm}^\dagger \tag{E2}
\]

\[
H_C = \hat{\sigma}_+ \hat{F} + \hat{\sigma}_- \hat{F}_m^\dagger \tag{E3}
\]

\[
\hat{F} = \sum_{klm} T_{klm} \hat{c}_{km}^\dagger \hat{d}_{lm}^\dagger . \tag{E4}
\]

Here the operators \( \hat{c}^{(\dagger)} \) and \( \hat{d}^{(\dagger)} \) annihilate (create) an electron in the system and in the bath, correspondingly. This model can be used to describe, for example, electron transport across small metallic islands with strong Coulomb interaction [41]. Here the transverse channel \( m \) is conserved in the transport. The island charge is described by the spin degree of freedom, assuming that only two charge numbers are relevant due to a strong Coulomb repulsion.

We first note that the coupling operators satisfy a bosonic commutation relation

\[
[\hat{c}_{km}^\dagger, \hat{d}_{lm}^\dagger, \hat{c}_{k'm'}] = 0 , \tag{E5}
\]

if the longitudinal channels differ, \( k \neq k' \) and \( l \neq l' \), or if the transverse channels differ \( m \neq m' \). The bath coupling operator can be treated to be bosonic in the limit of a large number of transverse channels, \( \sum_m 1 \gg 1 \). It is also possible when the bath memory time is shorter than the average time between electron hoppings. In such situations the bath behaves similarly as a bosonic field, when observing from the system.

In Sec. IV C, we study the steady state and relaxation dynamics of he island charge when the source-drain voltage is zero and the gate voltage \( (\propto \Delta) \) is varied. The relevant spectral function is

\[
S(\omega) = \left\langle \hat{F}^\dagger(t) \hat{F}(0) \right\rangle_\omega \approx \left\langle \hat{F}(t) \hat{F}^\dagger(0) \right\rangle_\omega \\
= 2\pi \sum_m \sum_k \sum_l [T_{klm}]^2 \delta(\omega - E_{lm}/\hbar + E_{km}/\hbar) \\
\times f(E_{lm}) |1 - f(E_{km})| , \tag{E6}
\]

where \( f(E) \) is the Fermi function. In the example, we choose a structured spectral function that is ohmic at low frequencies and resonant at frequencies \( \omega_0 \) and \( \omega_1 \),

\[
S(\omega) = \sum_{k=0}^1 \frac{\alpha \omega}{1 - \exp \left( -\frac{\omega}{\omega_0} \right)} \frac{1}{2\pi} \left( \frac{\omega - \omega_1}{\frac{\pi}{2}} \right)^2 + (\omega - \omega_1)^2 . \tag{E7}
\]

We use \( \alpha = 0.25, \kappa' = 0.4 \omega_0, \omega_1 = 2 \omega_0 \), and a cut-off function \( 1/[1 + (\omega/\omega_c)^4] \) with \( \omega_c = \sqrt{3} \omega_0 \).

When writing down the corresponding spin-boson model, we need to account for that the coupling operators \( \hat{F} \) are not Hermitian and

\[
\left\langle \hat{F}(t) \hat{F}(0) \right\rangle = \left\langle \hat{F}^\dagger(t) \hat{F}^\dagger(0) \right\rangle = 0 . \tag{E8}
\]

Furthermore, the opposite-direction spin-flips are associated with the same spectral function \( S(\omega) \). A spin-boson model that satisfies the corresponding properties is

\[
H_S = \frac{\hbar \Delta}{2} \sigma_z \tag{E9}
\]

\[
H_B = \sum_k \hbar \omega_k \hat{B}_1^\dagger \hat{B}_1 + \sum_k \hbar \omega_k \hat{B}_2^\dagger \hat{B}_2 \tag{E10}
\]

\[
H_C = \hat{\sigma}_+ \sum_k v_k \left( \hat{B}_1 + \hat{B}_1^\dagger \right) + \hat{\sigma}_- \sum_k v_k \left( \hat{B}_2 + \hat{B}_2^\dagger \right) . \tag{E11}
\]

Here we have introduced two independent bosonic fields with annihilation (creation) operators \( \hat{B}_1^\dagger \) and \( \hat{B}_2^\dagger \). The two bosonic fields have identical mode structure, i.e., fre-
quencies $\omega_k > 0$ and couplings $v_k$. A spin flip $\hat{\sigma}_z$ absorbs a boson from field 1 or creates a boson into field 2. The corresponding spectral function is in thermal equilibrium

$$S(\omega) = \sum_k \left\langle \hat{B}_{1k}(t) \hat{B}_{1k}(0) \right\rangle + \sum_k \left\langle \hat{B}_{2k}(t) \hat{B}_{2k}(0) \right\rangle \omega$$

$$= 2\pi \sum_k \frac{v_k^2 \delta(\omega_k - \omega)}{1 - \exp \left(-\frac{\hbar \omega_k}{k_B T}\right)} \text{sign}(\omega). \quad (E12)$$

The spin-boson model parameters $v_k$ are (formally) chosen so that the spectral function of the fermionic problem is reproduced. The spectral function $S(\omega)$ is then the target function in the coarse graining. The auxiliary boson modes are finally represented by auxiliary spins.

The form of coupling Hamiltonian (E11) supports the use of the variable iSWAP two-qubit decomposition, since it is the native gate of (system-bath) coupling $\hat{\sigma}_+ \hat{\sigma}_+^x + \hat{\sigma}_- \hat{\sigma}_-^x$. The counter-rotating coupling terms $\hat{\sigma}_+ \hat{\sigma}_+^\dagger + \hat{\sigma}_- \hat{\sigma}_-^\dagger$ can be created by surrounding the variable iSWAP by X-gates, see Appendix C.

Alternatively, an equivalent spin-boson Hamiltonian, supporting the variable MS decomposition, can be derived by defining new bosonic operators

$$\hat{a}_k \equiv \frac{1}{\sqrt{2}} (\hat{B}_{1k} + \hat{B}_{2k}) \quad (E13)$$

$$\hat{b}_k \equiv \frac{i}{\sqrt{2}} (-\hat{B}_{1k} + \hat{B}_{2k}) \quad (E14)$$

This changes the form of the coupling Hamiltonian,

$$H_B = \sum_k \hbar \omega_k \hat{a}_k \hat{a}_k + \sum_k \hbar \omega_k \hat{b}_k \hat{b}_k \quad (E15)$$

$$H_C = \hat{\sigma}_x \sum_k \frac{v_k}{\sqrt{2}} (\hat{a}_k + \hat{a}_k^\dagger) + \hat{\sigma}_y \sum_k \frac{v_k}{\sqrt{2}} (\hat{b}_k + \hat{b}_k^\dagger) \quad (E16)$$

When representing this with spin-spin Hamiltonian, the first coupling-term is replaced by $\hat{\sigma}_x \hat{\sigma}_x^\dagger$-interaction and the second coupling-term by $\hat{\sigma}_y \hat{\sigma}_y^\dagger$-interaction. The first coupling type is native to variable MS, whereas the second one can be created by surrounding the variable MS by $\pi/2$ Z-rotations, see Appendix C. It follows that the circuit depth, when time-propagating the system with variable MS according to this Hamiltonian, will be the same as when time-propagating the system with variable iSWAP according to the preceding form of the Hamiltonian. The Hamiltonian presented in the main text corresponds to Eq. (E16) with redefined couplings, $v_k/\sqrt{2} \rightarrow v_k/2$.

When time-evolving the open-system model on the quantum computer, system-qubit X-gates are introduced between Trotter steps in order to transform physical system-qubit decay into effective excitation, see Appendix C. From Eq. (C7) we see that the damping noise after this symmetrization corresponds to coupling to two independent baths, via coupling operators $\hat{\sigma}_x$ and $\hat{\sigma}_y$. It has exactly the same form as the considered open-system model. It follows that system noise can be added as a constant background to the spectral functions, as in Eq. (11). This mapping between the system-qubit noise and the spectral-function background is demonstrated in the example of Sec. IV C.

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