Reconstructing the ideal results of a perturbed analog quantum simulator

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Well-controlled quantum systems can potentially be used as quantum simulators. However, a quantum simulator is inevitably perturbed by coupling to additional degrees of freedom. This constitutes a major roadblock to useful quantum simulations. So far there are only limited means to understand the effect of perturbation on the results of quantum simulation. Here we present a method which, in certain circumstances, allows for the reconstruction of the ideal result from measurements on a perturbed quantum simulator. We consider extracting the value of the correlator $\langle \hat{O}^i(t)\hat{O}^j(0)\rangle$ from the simulated system, where $\hat{O}^i$ are the operators which couple the system to its environment. The ideal correlator can be straightforwardly reconstructed by using statistical knowledge of the environment, if any n-time correlator of operators $\hat{O}^i$ of the ideal system can be written as products of two-time correlators. We give an approach to verify the validity of this assumption experimentally by additional measurements on the perturbed quantum simulator. The proposed method can allow for reliable quantum simulations with systems subjected to environmental noise without adding an overhead to the quantum system.

I. INTRODUCTION AND CENTRAL RESULTS

Today we possess in principle the full knowledge to describe all processes of interest in a wide range of fields, such as chemistry, biology, and solid state physics. In all these fields a truly microscopic description is possible using quantum mechanics. However, it is also well understood that in practice full quantum mechanical simulations of even modestly sized systems are impossible [1]. To efficiently study quantum problems, we need to use other, well-controlled quantum mechanical systems [2–5]. In recent years unprecedented direct control over quantum systems has been achieved [3,6–9]. Precise experiments in the quantum regime have been performed using atomic systems [10–12], superconducting qubits [13–17], photonic circuits [18–20], and nuclear spins [21,22]. Larger systems have been demonstrated using trapped ions [23,24] and the equilibration of interacting bosons has been studied in cold gases [25,26].

A promising approach to understanding quantum systems is analog quantum simulation [27], where the goal is to create an artificial system with a Hamiltonian that is equivalent to the system we intend to study. Apart from quantum simulations using cold gases [28,29] and trapped ions [30,31], there are many proposals for analog quantum simulation with superconducting circuits [32–35], exploiting the controllability of superconducting systems, which in principle allows the creation of a large class of Hamiltonians. While most current superconducting systems are relatively small [36,37], larger networks of superconducting nonlinear elements are now being explored [38–40]. Other architectures for analog quantum simulation have also been investigated [41,42].

In this article we study an analog quantum simulator with the ideal Hamiltonian H_S. To understand the properties of the simulated system, we would like to use a measurement to extract a time-ordered correlation function (Green's function)

$$iG_{S0}(t) = \langle \mathcal{T}\hat{O}(t)\hat{O}(0)\rangle_0 = \langle 0|\mathcal{T}e^{iH_S t}\hat{O}e^{-iH_S t}\hat{O}|0\rangle, \quad (1)$$

where $\mathcal{T}$ is the time-ordering operator. The index $S0$ indicates that we are considering the ideal Green's function of the unperturbed Hamiltonian H_S, without coupling to additional degrees of freedom, and $|0\rangle$ is the ground state of H_S (zero-temperature limit). We start our analysis from this simple example and later in Sec. IV extend the theory to multiple operators $\hat{O}^i$ and to finite temperatures. We consider time-ordered Green's functions, since these are in general connected to numerous quantities of interest in experiments, such as heat or electric transport coefficients. There are several proposals which describe methods to measure the relevant correlators in the context of analog quantum simulation [43–46]. Thus, we assume that Green's functions play a central role in extracting results from a quantum simulator.

However, if we want to use measurements on a quantum simulator to study the properties of an ideal Hamiltonian, the key challenge remains: What is the role of errors and imperfections of the artificial system in a real measurement [5,47–49]? Usually we quantify the influence of external degrees of freedom by comparing measurements to theoretical predictions. However, by definition, for quantum simulation it should not be possible to predict the result either analytically or numerically using classical computers. Some proposals exist to analyze [50] or mitigate [51,52] errors for small noise in analog or digital quantum simulators. The approach we introduce in this paper works potentially also for intermediate levels of noise strength. It is based on connecting the ideal Green's function (1) to the perturbed Green's function we measure using a quantum simulator. We consider Green's functions where $\hat{O}$ is also the operator by which the quantum simulator couples to additional degrees of freedom (which cause the
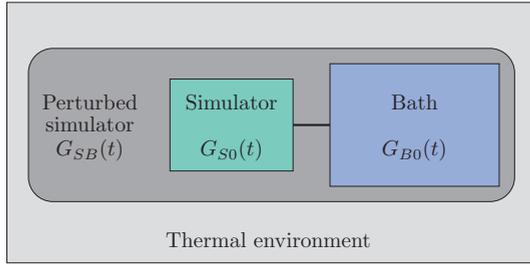
FIG. 1. The quantum simulator is coupled to a perturbative bath. The simulator-bath system is coupled weakly to an environment that establishes thermal equilibrium. For each subcomponent of the system we define a free correlator: the ideal correlator of the simulator $iG_{S0}(t) = \langle \mathcal{T}\hat{O}(t)\hat{O}(0)\rangle_0$ as defined in Eq. (1) and the free correlator of the bath $iG_{B0}(t) = \langle \mathcal{T}\hat{X}(t)\hat{X}(0)\rangle_0$. The full correlator $iG_{SB}(t) = \langle \mathcal{T}\hat{O}(t)\hat{O}(0)\rangle$ accounts for the coupling in the full Hamiltonian (2).

errors). This restricts the generality of the approach, but in reality it is actually very likely that the same mechanism which connects the system to its bath also allows for the readout of the system. For example, readout via a resonator for modern superconducting qubits can be done dispersively (via σ_z) or resonantly (via σ_x). In the case of T_1 limited qubits with resonant readout or T_2 limited qubits with dispersive readout [53] our requirement is fulfilled. So it is reasonable to assume that this is one of the Green's functions to which we have easy access in experiments.

We show that under specific conditions it is in fact possible to extract the ideal correlator of the operator $\hat{O}$ even from a perturbed system. One ingredient in our approach is good statistical knowledge of the additional degrees of freedom which act on H_S. This assumption is justified, for example, for a quantum simulator build from tunable qubits, where qubits can be decoupled and the properties of the baths of individual qubits can be probed by established spectroscopical methods. Apart from this, only one assumption is necessary about the properties of the ideal correlators. We need that any n-time correlation function can be expressed as the product of two-time correlation functions. This condition will be discussed in more detail in Sec. I A. In the present paper we describe this method assuming $\hat{O}$ and that the additional degrees of freedom are bosonic, but the method can also be directly transferred to fermionic operators $\hat{O}$ and fermionic baths.

A. Principal idea

We start by presenting a simple example of our approach, where we show how to extract the ideal properties from an imperfect simulator in equilibrium. In Sec. IV we extend this result to more general situations.

The full system we consider can be described by the Hamiltonian

$$H = H_S + H_C + H_B, \quad H_C = \hat{O}\hat{X}. \tag{2}$$

Here the ideal Hamiltonian of the simulator H_S is coupled via the Hamiltonian H_C to the additional degrees of freedom contained in the bath Hamiltonian H_B. The system operator in H_C is $\hat{O}$, which is the same as what we used to define the ideal correlator in Eq. (1), and the bath operator is $\hat{X}$.

The bath can usually be described by a set of bosonic modes and we assume that the free correlator of the bath $G_{B0}(t)$ is known, for example, from spectroscopic measurements. For the definition of all relevant Green's functions see Fig. 1 and its caption. In Sec. IV, we give a more precise definition.

The total system described by H is in thermal equilibrium. It should be emphasized that if coupling to the thermal bath is not infinitely weak it cannot be assumed that the only result of this coupling is the creation of equilibrium [54–56]. In the main part of this paper we focus on the situation at zero temperature and in Sec. IV D extend our method to finite temperatures.

We want to connect the spectral function of the bath to the properties of the perturbed quantum simulator. Standard many-body physics techniques exist which can be used to expand the full Green's function $G_{SB}(\omega)$ in terms of the ideal Green's functions $G_{S0}(\omega)$ and $G_{B0}(\omega)$ [57]. However, to apply these techniques there is one key assumption that is absolutely crucial: Wick's theorem needs to apply in some form. Using this theorem, it is possible to connect a single correlator of $2n$ operators with n two-time correlators. Wick's theorem for the system operator $\hat{O}$ takes the form

$$\begin{aligned}
&\langle \mathcal{T}\hat{O}(t_1)\hat{O}(t_2)\cdots\hat{O}(t_{n-1})\hat{O}(t_n)\rangle_0 \\
&= \langle \mathcal{T}\hat{O}(t_1)\hat{O}(t_2)\rangle_0 \langle \mathcal{T}\hat{O}(t_3)\cdots\hat{O}(t_{n-1})\hat{O}(t_n)\rangle_0 \\
&\quad + \langle \mathcal{T}\hat{O}(t_1)\hat{O}(t_3)\rangle_0 \langle \mathcal{T}\hat{O}(t_2)\cdots\hat{O}(t_{n-1})\hat{O}(t_n)\rangle_0 \\
&\quad + \cdots + \langle \mathcal{T}\hat{O}(t_1)\hat{O}(t_n)\rangle_0 \langle \mathcal{T}\hat{O}(t_2)\cdots\hat{O}(t_{n-1})\rangle_0. \tag{3}
\end{aligned}$$

This relation can be applied repeatedly until only two-time correlators remain. For the bath operator $\hat{X}$ it is natural to assume that Wick's theorem applies, in accordance with numerous system-bath descriptions. However, for the system operator $\hat{O}$ this is not in general true. A well known case where Eq. (3) holds is if the system H_S can be described as a system of noninteracting quasiparticles and $\hat{O}$ can be written as a linear combination of the annihilation and creation operators of these quasiparticles. More generally, Eq. (3) is valid if the fluctuations of $\hat{O}(t)$ have a Gaussian distribution. The expansion of n-time correlators in pair and higher correlators has been studied extensively for spin systems [58–60] and deviations from Gaussian statistics have been studied in the field of full-counting statistics [61–64]. From relatively general considerations, such as the central limit theorem [65], we expect that fluctuations become more Gaussian as the system size increases, which is also the most interesting limit for a quantum simulator. However, in some systems non-Gaussian fluctuations are known to persist even at large system size [66,67] or become even size independent [68]. For different expansions it could also be useful to map qubits coupled to bosonic baths to an effective electron-phonon model [69]. In Sec. II we discuss how Eq. (3) can be checked, to some extent, by making appropriate measurements on the perturbed quantum simulator.

Assuming Eq. (3) holds, we find an exact relation between the Green's functions

$$G_{SB}(\omega) = G_{S0}(\omega) + G_{S0}(\omega)G_{B0}(\omega)G_{SB}(\omega). \tag{4}$$

This is the well-known Dyson equation that defines the total Green's function as a function of the free system and bath Green's functions.

B. Central result

From Eq. (4) we see that the perturbed quantum simulator can be used to find the correlator of the unperturbed simulator $G_{S0}(\omega)$ as long as we know the free Green's function of the bath $G_{B0}(\omega)$, since

$$G_{S0}(\omega) = \frac{G_{SB}(\omega)}{1 + G_{B0}(\omega)G_{SB}(\omega)}. \quad (5)$$

This states the central idea of this paper in the simplest form. To derive Eq. (5) we use an important assumption, that Wick's theorem in the form in Eq. (3) applies for the system operator $\hat{O}$. This condition will be discussed in more detail in Sec. II, where we also show how to extract the lowest-order correction to this result from the perturbed simulator. Apart from this, the quality of the reconstruction is also restricted by the precision of the knowledge of the correlators, which is the subject of Sec. III. In particular, we presume that the properties of the bath are measured independently of the system, which will be discussed more detailed in Sec. IV. In Sec. IV we also consider the case where multiple baths couple to system via operators $\hat{O}^i$ and extend the reconstruction method to finite temperatures. Finally, we discuss a simple example, which can be solved analytically, to validate our result.

II. VERIFYING WICK'S THEOREM

The validity of Wick's theorem for the system operator $\hat{O}$ is crucial for the derivation of Eq. (5); however, for nontrivial systems we cannot in general predict if Wick's theorem holds. Therefore, we describe a method to verify the validity of Wick's theorem using the quantum simulator itself. A detailed derivation is given in Appendix B.

We introduce the lowest-order correction to Wick's theorem $G_4(t_1, t_2, t_3, t_4)$,

$$
\begin{aligned}
G_4(t_1, t_2, t_3, t_4) \\
= \langle \mathcal{T}\hat{O}_1\hat{O}_2\hat{O}_3\hat{O}_4 \rangle_{0,F} - \langle \mathcal{T}\hat{O}_1\hat{O}_2\hat{O}_3\hat{O}_4 \rangle_0 \\
= \langle \mathcal{T}\hat{O}_1\hat{O}_2\hat{O}_3\hat{O}_4 \rangle_{0,F} - \sum_{\substack{3 \text{ perm} \\ a,b,c,d \\ \in \{1,2,3,4\}}} \langle \mathcal{T}\hat{O}_a\hat{O}_b \rangle_0 \langle \mathcal{T}\hat{O}_c\hat{O}_d \rangle_0,
\end{aligned}
$$
$$(6)$$

where we make use of the abbreviation $\hat{O}_i = \hat{O}(t_i)$. The summation runs over all indistinguishable permutations. With $\langle \cdots \rangle_0$ and $\langle \cdots \rangle$ we refer to correlators for which we assume Wick's theorem to be exactly valid. The index 0 indicates that the system is considered without perturbation by the bath. In contrast to this, $\langle \cdots \rangle_F$ ($\langle \cdots \rangle_{0,F}$) describes the (un)perturbed correlators including the corrections to Wick's theorem. In this paper we consider corrections up to first order in G_4.

With measurements on the quantum simulator we have access to n-time correlators $\langle \ldots \rangle_F$ of $\hat{O}$. Measuring two- and four-time correlators

$$\langle \mathcal{T}\hat{O}_1\hat{O}_2\hat{O}_3\hat{O}_4 \rangle_F - \sum_{\substack{3 \text{ perm} \\ a,b,c,d \\ \in \{1,2,3,4\}}} \langle \mathcal{T}\hat{O}_a\hat{O}_b \rangle_F \langle \mathcal{T}\hat{O}_c\hat{O}_d \rangle_F = \mathtimes,$$
$$(7)$$

we get access to the quantity

$$(8)$$

where the thin cross represents the correction G_4 and the sinuous lines stand for the bath correlation function (see Table I). The central result here is that the correction to the perturbed two-time correlator can be expressed as

$$\langle \mathcal{T}\hat{O}_1\hat{O}_2 \rangle_F = \langle \mathcal{T}\hat{O}_1\hat{O}_2 \rangle + \mathbf{\times}. \quad (9)$$

Equations (7) and (9) show that it is possible to estimate the deviation from Wick's theorem by measuring the two- and four-time correlators and combining the measured result with our knowledge of the bath correlator. This allows us to check whether the assumption of Wick's theorem is justified and the result of the reconstruction is reliable.

III. IMPERFECT KNOWLEDGE

A fundamental prerequisite for the reconstruction of the unperturbed correlator is the knowledge of the perturbed correlator of the system G_{SB} and the correlator of the bath G_{B0}. In reality, we will not receive these quantities with full accuracy. In this section we address the question how imperfect knowledge affects the reconstruction of the ideal Green's function.

A. Bath correlator

We consider a variation of the Green's function of the bath $G_{B0}(\omega) + \delta G_{B0}(\omega)$. With this Green's function, we reconstruct the correlator of the simulator using Eq. (5) with

$$\tilde{G}_{S0}(\omega) = \frac{G_{SB}(\omega)}{1 + G_{B0}(\omega)G_{SB}(\omega) + \delta G_{B0}(\omega)G_{SB}(\omega)}. \quad (10)$$

For $|\delta G_{B0}(\omega)| \ll |G_{SB}^{-1}(\omega) + G_{B0}(\omega)|$, we find

$$\tilde{G}_{S0}(\omega) \approx G_{S0}(\omega)[1 - G_{S0}(\omega)\delta G_{B0}(\omega)]. \quad (11)$$

Hence, the impact of $\delta G_{B0}(\omega)$ is large at the peaks of $G_{S0}(\omega)$. The influence of $\delta G_{B0}(\omega)$ is independent of the value of $G_{B0}(\omega)$. This means that the quality of the reconstruction is defined by the absolute error $\delta G_{B0}(\omega)$ only.

B. Full system correlator

For a deviation of the full system correlator $G_{SB}(\omega) + \delta G_{SB}(\omega)$, we have

$$\tilde{G}_{S0}(\omega) = \frac{G_{SB}(\omega) + \delta G_{SB}(\omega)}{1 + G_{B0}(\omega)G_{SB}(\omega) + G_{B0}(\omega)\delta G_{SB}(\omega)}. \quad (12)$$

For $|\delta G_{SB}(\omega)| \ll |G_{B0}^{-1}(\omega) + G_{SB}(\omega)|$, we find

$$\tilde{G}_{S0}(\omega) \approx G_{S0}(\omega)\left(1 + \frac{G_{S0}(\omega)}{G_{SB}(\omega)}\frac{\delta G_{SB}(\omega)}{G_{SB}(\omega)}\right). \quad (13)$$

TABLE I. Summary of all relevant correlators and their diagrammatic representation.

Green's function	Matrix form	Diagram	Definition
$G_{SB}^{ij}(t) = -i\langle \mathcal{T}\hat{O}^i(t)\hat{O}^j(0)\rangle$	$[\mathbf{G}_{SB}]_{ij} = G_{SB}^{ij}$	━━━━━━	full correlator of the system operators, including the effects of the bath ($\lambda_B = 1$)
$G_{S0}^{ij}(t) = -i\langle \mathcal{T}\hat{O}^i(t)\hat{O}^j(0)\rangle_0$	$[\mathbf{G}_{S0}]_{ij} = G_{S0}^{ij}$	─────	free correlator of the system operators, without the effects of the bath ($\lambda_B = 0$)
$G_{B0}^{ij}(t) = -i\langle \mathcal{T}\hat{X}^i(t)\hat{X}^j(0)\rangle_0$	$[\mathbf{G}_{B0}]_{ij} = G_{B0}^{ij}$	∿∿∿∿	free correlator of the bath, without the effects of the system ($\lambda_B = 0$)

The ratio of $G_{S0}(\omega)$ and $G_{SB}(\omega)$ implies that the variation of the full system correlator $G_{S0}(\omega)$ is large at the peaks of this function. In contrast to the variation of the bath correlator in Eq. (11), the relative error $\delta G_{SB}(\omega)/G_{SB}(\omega)$ enters here.

In addition, this equation shows the limit of our reconstruction method. Consider the limit of large coupling of the bath to the system. Equation (5) is still valid, but a reconstruction is no longer possible if the bath widens the peaks of $G_{S0}(\omega)$ significantly. In this case $G_{S0}(\omega)/G_{SB}(\omega) \gg 1$ at the peaks. Therefore, even a small relative error in the measurement of $G_{SB}(\omega)$ makes the reconstruction of $G_{S0}(\omega)$ practically impossible.

IV. FULL MODEL AND DISCUSSION

A. Extended model

In this section we extend the model to a more general scenario and discuss the derivation of our results in detail. To make our model more realistic, we consider multiple baths. In practice, a system consisting of N coupled qubits or resonators arranged in a certain two-dimensional geometry does not couple to a single bath. Instead, we consider a system with multiple independent baths $H_B = \sum_{i=1}^{N} H_B^i$ with $[H_B^i, H_B^j] = 0$ and a similarly adjusted coupling term. The full Hamiltonian can now be written in the form

$$H = H_S + H_C + \sum_{i=1}^{N} H_B^i. \qquad (14)$$

The coupling H_C between the system and the additional degrees of freedom contained in $\sum_i H_B^i$ is assumed to be of the form

$$H_C = \lambda_B \sum_{i=1}^{N} \hat{O}^i \hat{X}^i. \qquad (15)$$

The system and bath variables satisfy the commutation relation $[\hat{X}^i, H_S] = [\hat{O}^i, H_B] = [\hat{X}^i, \hat{X}^j] = 0$. We have now N system operators $\hat{O}^i$ which couple the system to N baths via the corresponding bath operators $\hat{X}^i$. We have introduced the dimensionless constant $\lambda_B \in \{0,1\}$, which allows us to define the free and perturbed correlators in a more rigorous way (see Table I).

To perform the reconstruction of the unperturbed Green's function of the system, we need to characterize the properties of the baths independently of the system [70]. This assumption is justified, for example, for a large network of superconducting flux qubits coupled in a two-dimensional (2D) structure to simulate a spin system. Such systems have been realized with up to 1000 qubits [39,40]. The ideal Hamiltonian in this case would be, e.g., $H_S = \frac{1}{2}\sum_i h_i \sigma_x^i + \sum_{ij} J_{ij} \sigma_z^i \sigma_z^j$. Here h_i and J_{ij} are adjustable parameters which define the model under investigation and σ_k^i are the Pauli matrices acting on qubit i.

Under the assumption that the effect of the noise on a single qubit is almost Markovian, it is possible to characterize the noise spectral density of the decoupled qubits using the method described in [71]. The qubits are coupled to individual baths, whose bath correlators $\langle \hat{X}^i(t)\hat{X}^i(0)\rangle_0$ are known relatively well, as estimated in Ref. [72]. From a multitude of similar experiments we know that the system operator that couples to the bath corresponds to $\hat{O}^i = \sigma_z^i$. Thus, for such a quantum simulator the characterization of the bath correlator is possible independently of the properties of the simulator. Furthermore, the applicability of Wick's theorem has been studied broadly [58–60] in context of spin systems. Devices such as large networks of superconducting flux qubits coupled in a 2D structure can also be tuned into alternative regimes, e.g., into a weakly nonlinear regime where proposals exist on how to use such devices for the simulation of vibronic transitions [73]. In this limit, the application of Wick's theorem would also be more straightforward.

B. Full Green's function

In Eq. (1) we introduced the Green's function of the system without coupling to external degrees of freedom. In this section we consider the Green's function $\mathbf{G}_{SB}$ of the system coupled to its bath in matrix form with the elements

$$G_{SB}^{ij}(t) = -i\langle \mathcal{T}\hat{O}^i(t)\hat{O}^j(0)\rangle, \qquad (16)$$

where $\langle \cdots \rangle$ is an expectation value of the ground state of the full system. Using the standard technique for Green's functions at zero temperature, we expand $G_{SB}^{ij}(t)$ in orders of H_C. Therefore, the zeroth-order Hamiltonian is given by $H_0 = H_S + \sum_i H_B^i$. We define the time evolution

$$S_{\lambda_B}(t) = e^{-iHt} \qquad (17)$$

and transform all operators $\hat{A}$ into the appropriate picture using the definition

$$\hat{A}(t) = S_{\lambda_B}^{-1}(t)\hat{A}S_{\lambda_B}(t). \qquad (18)$$

For unperturbed correlators $\langle \cdots \rangle_0$ this transformation with $S_{\lambda_B=0}(t) = e^{-iH_0 t}$ defines operators in the interaction picture, while $\lambda_B = 1$ denotes the full time evolution in the Heisenberg picture for the perturbed correlators $\langle \cdots \rangle$. The full Green's function can be written in the form

$$G_{SB}^{ij}(t) = -i\frac{\langle \mathcal{T}S(\infty)\hat{O}^i(t)\hat{O}^j(0)\rangle_0}{\langle \mathcal{T}S(\infty)\rangle_0}, \qquad (19)$$

with the time evolution operator

$$S(\infty) = \mathcal{T}\exp\left(-i\int_{-\infty}^{\infty} dt\, H_C(t)\right), \qquad (20)$$

where we use the coupling Hamiltonian in the interaction picture. We introduce the Fourier transform of the Green's

TABLE II. Each circle represents a term of the expansion in H_C.

Interaction	Diagram	Definition
$\sum_{i=1}^{N} \hat{O}_i \hat{X}^i$	——◦〰	interaction between bath and system

function

$$G_X^{ij}(\omega) = \int_{-\infty}^{\infty} dt \, e^{i\omega t} G_X^{ij}(t).$$ (21)

C. Diagrammatic expansion

We show now the diagrammatic expansion that leads to expressions such as Eq. (4) if Wick's theorem is valid for the coupling operators. All relevant correlators and their diagrammatic representations are shown in Table I and the interaction term is shown in Table II.

Using an expansion of $S(\infty)$ in H_C, we can directly show the connection between the Green's function of the simulator perturbed by a bath G_{SB}^{ij} and the unperturbed ideal Green's functions

$$
\begin{aligned}
\text{═══} &= \text{──} + \text{──◦〰◦──} + \text{──◦〰◦──◦〰◦──} + \cdots \\
&= \text{──} + \text{──◦〰◦}(\text{──} + \text{──◦〰◦──} \cdots) \\
&= \text{──} + \text{──◦〰□═══} .
\end{aligned}
$$ (22)

Here all disconnected diagrams are canceled by the vacuum diagrams in $\langle \mathcal{T} S(\infty) \rangle_0$ (see Appendix A). Therefore we can write the Dyson equation in matrix form as

$$\mathbf{G}_{SB}(\omega) = \mathbf{G}_{S0}(\omega) + \mathbf{G}_{S0}(\omega)\mathbf{G}_{B0}(\omega)\mathbf{G}_{SB}(\omega).$$ (23)

If all Green's functions $G_{SB}^{ij}(\omega)$ and $G_{B0}^{ij}(\omega)$ are known, this equation can be solved for $\mathbf{G}_{S0}$:

$$\mathbf{G}_{S0}(\omega) = \mathbf{G}_{SB}(\omega)[1 + \mathbf{G}_{B0}(\omega)\mathbf{G}_{SB}(\omega)]^{-1}.$$ (24)

If we reduce the system to a single-bath situation, this result transforms to Eq. (5). It connects the ideal correlator in Eq. (1) to quantities which can be readily measured.

D. Extension to finite temperatures

The diagrammatic expansion in Sec. IV C can also be applied to the Matsubara Green's functions $\mathcal{G}_{M,X}$, which are connected to the retarded Green's functions for finite temperatures $\mathcal{G}_X^R$. This is a way to extend this method to systems in thermal equilibrium. The analog of Eq. (5) for finite temperatures is given by

$$\mathcal{G}_{S0}^R(i\omega_n) = \frac{\mathcal{G}_{SB}^R(i\omega_n)}{1 + \mathcal{G}_{B0}^R(i\omega_n)\mathcal{G}_{SB}^R(i\omega_n)}.$$ (25)

Below we introduce the Matsubara Green's functions and explain the connection to the spectral function.

1. Expansion in imaginary time

As we consider the whole system to be in thermal equilibrium, it is reasonable to use the standard Matsubara Green's function method. Therefore, we define the imaginary time

$\tau = it$ where we require $0 < \tau < \beta$. The Matsubara Green's function equivalent to Eq. (16) is

$$\mathcal{G}_{M,SB}^{ij}(\tau) = -\langle \mathcal{T} \hat{O}^i(\tau) \hat{O}^j(0) \rangle,$$ (26)

where $\mathcal{T}$ is the time-ordering operator for τ. In the case of finite temperatures, $\langle \cdots \rangle$ refers to the equilibrium expectation value $\text{Tr}(\frac{1}{Z} e^{-\beta H} \cdots)$, with $Z = \text{Tr}(e^{-\beta H})$. The time evolution in imaginary time is given by

$$U_{\lambda_B}(\tau) = e^{-H\tau}.$$ (27)

We transform all operators $\hat{A}$ into the appropriate picture in imaginary time using the definition

$$\hat{A}(\tau) = U_{\lambda_B}^{-1}(\tau)\hat{A}U_{\lambda_B}(\tau).$$ (28)

The full correlator can be written in the form

$$\mathcal{G}_{M,SB}(\tau) = -\frac{\langle \mathcal{T} U(\beta)\hat{O}^i(\tau)\hat{O}^j(0) \rangle_0}{\langle \mathcal{T} U(\beta) \rangle_0},$$ (29)

with evolution operator

$$U(\tau) = \mathcal{T} \exp\left(-\int_0^\tau d\tau' H_{C,I}(\tau')\right).$$ (30)

As for zero temperature, all disconnected diagrams are canceled by the factor $\langle \mathcal{T} U(\beta) \rangle_0$, the so-called vacuum diagrams.

The correlator in imaginary time is periodic in τ with period β. It is convenient to transform it to frequency space using the discrete Fourier transform

$$\mathcal{G}_{M,X}^{ij}(\tau) = \frac{1}{\beta} \sum_n \mathcal{G}_{M,X}^{ij}(\omega_n)e^{-i\omega_n \tau}$$ (31)

with the Matsubara frequencies $\omega_n = 2\pi n/\beta$.

2. Connecting a real-time correlator to the Matsubara Green's function

Now we discuss the connection of the Matsubara Green's function to measurable quantities such as the spectral function or correlators. As an example we focus on the Green's function of the bath.

We define the correlation function

$$C^i(t) = [\langle \hat{X}^i(t)\hat{X}^i(0) \rangle_0 - \langle \hat{X}^i(0)\hat{X}^i(t) \rangle_0]\theta(t).$$ (32)

The eigenstates of the bath are given by $|n\rangle$, with $H_B|n\rangle = E_n|n\rangle$. This allows us to rewrite the correlator

$$C^i(t) = \frac{\theta(t)}{Z_B} \sum_{nm} |\langle n|\hat{X}^i|m\rangle|^2 e^{i(E_n - E_m)t}(e^{-\beta E_n} - e^{-\beta E_m}),$$ (33)

with the partition function $Z_B = \text{Tr}(e^{-\beta H_B})$. The real part of the Fourier transform of the correlator gives us the spectral function

$$A^i(\omega) = \frac{1}{\pi}\text{Re}\left(\int_{-\infty}^\infty dt \, e^{i\omega t} C^i(t)\right) = \frac{1}{Z_B} \sum_{nm} |\langle n|\hat{X}^i|m\rangle|^2$$

$$\times (e^{-\beta E_m} - e^{-\beta E_n})\delta(\omega - (E_n - E_m)).$$ (34)

Apart from a factor -1, the imaginary part of the retarded Green's function $\mathcal{G}_{B0}^R(t)$ is equivalent to the correlation function $C^i(t)$, since

$$\mathcal{G}_{B0}^{R,ii}(t) = -i\langle [\hat{X}^i(t), \hat{X}^i(0)] \rangle_0 \theta(t).$$ (35)

Assuming that $A^i(\omega)$ has been measured, the retarded Green's function $\mathcal{G}_{B0}^R(\omega)$ of the bath can be calculated using

$$\mathcal{G}_{B0}^{R,ii}(\omega) = \int_{-\infty}^{\infty} d\omega_1 \frac{A^i(\omega_1)}{\omega - \omega_1 + i0}. \tag{36}$$

Describing the Matsubara Green's function in terms of the spectral function shows a connection to the retarded Green's function for finite temperatures $\mathcal{G}_P^R$,

$$\mathcal{G}_{M,P}^{ij}(\omega_n) = \mathcal{G}_P^{R,ij}(i\omega_n), \quad \omega_n > 0, \tag{37}$$

with $P \in \{B0, S0, SB\}$. This requires an analytic continuation of $\mathcal{G}_P^R$ in the complex plane. Via the spectral function we can derive the Kramers-Kronig relation

$$\mathcal{G}_P^{ij}(\omega) = \text{Re}\mathcal{G}_P^{R,ij}(\omega) + i[1 + 2\bar{n}(\omega)]\text{Im}\mathcal{G}_P^{R,ij}(\omega), \tag{38}$$

with $\bar{n}(\omega) = (e^{\beta\omega} - 1)^{-1}$. Starting from the Matsubara Green's function, we obtain information about the retarded Green's function at the points $i\omega_n$. We would like to have the ideal Green's function $\mathcal{G}_{S0}^R$, i.e., the spectral function, for the complete real axis. This can be achieved by using numerical methods like the Padé approximation approach [74,75]. However, it should be emphasized that the numerical transformation of a Green's function at the Matsubara frequencies to the real axis is still a nontrivial problem and an active research field [76].

E. Model system: Chain of resonators with individual baths

In this section we give an explicit example of our method and particularly of the validity of Eq. (24). We consider a system of coupled harmonic oscillators

$$H_S = \sum_{j=1}^{N} \left(\frac{1}{2}m\omega_r^2 q_j^2 + \frac{1}{2m}p_j^2 + \frac{m\Omega^2}{2}(q_{j+1} - q_j)^2 \right), \tag{39}$$

where N is the number of resonators, m refers to the mass, ω_r is the eigenfrequency of an uncoupled resonator, and Ω describes the coupling between neighboring oscillators. We assume periodic boundary conditions. For a system of coupled resonators, Wick's theorem stated in Eq. (3) is clearly valid. Here we show the validity of our previously derived results. We validate our results for the connection between the ideal and perturbed correlators by using the quantum regression theorem (QRT) [77]. While the system of bare coupled resonators would not make for a good quantum simulator, proposals exist for modeling the Bose-Hubbard model using coupled nonlinear resonators [78]. Similarly, limiting cases from noninteracting bosons to hard-core bosons have been studied in the context of analog quantum simulation [79].

We assume that each of the resonators is coupled to an individual bosonic bath

$$H_C = \sum_j \hat{O}^j \hat{X}^j, \quad H_B = \sum_{j,m} \bar{\omega}_m^{(j)} b_m^{(j)\dagger} b_m^{(j)}, \tag{40}$$

with $\hat{O}^j = q_j$ and $\hat{X}^j = \sum_m t_m^{(j)}(b_m^{(j)\dagger} + b_m^{(j)})$. We assume the baths to be identical, i.e.,

$$\bar{\omega}_m^{(j)} = \bar{\omega}_m, \quad t_m^{(j)} = t_m, \tag{41}$$

but independent

$$\langle \hat{X}^{j_1}(t_1)\hat{X}^{j_2}(t_2)\rangle_0 = 0 \quad \text{for } j_1 \neq j_2. \tag{42}$$

Diagonalizing the system Hamiltonian results in

$$H_S = \sum_k \Omega_k a_k^\dagger a_k \quad \text{with } \Omega_k = \sqrt{\left[2\Omega \sin\left(k\frac{\varphi_0}{2}\right)\right]^2 + \omega_r^2}, \tag{43}$$

where $\varphi_0 = \frac{2\pi}{N}$. The connection of annihilation and creation operators of system eigenstates, a_k and $a_k^\dagger$, to the original operators has the form

$$q_j = \sqrt{\frac{1}{2m\omega_r}}(d_j^\dagger + d_j), \tag{44}$$

$$d_j = \frac{1}{2\sqrt{N}} \sum_{k=1}^{N} \left[e^{-ikj\varphi_0}\left(\sqrt{\frac{\omega_r}{\Omega_K}} - \sqrt{\frac{\Omega_K}{\omega_r}}\right)a_k^\dagger \right.$$
$$\left. + e^{ijk\varphi_0}\left(\sqrt{\frac{\omega_r}{\Omega_K}} + \sqrt{\frac{\Omega_K}{\omega_r}}\right)a_k \right]. \tag{45}$$

We consider finite temperatures. Therefore, the spectral density of the bath is given by

$$A^i(\omega) \approx \frac{1}{2\pi}\text{sgn}(\omega)J^i(|\omega|), \tag{46}$$

with $J^i(\omega) = J(\omega) = 2\pi \sum_m t_m^2 \delta(\omega - \bar{\omega}_m)$.

To compare Eq. (24) to correlators calculated using a master-equation approach, we calculate the full Green's function $\mathcal{G}_{M,SB}^{j_1,j_2}$ using the QRT. To this end we assume the dynamics of the full system to be approximately described by the Lindblad equation

$$\dot{\rho}(t) = \mathcal{L}\rho(t), \tag{47}$$

with the Lindblad terms

$$\mathcal{L}\rho = -i[H_S, \rho]$$
$$+ \sum_{k=1}^{N} \frac{\Gamma_k}{2}(\bar{n}_k + 1)(2a_k\rho a_k^\dagger - a_k^\dagger a_k\rho - \rho a_k^\dagger a_k)$$
$$+ \sum_{k=1}^{N} \frac{\Gamma_k}{2}\bar{n}_k(2a_k^\dagger\rho a_k - a_k a_k^\dagger\rho - \rho a_k a_k^\dagger), \tag{48}$$

where $\bar{n}_k = (e^{\beta\Omega_k} - 1)^{-1}$. Assuming the spectral density of the bath to be smooth, we find the effective rates

$$\Gamma_k = \frac{1}{2m\Omega_k}J(\Omega_k), \tag{49}$$

where the prefactor $(2m\omega_r)^{-1}$ arises from $\hat{O}^i = \sqrt{2m\omega_r}^{-1}(d_j^\dagger + d_j)$ and $\frac{\omega_r}{\Omega_k}$ is a result of the transition from $d_j^\dagger + d_j$ to $a_k^\dagger + a_k$. In accordance with the assumptions used for the Lindblad equation, Eq. (36) reduces to

$$i\mathcal{G}_{B0}^{R,ij}(\omega) \approx \delta_{ij}\frac{1}{2}\text{sgn}(\omega)J^i(|\omega|). \tag{50}$$

For the Lindblad equation to be valid, some assumptions have to be made about the spectral density of the bath.

With the QRT, the Lindblad terms fulfill the following equation for an arbitrary operator $\hat{A}$ and all k [77]:

$$\text{Tr}[a_k\mathcal{L}\hat{A}] = -\left(i\Omega_k + \frac{\Gamma_k}{2}\right)\text{Tr}[a_k\hat{A}]. \tag{51}$$

For $t > 0$ we get

$$\langle \hat{A}(t_0) a_k(t + t_0) \rangle = e^{-i\Omega_k t} e^{-(\Gamma_k/2)t} \langle \hat{A}(t_0) a_k(t_0) \rangle, \quad (52)$$

$$\langle a_k(t + t_0) \hat{A}(t_0) \rangle = e^{-i\Omega_k t} e^{-(\Gamma_k/2)t} \langle a_k(t_0) \hat{A}(t_0) \rangle, \quad (53)$$

$$\langle \hat{A}(t_0) a_k^\dagger(t + t_0) \rangle = e^{+i\Omega_k t} e^{-(\Gamma_k/2)t} \langle \hat{A}(t_0) a_k^\dagger(t_0) \rangle, \quad (54)$$

$$\langle a_k^\dagger(t + t_0) \hat{A}(t_0) \rangle = e^{+i\Omega_k t} e^{-(\Gamma_k/2)t} \langle a_k^\dagger(t_0) \hat{A}(t_0) \rangle. \quad (55)$$

The stationary solution of the Lindblad equation is proportional to $\exp(-\beta \sum_k \Omega_k a_k^\dagger a_k)$. Using this, we calculate the initial values for $\langle a_k^{(\dagger)}(t_0) a_k^{(\dagger)}(t_0) \rangle$ and find

$$\langle a_k(t_1) a_{k'}(t_2) \rangle = 0, \quad (56)$$

$$\langle a_k^\dagger(t_1) a_{k'}(t_2) \rangle = \delta_{k,k'} \bar{n}_k e^{i\Omega_k(t_1-t_2)} e^{-(\Gamma_k/2)|t_1-t_2|}, \quad (57)$$

$$\langle a_k(t_1) a_{k'}^\dagger(t_2) \rangle = \delta_{k,k'} (\bar{n}_k + 1) e^{i\Omega_k(t_1-t_2)} e^{-(\Gamma_k/2)|t_1-t_2|}, \quad (58)$$

$$\langle a_k^\dagger(t_1) a_{k'}^\dagger(t_2) \rangle = 0. \quad (59)$$

A direct calculation of the free correlators results in

$$\langle a_k(t_1) a_{k'}(t_2) \rangle_0 = 0, \quad (60)$$

$$\langle a_k^\dagger(t_1) a_{k'}(t_2) \rangle_0 = \delta_{k,k'} \bar{n}_k e^{i\Omega_k(t_1-t_2)}, \quad (61)$$

$$\langle a_k(t_1) a_{k'}^\dagger(t_2) \rangle_0 = \delta_{k,k'} (\bar{n}_k + 1) e^{i\Omega_k(t_1-t_2)}, \quad (62)$$

$$\langle a_k^\dagger(t_1) a_{k'}^\dagger(t_2) \rangle_0 = 0. \quad (63)$$

From this result we calculate the retarded Green's functions $\mathcal{G}_{S0}^{R,j_1 j_2}(t)$, $\mathcal{G}_{SB}^{R,j_1 j_2}(t)$ and perform the Fourier transform. With an analytic continuation and Eq. (37) we finally arrive at the Matsubara Green's functions for $\omega_n > 0$:

$$\mathcal{G}_{M,S0}^{j_1 j_2}(\omega_n) = \frac{1}{N} \sum_{k=1}^{N} \frac{1}{2m\Omega_k}$$
$$\times [e^{-ik(j_1-j_2)\varphi_0} \bar{n}_k - e^{ik(j_1-j_2)\varphi_0} (\bar{n}_k + 1)]$$
$$\times \left(\frac{1}{i\omega_n + \Omega_k + i0} - \frac{1}{i\omega_n - \Omega_k + i0} \right), \quad (64)$$

$$\mathcal{G}_{M,SB}^{j_1 j_2}(\omega_n) = \frac{1}{N} \sum_{k=1}^{N} \frac{1}{2m\Omega_k}$$
$$\times [e^{-ik(j_1-j_2)\varphi_0} \bar{n}_k - e^{ik(j_1-j_2)\varphi_0} (\bar{n}_k + 1)]$$
$$\times \left(\frac{1}{i\omega_n + \Omega_k + i\frac{\Gamma_k}{2}} - \frac{1}{i\omega_n - \Omega_k + i\frac{\Gamma_k}{2}} \right). \quad (65)$$

To calculate the bath Green's function using Eq. (24) we introduce the transformation

$$\mathcal{G}_{M,S0}^k(\omega_n) = \sum_{j_1,j_2} \mathcal{G}_{M,S0}^{j_1 j_2} e^{ik(j_1-j_2)k\varphi_0}$$
$$= \frac{N}{2m\Omega_k} \left(\frac{1}{i\omega_n - \Omega_k + i0} - \frac{1}{i\omega_n + \Omega_k + i0} \right), \quad (66)$$

$$\mathcal{G}_{M,SB}^k(\omega_n) = \sum_{j_1,j_2} \mathcal{G}_{M,SB}^{j_1 j_2} e^{ik(j_1-j_2)k\varphi_0}$$
$$= \frac{N}{2m\Omega_k} \left(\frac{1}{i\omega_n - \Omega_k + i\frac{\Gamma_k}{2}} - \frac{1}{i\omega_n + \Omega_k + i\frac{\Gamma_k}{2}} \right). \quad (67)$$

With this Eq. (24) results in

$$\mathcal{G}_{M,SB}^k(\omega_n) = \mathcal{G}_{M,S0}^k(\omega_n) + \mathcal{G}_{M,S0}^k(\omega_n) \mathcal{G}_{M,SB}^k(\omega_n)$$
$$\times \sum_j \mathcal{G}_{M,BO}^{jj}(\omega_n) \frac{1}{N^2}. \quad (68)$$

In the Lindblad equation we take into account the spectral density of the bath at Ω_k. Since the bath Green's function depends on the spectral density of the bath, the relation is true for $\omega_n \approx \Omega_k$. Using the assumption of identical and independent baths we arrive at

$$\mathcal{G}_{M,BO}^{j_1 j_2}(\omega_n \approx \Omega_k) \approx \delta_{j_1,j_2} m\Gamma_k \left(\Omega_k + \frac{\Gamma_k}{4} \right). \quad (69)$$

In the limit of small coupling to the bath $\Gamma_k \ll \Omega_k$, we are left with

$$\mathcal{G}_{M,BO}^{j_1 j_2}(\omega_n \approx \Omega_k) \approx \delta_{j_1,j_2} \frac{1}{2} J(\Omega_k). \quad (70)$$

From a comparison to Eq. (50), we conclude that Eq. (24) holds for this example. For an Ohmic spectral density and with $\Omega_k \to i\omega$ the Matsubara Green's function of the bath coincides with Eq. (50).

V. CONCLUSION

The main result we presented in this paper is twofold. On the one hand, we introduced a method that can be used to reconstruct certain unperturbed (ideal) Green's functions from the perturbed ones, measured by a quantum simulator coupled to additional degrees of freedom. To achieve this, we assumed that any n-time correlator of the coupling operator of the ideal system can be written as a product of two-time correlators. This is known as Wick's theorem. On the other hand, we explained how to verify this assumption by a measurement. Furthermore, we assumed good knowledge of the bath correlators to perform the reconstruction. In particular, we presumed that these correlators are measured independently when not coupled to the ideal system. We also clarified how imperfect measurements of the bath and of the full correlator affect the reconstruction. For example, in the case of strong coupling to the bath our result is still valid, but the reconstruction fails even in the presence of small noise during the measurement.

Presently, the applicability of analog quantum simulation is severely restricted, since the influence of sources of errors is not well understood. The approach presented in this paper leads the way to quantify and even correct errors in quantum simulation. Since the reconstruction method is based on classical postprocessing, this method helps to make the results of quantum simulation reliable without adding an overhead to the quantum system. Therefore, the promising potential of quantum simulation to yield interesting results even using small quantum systems remains.

APPENDIX A: DISCONNECTED DIAGRAMS

In this Appendix we explain how the so-called vacuum diagrams $\langle \mathcal{T} S(\infty) \rangle_0$ cancel the disconnected diagrams in the free two-time correlator $\langle \mathcal{T} S(\infty) \hat{O}_I(t) \hat{O}_I(0) \rangle_0$. To shorten the equations we use $\hat{A}_i$ as an abbreviation for $\hat{A}(t_i)$. For simplicity we base our discussion on a coupling Hamiltonian of the form $H_C = \hat{O} \hat{X}$. It is straightforward to extend this calculations on the full model described in Sec. IV. The vacuum diagrams are given by

$$\langle \mathcal{T} S(\infty) \rangle_0 = \sum_n \frac{1}{n!} (-i)^n \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \langle \mathcal{T} \hat{O}_1 \cdots \hat{O}_n \rangle_0 \langle \mathcal{T} \hat{X}_1 \cdots \hat{X}_n \rangle_0 = \sum_n V_n, \tag{A1}$$

where we assume

$$\langle \hat{O}_I(t) \rangle_0 = 0, \quad \langle \hat{X}_I(t) \rangle_0 = 0 \tag{A2}$$

so that terms with n being an odd number are zero. We have introduced V_n, the vacuum diagrams of order n. Now we elaborate the connection between the free correlator and the vacuum diagrams. The free two-time correlator is given by

$$\langle \mathcal{T} S(\infty) \hat{O}_a \hat{O}_b \rangle_0 = \sum_n \frac{1}{n!} (-i)^n \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \langle \mathcal{T} \hat{O}_a \hat{O}_b \hat{O}_1 \cdots \hat{O}_n \rangle_0 \langle \mathcal{T} \hat{X}_1 \cdots \hat{X}_n \rangle_0. \tag{A3}$$

From this we apply Wick's theorem and take out the two-time correlators which form a connected diagram and recombine the surplus correlators in a higher-order correlator. There are $\frac{n!}{(n-m)!}$ possibilities to choose m vertices out of n. Therefore, a connected diagram with m vertices occurs $\frac{n!}{(n-m)!}$ times

$$\langle \mathcal{T} S(\infty) \hat{O}_a \hat{O}_b \rangle_0 = \sum_n \frac{1}{n!} (-i)^n \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \sum_m^n \langle \mathcal{T} \hat{O}_a \hat{O}_1 \rangle_0 \langle \mathcal{T} \hat{X}_1 \hat{X}_2 \rangle_0 \langle \mathcal{T} \hat{O}_2 \hat{O}_3 \rangle_0 \cdots \langle \mathcal{T} \hat{X}_{m-1} \hat{X}_m \rangle_0 \langle \mathcal{T} \hat{O}_m \hat{O}_b \rangle_0$$
$$\times \frac{n!}{(n-m)!} \langle \mathcal{T} \hat{O}_{m+1} \cdots \hat{O}_n \rangle_0 \langle \mathcal{T} \hat{X}_{m+1} \cdots \hat{X}_n \rangle_0. \tag{A4}$$

By resorting the factors we can identify the vacuum diagrams of order $n - m$,

$$\langle \mathcal{T} S(\infty) \hat{O}_a \hat{O}_b \rangle_0 = \sum_n \sum_m^n \underbrace{(-i)^m \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_m \langle \mathcal{T} \hat{O}_a \hat{O}_1 \rangle_0 \langle \mathcal{T} \hat{X}_1 \hat{X}_2 \rangle_0 \langle \mathcal{T} \hat{O}_2 \hat{O}_3 \rangle_0 \cdots \langle \mathcal{T} \hat{X}_{m-1} \hat{X}_m \rangle_0 \langle \mathcal{T} \hat{O}_m \hat{O}_b \rangle_0}_{=C_m^{a,b}}$$

$$\times \overbrace{\frac{1}{(n-m)!} (-i)^{n-m} \int_{-\infty}^{\infty} dt_{m+1} \cdots \int_{-\infty}^{\infty} dt_n \langle \mathcal{T} \hat{O}_{m+1} \cdots \hat{O}_n \rangle_0 \langle \mathcal{T} \hat{X}_{m+1} \cdots \hat{X}_n \rangle_0}^{=V_{n-m}}, \tag{A5}$$

and find the connected diagrams of order m, which we will call $C_m^{a,b}$, with $C_0^{a,b} = \langle \mathcal{T} \hat{O}_a \hat{O}_b \rangle_0$. One can factor out $\langle \mathcal{T} S(\infty) \rangle_0$ by using the Cauchy product formula

$$\langle \mathcal{T} S(\infty) \hat{O}_a \hat{O}_b \rangle_0 = \sum_n^{\infty} \sum_m^n C_m^{a,b} V_{n-m} = \sum_m^{\infty} C_m^{a,b} \sum_n^{\infty} V_n = \langle \mathcal{T} S(\infty) \rangle_0 \sum_m^{\infty} C_m^{a,b}. \tag{A6}$$

This means that the vacuum diagrams cancel all disconnected diagrams, i.e.,

$$\frac{\langle \mathcal{T} S(\infty) \hat{O}_a \hat{O}_b \rangle_0}{\langle \mathcal{T} S(\infty) \rangle_0} = \text{———} + \text{—o∿o—} + \text{—o∿o— —o∿o—} + \cdots . \tag{A7}$$

APPENDIX B: FOUR-TIME CORRELATOR

In this Appendix we consider a system where Wick's theorem is not exactly valid. The goal is to derive Eqs. (7) and (9) in order to quantify the deviation from Wick's theorem. We define the lowest-order correction to Wick's theorem as

$G_4(t_1, t_2, t_3, t_4)$,

$$G_4(t_1, t_2, t_3, t_4) = \langle \mathcal{T} \hat{O}_1 \hat{O}_2 \hat{O}_3 \hat{O}_4 \rangle_{0,F} - \langle \mathcal{T} \hat{O}_1 \hat{O}_2 \hat{O}_3 \hat{O}_4 \rangle_0 = \langle \mathcal{T} \hat{O}_1 \hat{O}_2 \hat{O}_3 \hat{O}_4 \rangle_{0,F} - \sum_{\substack{3 \text{ perm} \\ a,b,c,d}} \langle \mathcal{T} \hat{O}_a \hat{O}_b \rangle_0 \langle \mathcal{T} \hat{O}_c \hat{O}_d \rangle_0, \tag{B1}$$

where the summation runs over all three indistinguishable permutations. With $\langle \cdots \rangle$ ($\langle \cdots \rangle_0$) we refer to (un)perturbed correlators for which we assume Wick's theorem to be exactly valid. In contrast to this, $\langle \cdots \rangle_F$ ($\langle \cdots \rangle_{0,F}$) describe the (un)perturbed correlators including the corrections to Wick's theorem. In this paper we only consider the lowest-order correction to Wick's theorem (G_4). All higher-order corrections are neglected. To shorten the equations we use the abbreviation $G_4(1,2,3,4) = G_4(t_1,t_2,t_3,t_4)$. An n-time correlator is then given by

$$\langle \mathcal{T} \hat{O}_1 \cdots \hat{O}_n \rangle_{0,F} = \langle \mathcal{T} \hat{O}_1 \cdots \hat{O}_n \rangle_0 + \sum_{\substack{\text{perm.} \\ \alpha,\beta,\gamma,\delta}} G(\alpha,\beta,\gamma,\delta) \left\langle \mathcal{T} \prod_{k \in \{1,\ldots,n\} \setminus \{\alpha,\beta,\gamma,\delta\}} \hat{O}_k \right\rangle_0. \tag{B2}$$

At first we show for the four-time correlator that if Wick's theorem is valid for the unperturbed correlator, it is also valid for the perturbed one. We start with

$$\langle \mathcal{T} \hat{O}_\mathrm{I} \hat{O}_\mathrm{II} \hat{O}_\mathrm{III} \hat{O}_\mathrm{IV} \rangle = \frac{\langle \mathcal{T} S(\infty) \hat{O}_\mathrm{I} \hat{O}_\mathrm{II} \hat{O}_\mathrm{III} \hat{O}_\mathrm{IV} \rangle_0}{\langle \mathcal{T} S(\infty) \rangle_0} \tag{B3}$$

$$= \sum_n \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \frac{1}{\langle \mathcal{T} S(\infty) \rangle_0} \langle \mathcal{T} \hat{O}_\mathrm{I} \hat{O}_\mathrm{II} \hat{O}_\mathrm{III} \hat{O}_\mathrm{IV} \hat{O}_1 \cdots \hat{O}_n \rangle_0 \langle \mathcal{T} \hat{X}_1 \cdots \hat{X}_n \rangle_0. \tag{B4}$$

We focus on a coupling Hamiltonian of the form $H_C = \hat{O} \hat{X}$. We proceed as in Appendix A and identify connected diagrams $C_m^{a,b}$ with m vertices. Such diagrams occur $\frac{n!}{(n-m)!}$ times. There are six indistinguishable possibilities to choose a and b. Out of the remaining $n - m$ operators we choose a connected diagram $C_k^{c,d}$ with k vertices. This occurs $\frac{(n-m)!}{(n-m-k)!}$ times. As, for example, $C_m^{\mathrm{I,II}}$ and $C_k^{\mathrm{I,II}}$ for $m = k$ are indistinguishable, we have in fact three indistinguishable permutations to take into account:

$$\langle \mathcal{T} \hat{O}_\mathrm{I} \hat{O}_\mathrm{II} \hat{O}_\mathrm{III} \hat{O}_\mathrm{IV} \rangle = \sum_n \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \frac{1}{\langle \mathcal{T} S(\infty) \rangle_0} \sum_{\substack{3 \text{ perm} \\ a,b}} \sum_m^n \frac{n!}{(n-m)!} \langle \mathcal{T} \hat{O}_a \hat{O}_1 \rangle_0 \langle \mathcal{T} \hat{X}_1 \hat{X}_2 \rangle_0 \langle \mathcal{T} \hat{O}_2 \hat{O}_3 \rangle_0 \cdots \langle \mathcal{T} \hat{O}_m \hat{O}_b \rangle_0$$

$$\times \sum_k^{n-m} \frac{(n-m)!}{(n-m-k)!} \langle \mathcal{T} \hat{O}_c \hat{O}_{m+1} \rangle_0 \langle \mathcal{T} \hat{X}_{m+1} \hat{X}_{m+2} \rangle_0 \langle \mathcal{T} \hat{O}_{m+2} \hat{O}_{m+3} \rangle_0 \cdots \langle \mathcal{T} \hat{O}_{m+k} \hat{O}_d \rangle_0$$

$$\times \langle \mathcal{T} \hat{O}_{m+k+1} \cdots \hat{O}_n \rangle_0 \langle \mathcal{T} \hat{X}_{m+k+1} \cdots \hat{X}_n \rangle_0 \tag{B5}$$

$$= \sum_{\substack{3 \text{ perm} \\ a,b}} \frac{1}{\langle \mathcal{T} S(\infty) \rangle_0} \sum_n^\infty \sum_m^n C_m^{a,b} \sum_k^{n-m} C_k^{c,d} V_{n-m-k} = \sum_{\substack{3 \text{ perm} \\ a,b}} \frac{1}{\langle \mathcal{T} S(\infty) \rangle_0} \sum_n^\infty V_n \sum_m^\infty C_m^{a,b} \sum_k^\infty C_k^{c,d} \tag{B6}$$

$$= \sum_{\substack{3 \text{ perm} \\ a,b}} \langle \mathcal{T} \hat{O}_a \hat{O}_b \rangle \langle \mathcal{T} \hat{O}_c \hat{O}_d \rangle. \tag{B7}$$

The resummation in Eq. (B6) represents the Cauchy product formula for three series followed by an index shift. Hence, we expressed the full four-time correlator in terms of full two-time correlators.

Now we include the corrections to Wick's theorem and only consider the lowest-order correction G_4. We introduce the correction to the normalization $\langle \mathcal{T} S(\infty) \rangle_{0,\mathrm{corr}}$,

$$\frac{1}{\langle \mathcal{T} S(\infty) \rangle_{0,F}} = \frac{1}{\langle \mathcal{T} S(\infty) \rangle_0 + \langle \mathcal{T} S(\infty) \rangle_{0,\mathrm{corr}}} \approx \frac{1}{\langle \mathcal{T} S(\infty) \rangle_0} \left(1 - \frac{\langle \mathcal{T} S(\infty) \rangle_{0,\mathrm{corr}}}{\langle \mathcal{T} S(\infty) \rangle_0} \right). \tag{B8}$$

With this and Eq. (B2) we can identify the corrections to the full four-time correlator. For that we use the following abbreviation to describe on which set of operators we apply Wick's theorem:

$$\mathrm{Wick}(A, \pi_n \setminus B, C) = \left\langle \mathcal{T} \prod_{k \in A \cup \pi_n \setminus B} \hat{O}_k \right\rangle_0 \left\langle \mathcal{T} \prod_{l \in \pi_n \cup C} \hat{X}_l \right\rangle_0, \tag{B9}$$

where $\pi_n = \{1, \ldots, n\}$ describes the initial set of operators $\hat{O}_i$ and $\hat{X}_i$. With this notation we keep in mind which additional operators $\hat{O}_i$ we have and which operators $\hat{O}_i$ are missing. The full four-time correlator with corrections reads

$$
\langle \mathcal{T} \hat{O}_\mathrm{I} \hat{O}_\mathrm{II} \hat{O}_\mathrm{III} \hat{O}_\mathrm{IV} \rangle_F = \sum_{\substack{3\,\mathrm{perm} \\ a,b,c,d}} \langle \mathcal{T} \hat{O}_a \hat{O}_b \rangle \langle \mathcal{T} \hat{O}_c \hat{O}_d \rangle - \sum_{\substack{3\,\mathrm{perm} \\ a,b,c,d}} \langle \mathcal{T} \hat{O}_a \hat{O}_b \rangle \langle \mathcal{T} \hat{O}_c \hat{O}_d \rangle \frac{\langle \mathcal{T} S(\infty) \rangle_{0,\mathrm{corr}}}{\langle \mathcal{T} S(\infty) \rangle_0} + G_4(\mathrm{I},\mathrm{II},\mathrm{III},\mathrm{IV})
$$

$$
+ \sum_n \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \frac{1}{\langle \mathcal{T} S(\infty) \rangle_0} \left(\sum_{\substack{4\,\mathrm{perm} \\ a-d}} \sum_{\substack{\mathrm{perm} \\ \delta}} G_4(a,b,c,\delta) \mathrm{Wick}(\{d\}, \pi_n \backslash \{\delta\}) \right.
$$

$$
+ \sum_{\substack{6\,\mathrm{perm} \\ a-d}} \sum_{\substack{\mathrm{perm} \\ \gamma,\delta}} G_4(a,b,\gamma,\delta) \mathrm{Wick}(\{c,d\}, \pi_n \backslash \{\gamma,\delta\}) + \sum_{\substack{\mathrm{perm} \\ \alpha - \delta}} G_4(\alpha,\beta,\gamma,\delta) \mathrm{Wick}(\{a-d\}, \pi_n \backslash \{\alpha - \delta\})
$$

$$
\left. + \sum_{\substack{4\,\mathrm{perm} \\ a-d}} \sum_{\substack{\mathrm{perm} \\ \beta,\gamma,\delta}} G_4(a,\beta,\gamma,\delta) \mathrm{Wick}(\{b,c,d\}, \pi_n \backslash \{\beta,\gamma,\delta\}) \right). \tag{B10}
$$

The summations go over all distinguishable permutations. In addition, the correction to the vacuum diagrams reads

$$
\frac{\langle \mathcal{T} S(\infty) \rangle_{0,\mathrm{corr}}}{\langle \mathcal{T} S(\infty) \rangle_0} = \sum_n \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \frac{1}{\langle \mathcal{T} S(\infty) \rangle_0} \sum_{\substack{\mathrm{perm} \\ \alpha - \delta}} G_4(\alpha,\beta,\gamma,\delta) \mathrm{Wick}(\pi_n \backslash \{\alpha - \delta\}). \tag{B11}
$$

We can do the same for a two-time correlator

$$
\langle \mathcal{T} \hat{O}_a \hat{O}_b \rangle_F = \langle \mathcal{T} \hat{O}_a \hat{O}_b \rangle - \langle \mathcal{T} \hat{O}_a \hat{O}_b \rangle \frac{\langle \mathcal{T} S(\infty) \rangle_{0,\mathrm{corr}}}{\langle \mathcal{T} S(\infty) \rangle_0} + \sum_n \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \frac{1}{\langle \mathcal{T} S(\infty) \rangle_0}
$$

$$
\times \left(\sum_{\substack{\mathrm{perm} \\ \gamma,\delta}} G_4(a,b,\gamma,\delta) \mathrm{Wick}(\pi_n \backslash \{\gamma,\delta\}) + \sum_{\substack{2\,\mathrm{perm} \\ k,l}} \sum_{\substack{\mathrm{perm} \\ \beta,\gamma,\delta}} G_4(k,\beta,\gamma,\delta) \mathrm{Wick}(l, \pi_n \backslash \{\beta,\gamma,\delta\}) \right.
$$

$$
\left. + \sum_{\substack{\mathrm{perm.} \\ \alpha - \delta}} G_4(\alpha,\beta,\gamma,\delta) \mathrm{Wick}(a,b, \pi_n \backslash \{\alpha - \delta\} \right). \tag{B12}
$$

With these relations we calculate

$$
\langle \mathcal{T} \hat{O}_\mathrm{I} \hat{O}_\mathrm{II} \hat{O}_\mathrm{III} \hat{O}_\mathrm{IV} \rangle_F - \sum_{\substack{3\,\mathrm{perm} \\ a,b}} \langle \mathcal{T} \hat{O}_a \hat{O}_b \rangle_F \langle \mathcal{T} \hat{O}_c \hat{O}_d \rangle_F. \tag{B13}
$$

We have to compare terms with the same type of G_4, because only these terms can cancel each other. As an example we explain the procedure for $G_4(a,b,\gamma,\delta)$. Focusing on $G_4(a,b,\gamma,\delta)$ we obtain

$$
\sum_n \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \frac{1}{\langle \mathcal{T} S(\infty) \rangle_0}
$$

$$
\times \left(\sum_{\substack{6\,\mathrm{perm} \\ a-d}} \sum_{\substack{\mathrm{perm} \\ \gamma,\delta}} G_4(a,b,\gamma,\delta) \mathrm{Wick}(\{c,d\}, \pi_n \backslash \{\gamma,\delta\}) - \sum_{\substack{6\,\mathrm{perm} \\ a-d}} \sum_{\substack{\mathrm{perm} \\ \gamma,\delta}} G_4(a,b,\gamma,\delta) \mathrm{Wick}(\pi_n \backslash \{\gamma,\delta\}) \langle \mathcal{T} \hat{O}_c \hat{O}_d \rangle \right). \tag{B14}
$$

In the last term we have to take into account six permutations, since the $G_4(a,b,\gamma,\delta)$ occurs in both two-time correlators. The summation over the permutations for γ,δ yields a factor $\frac{n!}{(n-2)!}$. Since the first contribution arises for $n = 2$ we define $\tilde{n} = n - 2$,

which yields

$$\sum_{\substack{6\,\text{perm} \\ a-d}} (-i)^2 \int_{-\infty}^{\infty} dt_{x_1} \int_{-\infty}^{\infty} dt_{x_2} G_4(a,b,x_1,x_2) \frac{1}{\langle \mathcal{T} S(\infty)\rangle_0} \sum_{\tilde{n}} \frac{(-i)^{\tilde{n}}}{\tilde{n}!}$$

$$\times \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_{\tilde{n}} [\text{Wick}(\{c,d\},\pi_{\tilde{n}},\{x_1,x_2\}) - \text{Wick}(\pi_{\tilde{n}},\{x_1,x_2\})\langle \mathcal{T}\hat{O}_c \hat{O}_d\rangle]. \tag{B15}$$

The possible types of diagrams in these constellations are

$$(\text{I}): \quad \text{} \quad\quad (\text{II}): \quad \text{} \quad\quad \text{} \quad , \tag{B16}$$

multiplied by an appropriate vacuum diagram. The cross represents G_4. Both kinds appear in the first term. However, all contributions in the second term are of the form II. We define the following abbreviations that describe the leg- and ring-type structures in the above diagrams:

$$L_m^{x_1,a} = (-i)^m \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_m \langle \mathcal{T}\hat{X}_{x_1}\hat{X}_1\rangle_0 \langle \mathcal{T}\hat{O}_1\hat{O}_2\rangle_0 \langle \mathcal{T}\hat{X}_2\hat{X}_3\rangle_0 \cdots \langle \mathcal{T}\hat{O}_m\hat{O}_a\rangle_0, \quad L_0^{x_1,a} = 0 \tag{B17}$$

$$R_m^{x_1,x_2} = (-i)^m \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_m \langle \mathcal{T}\hat{X}_{x_1}\hat{X}_1\rangle_0 \langle \mathcal{T}\hat{O}_1\hat{O}_2\rangle_0 \langle \mathcal{T}\hat{X}_2\hat{X}_3\rangle_0 \cdots \langle \mathcal{T}\hat{X}_m\hat{X}_{x_2}\rangle_0. \tag{B18}$$

Now we proceed analogously with Eq. (B15) and identify similar structures, get combinational factors, and do the resummation using the Cauchy product formula. It turns out that the terms of type II fully cancel out. So we are left with

$$\sum_{\substack{6\,\text{perm} \\ a-d}} (-i)^2 \int_{-\infty}^{\infty} dt_{x_1} \int_{-\infty}^{\infty} dt_{x_2} G_4(a,b,x_1,x_2) \sum_{l}^{\infty} \sum_{k}^{\infty} L_l^{x_1,c} L_k^{x_2,d}. \tag{B19}$$

Repeating this procedure for all kinds of G_4 terms, we find

$$\langle \mathcal{T}\hat{O}_\text{I}\hat{O}_\text{II}\hat{O}_\text{III}\hat{O}_\text{IV}\rangle_F = \sum_{\substack{3\,\text{perm} \\ a,b}} \langle \mathcal{T}\hat{O}_a\hat{O}_b\rangle_F \langle \mathcal{T}\hat{O}_c\hat{O}_d\rangle_F + G_4(\text{I},\text{II},\text{III},\text{IV}) - i \sum_{\substack{4\,\text{perm} \\ a-d}} \int_{-\infty}^{\infty} dt_{x_1} G_4(a,b,c,x_1) \sum_{k}^{\infty} L_k^{x_1,d}$$

$$- \sum_{\substack{6\,\text{perm} \\ a-d}} \int_{-\infty}^{\infty} dt_{x_1} \int_{-\infty}^{\infty} dt_{x_2} G_4(a,b,x_1,x_2) \sum_{l}^{\infty} \sum_{k}^{\infty} L_l^{x_1,c} L_k^{x_2,d}$$

$$+ i \sum_{\substack{4\,\text{perm} \\ a-d}} \int_{-\infty}^{\infty} dt_{x_1} \int_{-\infty}^{\infty} dt_{x_2} \int_{-\infty}^{\infty} dt_{x_3} G_4(a,x_1,x_2,x_3) \sum_{l}^{\infty} \sum_{k}^{\infty} \sum_{m}^{\infty} L_l^{x_1,b} L_k^{x_2,c} L_m^{x_3,d}$$

$$+ \int_{-\infty}^{\infty} dt_{x_1} \int_{-\infty}^{\infty} dt_{x_2} \int_{-\infty}^{\infty} dt_{x_3} \int_{-\infty}^{\infty} dt_{x_4} G_4(x_1,x_2,x_3,x_4) \sum_{l}^{\infty} \sum_{k}^{\infty} \sum_{m}^{\infty} \sum_{n}^{\infty} L_l^{x_1,a} L_k^{x_2,b} L_m^{x_3,c} L_m^{x_4,d}. \tag{B20}$$

We define a diagrammatic representation for these corrections,

$$\text{} = \text{} + \text{} + \text{} + \text{} + \dots, \tag{B21}$$

and are left with

$$\langle \mathcal{T}\hat{O}_\text{I}\hat{O}_\text{II}\hat{O}_\text{III}\hat{O}_\text{IV}\rangle_F = \sum_{\substack{3\,\text{perm} \\ a,b,c,d}} \langle \mathcal{T}\hat{O}_a\hat{O}_b\rangle_F \langle \mathcal{T}\hat{O}_c\hat{O}_d\rangle_F + \text{}. \tag{B22}$$

With the above it is easy to derive the equation

$$\langle \mathcal{T}\hat{O}_{\mathrm{I}}\hat{O}_{\mathrm{II}}\rangle_F = \langle \mathcal{T}\hat{O}_{\mathrm{I}}\hat{O}_{\mathrm{II}}\rangle - \int_{-\infty}^{\infty} dt_{x_1} \int_{-\infty}^{\infty} dt_{x_2} G_4(\mathrm{I,II},x_1,x_2) \sum_k R_k^{x_1,x_2} + i \sum_{\substack{2\ \mathrm{perm}\\a,b}} \int_{-\infty}^{\infty} dt_{x_1} \int_{-\infty}^{\infty} dt_{x_2} \int_{-\infty}^{\infty} dt_{x_3} G_4(a,x_1,x_2,x_3)$$

$$\times \sum_l \sum_k R_k^{x_1,x_2} L_l^{x_3,b} + \int_{-\infty}^{\infty} dt_{x_1} \int_{-\infty}^{\infty} dt_{x_2} \int_{-\infty}^{\infty} dt_{x_3} \int_{-\infty}^{\infty} dt_{x_4} G_4(x_1,x_2,x_3,x_4) \sum_l \sum_k \sum_m R_k^{x_1,x_2} L_l^{x_3,\mathrm{I}} L_m^{x_4,\mathrm{II}}$$

$$\text{(B23)}$$

$$= \langle \mathcal{T}\hat{O}_{\mathrm{I}}\hat{O}_{\mathrm{II}}\rangle + \bowtie .$$

$$\text{(B24)}$$

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