Thermalization and ergodicity in one-dimensional many-body open quantum systems

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Using an approach based on the time-dependent density-matrix renormalization-group method, we study the thermalization in spin chains locally coupled to an external bath. Our results provide evidence that quantum chaotic systems do thermalize, that is, they exhibit relaxation to an invariant ergodic state which, in the bulk, is well approximated by the grand canonical state. Moreover, the resulting ergodic state in the bulk does not depend on the details of the baths. On the other hand, for integrable systems we found that the invariant state in general depends on the bath and is different from the grand canonical state.

The emergence of canonical ensembles in quantum statistical mechanics from first principles is one of the key remaining old questions of theoretical physics. Even the definition of the temperature at the nanoscale poses a challenge [1]. Namely, the main question is how to "derive" the canonical distribution? It has been realized that the canonical distribution is in a way "typical:" provided the overall system describing the environment plus a central system is in a generic pure state, the reduced state of the central system is with high probability canonical [2]. However, how precisely the canonical distribution arises from dynamical laws, without *a priori* statistical assumptions, is still unclear. The motivation in the study of this fundamental aspect of nonequilibrium physics also comes from some recent experiments with ultracold bosonic gases, where absence of thermalization in closed integrable strongly correlated quantum systems has been observed [3].

For closed many-body systems, integrability is believed to play a crucial role in the relaxation to the steady state (SS): the nonequilibrium dynamics of a chaotic system is expected to thermalize at the level of individual eigenstates [4] as numerically observed in several physical models [5]. By contrast, for systems with non trivial integrals of motion, SSs usually carry memory of the initial conditions and are not canonical: maximizing the entropy while keeping the values of constants of motion fixed results in a generalized Gibbs ensemble [6]. Much less is known about the relaxation to the SS for *open quantum systems* [7]; this is what we are going to address in this paper. We provide numerical evidence that, analogously to closed systems, the occurrence of thermalization is strictly related to system's integrability, irrespective of the fine details of the baths. In particular we show that *locally* coupling a quantum chaotic many-body system to an environment is enough for a SS of the central system to be very close, in the bulk, to the canonical or grand canonical

state (GCS). On the contrary, if the system is integrable, the constants of motion in general prevent thermalization and the form of the SS sensitively depends on the bath coupling operators.

We will treat open systems within the Lindblad master equation approach, in the rotating wave approximation. The reason for choosing such a Lindblad formulation is twofold. On one hand, we are explicitly interested in understanding if a completely positive map that acts *locally* at each small time step can induce thermalization. This would result in a minimal modification of closed system's dynamics, for which a number of significant and widely applicable findings has been established, such as a general nonthermal behavior for integrable systems. On the other hand, this approach provides us a practical way to devise and test an efficient numerical method for simulating strongly interacting quantum systems in equilibrium at finite temperatures, as well as in nonequilibrium settings. We are going to show that the numerical description of an open quantum system in terms of a Lindblad equation with *local* coupling to the reservoirs is in some sense a *computationally efficient minimal model of thermalization*. Such result paves the way for future simulations of quantum transport in large many-body quantum systems.

It is worth pointing out that the master-equation formulation for the treatment of open systems is not unique: in principle one could also use a Redfield approach. In this way an asymptotic "thermal" state would be achieved in an arbitrary system [8], so to speak, by construction. Unfortunately, the Redfield formulation is very difficult to treat both theoretically and numerically. Namely, numerical simulations of the Redfield equation in strongly interacting system are very demanding since the relaxation tensor scales with the fourth power of the Hilbert-space dimension [9].

The time evolution for a generic state ρ of an open quantum system can be described, under certain approximations, by a Lindblad master equation [8], being the most general form of a completely positive trace preserving dynamical semigroup,

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$$\frac{d}{dt}\rho = \frac{i}{\hbar}[\rho, \mathcal{H}] + \hat{\mathcal{L}}_B\rho, \tag{1}$$

where $\mathcal{H}$ is the Hamiltonian of the autonomous system, while the dissipation $\hat{\mathcal{L}}_B = \gamma\Sigma_k([L_k\rho, L_k^\dagger] + [L_k, \rho L_k^\dagger])$ is parametrized by Lindblad operators L_k (hereafter we set $\hbar = k_B = 1$ and, unless noted otherwise, $\gamma = 1$). The derivation of Eq. (1) from first principles, i.e., from the Hamiltonian evolution of a system plus environment is rather tricky [8]. For instance, for weakly coupled system one can end up with a Lindblad equation that fails to correctly account for a nonequilibrium current [10]. Our approach though will be top-down, taking the Lindblad equation for granted, we ask ourselves if, within this approximation, a *finite* many-body system can thermalize when coupled via some Lindblad operators L_k acting only *locally* just on *few* degrees of freedom.

To elucidate the role covered by chaoticity in the thermalization process, we consider prototype one-dimensional spin-1/2 chain models with nearest-neighbor interactions:

$$\mathcal{H} = \sum_{l=0}^{n-2} h_{l,l+1}, \tag{2}$$

where $h_{l,l+1}$ denotes the local energy density and n denotes the chain length. As we shall see, the chosen models exhibit a crossover from integrable to chaotic regime when a suitable parameter in their Hamiltonians is varied. With the term "chaotic" we refer, as usual, to a system whose bulk energy spectrum of highly excited levels obeys a random matrix statistics [11]; in particular, the level spacing statistics (LSS) $p(s)$ is well approximated by the Wigner-Dyson distribution $p_{WD}(s)$ [11], whereas in an integrable system LSS typically turns out to be Poissonian, $p_P(s)$.

We assume local coupling to the reservoirs, i.e., the dissipator $\hat{\mathcal{L}}_B$ acts only on the m ($\ll n$) leftmost (l) and rightmost (r) spins: $\hat{\mathcal{L}}_B = \hat{\mathcal{L}}_B^l \otimes \hat{\mathbb{1}}_{\text{bulk}} \otimes \hat{\mathcal{L}}_B^r$. We construct $\hat{\mathcal{L}}_B$ by generalizing the method discussed in Ref. [12]. For this purpose, we first consider the GCS for the spin chain,

$$\rho_{\mathcal{G}}(T, \mu) = Z^{-1}\exp[-(\mathcal{H} - \mu\Sigma^z)/T], \tag{3}$$

where $\Sigma^z = \Sigma_{l=0}^{n-1}\sigma_l^z$ is the total magnetization [$\sigma_j^\alpha (\alpha = x, y, z)$ being the Pauli operators for the jth spin], T is the temperature, μ is the "chemical potential," and $Z = \text{tr}[\exp(-(\mathcal{H} - \mu\Sigma^z)/T)]$ is the partition function. Given a target temperature T_{targ} and a chemical potential μ_{targ}, the reduced m-spin target density matrix $\rho_{\text{targ}}^\lambda$, $\lambda \in \{l, r\}$, is obtained after tracing $\rho_{\mathcal{G}}(T_{\text{targ}}, \mu_{\text{targ}})$ over all but the m leftmost/rightmost spins. We finally require that $\rho_{\text{targ}}^\lambda$ is the unique eigenvector of $\hat{\mathcal{L}}_B^\lambda$ with eigenvalue 0, while all other eigenvalues are equal to -1. Such a choice produces, in absence of $\mathcal{H}$ and for a given spectral norm of $\hat{\mathcal{L}}_B^\lambda$, the *fastest* convergence to $\rho_{\text{targ}}^\lambda$ [13]. In the presence of $\mathcal{H}$ we obtain, for up to $n \approx 100$ spins, the SS solution of Eq. (1) numerically by using a time-dependent density-matrix renormalization-group (tDMRG) method with a matrix product operator (MPO) ansatz [14].

In the following we are interested in the asymptotic state that is reached after a long time, independently of the initial
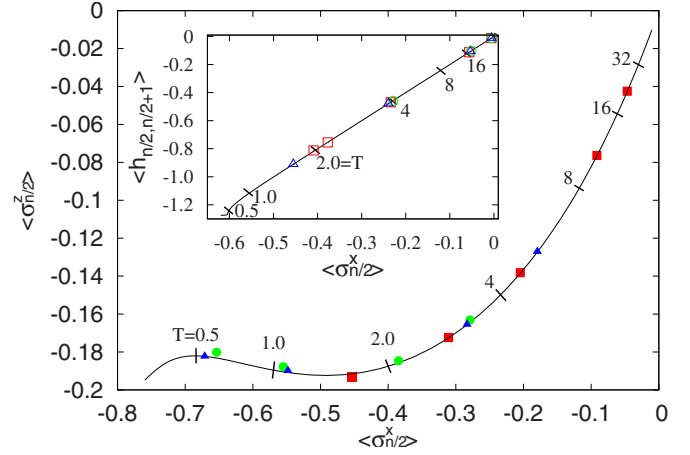

FIG. 1. (Color online) One-spin observables for the SS (symbols) agree with the theoretical canonical ones (full curve) to less than 0.5% for the chaotic Ising model (main plot). For the integrable model (inset) a comparable agreement is observed by looking at energy density vs $\langle\sigma_{n/2}^x\rangle$ (note that, in this specific case, one has $\langle\sigma_{n/2}^z\rangle \equiv 0$). Squares are for $n = 16$ and uniform couplings; circles (triangles) for $n = 16$ ($n = 40$) and couplings J_l switched on over a layer of thickness $\tau = 4$, with $\gamma = 0.2$. Marks on theoretical curves show the temperature.

conditions: $\rho_{SS} \equiv \lim_{t\to\infty}\rho(t)$. In all the simulations we carefully checked that the simulation time was long enough to reach convergence, which is exponential. Since Lindblad operators act only locally and $\rho_{\mathcal{G}}(T, \mu)$ is invariant for the unitary part of Eq. (1), ρ_{SS} cannot be equal to the GCS, unless it is also an eigenstate of the dissipator $\hat{\mathcal{L}}_B$. In other words, one can have $\rho_{SS} = \rho_{\mathcal{G}}(T, \mu)$ only if $\rho_{\mathcal{G}}(T, \mu) = \rho_{\text{targ}}^l \otimes \rho_{\text{bulk}} \otimes \rho_{\text{targ}}^r$, i.e., if the GCS is separable with respect to the border m spins which are used in the coupling. Nevertheless for chaotic systems, as we shall see, sufficiently far from the boundaries the state is arbitrarily close to $\rho_{\mathcal{G}}(T, \mu)$, regardless of the entanglement with the coupled parts.

Let us start our numerical investigations by considering a spin-1/2 Ising chain in a tilted magnetic field, described by the energy density

$$h_{l,l+1} = J_l\sigma_l^z\sigma_{l+1}^z + \frac{b_x}{2}(\sigma_l^x + \sigma_{l+1}^x) + \frac{b_z}{2}(\sigma_l^z + \sigma_{l+1}^z). \tag{4}$$

Its only conserved quantity is the total energy, therefore the expected invariant state is the canonical one $\rho_{\mathcal{G}}(T, 0)$. To check thermalization, we solved the master equation for two different sets of parameters: (i) a transverse field $b_x = 1$, $b_z = 0$, for which the model is integrable and exhibits a Poissonian LSS; (ii) a tilted field $b_x = 1$, $b_z = 1$, for which it is chaotic with a Wigner-Dyson LSS [15] (if not specified, we take $J_l = 1$ and couple two border spins, $m = 2$). With the obtained ρ_{SS}, we evaluated expectation values of several one- and two-spin observables in the bulk of the chain and compared them to the theoretical ones as given by the canonical state $\rho_{\mathcal{G}}(T, 0)$.

In the main plot of Fig. 1 we show one-spin expectation values $\langle\sigma_{n/2}^\alpha\rangle = \text{tr}(\rho_{SS}\sigma_{n/2}^\alpha)$ for the chaotic case: all numerical points fall on the curve given by theoretical expectation val-
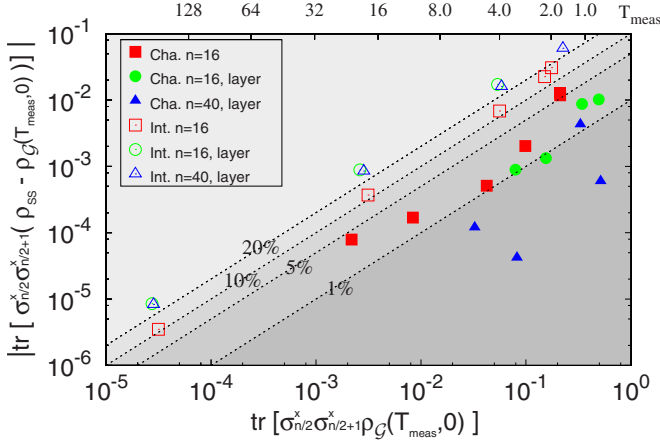
FIG. 2. (Color online) Absolute differences in the expectation value of a two-spin observable $\sigma_{n/2}^x \sigma_{n/2+1}^x$ between the SS and the theoretical canonical state, in the case of chaotic (full symbols) and integrable Ising model (empty symbols). Dashed lines denote constant relative error.
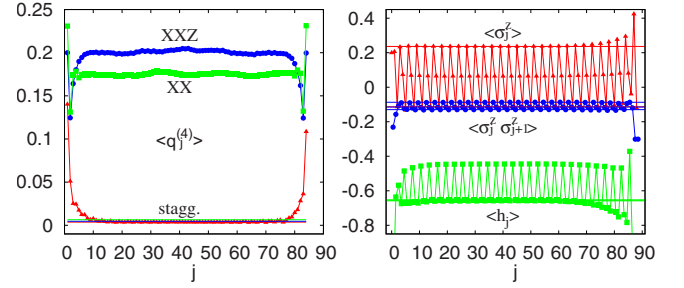

FIG. 3. (Color online) SS (symbols) and GCS (full lines) expectation values of $q_j^{(4)}$ (left panel), σ_j^z, $\sigma_j^z \sigma_{j+1}^z$, and h_j (right panel) for the Heisenberg model with $n=89$ spins, $T_{\text{targ}}=4$, $q_{\text{targ}}=2$, $m=3$, $J_l =1$. In the left panel, "*XX*" and "*XXZ*" refer to two integrable cases without magnetic field (respectively at $\Delta=0,0.5$), "stagg." to the chaotic case with $\Delta=0.5$ and period-3 staggered field with $B=2$. The curves in the right panel are for the chaotic case only. The GCS $\rho_{\mathcal{G}}(T_{\text{meas}}=5.851, \mu_{\text{meas}}=-0.534)$ for the chaotic case is obtained by matching $\langle h_{3l+1,3l+2} \rangle$ and $\langle \sigma_{3l+1}^z \rangle$ for which lines are not shown in the right panel.

ues for a canonical state. The same happens in the integrable Ising model. Such irrelevance of integrability is a peculiarity of certain few-body observables, similarly to what observed in a different context of out-of-equilibrium dynamics in closed systems [16]. Quite remarkably, we could not reach temperatures in the bulk below ≈ 1.7 (see squares in Fig. 1), even by using very small $T_{\text{targ}} \approx 0$. The reason resides in the already mentioned boundary effects due to entanglement between the boundary two spins and the bulk chain, which makes the cooling difficult. This must be contrasted with a zero attainable temperature in the case of separable states [17]. For entangled states though, our results show that to lower the minimal attainable temperature one has to reduce the effect of interaction at the boundaries which is responsible for entanglement. A possible way to do this is by switching on the interaction gently over a boundary layer of certain thickness τ, $J_l=\sin(\frac{l}{\tau}\frac{\pi}{2})$ $[J_{n-2-l}=\sin(\frac{l}{\tau}\frac{\pi}{2})]$, for $l=0,\dots,\tau-1$, at the left (right) end and using a weaker coupling γ (circles and triangles in Fig. 1). One could reasonably ask whether such method would be the most efficient way to achieve the lowest temperatures; the answer to such question is at present not clear and would demand a separate study that goes beyond our purposes. Here we surmise that chaoticity plays a major role in the thermalization process of open systems; on this basis, one could perhaps expect to be able to reach lower temperatures for larger systems because chaos would set in at lower temperatures [5].

To make comparison between ρ_{SS} and $\rho_{\mathcal{G}}(T,0)$ quantitative, we determined the "measured" temperature T_{meas} to which ρ_{SS} corresponds, which is in general different from T_{targ}, due to boundary effects. Assuming that the SS is canonical in the bulk, one can extract T_{meas} by comparing observables that uniquely set the temperature. For the Ising model [Eq. (4)], the energy density is sufficient, therefore we used the condition $\text{tr}[h_{n/2-1,n/2}\rho_{\text{SS}}] \equiv \text{tr}[h_{n/2-1,n/2}\rho_{\mathcal{G}}(T_{\text{meas}},0)]$ to compute T_{meas}. We then calculated theoretical expectation values of other observables, through $\rho_{\mathcal{G}}(T_{\text{meas}},0)$; a comparison with the corresponding values for the reached SS may

serve as an indicator of the *quality of thermalization*. In Fig. 2 we show differences between expectation values of $\sigma_l^x \sigma_{l+1}^x$, computed with ρ_{SS} and $\rho_{\mathcal{G}}(T_{\text{meas}},0)$, for both chaotic and integrable Ising chains. A marked distinction between the two cases appears. First, in the chaotic model errors are much smaller than in the integrable one; second, switching J_l gradually, which should decrease errors due to smaller boundary effects, in the integrable case even worsens the situation. The integrable Ising model therefore does not relax to a canonical state in the bulk. Similar results are obtained for other few-spin observables, as well as for the lowest moments of the energy distribution: we evaluated $\langle [(\mathcal{H}_6 -\langle\mathcal{H}_6\rangle)/5]^p\rangle$ ($p=2,\dots,5$ and $\mathcal{H}_6$ is the Hamiltonian of the six central spins) on the states ρ_{SS} and $\rho_{\mathcal{G}}(T_{\text{meas}},0)$. In a chain of $n=40$ spins relative errors are never greater than 1% in the chaotic case, and are typically an order of magnitude larger in the integrable case.

To corroborate the importance of system's integrability on the convergence to invariant statistical ensembles, we consider another prototype model of interacting spins: the Heisenberg *XXZ* chain in a magnetic field, described by the energy density

$$h_{l,l+1} = J_l(\sigma_l^x\sigma_{l+1}^x + \sigma_l^y\sigma_{l+1}^y + \Delta\sigma_l^z\sigma_{l+1}^z) + \frac{b_l}{2}\sigma_l^z + \frac{b_{l+1}}{2}\sigma_{l+1}^z.$$

(5)

If the field is homogeneous the model is integrable and possesses, besides energy and magnetization, an infinite sequence of conserved quantities [18]. On the other hand, integrability can be broken, e.g., simply by means of a period-3 staggered magnetic field, $b_{3k}=-B$, $b_{3k+1} =-B/2$, $b_{3k+2}=0$. In order to highlight the lack of thermalization in the integrable regime $B=0$, we target a non-Gibbsian state different from the GCS; namely, we use $\rho_{\text{non-}\mathcal{G}}(T,q) \sim \exp(-\mathcal{H}/T+qQ_4)$, with $Q_4=-h_{0,1}-h_{n-2,n-1} +\Sigma_{l=0}^{n-4}q_l^{(4)}$, $q_l^{(4)}=\sigma_l^x\sigma_{l+1}^z\sigma_{l+2}^z\sigma_{l+3}^x + \sigma_l^y\sigma_{l+1}^z\sigma_{l+2}^z\sigma_{l+3}^y$, being a conserved charge for an open chain with $\Delta=0$ and $b_l=0$ [18].
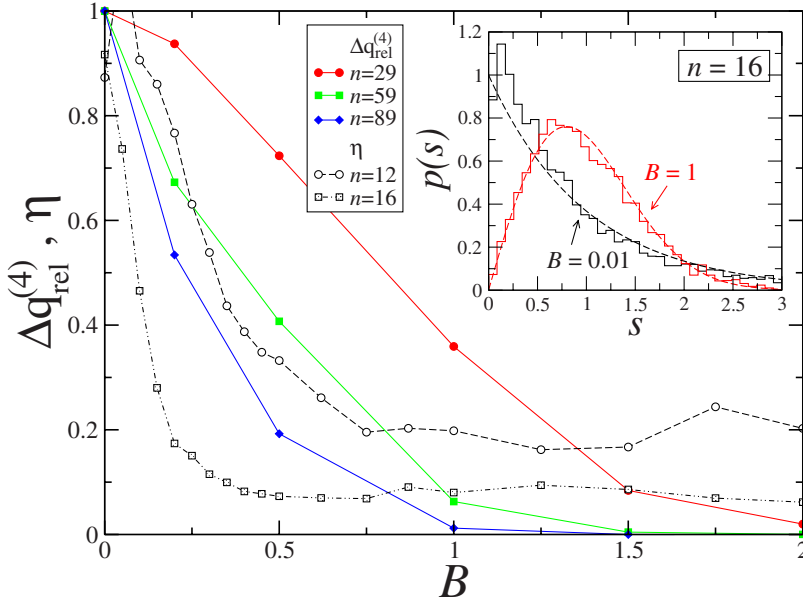
FIG. 4. (Color online) Relative differences $\Delta q_{rel}^{(4)} = \Delta q^{(4)}(B)/\Delta q^{(4)}(0)$ in $q^{(4)}$ expectation values on the SS and the GCS evaluated in the bulk of the Heisenberg model with $\Delta = 0.5$, as the staggering strength B is varied (full curves). Also shown is dependence of the η function (dashed curves), characterizing the integrable-chaotic crossover. For both quantities the crossover takes place at smaller B with increasing n. Inset: two examples of LSS in the integrable ($B=0.01$) and chaotic ($B=1$) regimes; dashed lines denote Poissonian and Wigner-Dyson statistics [11], respectively.

The idea is that, using a $q_{targ} \neq 0$, in the integrable regime the SS exhibits strong deviations from the GCS, corresponding to $q=0$, while we expect chaotic dynamics to drive the bulk toward the GCS. Such expectation is confirmed by our numerical data. In Fig. 3 we show the spatial dependence of various observables for integrable, as well as for chaotic cases. In the integrable cases deviations from the GCS expectations are large, while they become very small for a chaotic system. Analogously to the Ising model, we checked this statement also for other few-spin observables (we found that, in presence of chaos, the largest discrepancy among all the one- and two-spin observables amounts to 2×10^{-4}); layered interactions in the integrable model do not help in thermalizing the system.

A further confirmation of the role of integrability comes from a direct analysis of the quality of thermalization after gradually switching on the perturbation that drives the crossover from integrability to chaos: the longitudinal field b_z in Eq. (4) or the staggering intensity B in Eq. (5). As shown in Fig. 4 for the Heisenberg model, such crossover is conveniently detected by the parameter $\eta \equiv \int |p(s) - p_{WD}(s)| ds / \int |p_P(s) - p_{WD}(s)| ds$; $\eta = 1$ and $\eta = 0$ correspond to Poissonian and Wigner-Dyson distributions, respectively. In the same figure we also plot deviations in $\langle q^{(4)} \rangle$ evaluated on the SS and on the corresponding GCS: $\Delta q^{(4)} = \text{tr}[q_l^{(4)}(\rho_{SS} - \rho_{\mathcal{G}}(T_{meas}, \mu_{meas}))]$ as the strength B of the staggered magnetic field is increased. The progressive onset of chaos

gradually improves the quality of thermalization, being $\Delta q^{(4)}$ a monotonic decreasing function of B. Moreover, the strength of the staggered field required to converge to the GC expectation value drops with the system size.

In conclusion, we have shown that, within the Lindblad equation formalism, coupling a one-dimensional quantum chaotic system locally to a bath results in a SS being equal to the invariant (grand) canonical state, far away from the coupled sites. In contrast, integrable systems do not thermalize and their SSs exhibit strong deviations from the (grand)canonical state, depending on the details of the coupling. The fact that for chaotic systems the SS does not depend on the details of the coupling, shows that very likely the same result would be obtained even for a harder-to-treat Hamiltonian evolution of a system plus environment or for higher dimensional systems. Our method should be applicable also to nonequilibrium situations. Indeed, by locally coupling a system to two or several baths at different values of temperature and chemical potentials, one should be able to efficiently control local thermalization. Thus, our results might open significant new perspectives in the simulation of quantum transport in many-body quantum systems in contact with thermal and chemical baths.

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[13] To construct such $\hat{\mathcal{L}}_B^l$ (and similarly for $\hat{\mathcal{L}}_B^r$), we first diagonalize ρ_{targ}^l, thus getting eigenvalues d_i and eigenvectors, $\rho_{\text{targ}}^l = V^\dagger dV$. Then we obtain $\hat{\mathcal{L}}_B^l$ after rotating the "diagonal" Lindblad superoperator $\hat{\mathcal{L}}_B^{\text{diag}}$, $\hat{\mathcal{L}}_B^l = R\hat{\mathcal{L}}_B^{\text{diag}}R^{\text{T}}$, with the orthogonal matrix $R_{\alpha,\beta} = \text{tr}(V^\dagger \sigma^\alpha V \sigma_-^\beta)/4$ ($\sigma^\alpha = \sigma^{\alpha_1} \otimes \cdots \otimes \sigma^{\alpha_m}$). A set of 4^m Lindblad operators leading to the diagonal superoperator $\hat{\mathcal{L}}_B^{\text{diag}}$ is given by $L_{i_1 i_2 \cdots i_m} = \sqrt{\frac{d_k}{2 \cdot 4^m}} r^{i_1} \otimes r^{i_2} \otimes \cdots \otimes r^{i_m}$, with $i_j \in \{0,1,2,3\}$, $k = \Sigma_{j=1}^m (i_j \bmod 2) \cdot 2^{j-1}$, and $r^0 = \sigma^x + i\sigma^y$, $r^1 = \sigma^x - i\sigma^y$, $r^2 = 1 + \sigma^z$, $r^3 = 1 - \sigma^z$.

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