Simulation methods for open quantum many-body systems

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Coupling a quantum many-body system to an external environment dramatically changes its dynamics and offers novel possibilities not found in closed systems. Of special interest are the properties of the steady state of such open quantum many-body systems, as well as the relaxation dynamics toward the steady state. However, new computational tools are required to simulate open quantum many-body systems, as methods developed for closed systems cannot be readily applied. Several approaches to simulating open many-body systems are reviewed, and advances made in recent years toward the simulation of large system sizes are pointed out.

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CONTENTS

I. INTRODUCTION

A. The open quantum many-body problem

Open quantum many-body systems have witnessed a surge of interest in recent years, chiefly for two reasons. On the one hand, these systems offer the possibility of using controlled dissipation channels to engineer interesting quantum many-body states as the stationary state of their dynamics (Diehl *et al.*, 2008; Verstraete, Wolf, and Ignacio Cirac, 2009; Weimer *et al.*, 2010). On the other hand, open quantum many-body systems are attractive from a fundamental perspective, as their dynamics exhibits a wide range of features not found in equilibrium systems. As in the case of closed quantum systems, the complexity of the problem scales exponentially with the size of the system, requiring the use of sophisticated simulation methods to obtain useful results. An additional important reason is that systems in nature are not perfectly isolated. They are constantly interacting with their environment in the form of heat transfer, decoherence (Schlosshauer, 2005; Vinjanampathy and Anders, 2016), etc. In practice, modeling the effect of the environment can be

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quite complex, implying that the mathematical description of open systems is more complex than that of isolated ones. Thus, to realistically mimic nature through quantum simulation experiments, numerical methods, etc., one needs to take into account the effects of dissipation.

Open quantum many-body systems are even harder to simulate on classical computers than closed systems, while at the same time the stationary state of an open quantum system is much easier to experimentally prepare than the ground state of a closed system. These properties make open quantum systems one of the prime candidates to show a quantum advantage of quantum simulators over classical methods within noisy intermediate-scale quantum devices (Preskill, 2018). However, this requires a thorough assessment of the capabilities of classical simulation methods, which we provide in this review.

In our review, we first provide a general introduction to open quantum many-body systems, placing particular emphasis on the key differences relative to simulating closed quantum systems and on the paradigmatic models that have emerged in benchmarking simulation methods for open systems. In the main part, we first review stochastic methods commonly known as wave-function Monte Carlo techniques, which are based on a numerical exact treatment of the total Hilbert space of the problem. We then turn to tensor network simulation techniques aiming to describe the "physical corner" of the Hilbert space, i.e., the quantum states that are most relevant for describing the dynamical evolution and steady states of open quantum many-body systems. Subsequently, we review variational methods that employ similar strategies, including variational methods that are based on a tensor network description. We also cover phase-space methods and closely related counterparts. Finally, we include a section on linked-cluster expansion. Within our review, we do not cover methods derived from a field-theoretical description of open quantum systems within the Keldysh formalism, as this was already extensively covered in a previous review (Sieberer, Buchhold, and Diehl, 2016). We also do not cover integrable models (Prosen, 2008, Prosen, 2011a; 2011b; Medvedyeva, Essler, and Prosen, 2016; Foss-Feig *et al.*, 2017; Guo and Poletti, 2018) for which analytical techniques such as the Bethe ansatz can be employed.

B. The Markovian quantum master equation

The state of an open system is described by its density operator ρ, which can be described as a statistical ensemble of pure states

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \tag{1}$$

where p_i denotes the probability of finding the system in the state $|\psi_i\rangle$. Note that the decomposition into pure states is not unique. In our review, we limit ourselves to the discussion of Markovian systems, i.e., dynamical systems in which the generator of the dynamics $\mathcal{L}[\rho]$ (commonly called the Liouvillian) depends only on the state at the present time t, not on the state at earlier times. For an introduction to the Markovian master equation, see Manzano (2020) or the lecture notes given by Preskill (2020). Such Markovian systems form a dynamical semigroup and can be described by a quantum master equation in Lindblad form

$$\frac{d}{dt}\rho = \mathcal{L}[\rho] = -i[H,\rho] + \sum_\mu \left(L_\mu \rho L_\mu^\dagger - \frac{1}{2} L_\mu^\dagger L_\mu \rho - \frac{1}{2} \rho L_\mu^\dagger L_\mu \right), \tag{2}$$

where H is the Hamiltonian of the system and $\{L_\mu, L_\mu^\dagger\}$ are the Lindblad operators responsible for the incoherent dynamics arising from the coupling to an external environment, which are also known as the jump operators (Gorini, Kossakowski, and Sudarshan, 1976; Lindblad, 1976) acting at site μ.

The validity of the Lindblad master equation (2) for a concrete physical system depends on the separation of several timescales. Considering a system of interest coupled to a larger environment, one first assumes a weak coupling between system and environment, such that the entanglement between system and environment remains low. Furthermore, the environment must not retain any memory of the system degrees of freedom. The approximations related to these conditions are commonly referred to as the Born-Markov approximation (Breuer and Petruccione, 2002) and require that the correlation time of the environment τ_E is much smaller than the relaxation time of the system τ_R. Finally, the differences in eigenfrequencies in the system ω_s have to be large relative to the inverse relaxation time τ_R^{-1}.

These approximations are well justified in quantum optical systems, in particular, atoms coupled to electronically excited states (Raitzsch *et al.*, 2009; Baumann *et al.*, 2010; Barreiro *et al.*, 2011; Krauter *et al.*, 2011; Malossi *et al.*, 2014). There the optical frequencies of the transition leave a large timescale to observe the complete relaxation to its equilibrium state. Additionally, the relaxation of the electronic excitation into the vacuum of the radiation field as the correlation time of the radiation field is related to the photon frequency (Breuer and Petruccione, 2002), which again is much larger than the relaxation rate τ_R^{-1}. Artificial atomic systems such as the nitrogen-vacancy center in diamond (Jelezko *et al.*, 2004; Dutt *et al.*, 2007; Robledo *et al.*, 2011) offer similar benefits.

Another advantage of quantum optical systems for studying open quantum many-body systems is the possibility to drive them with time-dependent laser fields. If all the jump operators in the master equation describe transitions between the eigenstates of the Hamiltonian, the resulting steady state of the system is guaranteed to be a thermal state (Breuer and Petruccione, 2002). However, if an oscillatory driving term is added to the system Hamiltonian, it is possible to observe nonequilibrium steady states in the rotating frame of the driving. Optically excited atoms can also exhibit strong interactions when excited to Rydberg states (Saffman, Walker, and Mølmer, 2010), which can be used to realize a variety of driven-dissipative quantum many-body systems (Lee, Häffner, and Cross, 2011; Ates *et al.*, 2012; Glaetzle *et al.*, 2012; Carr and Saffman, 2013; Lemeshko and Weimer, 2013; Rao and Mølmer, 2013).

There are also interesting solid-state platforms to study strong interaction and dissipation. One example is that of

semiconductor polaritonic systems [see Carusotto and Ciuti (2013)], where semiconductor microstructures are used to embed quantum wells or quantum dots, becoming a photonic resonator where strong interactions can be induced. Another example is that of circuit-quantum electrodynamics (QED) systems (Fitzpatrick *et al.*, 2017; Ma *et al.*, 2019), where superconducting circuits can be used to construct Bose-Hubbard lattices of microwave photons and dissipation can be engineered, so that one can have a tailored reservoir.

It is important to remark that the Lindblad operators are usually considered to be local, but this approximation holds only in the weak-coupling limit. To be more precise, a Markovian master equation with quasilocal Lindblad operators holds as long as the coupling between the system and the environment is weak, which in practice amounts to (1) a slow development of correlations between system and environment, (2) fast decay of excitations of the environment, and (3) neglect of fast-oscillating terms when making a comparison to the typical system timescale. One should be careful, however, since when dealing with strongly correlated systems, strong interactions within the system of interest may lead to a breakdown of the local Lindblad dissipation (Wichterich *et al.*, 2007; Beaudoin, Gambetta, and Blais, 2011). In these cases, it may be necessary to consider additional steps to derive the correct Lindblad operators (Reiter and Sørensen, 2012). For the purpose of our review, we assume that the correct Lindblad form has already been derived.

Although the Lindblad master equation is widely used to describe open quantum many-body systems and can also handle extensions such as time-dependent Hamiltonian driving, the approximations made in its derivation signal that there are physical systems that have to be described by other means. This refers to non-Markovian dynamics (de Vega and Alonso, 2017), where the system retains a memory of its previous state. One particular area where this plays an important role is the behavior of systems under continuous measurement and feedback: while *instantaneous* feedback gives rise to a feedback master equation in Lindblad form (Hofer *et al.*, 2013; Hofer and Hammerer, 2015; Lammers, Weimer, and Hammerer, 2016), *delayed* feedback generically results in non-Markovian dynamics.

C. Steady-state solution versus time evolution

Typically there are two different aspects that are of interest when studying open quantum many-body systems. First, one wants to understand the properties of one or several steady states that the system reaches in the long time limit. This is similar to understanding the ground state properties of a closed many-body system. Second, one is interested in the dynamical evolution of the system toward the steady state. The latter is particularly interesting when the system exhibits several steady states that can be reached depending on the initial condition of the system.

While the requirements for the appearance of a unique steady state are well understood for finite systems (Spohn, 1976), many-body systems add the additional complication that the long time limit and the thermodynamic limit do not necessarily commute. In some cases, even when chiefly interested in the steady state, it is more efficient to compute the full time evolution of the system. This is comparable to imaginary time evolution algorithms to find the ground state of a closed many-body system. In our review, we contrast the two approaches and address this distinction when discussing individual simulation methods in the main part of our review.

Investigating the full time evolution also offers the possibility to investigate interesting many-body effects during the relaxation dynamics. For instance, it is possible for open many-body systems exhibiting a trivial steady state, while the relaxation behavior is dominated by complex glassy quantum dynamics (Olmos, Lesanovsky, and Garrahan, 2012).

D. Differences to equilibrium problems

To find the steady state of an open quantum many-body system, it might first be tempting to take well established methods for ground state calculations for closed systems and try to adapt it to the open case. This approach fails in many cases. For example, quantum Monte Carlo methods that are highly successful for ground state calculations require one to rewrite the partition function of the quantum system to a corresponding classical system. However, for the steady state of an open system it is unclear *a priori* [and often incorrect (Sieberer *et al.*, 2013)] whether the steady state of the system is a thermal state that can be described in terms of a partition function. The same argument holds for density functional theory approaches trying to minimize the ground state energy; usually, the steady state of an open system is completely different than the ground state of the Hamiltonian. This is even true in the limit of infinitely weak dissipation, as the strength of the dissipation predominantly controls the relaxation rate rather than the properties of the steady state.

Some methods from the study of closed quantum systems out of equilibrium can be adopted to open systems; we discuss these cases in detail here. In general, the simulation of an open quantum system is computationally much harder than for a closed system due to the statistical nature of the state.

Additionally, one can benefit to some extent from the vast body of work committed to the study of classical nonequilibrium dynamics. For example, the importance of the symmetries of the open quantum many-body dynamics is just as important as in the classical case (Hohenberg and Halperin, 1977) and allows for the classification of dissipative phase transitions in terms of their universality classes.

E. Paradigmatic models

Within the analysis of ground state many-body problems, there are a number of particular models that have found especially wide interest and are often used as a first example to benchmark a numerical method. These models include the Ising model in a transverse field, the Heisenberg model, and the Hubbard model (both bosonic and fermionic). A similar observation can be made about open quantum many-body problems, where these paradigmatic models are often derived from the corresponding ground state counterparts; i.e., the Hamiltonian dynamics is the same. However, adding dissipation to a closed many-body model can be done in different ways and can lead to drastically different results. In the following, we present and briefly discuss the two most

prominent dissipative many-body models; we provide a more detailed discussion in later sections when referring to particular numerical strategies to tackle them.

1. Dissipative Ising model

One of the most widely studied open many-body models in recent years is the transverse field Ising model with longitudinal dissipation (Lee, Häffner, and Cross, 2011). Its Hamiltonian is of the form of the conventional Ising model, given in terms of Pauli matrices σ_α by

$$H = \frac{h}{2}\sum_i \sigma_x^{(i)} + \frac{V}{4}\sum_{\langle ij\rangle}\sigma_z^{(i)}\sigma_z^{(j)}, \tag{3}$$

where h is the strength of the transverse field and V accounts for the Ising interaction limited to nearest neighbor only. The dissipation is incorporated in terms of jump operators of the form $c_i = \sqrt{\gamma}\sigma_-$, with γ the rate of dissipative flips from the spin up to the spin down state described by the spin lowering operator $\sigma_- = \sigma_x - i\sigma_y$. An important aspect is that the dissipation breaks the Z_2 Ising symmetry of the Hamiltonian; i.e., the quantum master equation does not exhibit such a symmetry. The model is also relevant to ongoing experiments in the field of interacting Rydberg atoms (Carr *et al.*, 2013; Malossi *et al.*, 2014).

Within a mean-field calculation (Lee, Häffner, and Cross, 2011), the model is predicted to support a large range of h values for which the system exhibits two stable steady states. We discuss in later sections of our review how different numerical approaches address the question on the existence of such a bistable thermodynamic phase. According to mean-field theory, the bistable region ends in a critical point that belongs to the Ising universality class (Marcuzzi *et al.*, 2014).

2. Driven-dissipative Bose-Hubbard model

Another important dissipative model is the driven-dissipative Bose-Hubbard model. While there are different ways to generalize the famous Bose-Hubbard model (Fisher *et al.*, 1989) to the dissipative case, the most commonly studied one involves a dissipative particle loss that can be countered by a coherent driving term (Carusotto and Ciuti, 2013; Le Boité, Orso, and Ciuti, 2013). Its Hamiltonian is given by

$$H = -J\sum_{\langle i,j\rangle} b_i^\dagger b_j + \sum_i \left[\frac{U}{2}n_i^2 - \Delta\omega n_i + F(b_i + b_i^\dagger)\right]. \tag{4}$$

In this model, J describes the hopping of bosons between neighboring sites, while the on-site interaction U involves the square of the density operator $n_i = b_i^\dagger b_i$, where $b_i^\dagger$ and b_i correspond to the bosonic creation and annihilation operators at site i. Furthermore, $\Delta\omega$ is the chemical potential for the bosons, and F describes the aforementioned coherent driving. Finally, the quantum jump operators capturing the loss of a single boson are given by $c_i = \sqrt{\gamma}b_i$. While the dissipation term also breaks the U(1) symmetry of the conventional Bose-Hubbard model, here the symmetry is already broken on the level of the Hamiltonian by the inclusion of the driving term F.

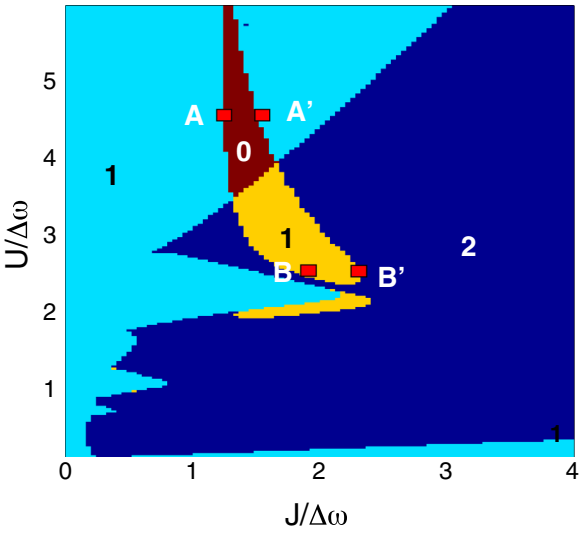

FIG. 1. Mean-field phase diagram of the driven-dissipative Bose-Hubbard model. The numbers inside the plot represent the number of stable mean-field solutions. The yellow region exhibits two mean-field solutions, one of which is unstable. From Le Boité, Orso, and Ciuti, 2013.

As with the dissipative Ising model, the driven-dissipative Bose-Hubbard model has an intriguing mean-field phase diagram where several islands of multistability occur in a way that is somewhat reminiscent of Mott lobes (Le Boité, Orso, and Ciuti, 2013); see Fig. 1. The stability of the mean-field solutions has been evaluated by considering density matrices of the form

$$\rho = \prod_i (\rho_i^{\mathrm{MF}} + \delta\rho_i), \tag{5}$$

with ρ_i^{MF} the mean-field solution for the steady state. Expanding the quantum master equation up to first order in $\delta\rho_i$ allows one to evaluate the stability by checking whether none of eigenvalues of the Liouvillian have a positive real part.

II. STOCHASTIC METHODS

The statistical nature inherent in open quantum systems makes them especially amendable to treating their dynamics as stochastic processes. For an introduction to the probability-theoretic concepts and some of the numerical methods discussed here, see Breuer and Petruccione (2002).

At first glance, the computational complexity of an open quantum system in terms of the Hilbert space dimension d appears to be at least $O(d^2)$, as there are $O(d^2)$ independent entries in the density matrix ρ. However, the density matrix at an initial time t_0 can be written as a statistical ensemble of pure states $\rho(t_0) = \sum_i p_i|\psi_i(t_0)\rangle\langle\psi_i(t_0)|$. Instead of propagating the entire density matrix, the key strategy is to propagate the individual trajectories consisting of pure states $|\psi_i\rangle$ to the time t and then calculate observables according to

$$\langle O\rangle = \mathrm{Tr}\{O\rho\} = \sum_i p_i\langle\psi_i|O|\psi_i\rangle, \tag{6}$$

where O is an operator whose expectation value we want to compute. The probability distribution p_i can then be sampled using standard Monte Carlo techniques, which is why the approach is often called the wave-function Monte Carlo method. In most cases, one starts from an initial pure state $|\psi_0\rangle$, which is the same for all trajectories. For M trajectories, the probabilities p_i are then simply given by $p_i = 1/M$. Since the trajectories $|\psi_i\rangle$ are independent from each other, the statistical error associated with the observable behaves as $\Delta O \sim 1/\sqrt{M}$. The entire computational cost is $O(Md)$, which is already considerably lower than d^2 for modest system sizes. The requirement to repeat the simulation M times results in the simulation time being significantly longer than for a comparable closed quantum system. Depending on the observable, $M \approx 1000$ is a reasonable choice to get the statistical error down to a few percent. For spin $1/2$ systems, this essentially means that the system sizes that can be studied in an open system consist of $\log_2 M \approx 10$ particles fewer than in a closed system.

A. Quantum state diffusion

The central question now is how a single trajectory $|\psi_i\rangle$ can be propagated such that the ensemble of all trajectories satisfies $\rho(t) = \sum_i p_i |\psi_i(t)\rangle\langle\psi_i(t)|$. One possibility is to describe the evolution of the density operator in terms of a quantum state diffusion approach (Gisin and Percival, 1992; Percival, 1998), in which the incoherent dynamics from the Lindblad operators is captured in terms of a stochastic Schrödinger equation

$$d\psi_i(t) = -iH_{\text{eff}}|\psi_i(t)\rangle dt + \sum_j M_j|\psi_i(t)\rangle dW_j, \tag{7}$$

where dW_j refers to the Wiener increments. The effective Hamiltonian H_{eff} describes the drift of the state vector in the Hilbert space

$$H_{\text{eff}} = H + \sum_j 2\langle c_j^\dagger\rangle c_j - c_j^\dagger c_j - \langle c_j^\dagger\rangle\langle c_j\rangle. \tag{8}$$

The diffusion operators M_j describe the random fluctuations arising from each associated jump operator c_j:

$$M_j = c_j - \langle c_j\rangle. \tag{9}$$

This stochastic Schrödinger equation conserves the norm of the state vector and can be solved by standard techniques for stochastic differential equations.

B. Quantum jump method

An alternative strategy to propagate a single trajectory is the quantum jump method (Dalibard, Castin, and Mølmer, 1992; Dum, Zoller, and Ritsch, 1992; Mølmer, Castin, and Dalibard, 1993; Plenio and Knight, 1998). This approach was reviewed extensively by Daley (2014), so we cover only the basic strategy here. Within the quantum jump method, the dynamics is split into two parts. First, the state $|\psi_i\rangle$ is propagated under an effective non-Hermitian Hamiltonian H_{NH},

$$H_{\text{NH}} = H - \frac{i}{2}\sum_j c_j^\dagger c_j. \tag{10}$$

Once the norm of the state drops below a previously drawn random number r, a quantum jump occurs. Which quantum jump occurs is drawn from the probability distribution

$$p_j = \mathcal{N}\langle\psi_i|c_j^\dagger c_j|\psi_i\rangle, \tag{11}$$

with $\mathcal{N}$ a normalization factor. While the high-order integration of H_{NH} is straightforward, a high-order simulation of the quantum jumps requires a more subtle identification of the time the jump operator needs to be applied. For instance, the popular `QuTiP` library (Johansson, Nation, and Nori, 2012, 2013) uses a logarithmic secant method to numerically solve the equation $\langle\psi_i(t)|\psi_i(t)\rangle = r$ for the time t.

No matter which approach is used to propagate a single trajectory, the computations can be highly parallelized since the trajectories are independent from each other by construction. Doing so, it is possible to simulate open many-body spin $1/2$ models with up to 20 spins (Raghunandan, Wrachtrup, and Weimer, 2018). The relatively small system sizes relative to equilibrium problems demand the development of new data analysis techniques, such as those concerning finite-size scaling methods. One possibility is to use anisotropic system sizes to obtain more data points for a reliable finite-size scaling extrapolation. Close to a phase transition, the susceptibility χ of a system may be expressed as

$$\chi = N^\alpha \tilde{\chi}(\lambda), \tag{12}$$

where N is the number of particles and α is an exponent associated with the underlying phase transition (Binder and Wang, 1989). The reduced susceptibility $\tilde{\chi}$ is only a function of the anisotropy λ of the system and can be determined by symmetry considerations as well as numerical data (Raghunandan, Wrachtrup, and Weimer, 2018).

The wave-function Monte Carlo method has been used to analyze the one-dimensional dissipative Ising model of Eq. (3) (Ates *et al.*, 2012; Hu, Lee, and Clark, 2013). While previous works have not found a bistable phase as predicted by mean-field theory, a significant increase in the spin correlations has been reported in the same region (Hu, Lee, and Clark, 2013). Additionally, finite-size scaling of a similar two-dimensional model believed to lie in the same universality class as the dissipative Ising model has produced evidence of a first-order transition (Raghunandan, Wrachtrup, and Weimer, 2018).

III. TENSOR NETWORK METHODS

Tensor network techniques are state-of-the-art numerical methods for studying strongly correlated, quantum many-body systems. They are built on genuine quantum correlations and therefore automatically go beyond the mean-field approximations. Other advantages of these techniques include the ability to access large system size, no sign problem for fermionic or frustrated systems, etc. For an introduction to tensor network techniques and their diagrammatic notation, see Verstraete, Murg, and Cirac (2008), Cirac and Verstraete

(2009), Eisert (2013), and Orus (2014, 2019). In the following, we discuss how these techniques have been used for studying open quantum systems.

A. One spatial dimension

We first describe the important numerical techniques that have been developed for studying open quantum many-body systems using matrix product states (MPSs), which are a one-dimensional ansatz of the tensor network (TN) family. MPSs are by far the most successful and widely used ansatz in comparison to other ansatz of the tensor network family, thanks to the success of the density matrix renormalization group (DMRG) (White, 1992, 1993) and related techniques (Vidal, 2003, 2004). Not only are its properties well understood, but contraction of MPS tensors can be done efficiently and exactly unlike the case for its higher-dimensional counterparts (Schuch *et al.*, 2007; Haferkamp *et al.*, 2020). For these reasons, MPSs have been used extensively and produce extremely accurate results, however, mostly in the context of ground state calculations of many-body systems (Schollwöck, 2005). The application to open quantum systems, meanwhile, is more rare and there are only a few known approaches that one can take for such systems. Not only are open systems more computationally challenging (since we need to deal with matrices in place of vectors for the pure states), but there are also several intrinsic bottlenecks such as the positivity Hermiticity in the numerical optimization of the density matrix. Nevertheless, many of the ideas in the pure state formalism have been successfully applied in the context of open systems using the concept of matrix product operators (MPOs) or matrix product density operators (MPDOs) (Pirvu *et al.*, 2010; Cirac *et al.*, 2017). These approaches have also been used to study thermodynamic properties of 1D systems. We discuss them next.

1. Matrix product density operators

In 2004, Verstraete, García-Ripoll, and Cirac (2004) introduced the concept of MPDOs, which extended the MPS formalism from pure to mixed states. We recall that an MPS can be written in the following form:

$$|\psi\rangle = \sum_{s_1,\ldots,s_N=1}^{d} A_1^{s_1},\ldots,A_N^{s_N}|s_1,\ldots,s_N\rangle, \tag{13}$$

where the A's are matrices whose dimension is bounded by some fixed number D (also called the bond dimension χ) and d is the physical dimension of the local Hilbert space labeled by $s_1,\ldots,s_N$. A MPDO ρ of N d-level particles with $(D_1, D_2, \ldots, D_N)$-dimensional bonds is then defined as

$$\rho = \sum_{s_1,s_1',\ldots,s_N,s_N'=1}^{d} (M_1^{s_1,s_1'},\ldots,M_N^{s_N,s_N'})|s_1,\ldots,s_N\rangle\langle s_1',\ldots,s_N'|, \tag{14}$$

where $M_k^{s_k,s_k'}$ are $D_k^2 \times D_{k+1}^2$ matrices that can be decomposed as

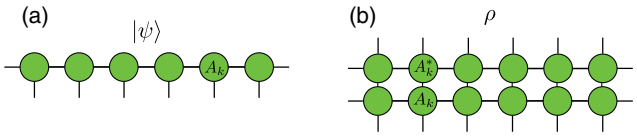

FIG. 2. (a) Writing a wave function $|\psi\rangle$ as a MPS for six sites. Each site has a physical dimension d. (b) A density matrix ρ can be written as a MPDO, an extension of the MPS formalism. Such a construction automatically ensures positivity of the density matrix.

$$M_k^{s,s'} = \sum_{a=1}^{d_k} A_k^{s,a} \otimes (A_k^{s',a})^*, \tag{15}$$

where d_k is at most dD_kD_{k+1} and the matrices $A_k^{s,k}$ are of size $D_k \times D_{k+1}$. Such a construction of MPDOs automatically ensures the positivity of the reduced density matrix ρ. This is shown in Fig. 2. This MPDO can be expressed in terms of a pure state MPS by defining it over a larger Hilbert space and using the concept of purification (Nielsen and Chuang, 2000). This can be done by associating an ancilla with a Hilbert space of dimension d_k with each physical system. One can then choose an orthonormal basis $|s_k, a_k\rangle$ for these physical and ancilla indices. The corresponding MPS for this system can be written as

$$|\Psi\rangle = \sum_{s_1,\ldots,s_N} \sum_{a_1,\ldots,a_N} A_1^{s_1,a_1},\ldots,A_N^{s_N,a_N}|s_1a_1,\ldots,s_Na_N\rangle. \tag{16}$$

The MPDO ρ can be obtained by tracing over the ancillas, i.e., $\rho = \mathrm{Tr}_a(|\Psi\rangle\langle\Psi|)$. This process is illustrated in Fig. 3. The original A_k matrices can be recovered from M_k by doing some eigenvalue decomposition. To determine the evolution of a Hamiltonian of a mixed state in real and imaginary time, Verstraete, García-Ripoll, and Cirac (2004) simply simulated the evolution of the purification by updating the A_k matrices using an iterative procedure similar to the standard DMRG in this technique. The purification could then be used to reconstruct the density operator at any time and compute the expectation values of the observables. Such a purification scheme can be used for mixed state evolution under dissipation as well as for thermal equilibrium and can be implemented irrespective of periodic or open boundary conditions and finite or infinite systems. The main source of errors in this procedure, as in most other TN techniques are

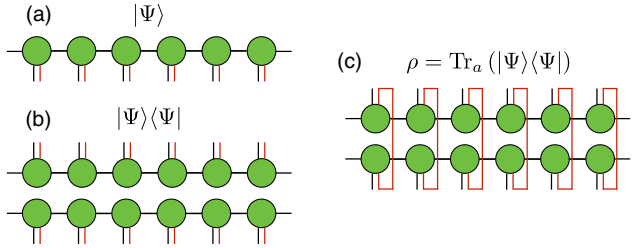

FIG. 3. (a) Defining a MPS $|\Psi\rangle$ over the enlarged Hilbert space using ancillas (in red). (b) Taking the projector of the MPS with ancillas. (c) Tracing out the ancillas from the projector to obtain the MPDO ρ.

(i) Trotter error and (ii) truncation error. Such an approach with ancillas was also applied to study the thermodynamic properties of several spin chains by Feiguin and White (2005). Although the MPDOs given by Verstraete, García-Ripoll, and Cirac (2004) are positive by construction, it was shown by De las Cuevas *et al.* (2013) that such a MPDO description of mixed states is not exactly equivalent to that obtained using local purification schemes. In particular, it was shown that the bond dimension of the locally purified MPS D' is not upper bounded by the bond dimension of the MPDO D. In fact, the local purification techniques can be much more costly than the MPDO form itself. Thus, De las Cuevas *et al.* (2013) concluded that a description of mixed states that is both efficient and locally positive semidefinite does not exist and that one can make only approximations.

2. Vectorized density matrices

Around the same time, Zwolak and Vidal (2004) proposed another technique to study the mixed state dynamics in one-dimensional lattice systems. Their technique, which is also based on MPSs, used the time-evolving block decimation (TEBD) to simulate the real time Markovian dynamics given by a master equation with nearest-neighbor couplings. At the heart of this algorithm lies the concept of a "Choi isomorphism." This is more of a mathematical trick, and it states that one can rewrite the coefficients of a matrix as those of a vector. In other words, this is simply turning a bra index into a ket index for a density matrix (understanding the coefficients of ρ as those of a vectorized density matrix denoted by $|\rho\rangle_\sharp$). And in the language of TN diagrams, it can be regarded as reshaping one of the legs and gluing it to the other (Fig. 4). Once vectorized, $|\rho\rangle_\sharp$ now lives in the n-fold tensor product of $\mathbb{C}_{d^2}$ and the master equation can be written in the vector form. The mixed state now looks as follows:

$$|\rho\rangle_\sharp = \sum_{i_1=0}^{d^2-1} \cdots \sum_{i_N=0}^{d^2-1} c_{i_1 \cdots i_N} |i_1\rangle_\sharp \otimes \cdots \otimes |i_N\rangle_\sharp, \qquad (17)$$

where $|i_l\rangle_\sharp$ is an orthonormal basis of $\mathbb{C}_{d^2}$ for site l. Further assuming that the Liouvillian superoperator $\mathcal{L}$ can be decomposed into terms involving at most nearest neighbors, i.e., $\mathcal{L}[\rho] = \sum_l \mathcal{L}_{l,l+1}[\rho]$, one could in principle use the usual TEBD algorithm to solve Eq. (2) by starting from some initial MPO (shown on the left side of Fig. 4). This was the basic idea behind the technique used by Zwolak and Vidal (2004). One of the first applications of this technique was the study of the driven-dissipative Bose-Hubbard model in the context of optical resonators (Hartmann, 2010). A more detailed explanation of this vectorization process is given later when we discuss the case for higher-dimensional systems. Although the technique has proven to be extremely simple and efficient, the issue of positivity still remains at large. In fact, checking the positivity of a reduced density matrix is known to be a difficult problem in physics (Kliesch, Gross, and Eisert, 2014).

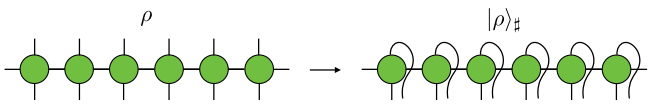

FIG. 4. Choi isomorphism: vectorizing a density matrix written in terms of an MPO. In a TN diagram, it is simply reshaping one of the indices and gluing it to the other, thereby giving us a MPS.

Another approach was taken by Werner *et al.* (2016) to solve the problem of positivity. In this approach, instead of expressing ρ directly as a MPO, at every stage of the algorithm ρ was kept in its locally purified $\rho = XX^\dagger$, where the purification operator X is decomposed as a variational tensor network:

$$[X]^{s_1,\ldots,s_N}_{r_1,\ldots,r_N} = \sum_{m_1,\ldots,m_{N-1}} A^{[1]s_1,r_1}_{m_1} A^{[2]s_2,r_2}_{m_1,m_2}, \ldots, A^{[N]s_N,r_N}_{m_{N-1}}, \qquad (18)$$

where $1 \le s_l \le d$, $1 \le r_l \le K$, and $1 \le m_l \le D$. $A^{[l]}$ are rank-4 tensors with physical dimension d, bond dimension D, and Kraus dimension K. Then a technique similar to the usual TEBD was used to update the tensors. Such an approach never required to contract the two TN layers (X and $X^\dagger$) together, thereby ensuring positivity at all times during the evolution. The technique also provided more control of the approximation error with respect to the trace norm.

3. Direct MPO approaches

Cui, Ignacio Cirac, and Bañuls (2015) took an interesting and different approach based on MPOs for finding the steady states of dissipative 1D systems governed by the master equation of the Lindbladian form $d\rho/dt = \mathcal{L}[\rho]$, where $\mathcal{L}$ is the Liouvillian superoperator. In this technique, instead of doing the full real time evolution of the Liouvillian, they proposed a variational method that searches for the null eigenvector of $\mathcal{L}$, which is by definition the steady state of the master equation in the Lindbladian form. Their results were based on the principle that if ρ_s is the steady state of the Lindbladian master equation satisfying $\hat{\mathcal{L}}|\rho_s\rangle_\sharp = 0$, then $|\rho_s\rangle_\sharp$ will also be the ground state of the nonlocal Hamiltonian $\hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}$ (since it is Hermitian and positive semidefinite), where $|\rho_s\rangle_\sharp$ is the vectorized form of the steady-state density matrix. Then using a variational algorithm, they directly targeted the ground state of $\hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}$ to find the steady state of the Lindbladian master equation for a finite chain. One of the reasons why directly targeting the ground state of $\hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}$ might be advantageous is that unlike imaginary time evolution, where the sequence of states visited by the algorithm is unimportant, the simulation of a master equation requires us to follow real time evolution. Therefore, if there are errors in the intermediate states visited by the algorithm, it may lead to problems in the convergence of our steady state. For example, some of the intermediate states may require large bond dimensions of the MPO, although it is known that the final steady state can be well represented by a MPO of small bond dimensions (Cai and Barthel, 2013; Bonnes, Charrier, and Läuchli, 2014). In addition, one does not need to worry about the large-entanglement growth of real time evolution. A similar approach was taken by Mascarenhas, Flayac, and Savona (2015), where the algorithm, instead of doing a time evolution, searched for the null eigenvalue of the Liouvillian superoperator $\mathcal{L}$ by sweeping along the system. Their method was

claimed to work even in the weakly dissipative regime by slowly tuning the dissipation rates along the sweeps. However, we note that such techniques, while advantageous numerically, cannot be used for obtaining the transient states.

Gangat, I, and Kao (2017) applied this idea to infinite 1D systems (i.e., the thermodynamic limit) using a hybrid technique of both imaginary and real time evolution. They took a local auxiliary Hamiltonian $\mathcal{H}$ whose ground state is a good approximation to the ground state of the nonlocal Hamiltonian $\hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}$ by taking its kth root as

$$\mathcal{H} = \sum_{r\in\mathbb{Z}} (\hat{\mathcal{L}}_r^\dagger \hat{\mathcal{L}}_r)^{1/k}, \tag{19}$$

where $\hat{\mathcal{L}} = \sum_{r\in\mathbb{Z}} \hat{\mathcal{L}}_r$ since $\hat{\mathcal{L}}$ is a translationally invariant local operator. The kth root was taken in order to yield faster convergence. The idea is that if the gap between the two lowest eigenvalues of $\hat{\mathcal{L}}_r^\dagger\hat{\mathcal{L}}_r$ is less than 1, then $k > 1$ will increase the gap since $\hat{\mathcal{L}}_r^\dagger\hat{\mathcal{L}}_r$ is positive semidefinite, thereby achieving faster convergence to the ground state. Gangat, I, and Kao then performed a real time evolution to obtain a more accurate steady state. In summary, the main steps of the algorithm are as follows:

(i) Imaginary time evolution of the auxiliary Hamiltonian $\mathcal{H}$ starting from some vectorized initial density matrix $|\rho_0\rangle$:

$$|\rho_G\rangle \approx \lim_{\tau\to\infty} \frac{e^{-\mathcal{H}\tau}|\rho_0\rangle}{\|e^{-\mathcal{H}\tau}|\rho_0\rangle\|}. \tag{20}$$

(ii) Real time evolution of the Liouvillian superoperator starting from $|\rho_G\rangle$:

$$|\rho_S\rangle \approx \lim_{T\to\infty} \frac{e^{\mathcal{L}T}|\rho_G\rangle}{\|e^{\mathcal{L}T}|\rho_G\rangle\|}. \tag{21}$$

$|\rho_S\rangle$ is the desired steady state of the Liouvillian master equation. Imaginary time evolution in step (i) ensures that one does not pass through a highly entangled transient regime. Step (ii) improves the accuracy of the stationary state since $|\rho_G\rangle$ is the ground state of $\mathcal{H}$, which is a truncated approximation of the nonlocal Hamiltonian $\hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}$.

In one spatial dimension, many of the previously mentioned techniques and their combinations have been used not only for studying other important dissipative models (Höning, Moos, and Fleischhauer, 2012; Pižorn, 2013; Mascarenhas, Flayac, and Savona, 2015; Carollo *et al.*, 2019), including the dissipative Ising model of Eq. (3) (Höning *et al.*, 2013; Mendoza-Arenas *et al.*, 2016), but also in the dissipative preparation of topologically ordered materials (Iemini *et al.*, 2016) as well as in the energy transport (Guo, Mukherjee, and Poletti, 2015). Recently MPO based techniques have been applied to the study of vibronic states, which has extended applications to quantum biology and organic photovoltaics (Somoza *et al.*, 2019), and also to the study of the dynamics of photonic circuits with time delays and quantum feedback (Pichler and Zoller, 2016). We do not discuss the last two works due to the non-Markovian nature of the problem, which is beyond the scope of this review. Similar MPS based techniques that go beyond the Lindblad master equation (Xu *et al.*, 2019) or the Markovian approximation (Guo *et al.*, 2018) are also not discussed here.

B. Extensions to higher dimensions

Unlike the case in one dimension, the generalization of MPS in higher dimensions, also known as projected entangled pair states (PEPSs) or tensor product states, comes with serious limitations and there are still many open problems (Cirac, Garre-Rubio, and Pérez-García, 2019). Not only does the PEPS algorithm require significant programming effort, but exact contraction of PEPSs is known to be a mathematically difficult problem (Schuch *et al.*, 2007; Haferkamp *et al.*, 2020). To achieve this, one requires additional PEPS contraction algorithms (Jordan *et al.*, 2008; Orús and Vidal, 2009; Orús, 2012) that are nevertheless known to give accurate results, particularly for gapped systems. Even for critical systems with algebraically decaying correlations, the PEPS contraction schemes are known to provide reasonably accurate results with sufficiently high bond dimension of the environment (Orús and Vidal, 2009). In fact, techniques have recently been introduced to capture the infinite correlation length of 2D critical systems using infinite-PEPS algorithm (iPEPS) based on finite correlation length scaling (Corboz *et al.*, 2018; Rader and Läuchli, 2018). Thus, despite the higher requirement of numerical dedications and limitations, PEPS algorithms are becoming state-of-the-art numerical tools for strongly correlated two-dimensional systems. PEPSs have provided the best variational energy for the 2D Hubbard model (Corboz, 2016a) and offered several new insights on paradigmatic models and real materials in the lab (Matsuda *et al.*, 2013; Corboz and Mila, 2014; Liao *et al.*, 2017; Kshetrimayum, Balz *et al.*, 2020). The successes of PEPS thus far, however, are confined mostly to ground state calculations and partially to thermal states (Czarnik, Cincio, and Dziarmaga, 2012; Czarnik and Dziarmaga, 2015; Czarnik, Dziarmaga, and Oleś, 2016; Dai *et al.*, 2017; Kshetrimayum *et al.*, 2019; Mondal, Kshetrimayum, and Mishra, 2020) using the concept of projected entangled pair operators (PEPOs) or tensor product operators, which we discuss in more detail later and, more recently, to time evolution (Czarnik, Dziarmaga, and Corboz, 2019; Hubig and Cirac, 2019; Kshetrimayum, Goihl *et al.*, 2020; Kshetrimayum, Goihl, and Eisert, 2020). For the context of open dissipative quantum systems, thus far there is only one known approach using PEPSs (Kshetrimayum, Weimer, and Orús, 2017) and another one using a corner space renormalization method (Finazzi *et al.*, 2015). We describe them next. We also discuss other potential implementation techniques and possible issues while using the PEPS formalism, particularly for such open systems.

1. Corner space renormalization method

The corner space renormalization method (Finazzi *et al.*, 2015) solves the master equation in a corner of the Hilbert space through an iterative procedure. It starts by finding the steady-state density matrix for small lattice systems (say, ρ^A and ρ^B for systems A and B, respectively). This can be done

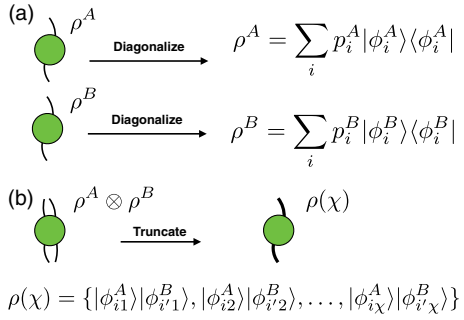

FIG. 5. (a) Steady-state density matrices of two systems A and B are first obtained using brute force. They are then expressed in their respective diagonal forms. (b) We then merge the two systems and keep only the χ most probable pair of states. The process is repeated for different χ's until we get some convergence. Larger systems can be simulated by merging more systems in step (b).

using a brute force integration of the master equation since the system size is small. The steady-state density matrices can be diagonalized and written as

$$\rho^A = \sum_i p_i^A |\phi_i^A\rangle\langle\phi_i^A|,$$
$$\rho^B = \sum_i p_i^B |\phi_i^B\rangle\langle\phi_i^B|, \tag{22}$$

where the states $|\phi_i^A\rangle$ form an orthonormal basis for $\mathcal{H}_A$ (the Hilbert space corresponding to system A) and p_i^A are the corresponding probabilities. A similar notation follows for system B. The two systems are then merged and the χ most probable product states spanning the so-called corner space are selected; i.e., we keep only the subspace generated by the orthonormal basis $\{|\phi_{i1}^A\rangle|\phi_{i'1}^B\rangle, |\phi_{i2}^A\rangle|\phi_{i'2}^B\rangle, \ldots, |\phi_{i\chi}^A\rangle|\phi_{i'\chi}^B\rangle\}$, where the products of the probabilities of the two systems are arranged in decreasing order of magnitude. In this way, we keep only the χ most probable pair of states. The steady state of the density matrix in this corner space can be determined by using either direct numerical integration in time (for small χ) or a stochastic wave-function Monte Carlo algorithm for large χ; see Sec. II. One can then increase the size of the corner χ until convergence in some observables is reached. Larger systems can be simulated by merging more systems, as we discussed in the initial steps. A simplified summary of the steps involved is shown in Fig. 5.

The proposed corner space renormalization method was used to study the driven-dissipative Bose-Hubbard model in two dimensions in both periodic and open boundary conditions for system sizes up to 16×16 lattice sites. The technique has also been used to study the critical Heisenberg model (Rota *et al.*, 2017) for system sizes up to 6×6 lattice sites and, more recently, the critical regime in the Bose-Hubbard model (Rota *et al.*, 2019) for up to 8×8 lattices. The size of the lattice that can be simulated using this technique depends on the entanglement of the steady state. Even if it is not obvious at first sight, the structure of the density operator generated by the corner space renormalization method amounts to that of a tree tensor network (Shi, Duan, and Vidal, 2006). As such, this particular method, even if understood in terms of TNs, is tailored to driven-dissipative systems of finite size. For generalizing it to the thermodynamic limit or for nondriven nondissipative systems, one needs to use more general TN techniques. We now discuss one such technique that we developed recently.

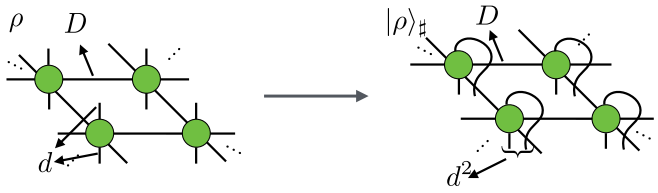

FIG. 6. TN diagram for the PEPO of ρ on a 2D square lattice with bond dimension D and physical dimension d. When vectorized, it can be understood as a PEPS for $|\rho\rangle_\sharp$ with physical dimension d^2.

2. Vectorized projected entangled pair operators

In 2017, we made use of the concept of PEPOs by vectorizing them (Kshetrimayum, Weimer, and Orús, 2017). PEPOs are simply the operator version of PEPSs, in the same way that a MPO is the operator version of MPS for the 1D case. Hence, PEPOs are used to represent mixed states ρ in two dimensions, even beyond dissipative systems, such as for thermal states (Czarnik, Cincio, and Dziarmaga, 2012; Czarnik and Dziarmaga, 2015; Czarnik, Dziarmaga, and Oleś, 2016; Kshetrimayum *et al.*, 2019). As mentioned earlier, such a construction of density matrices using PEPOs does not automatically guarantee the positivity of the density matrix. However, for simulations targeting the steady states, this lack of exact positivity is not a bottleneck if the fixed point is not highly entangled. For the moment, we restrict our discussion to this case. Once we have our PEPO, we vectorize it, i.e., rewrite the coefficients of the PEPO as a PEPS (also called Choi's isomorphism). Once vectorized, the PEPO ρ can be understood as a PEPS of physical dimension d^2 and bond dimension D (now called $|\rho\rangle_\sharp$), as shown in Fig. 6. The vectorized form of the Lindblad master equation (2) can be written as

$$\frac{d}{dt}|\rho\rangle_\sharp = \mathcal{L}_\sharp|\rho\rangle_\sharp, \tag{23}$$

where the vectorized Liouvillian operator is given by

$$\mathcal{L}_\sharp \equiv -i(H \otimes \mathbb{I} - \mathbb{I} \otimes H^T) + \sum_\mu \left(L_\mu \otimes L_\mu^* - \frac{1}{2} L_\mu^\dagger L_\mu \otimes \mathbb{I} - \frac{1}{2} \mathbb{I} \otimes L_\mu^* L_\mu^T \right). \tag{24}$$

H is the Hamiltonian of the system and $\mathbb{I}$ corresponds to the identity operator. L_μ and $L_\mu^\dagger$ correspond to the on-site Lindblad or jump operators responsible for dissipation. The tensor product $\otimes$ separates the operator acting on the ket and bra index of ρ before the vectorization. When the vectorized Liouvillian superoperator $\mathcal{L}_\sharp$ is independent of time, Eq. (23) can be integrated as

TABLE I. Ground state calculation in a closed quantum system (left column) and steady-state calculation in an open quantum system (right column). The former requires an imaginary time evolution, while the latter follows a real time evolution. Both the Hamiltonian H and the vectorized Liouvillian $\mathcal{L}_\sharp$ can be decomposed as a sum of local terms. $|e_0\rangle$ is the ground state of the many-body Hamiltonian with e_0 as its ground state. $|\rho_s\rangle_\sharp$ is the nonequilibrium steady state of the Liouvillian in their vectorized forms.

Ground states	Steady states
$H=\sum_{\langle i,j\rangle} h^{[i,j]}$	$\mathcal{L}_\sharp=\sum_{\langle i,j\rangle}\mathcal{L}_\sharp^{[i,j]}$
e^{-Ht}	$e^{\mathcal{L}_\sharp t}$
$\lvert e_0\rangle$	$\lvert\rho_s\rangle_\sharp$
$\langle e_0\lvert H\rvert e_0\rangle=e_0$	${}_\sharp\langle\rho_s\lvert\mathcal{L}_\sharp\rvert\rho_s\rangle_\sharp=0$
Imaginary time	Real time

$$|\rho(t)\rangle_\sharp = e^{\mathcal{L}_\sharp t}|\rho(0)\rangle_\sharp, \tag{25}$$

where $|\rho(0)\rangle_\sharp$ is some vectorized initial density matrix, written as a PEPS. In the limit of $t\to\infty$, we obtain the nonequilibrium steady state (NESS) as the fixed point of the master equation that we denote by $|\rho_s\rangle_\sharp$. From Eq. (23), it is also obvious that $|\rho_s\rangle_\sharp$ is the right eigenvector of $\mathcal{L}_\sharp$ with zero eigenvalue so that

$$\mathcal{L}_\sharp|\rho_s\rangle_\sharp = 0. \tag{26}$$

For a Liouvillian $\mathcal{L}$ consisting of local terms, say, $\mathcal{L}[\rho]=\sum_{\langle i,j\rangle}\mathcal{L}^{[i,j]}[\rho]$, the vectorized form of the Lindblad equation (2) yields a parallelism with the calculation of ground states of local Hamiltonians by imaginary time evolution, which we detail in Table I. Given this parallelism, one can adapt, at least in principle, the methods to compute imaginary time evolution of a pure state as generated by local Hamiltonians to compute also the real time evolution of a mixed state as generated by local Liouvillians. This was, in fact, the approach taken by Zwolak and Vidal (2004) for finite-size 1D systems, using MPOs to describe the 1D reduced density matrix and proceeding as in the TEBD algorithm for ground states of 1D local Hamiltonians (Vidal, 2003, 2004, 2007; Orús and Vidal, 2008), as previously discussed. In 2017, we extended this implementation for the case of 2D systems using the concept of PEPOs with physical dimension d and bond dimension D (Kshetrimayum, Weimer, and Orús, 2017); see Fig. 6. For the case of an infinite-size 2D system, this setting is actually equivalent to that of the iPEPS to compute ground states of local Hamiltonians in 2D in the thermodynamic limit. Thus, in principle, one can use the full machinery of the iPEPS to tackle the problem of 2D dissipation and steady states.

There is, however, one problem with this idea: unlike in imaginary-time evolution, we are now dealing with real time. In the master equation, part of the evolution is generated by a Hamiltonian H and part by the Lindblad operators L_μ. The Hamiltonian part corresponds actually to a unitary "Schrödinger-like" evolution in real time, which typically increases the "operator entanglement" in $|\rho\rangle_\sharp$, up to a point at which it may be too large to handle for a TN representation

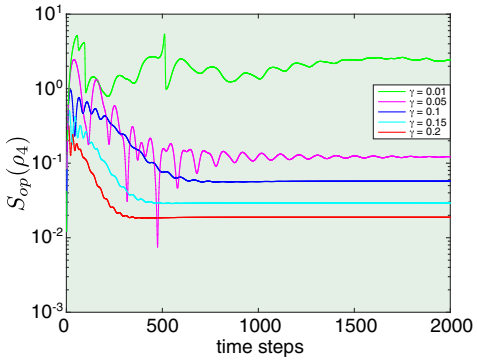

FIG. 7. Operator-entanglement entropy $S_{\rm op}$ for a block of 2×2 unit cells for real time evolution of the master equation for different values of dissipation strength. Stronger dissipation implies lower entanglement growth and faster convergence to the NESS. From Kshetrimayum, Weimer, and Orús, 2017.

(such as 1D MPOs or 2D PEPOs) with a reasonable bond dimension. In one dimension this is the reason why the simulations of master equations are only for only a finite amount of time. In two dimensions, simple numerical experiments indicate that in a typical simulation the growth of entanglement is even faster than in one dimension. This is not a dead end: if the dissipation is strong compared to the rate of entanglement growth, then the evolution drives the system into the steady state before hitting a large-entanglement region. In fact, even if there is too much entanglement for the TN at intermediate times, the dissipation may still drive the evolution toward a good approximation of the correct steady state. In short, dissipation limits the growth of entanglement if the fixed point attractor is strong enough. This can be verified numerically by plotting the operator-entanglement entropy for different dissipation strengths as it flows into the NESS. This is shown in Fig. 7. Details on how to compute this quantity were given by Kshetrimayum (2017) and Kshetrimayum, Weimer, and Orús (2017).

Hence, one can apply the iPEPS machinery to compute the time evolution in two dimensions with a local Liouvillian $\mathcal{L}$ and an initial state. This procedure was used to investigate the dissipative Ising and the XYZ model, confirming and offering several insights that were inaccessible before using mean-field and other techniques, for example, for the dissipative Ising model of Eq. (3) given by the Hamiltonian $H=(V/4)\sum_{\langle i,j\rangle}\sigma_z^{[i]}\sigma_z^{[j]}+(h_x/2)\sum_i\sigma_x^{[i]}$ and Lindblad operators $L_\mu=\sqrt{\gamma}\sigma_-^{[\mu]}$. The phase diagram is controversial with some researchers suggesting the existence of a bistable steady state (Lee, Häffner, and Cross, 2011; Marcuzzi *et al.*, 2014) and others supporting a first-order transition (Weimer, 2015a, 2015b; Maghrebi and Gorshkov, 2016). Our technique found bistability for low bond dimensions of the PEPO ($D=1,2$), which was replaced by a first-order transition for higher D's, thus confirming that the bistability is an artifact of the mean field. This is shown in Fig. 8. Furthermore, some studies suggested the existence of an antiferromagnetic region in the presence of the transverse field h_x (Lee, Häffner, and Cross, 2011; Weimer, 2015a). Once again, while our technique produced evidence of such an antiferromagnetic (AFM)

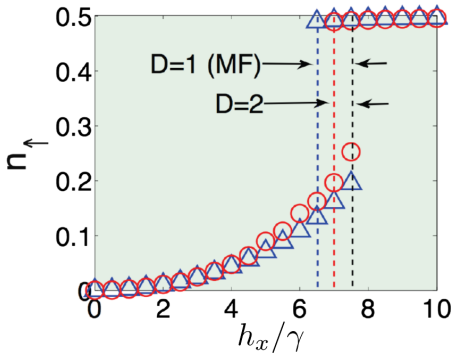

FIG. 8. Our study based on iPEPS found bistability in the phase diagram of the dissipative Ising model for low bond dimensions $D = 1, 2$. The bistability is replaced by a first-order transition for higher D's. From Kshetrimayum, Weimer, and Orús, 2017.

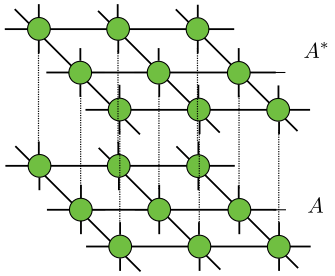

FIG. 9. TN diagram for the PEPDO of ρ on a 2D square lattice with bond dimension D and physical dimension d. When vectorized, it can be understood as a PEPS for $|\rho\rangle_\sharp$ with physical dimension d^2.

region, it eventually shrank with increasing bond dimension until it finally disappeared for large enough D. Results of the dissipative Ising model have been reproduced independently using a different update scheme (Czarnik, Dziarmaga, and Corboz, 2019) than that used by Kshetrimayum, Weimer, and Orús (2017). While the technique also employed vectorization along with the iPEPS, the update scheme is based on maximizing the fidelity between two consecutive steps of the update of the iPEPS tensors. For the case of the dissipative Heisenberg model (Lee, Gopalakrishnan, and Lukin, 2013) with the Hamiltonian

$$H = \sum_{\langle i,j\rangle} (J_x \sigma_x^i \sigma_x^j + J_y \sigma_y^i \sigma_y^j + J_z \sigma_z^i \sigma_z^j) \tag{27}$$

and the same Lindblad operators as before, our studies found no phenomenon of reemergence in the phase diagram, confirming a prediction by studies using cluster mean-field approaches (Jin *et al.*, 2016). Our extensive numerical experiments have revealed that although this technique, based on vectorization, does not explicitly preserve the positivity of the density matrix, it can still give accurate results for the nonequilibrium steady states of most models, especially when the steady state is not highly entangled. This is shown in Fig. 2(d) of Kshetrimayum, Weimer, and Orús (2017), where contributions of negative eigenvalues of the reduced density matrices are small in most of the regimes. Thus, the issue of positivity might be even less of a problem here than in the 1D case. One plausible explanation for this is the so-called entanglement monogamy (Coffman, Kundu, and Wootters, 2000; Koashi and Winter, 2004; Terhal, 2004; Osborne and Verstraete, 2006), where the correlation is spread out across several bonds in two dimensions, unlike in one dimension, and therefore one requires only a small bond dimension of the iPEPS for an accurate description of these steady states. The same is true in other settings, where it has been found that a small bond dimension of the PEPS is enough for accurate description of ground states of relevant and interesting 2D models (Verstraete, Murg, and Cirac, 2008; Orus, 2014).

3. Preserving positivity of the density matrix

To the best of our knowledge, we have discussed most of the state-of-the-art numerical techniques based on a TN for the study of open quantum many-body systems in both one and two spatial dimensions. We now discuss some ideas that could be helpful in improving the existing algorithm and possible new implementation techniques, especially in two dimensions. We first remark that the previously suggested 2D algorithm does not guarantee the positivity of the density matrices. This problem can be solved by starting from an initial state that is positive by construction, for example, by taking the product of two PEPOs that are the conjugates of each other (A and A^*). One can then think about using a positivity preserving algorithm such as the one given by Werner *et al.* (2016). Such an algorithm will ensure the positivity of the density matrix at all times of the evolution. We can call this initial density matrix the projected entangled pair density operator (PEPDO), as shown in Fig. 9. While such an approach may avoid the problem of negative eigenvalues of the density matrix, in practice it may require a high bond dimension of the PEPDO, and one therefore needs to consider the practical aspect of the implementation.

The other possibility would be to target the ground state of the Hermitian and positive semidefinite operator $\mathcal{L}_\sharp^\dagger \mathcal{L}_\sharp$. This ground state could be computed using an imaginary time evolution. However, there are two major hurdles associated with this approach. The crossed products in $\mathcal{L}_\sharp^\dagger \mathcal{L}_\sharp$ are nonlocal, and therefore the usual algorithms for time evolution are difficult to implement unless one introduces extra approximations in the range of the crossed terms. Another option is to approximate the ground state variationally via the density matrix renormalization group (White, 1992, 1993) in one dimension, or variational PEPS in two dimensions (Corboz, 2016b). In the thermodynamic limit, however, this approach does not look promising because of the previously mentioned nonlocality of $\mathcal{L}_\sharp^\dagger \mathcal{L}_\sharp$. In any case, one could always represent this operator as a PEPO (in two dimensions), which simplifies some of the calculations, but at the cost of introducing a large bond dimension in the representation of $\mathcal{L}_\sharp^\dagger \mathcal{L}_\sharp$. For instance, if a typical PEPO bond dimension for $\mathcal{L}_\sharp$ is ~ 4, then for $\mathcal{L}_\sharp^\dagger \mathcal{L}_\sharp$ it is ~ 16, which in two dimensions implies extremely slow calculations. Another option is to target the variational minimization of the real part for the expectation value of $\mathcal{L}$.

IV. VARIATIONAL METHODS

Variational techniques have a long history of finding approximate solutions to the ground state of quantum systems; see Schwabl (2010) for an introduction to the general concept. The successes of density functional theory (Kohn, 1999) and matrix product state approaches (Schollwöck, 2011) have made variational formulations a particularly powerful tool to analyze quantum many-body systems. As we discuss in this section, variational methods can also be successfully applied to open quantum many-body systems.

A. The variational principle for open quantum systems

1. Steady-state solution

Variational methods generically consist of two steps. The first step is a parametrization of the state of the system in terms of a set of variational parameters $\{\alpha_i\}$. For an open quantum system, it is convenient to parametrize the density matrix, i.e., $\rho = \rho(\{\alpha_i\})$, although parametrizations based on statistical ensembles of pure states are also possible (Transchel, Milsted, and Osborne, 2014). The second step is to identify a suitable functional that can be optimized by tuning the variational parameters. For open quantum systems, it is natural to apply a variational principle to find the steady state of the quantum master equation, which can be found by solving the equation $\dot{\rho} = 0$. The exact steady state can no longer be determined after the variational parametrization, as the steady state will generically lie outside the variational manifold. Hence, the best possible option is to find the variational parameters that will minimize the functional $\|\mathcal{L}\rho\|$ for a suitable norm (Weimer, 2015b).

The correct norm for the variational optimization can be identified as the trace norm $\|\mathcal{L}\rho\| = \mathrm{Tr}\{|\dot{\rho}|\}$, i.e., the sum of the absolute values of the eigenvalues of $\dot{\rho}$ (Weimer, 2015b). This choice can be motivated by different grounds. First, the trace distance, being the natural distance measure for density matrices (Nielsen and Chuang, 2000), is highly suggestive of the trace norm being the natural norm for the tangent space $\dot{\rho}$. This can be formalized in the sense that the trace norm describes an optimal measurement to distinguish $\dot{\rho}$ from the zero matrix (Gilchrist, Langford, and Nielsen, 2005). A second motivation for exploring the trace norm is to consider classes of possible alternatives. It can be shown that all Schatten p norms of the form $(|\dot{\rho}|^p)^{1/p}$ are inherently biased toward the maximally mixed state for all values of $p > 1$ (Weimer, 2015b). Since functionals with $p < 1$ do not constitute proper norms, this leaves the trace norm as the only valid choice. One can also understand the variational principle as a direct solution of the overdetermined steady-state equation $\mathcal{L}\rho = 0$ in terms of a trace norm minimization.

In general, the evaluation of the variational functional is still an exponentially difficult problem, as the computation of the trace norm requires the diagonalization of the matrix $\dot{\rho}$. However, it is possible to construct upper bounds to the variational norm that retain the variational character (Weimer, 2015b) and appear to introduce only small quantitative deviations even close to phase transitions (Weimer, 2015a). The upper bound depends on the variational manifold and its tangent space, i.e., the degree of additional correlations that can be built up by applying the Liouvillian to states within the variational manifold. For example, for a variational class of product states of the form $\rho = \prod_i \rho_i$, the upper bound D can be given as

$$D = \sum_{ij\in\mathcal{T}} \mathrm{Tr}\{|\dot{\rho}_{ij}|\}, \tag{28}$$

where $\mathcal{T}$ contains pairs of sites that are connected to each other by the Liouvillian (Weimer, 2015b).

The variational principle has been applied to find the steady states of the dissipative Ising and Bose-Hubbard models introduced in Eqs. (3) and (4), respectively (Weimer, 2015a, 2015b), as well as dissipative Ising models including a $\mathbb{Z}_2$ symmetry (Overbeck *et al.*, 2017), purely dissipative Heisenberg models (Weimer, 2017), dissipative Rydberg gases (Weimer, 2015a), dissipative ensembles of nitrogen-vacancy centers (Raghunandan, Wrachtrup, and Weimer, 2018), entanglement generation in cavity QED arrays (Lammers, Weimer, and Hammerer, 2016), and dissipative Fermi-Hubbard models (Kaczmarczyk, Weimer, and Lemeshko, 2016). In the last case, the study of fermionic models was realized by employing a two-dimensional Jordan-Wigner transformation, where the appearance of nonlocal Wigner strings was ruled out by the choice of the variational manifold.

2. Field-theoretical treatment of fluctuations

In the case where the steady state of the system is close to criticality, it is possible to construct a dissipative Ginzburg-Landau theory based on the variational principle (Overbeck *et al.*, 2017). The essential step is to perform a series expansion of the variational norm of Eq. (28) in terms of an order parameter field $\phi(x)$ and its spatial gradient $\nabla\phi(x)$, leading to

$$D[\phi] = \int dx \sum_m v_m [\nabla\phi(x)]^m + \sum_n u_n [\phi(x)]^n. \tag{29}$$

All the coefficients v_n and u_n can be calculated from the microscopic quantum master equation. The series can be truncated at low orders of m and n, as higher-order terms are irrelevant close to criticality. In the case of steady states with thermal statistics due to the presence of a dynamical symmetry (Sieberer *et al.*, 2013), it is possible to construct a Ginzburg-Landau-Wilson functional integral for an effective partition function (Hohenberg and Krekhov, 2015) given by

$$Z_{\mathrm{eff}} = \int \mathcal{D}\phi \exp\left(-\beta_{\mathrm{eff}} D[\phi]\right). \tag{30}$$

Here the effective inverse temperature β_{eff} can be derived from the u_0 coefficient, as this coefficient captures the strength of fluctuations beyond a spatially homogeneous order parameter field (Overbeck *et al.*, 2017). The subsequent statistical field theory of Eq. (30) can then be analyzed using standard techniques such as the perturbative renormalization group.

3. Time evolution

Finally, the variational principle can also be extended toward the full time evolution of open quantum systems (Overbeck and Weimer, 2016), following similar ideas to those discussed in the context of the time-dependent variational principle (Kraus and Osborne, 2012; Transchel, Milsted, and Osborne, 2014). There the variational functional is replaced by a variational integration of the quantum master equation for small time steps τ. For example, in the lowest-order Euler approximation, it is given by

$$D = \mathrm{Tr}\{|\rho(t+\tau) - \rho(t) - \tau\mathcal{L}\rho(t)|\}, \tag{31}$$

where $\rho(t+\tau)$ is the density matrix containing the variational parameters. Higher-order schemes exist as well, but constructing an upper bound similar to Eq. (28) requires one to consider higher-order correlations due to multiple applications of the Liouvillian to the density matrix. A good compromise is the implicit midpoint method, which is exact up to second order in τ while requiring only a single application of the Liouvillian (Overbeck and Weimer, 2016).

B. Comparison with mean-field methods

For equilibrium problems, the variational method based on product states is exactly equivalent to a mean-field decoupling of the interaction terms. This is not the case in open quantum systems. Within the mean-field approach to open systems (Diehl *et al.*, 2010; Tomadin *et al.*, 2010), a set of effective single site master equations that is obtained by tracing out the rest of the system is considered. For the ith site, the mean-field master equation reads as

$$\frac{d}{dt}\rho_i = \mathrm{Tr}_{i'}\left\{\frac{d}{dt}\rho\right\} = -i[H_i^{\mathrm{MF}}, \rho_i] + \mathcal{D}_i(\rho_i), \tag{32}$$

where H_i^{MF} and $\mathcal{D}_i$ are the mean-field Hamiltonian and the mean-field dissipators, respectively. This set of equation is then solved self-consistently, while for translationally invariant systems it is often sufficient to consider an effective single site problem.

1. Mean-field bistability

Because of the nonlinear structure of the mean-field equations of motion, it is possible to have two or more independent solutions for the steady state (Lee, Häffner, and Cross, 2011); see Fig. 10. This also occurs within mean-field theory for equilibrium systems close to first-order transitions. However, there one can always resort to the free energy, which has to be minimal in thermal equilibrium. Unless one invokes the variational principle, one cannot decide which of the solutions of mean-field theory are stable and which ones are not. The solutions according to the variational principle and mean-field theory are identical only in the limit of infinite dimensions, where both approaches become exact (Weimer, 2015b).

Mean-field theory predicts bistability for a wide range of models, including the dissipative Ising model (Lee, Häffner, and Cross, 2011; Lee and Cross, 2012; Marcuzzi *et al.*, 2014)

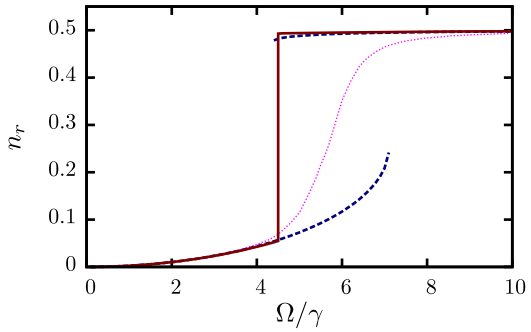

FIG. 10. Comparison of the solutions according to the variational principle (solid line), the mean-field decoupling (dashed line), and wave-function Monte Carlo simulations for 4×4 lattices for the up-spin density n_r of the dissipative Ising model. The mean-field solution displays a region of bistability, while the variational solution correctly predicts a first-order transition. From Weimer, 2015a.

or extended spin models (Parmee and Cooper, 2018), as well as driven-dissipative Bose-Hubbard models (Jin *et al.*, 2013; Le Boité, Orso, and Ciuti, 2013, 2014; Mertz *et al.*, 2016). To date mean-field bistability has been found in the absence of symmetries in the underlying master equation; i.e., the two solutions are not connected by a symmetry transformation. These properties have led to speculation that bistability could be a genuine nonequilibrium phase, which has stimulated several investigations into whether this could indeed be the case. However, the results of these investigations have all been negative thus far. Specifically, the variational principle predicts that bistability will be replaced by a first-order transition both in the dissipative Ising and in the driven-dissipative Bose-Hubbard model (Weimer, 2015b). For the dissipative Ising model, the existence of the first-order transition has been confirmed in tensor network simulations, where bistability is found for low bond dimensions, but a first-order transition appears for higher bond dimensions (Kshetrimayum, Weimer, and Orús, 2017); see Sec. III.B. In the case of the driven-dissipative Bose-Hubbard model, the first-order transition has also been found in a field-theoretic treatment based on the Keldysh formalism (Maghrebi and Gorshkov, 2016), again confirming the variational prediction. These results underscore that the conventional argument of mean-field theory becoming qualitatively correct if the spatial dimension becomes large enough appears to be incorrect for open quantum systems. On the other hand, this argument seems to be much more justified when applied to the variational principle [especially when considering the connection to equilibrium statistical physics through the existence of the dissipative Ginzburg-Landau theory of Eq. (29)]; however, even there one may have possible counterexamples (Mesterházy and Hebenstreit, 2017) that are not yet fully understood.

Nevertheless, these findings do not rule out genuine bistability in open quantum systems *per se*, but only that such mean-field results need to be taken with caution. Classical models exhibiting extended coexistence regions (Muñoz, de los Santos, and Telo da Gama, 2005) might still exhibit bistability after including quantum fluctuations.

The situation is similar when it comes to limit cycles of open quantum many-body systems (Chan, Lee, and Gopalakrishnan, 2015), which have been predicted to exist in sufficiently high-dimensional systems (Owen *et al.*, 2018).

2. Extensions of mean-field theory

One systematic extension of mean-field theory is cluster mean-field theory, where the trace in Eq. (32) is not carried out over all but one site but results in a larger cluster that again has to be solved self-consistently (Jin *et al.*, 2016). This strategy is in close analogy to the cluster mean-field theory for statistical mechanics and ground state problems (Bethe, 1935; Oguchi, 1955). Essentially, cluster mean-field approaches treat the short-range physics more accurately than bare mean-field theory, leading to better quantitative estimates for phase transitions. However, the qualitative limitations of bare mean-field theory remains, as these are the result of long-range fluctuations in the system. For open quantum many-body models, cluster mean-field theory has been used to calculate the phase diagram of the dissipative Heisenberg model given by Eq. (27) (Jin *et al.*, 2016) and dissipative Ising models with and without a $\mathbb{Z}_2$ symmetry (Jin *et al.*, 2018).

Finally, it is also possible to systematically go beyond the mean-field approximation using open system dynamical mean-field theory (DMFT). DMFT is a mapping of a many-body lattice model onto a single impurity problem that has to be solved in a self-consistent way (Georges *et al.*, 1996). Within DMFT, the approach is to start with an effective dynamical Green's function $\mathcal{G}_0$, which serves as a time-dependent version of a mean-field coupling. Considering the Fermi-Hubbard model as an example, $\mathcal{G}_0$ can be used to express the effective action of a single site as

$$S_{\mathrm{eff}} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma f_\sigma^\dagger(\tau)\mathcal{G}_0^{-1} f_\sigma(\tau') + U\int_0^\beta f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow, \tag{33}$$

where f_σ annihilates a fermion with spin σ, β is the inverse temperature, and U is the on-site interaction. The central idea of DMFT is to consider a self-consistent solution that reproduces the dynamical Green's function $\mathcal{G}_0$. This constraint is satisfied by the solution to the DMFT equations for the local Green's function G_0, the dynamical Green's function $\mathcal{G}_0$, and the self-energy Σ evaluated at the Matsubara frequencies $\omega_n = (2n+1)\pi/\beta$,

$$G_0(i\omega_n) = \langle c_\sigma(i\omega_n) c_\sigma^*(i\omega_n)\rangle_{S_{\mathrm{eff}}}, \tag{34}$$

$$G_0(i\omega_n) = [\mathcal{G}_0(i\omega_n)^{-1} - \Sigma(i\omega_n)]^{-1}, \tag{35}$$

$$G_0(i\omega_n) = \int d\epsilon \frac{N(\epsilon)}{i\omega_n + \mu - \Sigma(i\omega_n) - \epsilon}, \tag{36}$$

where μ is the chemical potential and $N(\epsilon)$ is the density of states (Kollar, 2011). The first step in bringing DMFT to open systems was to use effective Lindblad master equations to describe quantum transport in closed quantum systems using DMFT (Arrigoni, Knap, and Linden, 2013; Titvinidze *et al.*, 2015, 2016). Recently this approach was extended to the case where the initial many-body problem already describes an open quantum system (Panas *et al.*, 2019).

A different method to systematically extend mean-field theory is to use projection operator methods. The central idea is to consider a single site of the many-body problem, with the rest of the system forming a non-Markovian environment. This non-Markovian master equation is then solved using standard projection operator techniques such as the Nakajima-Zwanzig method or the time-convolutionless master equation (Breuer and Petruccione, 2002). Initially, this approach was used to describe the relaxation dynamics of local observables in a closed quantum system (Weimer *et al.*, 2008), and the approach was later extended to the Lindblad dynamics of open systems (Degenfeld-Schonburg and Hartmann, 2014). In the second approach, the initial step is to introduce corrections $\Delta\mathcal{L}$ to the mean-field Liouvillian $\mathcal{L}_{\mathrm{MF}}$ that are introduced according to

$$\mathcal{L} = \mathcal{L}_{\mathrm{MF}} + \Delta\mathcal{L}. \tag{37}$$

The projection $\mathcal{P}$ removes all correlations and projects the system onto a product state, i.e.,

$$\mathcal{P}\rho = \prod_i \rho_i. \tag{38}$$

If the initial state at time t_0 is also a product state, the projected Lindblad master equation may be formally written as

$$\mathcal{P}\frac{d}{dt}\rho(t) = \mathcal{L}_{\mathrm{MF}}\mathcal{P}\rho(t) + \mathcal{P}\Delta\mathcal{L}\int_0^t dt' \mathcal{K}(t,t')\mathcal{P}\rho(t'), \tag{39}$$

where the generator $\mathcal{K}$ is introduced (Degenfeld-Schonburg and Hartmann, 2014). The generator $\mathcal{K}$ may then be expanded in terms of a power series of the beyond mean-field corrections $\Delta\mathcal{L}$. This projection operator approach has been used to investigate both dissipative XY models (Degenfeld-Schonburg and Hartmann, 2014) and the dissipative Heisenberg model (Owen *et al.*, 2018). In the latter case a limit cycle behavior has been reported, which for sufficiently large spatial dimensions also survives under inclusion of the terms beyond mean field. Consequently, it would be interesting to learn whether the projection operator approach is also capable of correctly identifying the replacement of mean-field bistability by a first-order transition in the dissipative Ising model.

C. Variational tensor network methods

Given the successes of tensor network methods discussed in Sec. III, it is natural to combine them with variational methods for the study of open quantum many-body systems. However, the main challenge is that the natural trace norm for constructing the variational principle cannot be calculated efficiently in a tensor network representation. This has led to the use of different norms as possible alternatives (Cui, Ignacio Cirac, and Bañuls, 2015; Mascarenhas, Flayac, and Savona, 2015); see Sec. III.A.

On the one hand, the choice of the norm is not really relevant if the value of the norm is low (i.e., comparable to the

machine precision of the numerical simulation), as then the solution is almost exact from any point of view. On the other hand, choosing a non-natural norm is a potential source of errors that is not under the control of the variational algorithm. In practice, this difficulty will mostly manifest itself for higher-dimensional problems, as there the bond dimensions that can be reached are severely constrained by the computational resources (Kshetrimayum, Weimer, and Orús, 2017). But even for one-dimensional systems, there are computationally challenging problems involving long relaxation times (Carollo *et al.*, 2019), where an arbitrarily low variational norm might not be reachable.

A way out of this problem can be realized by representing the density matrix in terms of an ensemble of pure states and use a variational tensor network formulation for these pure states (Transchel, Milsted, and Osborne, 2014). In this case, the density matrix is parametrized according to

$$\rho = \int p(\alpha, \bar{\alpha}) |\psi(\alpha)\rangle\langle\psi(\alpha)| d\alpha d\bar{\alpha}, \tag{40}$$

where $|\psi(\alpha)\rangle$ is a variational wave function with variational parameters α and $p(\alpha, \bar{\alpha})$ is the associated probability distribution. The variational norm associated with the effective Hamiltonian of the master equation $H_{\text{eff}} = H - (i/2)\sum_i c_i^\dagger c_i$ can now be calculated as

$$D_H = |H_{\text{eff}}|\psi(\alpha)\rangle|^2. \tag{41}$$

This expression both can be computed efficiently using tensor network methods and corresponds to the natural trace norm when evaluated over the full ensemble. The quantum jump terms of the master equation can be treated in a similar fashion (Transchel, Milsted, and Osborne, 2014).

D. Variational quantum Monte Carlo methods

The central idea behind variational quantum Monte Carlo methods is to rewrite a quantum many-body problem in terms of a sampling over a classical probability distribution (Batrouni and Scalettar, 2011). However, the existence of destructive interference in quantum mechanics can lead to corresponding classical probabilities that are negative, which is the root of the famous sign problem. One common workaround is to sample over the absolute value of the probability distribution instead, but this comes at the price of the complexity of the computation increasing exponentially with the system size (Troyer and Wiese, 2005). Open quantum many-body systems are especially prone to the sign problem since the eigenvalues of the Liouvillian can be complex (Nagy and Savona, 2018). Nevertheless, Monte Carlo sampling can be useful even in the presence of the sign problem if the required resources for the Monte Carlo sampling are lower than for a full solution of the problem.

The first quantum Monte Carlo simulation of an open quantum many-body problem was based on a nonvariational full-configuration-interaction Monte Carlo algorithm (Nagy and Savona, 2018), which is better equipped to deal with the sign problem without completely negating it. For the magnetization of a dissipative XYZ model on small lattices, the quantum Monte Carlo simulation is in excellent agreement with wave-function Monte Carlo results.

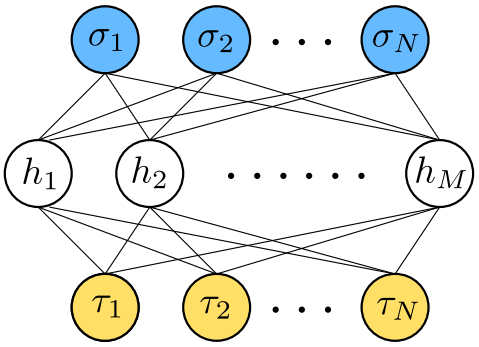

FIG. 11. Node structure of a restricted Boltzmann machine for open quantum systems. The vectorized density matrix is realized in terms of a physical layer σ_i corresponding to a set of spin 1/2 variables. These are coupled to the nodes of a hidden layer h_i, which are again coupled to the third layer τ_i, which represents the adjoint of the physical layer.

Recently variational Monte Carlo methods have been applied to open quantum systems (Hartmann and Carleo, 2019; Nagy and Savona, 2019; Vicentini, Biella *et al.*, 2019; Yoshioka and Hamazaki, 2019). These approaches were inspired by using variational wave functions corresponding to restricted Boltzmann machines (RBMs) (Carleo and Troyer, 2017), which were first introduced in the context of neural network simulations. The main idea behind RBM wave functions is shown in Fig. 11, where an additional hidden layer introduces variational parameters associated with the quantum correlations of the many-body state. The entries of the vectorized density matrix are then given by

$$\begin{aligned} {}_\sharp\langle \boldsymbol{\sigma}, \boldsymbol{\tau}\rangle \rho_\sharp = \frac{1}{Z}\sum_{\{h_j\}} \exp\left(\sum_{ij} W_{ij}\sigma_i h_j + W_{ij}^*\tau_i h_j\right) \\ \times \exp\left(\sum_i a_i\sigma_i + a_i^*\tau_i + \sum_j b_j h_j\right), \end{aligned} \tag{42}$$

where Z is the partition function for normalization, W_{ij}, a_i, and b_j are the variational parameters, and σ_i, τ_i, and h_j refer to the spins of the physical and the hidden layers, respectively; see Fig. 11. There is a close connection between RBM wave functions and matrix product states (Deng, Li, and Das Sarma, 2017; Chen *et al.*, 2018); however, RBMs are potentially also capable of describing long-range entangled quantum states.

For the variational Monte Carlo samplings, different norms have been put forward. One possibility is to consider the Hilbert-Schmidt norm of the time evolution (Hartmann and Carleo, 2019) or the steady state (Vicentini, Biella *et al.*, 2019). In the latter case, the variational norm D has been normalized according to the purity $\mathrm{Tr}\{\rho^2\}$, i.e.,

$$D = \frac{\mathrm{Tr}\{\dot{\rho}^2\}}{\mathrm{Tr}\{\rho^2\}}. \tag{43}$$

This norm is not biased toward the maximally mixed state, as mentioned earlier. An alternative approach to constructing a

suitable norm is to minimize the Hermitian $\mathcal{L}^\dagger\mathcal{L}$ in close analogy to a ground state problem (Yoshioka and Hamazaki, 2019). Finally, it is possible to consider the equivalent of an expectation value for vectorized density matrices according to ${}_\sharp\langle\rho|\mathcal{L}_\sharp|\rho\rangle_\sharp/{}_\sharp\langle\rho|\rho\rangle_\sharp$ (Nagy and Savona, 2019). With respect to the more natural trace norm for density matrices, the RBM approaches behave similarly to the tensor network simulations discussed in Sec. IV.C. However, since RBMs can be applied to two-dimensional models in a straightforward way, it will be interesting to see how these methods perform for the investigation of dissipative phase transitions, particularly in critical systems.

V. PHASE-SPACE AND RELATED METHODS

Other methods have also been used with relative success in the study of open quantum systems, such as phase-space methods, as well as methods based on hierarchy equations. In this section we explain two such examples, namely, truncated Wigner approximations and Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchies. On the one hand, the truncated Wigner approximation is a semiclassical approximation of the dynamics of an open system obtained by replacing Moyal's equation, which governs the dynamics of operators in phase space (Marzlin and Deering, 2015), with the classical Liouville's equation. On the other hand, the BBGKY hierarchy is a set of coupled equations of motion for the reduced density matrices of the system (Requist, 2012). The resulting methods are general in purpose and can be applied to a wide variety of systems, but in what follows we discuss concrete examples.

A. Truncated Wigner approximation

In the context of phase-space related methods, truncated Wigner approximations were first used by Carusotto and Ciuti (2005) in a driven-dissipative microcavity polariton system coherently driven into the optical parametric oscillator regime that was also reviewed by Carusotto and Ciuti (2013) and revisited in Dagvadorj *et al.* (2015) as an example of a 2D driven-dissipative nonequilibrium phase transition. We revisit this example here. The Hamiltonian for the system is given by

$$H_S = \int d\vec{r}(\psi_X^\dagger \psi_C^\dagger)\begin{pmatrix} -\nabla^2/2m_X + (g_X/2)|\psi_X|^2 & \Omega_R/2 \\ \Omega_R/2 & -\nabla^2/2m_C \end{pmatrix} \times \begin{pmatrix} \psi_X \\ \psi_C \end{pmatrix}, \tag{44}$$

with cavity and photon field operators $\psi_{X,C}(\vec{r},t)$, spatial coordinate $\vec{r}=(x,y)$, $m_{X,C}$ the exciton and photon masses, g_X the exciton-exciton interaction strength, and Ω_R the Rabi splitting. One introduces the effect of an external drive (pump) as well as incoherent decay by adding a system-bath (SB) Hamiltonian given by

$$H_{\mathrm{SB}} = \int d\vec{r}[F(\vec{r},t)\psi_C^\dagger(\vec{r},t) + \mathrm{H.c.}] + \sum_{\vec{k}}\sum_{l=X,C}\{\xi_{\vec{k}}^l[\psi_{l,\vec{k}}^\dagger(t)B_{l,\vec{k}} + \mathrm{H.c.}] + \omega_{l,\vec{k}}B_{l,\vec{k}}^\dagger B_{l,\vec{k}}\}, \tag{45}$$

with $\psi_{l,\vec{k}}(t)$ the Fourier transform of the field operators in real space and $B_{l,\vec{k}}$ and $B_{l,\vec{k}}^\dagger$ the bath's bosonic annihilation and creation operators with energy $\omega_{l,\vec{k}}$, which describes the decay for both excitons and cavity photons. The decay is compensated for by an external homogeneous coherent pump $F(\vec{r},t) = f_p e^{i(\vec{k}_p\cdot\vec{r}-\omega_p t)}$ injecting polaritons with momentum $\vec{k}_p$ and energy ω_p.

By using standard quantum optical methods, one can trace out the bath within the Markovian approximation and obtain a master equation for the system. There is, however, an alternative approach by means of phase-space techniques. In particular, one can represent the quantum fields as quasiprobability distribution functions. The Fokker-Planck partial differential equation that governs the dynamics of such distributions can be mapped to a stochastic differential equation, which can be solved using different techniques. For the example that we are discussing, one solves the equation on a finite grid with lattice spacing a. The most suitable quasiprobability distribution for this example is the Wigner representation, which is also the most suitable one for numerical implementation. By truncating the corresponding Fokker-Planck equation in the limit $g_X/\kappa_{X,C}a^2 \ll 1$, with $\kappa_{X,C}$ the exciton and photon decay rates, and keeping up to second-order derivatives only, one obtains the stochastic differential equation

$$id\begin{pmatrix}\psi_X \\ \psi_C\end{pmatrix} = \left[H'_{\mathrm{MF}}\begin{pmatrix}\psi_X \\ \psi_C\end{pmatrix} + \begin{pmatrix}0 \\ F\end{pmatrix}\right]dt + i\begin{pmatrix}\sqrt{\kappa_X}dW_X \\ \sqrt{\kappa_C}dW_C\end{pmatrix}. \tag{46}$$

In Eq. (46), $dW_{l=X,C}$ are Wiener noise terms and H'_{MF} is given by

$$H'_{\mathrm{MF}} = \begin{pmatrix} -\nabla^2/2m_X + g_X(|\psi_X|^2 - 1/a^2) - i\kappa_X & \Omega_R/2 \\ \Omega_R/2 & -\nabla^2/2m_C - i\kappa_C \end{pmatrix}, \tag{47}$$

with the different symbols as previously defined. The resulting stochastic differential equation can then be solved using standard methods and software packages designed for this purpose.

We add that this method has also recently been used to study critical slowing down in photonic lattices (Vicentini *et al.*, 2018) and extended to disordered quantum many-body system (the so-called optical stochastic unraveling for

disordered systems) (Vicentini, Minganti *et al.*, 2019). Moreover, additional developments include the discrete sampling of the Wigner function (Schachenmayer, Pikovski, and Rey, 2015b), together with the explicit calculation of the quantum corrections (Ivanov and Breuer, 2017). In the last case, the new formalism was applied explicitly to an exciton transport model. As such, these methods can also be generalized to other scenarios, such as spin systems (Khasseh *et al.*, 2020).

B. BBGKY hierarchy equations

It is also possible to study open quantum systems via the so-called Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy (Liboff, 2003). In a nutshell, this is a hierarchy of equations aimed to describe a system of a large number of interacting particles. As such, the idea is generic. But, as shown by Navez and Schützhold (2010), it can also be applied directly in the context of open dissipative systems to obtain a hierarchy of equations for the different reduced density matrices. The way this approach works is intuitive. Consider the reduced density matrices for one lattice site ρ_μ, two lattice sites $\rho_{\mu\nu}$, etc. We separate the correlated parts as $\rho_{\mu\nu}=\rho^c_{\mu\nu}+\rho_\mu\rho_\nu$, as well as $\rho_{\mu\nu\lambda}=\rho^c_{\mu\nu}\rho_\lambda+\rho^c_{\mu\lambda}\rho_\nu+\rho^c_{\nu\lambda}\rho_\mu+\rho_\mu\rho_\nu\rho_\lambda$, etc. The method discussed in what follows is based on the scaling hierarchy of correlations

$$\rho^c_{\mathcal{S}}=O(Z^{1-|\mathcal{S}|}), \tag{48}$$

with $|\mathcal{S}|$ the number of lattice sites in set $\mathcal{S}$. The different reduced density matrices can also be computed using the generating functional $\mathcal{F}(\alpha_\mu)=\log\mathrm{Tr}[\rho\prod_\mu(\mathbb{I}_\mu+\alpha_\mu)]$, with α_μ an arbitrary operator acting on an on-site μ. Using such a functional one has $\rho_\mu=\partial\mathcal{F}/\partial\alpha_\mu|_{\alpha=0}$, as well as $\rho^c_{\mu\nu}=\partial^2\mathcal{F}/\partial\alpha_\mu\partial\alpha_\nu|_{\alpha=0}$, etc. Next the Liouville operators $\mathcal{L}_\mu$ and $\mathcal{L}_{\mu\nu}$ acting on one and two sites are introduce via the dissipation equation $i\partial_t\rho=[H,\rho]+\sum_\mu\mathcal{L}_\mu\rho+\sum_{\mu\nu}\mathcal{L}_{\mu\nu}\rho/Z$, with Z the coordination number of the Hamiltonian (e.g., the number of tunneling neighbors at any given site for a Hubbard-like Hamiltonian). Following these equations, the time evolution of $\mathcal{F}$ is given by

$$i\frac{\partial}{\partial t}\mathcal{F}(\alpha)=\sum_\mu\mathrm{Tr}_\mu\left(\alpha_\mu\mathcal{L}_\mu\frac{\partial\mathcal{F}}{\partial\alpha_\mu}\right)+\frac{1}{Z}\sum_{\mu\nu}\mathrm{Tr}_{\mu\nu}\left[(\alpha_\mu+\alpha_\nu+\alpha_\mu\alpha_\nu)\mathcal{L}_{\mu\nu}\left(\frac{\partial^2\mathcal{F}}{\partial\alpha_\mu\partial\alpha_\nu}+\frac{\partial\mathcal{F}}{\partial\alpha_\mu}\frac{\partial\mathcal{F}}{\partial\alpha_\nu}\right)\right]. \tag{49}$$

Using this equation, one can take derivatives and obtain a set of equations for the correlated density matrices

$$\begin{aligned}i\frac{\partial}{\partial t}\rho^c_{\mathcal{S}}=&\sum_{\mu\in\mathcal{S}}\mathcal{L}_\mu\rho^c_{\mathcal{S}}+\frac{1}{Z}\sum_{\mu\nu\in\mathcal{S}}\mathcal{L}_{\mu\nu}\rho^c_{\mathcal{S}}+\frac{1}{Z}\sum_{k\notin\mathcal{S}}\sum_{\mu\in\mathcal{S}}\mathrm{Tr}_k\left(\mathcal{L}^S_{\mu k}\rho^c_{\mathcal{S}\cup k}+\sum_{\mathcal{P}\subseteq\mathcal{S}\setminus\{\mu\}}^{\mathcal{P}\cup\bar{\mathcal{P}}=\mathcal{S}\setminus\{\mu\}}\mathcal{L}^S_{\mu k}\rho^c_{\{\mu\}\cup\mathcal{P}}\rho^c_{\{k\}\cup\bar{\mathcal{P}}}\right)\\&+\frac{1}{Z}\sum_{\mu\nu\in\mathcal{S}}\sum_{\mathcal{P}\subseteq\mathcal{S}\setminus\{\mu,\nu\}}^{\mathcal{P}\cup\bar{\mathcal{P}}=\mathcal{S}\setminus\{\mu,\nu\}}\left\{\mathcal{L}_{\mu\nu}\rho^c_{\{\mu\}\cup\mathcal{P}}\rho^c_{\{\nu\}\cup\bar{\mathcal{P}}}-\mathrm{Tr}_\nu\left[\mathcal{L}^S_{\mu\nu}\left(\rho^c_{\{\mu,\nu\}\cup\bar{\mathcal{P}}}+\sum_{\mathcal{Q}\subseteq\bar{\mathcal{P}}}^{\mathcal{Q}\cup\bar{\mathcal{Q}}=\bar{\mathcal{P}}}\rho^c_{\{\mu\}\cup\mathcal{Q}}\rho^c_{\{\nu\}\cup\bar{\mathcal{Q}}}\right)\right]\rho^c_{\{\nu\}\cup\mathcal{P}}\right\},\end{aligned} \tag{50}$$

with $\mathcal{L}^S_{\mu\nu}=\mathcal{L}_{\mu\nu}+\mathcal{L}_{\nu\mu}$. This hierarchy of equations for the reduced density matrices is preserved in time. Moreover, it allows us to write explicit equations for the one- and two-site density matrices. For the one-site matrix one gets

$$i\frac{\partial}{\partial t}\rho_\mu=\mathcal{L}_\mu+\frac{1}{Z}\sum_k\mathrm{Tr}_k[\mathcal{L}^S_{\mu k}(\rho^c_{\mu k}+\rho_\mu\rho_k)], \tag{51}$$

and for the two-site matrix one has

$$i\frac{\partial}{\partial t}\rho_{\mu\nu}=\mathcal{L}_\mu\rho^c_{\mu\nu}\frac{1}{Z}\mathcal{L}_{\mu\nu}(\rho^c_{\mu\nu}+\rho_\mu\rho_\nu)+\frac{1}{Z}\sum_{k\neq\mu,\nu}\mathrm{Tr}_k[\mathcal{L}^S_{\mu k}(\rho^c_{\mu\nu k}+\rho^c_{\mu\nu}\rho_k+\rho^c_{\nu k}\rho_\mu)]-\frac{\rho_\mu}{Z}\mathrm{Tr}_\mu[\mathcal{L}^S_{\mu\nu}(\rho^c_{\mu\nu}+\rho_\mu\rho_\nu)]+(\mu\leftrightarrow\nu). \tag{52}$$

By combining Eqs. (51) and (52) with Eq. (48), one can expand in powers of $1/Z$ and obtain different approximations for the one- and two-particle behavior.

This approach can be implemented for a variety of systems (spins, bosons, fermions, etc.) and has the advantage of being independent of the dimensionality of the system. Navez and Schützhold (2010) applied it to a lattice Bose-Hubbard model. The method can be used to obtain analytical expansions, as well as to facilitate efficient numerical simulations.

VI. LINKED-CLUSTER EXPANSION METHODS

Methods based on linked-cluster expansions have also recently been put forward in the study of open quantum many-body systems. While the method has been broadly applied to isolated systems (Tang, Khatami, and Rigol, 2013), for open systems only the case of two-dimensional spin systems with incoherent spin relaxation (Biella *et al.*, 2018) has been considered. The method numerically targets expectation values of observables in the steady state at long times of the master equation.

Mathematically, the procedure is as follows: One expands the Liouvillian as a sum of quasilocal terms, i.e.,

$$\mathcal{L} = \sum_{\langle k \rangle} \alpha_k \mathcal{L}_k, \tag{53}$$

with α_k a local coupling strength and k a combined index that runs over all sites taking part in the respective interaction. For example, a nearest-neighbor two-body term would lead to a set of $k \equiv (i, j)$, with i and j adjacent sites. The expectation value O of an observable $\hat{O}$ can be expanded in terms of powers of α_k, i.e.,

$$O(\{\alpha_k\}) = \sum_{\{n_k\}} O_{\{n_k\}} \prod_k \alpha_k^{n_k}, \tag{54}$$

with n_k running over all non-negative integers for all k. It is clear that all possible polynomials in α_k are included in Eq. (54), which can be reorganized in clusters as follows:

$$O = \sum_c W_{[O]}(c), \tag{55}$$

with c a nonempty set of k indexes identifying the sites belonging to the cluster. The cluster weight $W_{[O]}(c)$ contains all terms in the expansion with at least one power of α_k, for all k in c, and no powers of α_k of k belong to c. These terms obey the recurrence relation

$$W_{[O]}(c) = O(c) - \sum_{s \subset c} W_{[O]}(s), \tag{56}$$

with

$$O(c) = \mathrm{Tr}[\hat{O}\rho_s(c)] \tag{57}$$

the expectation value of the observable in the steady state $\rho_s(c)$ for the finite cluster c. Taking into account symmetries in the system, the expectation value per site in the thermodynamic limit can be written as

$$\frac{O}{L} = \sum_{n=1}^{\infty} \left(\sum_{c_n} l(c_n) W_{[O]}(c_n) \right), \tag{58}$$

with $L \to \infty$ the size of the system, the outer sum running over all possible cluster sizes n, and the inner sum running over all topologically different clusters c_n of size n, with $l(c_n)$ their multiplicity. This series expansion can be truncated up to a cluster size R, thus giving rise to a plausible approximation method that is also valid for open systems.

The linked-cluster expansion works well for the dissipative Heisenberg model (Biella *et al.*, 2018), where an exact product state solution can be used as a starting point of the expansion. In this case, it is even possible to calculate phase boundaries and critical exponents of a dissipative phase transition between a paramagnet and a ferromagnet. The situation is quite different for the dissipative Ising model, where the expansion series failed to converge even for a tenth-order expansion (Jin *et al.*, 2018).

VII. SUMMARY AND OUTLOOK

The substantial effort to develop novel simulation methods to investigate open quantum many-body systems has enabled us to review a variety of numerical methods. Specifically, in this review we considered methods for the Markovian quantum master equation (assuming a weak-coupling limit), including mean-field stochastic methods, tensor networks, variational methods, quantum Monte Carlo methods, a truncated Wigner approximation, BBGKY hierarchy equations, and linked-cluster expansions. While no method has yet emerged that is universally optimal for all cases, there have been several promising developments with different methods for different regimes. Even with the major technical advances discussed in this review, there are still many open problems that are inaccessible with these state-of-the-art numerical techniques. To give concrete examples of actual physical problems, one may consider a common setting in the context of Rydberg atoms in which the interaction is often long range and cannot be approximated with just a nearest-neighbor Hamiltonian (Schachenmayer, Pikovski, and Rey, 2015a; Browaeys, Barredo, and Lahaye, 2016; Labuhn *et al.*, 2016). Even TN techniques will face a difficult challenge (especially in two dimensions) while encountering such problems, although there have been promising developments in this direction recently (O'Rourke and Chan, 2020). Other challenging problems include the existence of AFM order in the 3D dissipative Ising model, which is an open question that appears to be difficult to answer. This is again relevant to ongoing experiments with Rydberg atoms, which one cannot reliably simulate at the moment (Carr *et al.*, 2013; Malossi *et al.*, 2014; Helmrich, Arias, and Whitlock, 2018). Phase transitions and universality classes of dissipative models form another class of problem that has proven to be difficult for numerical techniques (Diehl *et al.*, 2010; Carmichael, 2015; Biondi *et al.*, 2017; Fink *et al.*, 2017).

The most confidence in a simulation result can be achieved if it is reproducible when using a complementary simulation approach. Despite these caveats, one can make several key observations about the particular methods covered in this review. The first observation is that mean-field methods are considerably less reliable for open systems than their counterparts for closed systems, although the reason for this discrepancy is still an open question. Furthermore, tensor network methods have demonstrated their ability to successfully tackle many hard problems surrounding open many-body systems and resolve long-standing open questions. A particularly interesting and promising case is that of open 2D systems, which are unexplored territory to a large extent. As for the variational methods discussed in this review, there appears to be a trade-off between the formal suitability of the norm and its efficient computability. It will be interesting to see if and how this trade-off will be resolved in future work. We provide a summary in Table II comparing the different techniques that we have discussed.

Progress in recent years in simulating open quantum systems has brought the field to a level where one has a wide range of tools at hand to systematically make a comparison to experimental results, particularly in the context of quantum simulations. Combined with the experimental ease

TABLE II. Comparison of the different simulation methods discussed in this review. We differentiate the methods by the system sizes that can be simulated, the spatial dimensions, constraints on the local Hilbert space dimension, whether or not fermionic systems can be treated, the simulation performance for inhomogeneous systems, and whether or not the correct critical exponents of phase transitions can be obtained.

	WFMC[a]	TN[b]	Variational principle	VQMC[c]	CMF[d]	TWA[e]
System size (in qubits)	20	TDL[f]	TDL	16	TDL	400
Dimensions	One, two	One, two	Any[g]	Any	Any[h]	Any
Local Hilbert space	Small	Small	Large	Large	Small	Large
Fermionic systems	Yes	Yes	Partially	No	Partially	Unknown
Inhomogeneous systems	Good	Good	Bad	Good	Good	Good
Critical exponents	Good	Good	Good[i]	Unknown	Bad	Unknown
Time-dependent $\mathcal{L}$	Yes	Yes	Yes	Yes	Yes	Yes

[a]Wave-function Monte Carlo.
[b]Tensor networks.
[c]Variational quantum Monte Carlo.
[d]Cluster mean field.
[e]Truncated Wigner approximation.
[f]Systems in the thermodynamic limit.
[g]Works better in higher dimensions.
[h]Works better in higher dimensions.
[i]For states with thermal statistics.

of preparing the steady state of an open quantum system, these are good reasons to believe that the study of strongly correlated open quantum many-body systems will become a research topic with an impact on other areas of science, such as material design and quantum computation.

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REFERENCES

Arrigoni, Enrico, Michael Knap, and Wolfgang von der Linden, 2013, "Nonequilibrium Dynamical Mean-Field Theory: An Auxiliary Quantum Master Equation Approach," Phys. Rev. Lett. **110**, 086403.

Ates, Cenap, Beatriz Olmos, Juan P. Garrahan, and Igor Lesanovsky, 2012, "Dynamical phases and intermittency of the dissipative quantum Ising model," Phys. Rev. A **85**, 043620.

Barreiro, Julio T., Markus Müller, Philipp Schindler, Daniel Nigg, Thomas Monz, Michael Chwalla, Markus Hennrich, Christian F. Roos, Peter Zoller, and Rainer Blatt, 2011, "An open-system quantum simulator with trapped ions," Nature (London) **470**, 486.

Batrouni, G. G., and R. T. Scalettar, 2011, "Quantum phase transitions", in *Ultracold Gases and Quantum Information*, edited by Christian Miniatura, Leong-Chuan Kwek, Martial Ducloy, Benot Grmaud, Berthold-Georg Englert, Leticia Cugliandolo, Artur Ekert, and Kok Khoo Phua (Oxford University Press, New York), pp. 356–394.

Baumann, K., C. Guerlin, F. Brennecke, and T. Esslinger, 2010, "Dicke quantum phase transition with a superfluid gas in an optical cavity," Nature (London) **464**, 1301–1306.

Beaudoin, Félix, Jay M. Gambetta, and A. Blais, 2011, "Dissipation and ultrastrong coupling in circuit QED," Phys. Rev. A **84**, 043832.

Bethe, H. A., 1935, "Statistical theory of superlattices," Proc. R. Soc. A **150**, 552–575, http://rspa.royalsocietypublishing.org/content/150/871/552.full.pdf.

Biella, Alberto, Jiasen Jin, Oscar Viyuela, Cristiano Ciuti, Rosario Fazio, and Davide Rossini, 2018, "Linked cluster expansions for open quantum systems on a lattice," Phys. Rev. B **97**, 035103.

Binder, Kurt, and Jian Sheng Wang, 1989, "Finite-size effects at critical points with anisotropic correlations: Phenomenological scaling theory and Monte Carlo simulations," J. Stat. Phys. **55**, 87–126.

Biondi, Matteo, Gianni Blatter, Hakan E. Türeci, and Sebastian Schmidt, 2017, "Nonequilibrium gas-liquid transition in the driven-dissipative photonic lattice," Phys. Rev. A **96**, 043809.

Bonnes, Lars, Daniel Charrier, and Andreas M. Läuchli, 2014, "Dynamical and steady-state properties of a Bose-Hubbard chain with bond dissipation: A study based on matrix product operators," Phys. Rev. A **90**, 033612.

Breuer, Heinz-Peter, and Francesco Petruccione, 2002, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford).

Browaeys, Antoine, Daniel Barredo, and Thierry Lahaye, 2016, "Experimental investigations of dipole-dipole interactions between a few Rydberg atoms," J. Phys. B **49**, 152001.

Cai, Zi, and Thomas Barthel, 2013, "Algebraic versus Exponential Decoherence in Dissipative Many-Particle Systems," Phys. Rev. Lett. **111**, 150403.

Carleo, Giuseppe, and Matthias Troyer, 2017, "Solving the quantum many-body problem with artificial neural networks," Science **355**, 602–606.

Carmichael, H. J., 2015, "Breakdown of Photon Blockade: A Dissipative Quantum Phase Transition in Zero Dimensions," Phys. Rev. X **5**, 031028.

Carollo, F., E. Gillman, H. Weimer, and I. Lesanovsky, 2019, "Critical Behavior of the Quantum Contact Process in One Dimension," Phys. Rev. Lett. **123**, 100604.

Carr, A. W., and M. Saffman, 2013, "Preparation of Entangled and Antiferromagnetic States by Dissipative Rydberg Pumping," Phys. Rev. Lett. **111**, 033607.

Carr, C., R. Ritter, C. G. Wade, C. S. Adams, and K. J. Weatherill, 2013, "Nonequilibrium Phase Transition in a Dilute Rydberg Ensemble," Phys. Rev. Lett. **111**, 113901.

Carusotto, Iacopo, and Cristiano Ciuti, 2005, "Spontaneous microcavity-polariton coherence across the parametric threshold: Quantum Monte Carlo studies," Phys. Rev. B **72**, 125335.

Carusotto, Iacopo, and Cristiano Ciuti, 2013, "Quantum fluids of light," Rev. Mod. Phys. **85**, 299–366.

Chan, Ching-Kit, Tony E. Lee, and Sarang Gopalakrishnan, 2015, "Limit-cycle phase in driven-dissipative spin systems," Phys. Rev. A **91**, 051601.

Chen, Jing, Song Cheng, Haidong Xie, Lei Wang, and Tao Xiang, 2018, "Equivalence of restricted Boltzmann machines and tensor network states," Phys. Rev. B **97**, 085104.

Cirac, J. I., D. Prez-Garca, N. Schuch, and F. Verstraete, 2017, "Matrix product density operators: Renormalization fixed points and boundary theories," Ann. Phys. (Amsterdam) **378**, 100–149.

Cirac, J. Ignacio, José Garre-Rubio, and David Pérez-García, 2019, "Mathematical open problems in projected entangled pair states," arXiv:1903.09439.

Cirac, J. Ignacio, and Frank Verstraete, 2009, "Renormalization and tensor product states in spin chains and lattices," J. Phys. A **42**, 504004.

Coffman, Valerie, Joydip Kundu, and William K. Wootters, 2000, "Distributed entanglement," Phys. Rev. A **61**, 052306.

Corboz, Philippe, 2016a, "Improved energy extrapolation with infinite projected entangled-pair states applied to the two-dimensional Hubbard model," Phys. Rev. B **93**, 045116.

Corboz, Philippe, 2016b, "Variational optimization with infinite projected entangled-pair states," Phys. Rev. B **94**, 035133.

Corboz, Philippe, Piotr Czarnik, Geert Kapteijns, and Luca Tagliacozzo, 2018, "Finite Correlation Length Scaling with Infinite Projected Entangled-Pair States," Phys. Rev. X **8**, 031031.

Corboz, Philippe, and Frédéric Mila, 2014, "Crystals of Bound States in the Magnetization Plateaus of the Shastry-Sutherland Model," Phys. Rev. Lett. **112**, 147203.

Cui, Jian, J. Ignacio Cirac, and Mari Carmen Bañuls, 2015, "Variational Matrix Product Operators for the Steady State of Dissipative Quantum Systems," Phys. Rev. Lett. **114**, 220601.

Czarnik, Piotr, Lukasz Cincio, and Jacek Dziarmaga, 2012, "Projected entangled pair states at finite temperature: Imaginary time evolution with ancillas," Phys. Rev. B **86**, 245101.

Czarnik, Piotr, and Jacek Dziarmaga, 2015, "Variational approach to projected entangled pair states at finite temperature," Phys. Rev. B **92**, 035152.

Czarnik, Piotr, Jacek Dziarmaga, and Philippe Corboz, 2019, "Time evolution of an infinite projected entangled pair state: An efficient algorithm," Phys. Rev. B **99**, 035115.

Czarnik, Piotr, Jacek Dziarmaga, and Andrzej M. Oleś, 2016, "Variational tensor network renormalization in imaginary time: Two-dimensional quantum compass model at finite temperature," Phys. Rev. B **93**, 184410.

Dagvadorj, G., J. M. Fellows, and S. Matyjaśkiewicz, F. M. Marchetti, I. Carusotto, and M. H. Szymańska, 2015, "Nonequilibrium Phase Transition in a Two-Dimensional Driven Open Quantum System," Phys. Rev. X **5**, 041028.

Dai, Yan-Wei, Qian-Qian Shi, Sam Young Cho, Murray T. Batchelor, and Huan-Qiang Zhou, 2017, "Finite-temperature fidelity and von Neumann entropy in the honeycomb spin lattice with quantum Ising interaction," Phys. Rev. B **95**, 214409.

Daley, Andrew J., 2014, "Quantum trajectories and open many-body quantum systems," Adv. Phys. **63**, 77–149.

Dalibard, Jean, Yvan Castin, and Klaus Mølmer, 1992, "Wave-Function Approach to Dissipative Processes in Quantum Optics," Phys. Rev. Lett. **68**, 580–583.

Degenfeld-Schonburg, Peter, and Michael J. Hartmann, 2014, "Self-consistent projection operator theory for quantum many-body systems," Phys. Rev. B **89**, 245108.

De las Cuevas, Gemma, Norbert Schuch, David Prez-Garca, and J. Ignacio Cirac, 2013, "Purifications of multipartite states: Limitations and constructive methods," New J. Phys. **15**, 123021.

Deng, Dong-Ling, Xiaopeng Li, and S. Das Sarma, 2017, "Quantum Entanglement in Neural Network States," Phys. Rev. X **7**, 021021.

de Vega, Inés, and Daniel Alonso, 2017, "Dynamics of non-Markovian open quantum systems," Rev. Mod. Phys. **89**, 015001.

Diehl, S., A. Micheli, A. Kantian, B. Kraus, H. P. Büchler, and P. Zoller, 2008, "Quantum states and phases in driven open quantum systems with cold atoms," Nat. Phys. **4**, 878–883.

Diehl, Sebastian, Andrea Tomadin, Andrea Micheli, Rosario Fazio, and Peter Zoller, 2010, "Dynamical Phase Transitions and Instabilities in Open Atomic Many-Body Systems," Phys. Rev. Lett. **105**, 015702.

Dum, R., P. Zoller, and H. Ritsch, 1992, "Monte Carlo simulation of the atomic master equation for spontaneous emission," Phys. Rev. A **45**, 4879–4887.

Dutt, M. V. G., L. Childress, L. Jiang, E. Togan, J. Maze, F. Jelezko, A. S. Zibrov, P. R. Hemmer, and M. D. Lukin, 2007, "Quantum register based on individual electronic and nuclear spin qubits in diamond," Science **316**, 1312–1316.

Eisert, J., 2013, "Entanglement and tensor network states," in *Emergent Phenomena in Correlated Matter*, Modeling and Simulation Vol. 3, edited by E. Pavarini, E. Koch, and U. Schollwöck (Schriften des Forschungszentrums, Jülich, Germany), Chap. 17, pp. 17.1–17.41.

Feiguin, Adrian E., and Steven R. White, 2005, "Finite-temperature density matrix renormalization using an enlarged Hilbert space," Phys. Rev. B **72**, 220401.

Finazzi, S., A. Le Boité, F. Storme, A. Baksic, and C. Ciuti, 2015, "Corner-Space Renormalization Method for Driven-Dissipative Two-Dimensional Correlated Systems," Phys. Rev. Lett. **115**, 080604.

Fink, J. M., A. Dombi, A. Vukics, A. Wallraff, and P. Domokos, 2017, "Observation of the Photon-Blockade Breakdown Phase Transition," Phys. Rev. X **7**, 011012.

Fisher, Matthew P. A., Peter B. Weichman, G. Grinstein, and Daniel S. Fisher, 1989, "Boson localization and the superfluid-insulator transition," Phys. Rev. B **40**, 546–570.

Fitzpatrick, Mattias, Neereja M. Sundaresan, Andy C. Y. Li, Jens Koch, and Andrew A. Houck, 2017, "Observation of a Dissipative Phase Transition in a One-Dimensional Circuit QED Lattice," Phys. Rev. X **7**, 011016.

Foss-Feig, Michael, Jeremy T. Young, Victor V. Albert, Alexey V. Gorshkov, and Mohammad F. Maghrebi, 2017, "Solvable Family of Driven-Dissipative Many-Body Systems," Phys. Rev. Lett. **119**, 190402.

Gangat, Adil A., Te I, and Ying-Jer Kao, 2017, "Steady States of Infinite-Size Dissipative Quantum Chains via Imaginary Time Evolution," Phys. Rev. Lett. **119**, 010501.

Georges, Antoine, Gabriel Kotliar, Werner Krauth, and Marcelo J. Rozenberg, 1996, "Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions," Rev. Mod. Phys. **68**, 13–125.

Gilchrist, Alexei, Nathan K. Langford, and Michael A. Nielsen, 2005, "Distance measures to compare real and ideal quantum processes," Phys. Rev. A **71**, 062310.

Gisin, N., and I. C. Percival, 1992, "The quantum-state diffusion model applied to open systems," J. Phys. A **25**, 5677–5691.

Glaetzle, A. W., R. Nath, B. Zhao, G. Pupillo, and P. Zoller, 2012, "Driven-dissipative dynamics of a strongly interacting Rydberg gas," Phys. Rev. A **86**, 043403.

Gorini, Vittorio, Andrzej Kossakowski, and E. C. G. Sudarshan, 1976, "Completely positive dynamical semigroups of N-level systems," J. Math. Phys. (N.Y.) **17**, 821–825.

Guo, Chu, Manas Mukherjee, and Dario Poletti, 2015, "Tuning energy transport using interacting vibrational modes," Phys. Rev. A **92**, 023637.

Guo, Chu, and Dario Poletti, 2018, "Analytical solutions for a boundary-driven xy chain," Phys. Rev. A **98**, 052126.

Guo, Chu, Ines de Vega, Ulrich Schollwöck, and Dario Poletti, 2018, "Stable-unstable transition for a Bose-Hubbard chain coupled to an environment," Phys. Rev. A **97**, 053610.

Haferkamp, Jonas, Dominik Hangleiter, Jens Eisert, and Marek Gluza, 2020, "Contracting projected entangled pair states is average-case hard," Phys. Rev. Research **2**, 013010.

Hartmann, Michael J., 2010, "Polariton Crystallization in Driven Arrays of Lossy Nonlinear Resonators," Phys. Rev. Lett. **104**, 113601.

Hartmann, Michael J., and Giuseppe Carleo, 2019, "Neural-Network Approach to Dissipative Quantum Many-Body Dynamics," Phys. Rev. Lett. **122**, 250502.

Helmrich, S., A. Arias, and S. Whitlock, 2018, "Uncovering the nonequilibrium phase structure of an open quantum spin system," Phys. Rev. A **98**, 022109.

Hofer, Sebastian G., and Klemens Hammerer, 2015, "Entanglement-enhanced time-continuous quantum control in optomechanics," Phys. Rev. A **91**, 033822.

Hofer, Sebastian G., Denis V. Vasilyev, Markus Aspelmeyer, and Klemens Hammerer, 2013, "Time-Continuous Bell Measurements," Phys. Rev. Lett. **111**, 170404.

Hohenberg, P. C., and B. I. Halperin, 1977, "Theory of dynamic critical phenomena," Rev. Mod. Phys. **49**, 435–479.

Hohenberg, P. C., and A. P. Krekhov, 2015, "An introduction to the Ginzburg-Landau theory of phase transitions and nonequilibrium patterns," Phys. Rep. **572**, 1–42.

Höning, M., M. Moos, and M. Fleischhauer, 2012, "Critical exponents of steady-state phase transitions in fermionic lattice models," Phys. Rev. A **86**, 013606.

Höning, Michael, Dominik Muth, David Petrosyan, and Michael Fleischhauer, 2013, "Steady-state crystallization of Rydberg excitations in an optically driven lattice gas," Phys. Rev. A **87**, 023401.

Hu, Anzi, Tony E. Lee, and Charles W. Clark, 2013, "Spatial correlations of one-dimensional driven-dissipative systems of Rydberg atoms," Phys. Rev. A **88**, 053627.

Hubig, C., and J. I. Cirac, 2019, "Time-dependent study of disordered models with infinite projected entangled pair states," SciPost Phys. **6**, 31.

Iemini, Fernando, Davide Rossini, Rosario Fazio, Sebastian Diehl, and Leonardo Mazza, 2016, "Dissipative topological superconductors in number-conserving systems," Phys. Rev. B **93**, 115113.

Ivanov, Anton, and Heinz-Peter Breuer, 2017, "Quantum corrections of the truncated Wigner approximation applied to an exciton transport model," Phys. Rev. E **95**, 042115.

Jelezko, F., T. Gaebel, I. Popa, A. Gruber, and J. Wrachtrup, 2004, "Observation of Coherent Oscillations in a Single Electron Spin," Phys. Rev. Lett. **92**, 076401.

Jin, Jiasen, Alberto Biella, Oscar Viyuela, Cristiano Ciuti, Rosario Fazio, and Davide Rossini, 2018, "Phase diagram of the dissipative quantum Ising model on a square lattice," Phys. Rev. B **98**, 241108.

Jin, Jiasen, Alberto Biella, Oscar Viyuela, Leonardo Mazza, Jonathan Keeling, Rosario Fazio, and Davide Rossini, 2016, "Cluster Mean-Field Approach to the Steady-State Phase Diagram of Dissipative Spin Systems," Phys. Rev. X **6**, 031011.

Jin, Jiasen, Davide Rossini, Rosario Fazio, Martin Leib, and Michael J. Hartmann, 2013, "Photon Solid Phases in Driven Arrays of Nonlinearly Coupled Cavities," Phys. Rev. Lett. **110**, 163605.

Johansson, J. R., P. D. Nation, and Franco Nori, 2012, "QuTiP: An open-source PYTHON framework for the dynamics of open quantum systems," Comput. Phys. Commun. **183**, 1760–1772.

Johansson, J. R., P. D. Nation, and Franco Nori, 2013, "QuTiP 2: A PYTHON framework for the dynamics of open quantum systems," Comput. Phys. Commun. **184**, 1234–1240.

Jordan, J., R. Orús, G. Vidal, F. Verstraete, and J. I. Cirac, 2008, "Classical Simulation of Infinite-Size Quantum Lattice Systems in Two Spatial Dimensions," Phys. Rev. Lett. **101**, 250602.

Kaczmarczyk, J., H. Weimer, and M. Lemeshko, 2016, "Dissipative preparation of antiferromagnetic order in the Fermi-Hubbard model," New J. Phys. **18**, 093042.

Khasseh, Reyhaneh, Angelo Russomanno, Markus Schmitt, Markus Heyl, and Rosario Fazio, 2020, "Discrete truncated Wigner approach to dynamical phase transitions in Ising models after a quantum quench," Phys. Rev. B **102**, 014303.

Kliesch, M., D. Gross, and J. Eisert, 2014, "Matrix-Product Operators and States: NP-Hardness and Undecidability," Phys. Rev. Lett. **113**, 160503.

Koashi, Masato, and Andreas Winter, 2004, "Monogamy of quantum entanglement and other correlations," Phys. Rev. A **69**, 022309.

Kohn, W., 1999, "Nobel lecture: Electronic structure of matter-wave functions and density functionals," Rev. Mod. Phys. **71**, 1253–1266.

Kollar, Marcus, 2011, "Introduction to dynamical mean-field theory," in *The LDA+DMFT Approach to Strongly Correlated Materials*, Modeling and Simulation Vol. 1, edited by E. Pavarini, E. Koch, A. Lichtenstein, and D. Vollhardt (Schriften des Forschungszentrums, Jülich, Germany), Chap. 5, pp. 5.1–5.20.

Kraus, Christina V., and Tobias J. Osborne, 2012, "Time-dependent variational principle for dissipative dynamics," Phys. Rev. A **86**, 062115.

Krauter, Hanna, Christine A. Muschik, Kasper Jensen, Wojciech Wasilewski, Jonas M. Petersen, J. Ignacio Cirac, and Eugene S. Polzik, 2011, "Entanglement Generated by Dissipation and Steady State Entanglement of Two Macroscopic Objects," Phys. Rev. Lett. **107**, 080503.

Kshetrimayum, A., 2017, "Quantum many-body systems and tensor network algorithms," Ph.D. thesis (Johannes Gutenberg-Universität Mainz).

Kshetrimayum, A., M. Rizzi, J. Eisert, and R. Orús, 2019, "Tensor Network Annealing Algorithm for Two-Dimensional Thermal States," Phys. Rev. Lett. **122**, 070502.

Kshetrimayum, A., H. Weimer, and R. Orús, 2017, "A simple tensor network algorithm for two-dimensional steady states," Nat. Commun. **8**, 1291.

Kshetrimayum, Augustine, Christian Balz, Bella Lake, and Jens Eisert, 2020, "Tensor network investigation of the double layer kagome compound $Ca_{10}Cr_7O_{28}$," Ann. Phys. (Amsterdam) **421**, 168292.

Kshetrimayum, Augustine, Marcel Goihl, and Jens Eisert, 2020, "Time evolution of many-body localized systems in two spatial dimensions," Phys. Rev. B **102**, 235132.

Kshetrimayum, Augustine, Marcel Goihl, Dante M. Kennes, and Jens Eisert, 2020, "Quantum time crystals with programmable disorder in higher dimensions," arXiv:2004.07267.

Labuhn, Henning, Daniel Barredo, Sylvain Ravets, Sylvain de Léséleuc, Tommaso Macrì, Thierry Lahaye, and Antoine Browaeys, 2016, "Tunable two-dimensional arrays of single Rydberg atoms for realizing quantum Ising models," Nature (London) **534**, 667–670.

Lammers, Jonas, Hendrik Weimer, and Klemens Hammerer, 2016, "Open-system many-body dynamics through interferometric measurements and feedback," Phys. Rev. A **94**, 052120.

Le Boité, Alexandre, Giuliano Orso, and Cristiano Ciuti, 2013, "Steady-State Phases and Tunneling-Induced Instabilities in the Driven Dissipative Bose-Hubbard Model," Phys. Rev. Lett. **110**, 233601.

Le Boité, Alexandre, Giuliano Orso, and Cristiano Ciuti, 2014, "Bose-Hubbard model: Relation between driven-dissipative steady states and equilibrium quantum phases," Phys. Rev. A **90**, 063821.

Lee, Tony E., and M. C. Cross, 2012, "Spatiotemporal dynamics of quantum jumps with Rydberg atoms," Phys. Rev. A **85**, 063822.

Lee, Tony E., Sarang Gopalakrishnan, and Mikhail D. Lukin, 2013, "Unconventional Magnetism via Optical Pumping of Interacting Spin Systems," Phys. Rev. Lett. **110**, 257204.

Lee, Tony E., H. Häffner, and M. C. Cross, 2011, "Antiferromagnetic phase transition in a nonequilibrium lattice of Rydberg atoms," Phys. Rev. A **84**, 031402.

Lemeshko, M., and H. Weimer, 2013, "Dissipative binding of atoms by non-conservative forces," Nat. Commun. **4**, 2230.

Liao, H. J., Z. Y. Xie, J. Chen, Z. Y. Liu, H. D. Xie, R. Z. Huang, B. Normand, and T. Xiang, 2017, "Gapless Spin-Liquid Ground State in the $s = 1/2$ Kagome Antiferromagnet," Phys. Rev. Lett. **118**, 137202.

Liboff, R. L., 2003, *Kinetic Theory: Classical, Quantum, and Relativistic Descriptions* (Springer, New York).

Lindblad, G., 1976, "On the generators of quantum dynamical semigroups," Commun. Math. Phys. **48**, 119–130.

Ma, R., B. Saxberg, C. Owens, N. Leung, Y. Lu, J. Simon, and D. I. Schuster, 2019, "A dissipatively stabilized Mott insulator of photons," Nature (London) **566**, 51–57.

Maghrebi, Mohammad F., and Alexey V. Gorshkov, 2016, "Nonequilibrium many-body steady states via Keldysh formalism," Phys. Rev. B **93**, 014307.

Malossi, N., M. M. Valado, S. Scotto, P. Huillery, P. Pillet, D. Ciampini, E. Arimondo, and O. Morsch, 2014, "Full Counting Statistics and Phase Diagram of a Dissipative Rydberg Gas," Phys. Rev. Lett. **113**, 023006.

Manzano, Daniel, 2020, "A short introduction to the Lindblad master equation," AIP Adv. **10**, 025106.

Marcuzzi, Matteo, Emanuele Levi, Sebastian Diehl, Juan P. Garrahan, and Igor Lesanovsky, 2014, "Universal Nonequilibrium Properties of Dissipative Rydberg Gases," Phys. Rev. Lett. **113**, 210401.

Marzlin, Karl-Peter, and Stephen Deering, 2015, "The Moyal equation for open quantum systems," J. Phys. A **48**, 205301.

Mascarenhas, Eduardo, Hugo Flayac, and Vincenzo Savona, 2015, "Matrix-product-operator approach to the nonequilibrium steady state of driven-dissipative quantum arrays," Phys. Rev. A **92**, 022116.

Matsuda, Y. H., N. Abe, S. Takeyama, H. Kageyama, P. Corboz, A. Honecker, S. R. Manmana, G. R. Foltin, K. P. Schmidt, and F. Mila, 2013, "Magnetization of $SrCu_2(BO_3)_2$ in Ultrahigh Magnetic Fields up to 118 T," Phys. Rev. Lett. **111**, 137204.

Medvedyeva, Mariya V., Fabian H. L. Essler, and Tomaž Prosen, 2016, "Exact Bethe Ansatz Spectrum of a Tight-Binding Chain with Dephasing Noise," Phys. Rev. Lett. **117**, 137202.

Mendoza-Arenas, J. J., S. R. Clark, S. Felicetti, G. Romero, E. Solano, D. G. Angelakis, and D. Jaksch, 2016, "Beyond mean-field bistability in driven-dissipative lattices: Bunching-antibunching transition and quantum simulation," Phys. Rev. A **93**, 023821.

Mertz, Thomas, Ivana Vasić, Michael J. Hartmann, and Walter Hofstetter, 2016, "Photonic currents in driven and dissipative resonator lattices," Phys. Rev. A **94**, 013809.

Mesterházy, D., and F. Hebenstreit, 2017, "Solvable Markovian dynamics of lattice quantum spin models," Phys. Rev. A **96**, 010104.

Mølmer, Klaus, Yvan Castin, and Jean Dalibard, 1993, "Monte Carlo wave-function method in quantum optics," J. Opt. Soc. Am. B **10**, 524–538.

Mondal, Suman, Augustine Kshetrimayum, and Tapan Mishra, 2020, "Two-body repulsive bound pairs in a multibody interacting Bose-Hubbard model," Phys. Rev. A **102**, 023312.

Muñoz, M. A., F. de los Santos, and M. M. Telo da Gama, 2005, "Generic two-phase coexistence in nonequilibrium systems," Eur. Phys. J. B **43**, 73–79.

Nagy, Alexandra, and Vincenzo Savona, 2018, "Driven-dissipative quantum Monte Carlo method for open quantum systems," Phys. Rev. A **97**, 052129.

Nagy, Alexandra, and Vincenzo Savona, 2019, "Variational Quantum Monte Carlo Method with a Neural-Network Ansatz for Open Quantum Systems," Phys. Rev. Lett. **122**, 250501.

Navez, Patrick, and Ralf Schützhold, 2010, "Emergence of coherence in the Mott-insulator–superfluid quench of the Bose-Hubbard model," Phys. Rev. A **82**, 063603.

Nielsen, Michael A., and Isaac L. Chuang, 2000, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England).

Oguchi, Takehiko, 1955, "A theory of antiferromagnetism, II," Prog. Theor. Phys. **13**, 148–159.

Olmos, Beatriz, Igor Lesanovsky, and Juan P. Garrahan, 2012,"Facilitated Spin Models of Dissipative Quantum Glasses," Phys. Rev. Lett. **109**, 020403.

O'Rourke, Matthew J., and Garnet Kin-Lic Chan, 2020, "Simplified and improved approach to tensor network operators in two dimensions," Phys. Rev. B **101**, 205142.

Orus, R., 2014, "A practical introduction to tensor networks: Matrix product states and projected entangled pair states," Ann. Phys. (Amsterdam) **349**, 117.

Orus, Roman, 2019, "Tensor networks for complex quantum systems," Nat. Rev. Phys. **1**, 538–550.

Orús, R., and G. Vidal, 2008, "Infinite time-evolving block decimation algorithm beyond unitary evolution," Phys. Rev. B **78**, 155117.

Orús, Román, 2012, "Exploring corner transfer matrices and corner tensors for the classical simulation of quantum lattice systems," Phys. Rev. B **85**, 205117.

Orús, Román, and Guifré Vidal, 2009, "Simulation of two-dimensional quantum systems on an infinite lattice revisited: Corner transfer matrix for tensor contraction," Phys. Rev. B **80**, 094403.

Osborne, Tobias J., and Frank Verstraete, 2006, "General Monogamy Inequality for Bipartite Qubit Entanglement," Phys. Rev. Lett. **96**, 220503.

Overbeck, Vincent R., Mohammad F. Maghrebi, Alexey V. Gorshkov, and Hendrik Weimer, 2017, "Multicritical behavior in dissipative Ising models," Phys. Rev. A **95**, 042133.

Overbeck, Vincent R., and Hendrik Weimer, 2016, "Time evolution of open quantum many-body systems," Phys. Rev. A **93**, 012106.

Owen, E. T., J. Jin, D. Rossini, R. Fazio, and M. J. Hartmann, 2018, "Quantum correlations and limit cycles in the driven-dissipative Heisenberg lattice," New J. Phys. **20**, 045004.

Panas, Jaromir, Michael Pasek, Arya Dhar, Tao Qin, Andreas Geißler, Mohsen Hafez-Torbati, Max E. Sorantin, Irakli Titvinidze, and Walter Hofstetter, 2019, "Density-wave steady-state phase of dissipative ultracold fermions with nearest-neighbor interactions," Phys. Rev. B **99**, 115125.

Parmee, C. D., and N. R. Cooper, 2018, "Phases of driven two-level systems with nonlocal dissipation," Phys. Rev. A **97**, 053616.

Percival, I., 1998, *Quantum State Diffusion* (Cambridge University Press, Cambridge, England).

Pichler, Hannes, and Peter Zoller, 2016, "Photonic Circuits with Time Delays and Quantum Feedback," Phys. Rev. Lett. **116**, 093601.

Pirvu, B., V. Murg, J. I. Cirac, and F. Verstraete, 2010, "Matrix product operator representations," New J. Phys. **12**, 025012.

Pižorn, Iztok, 2013, "One-dimensional Bose-Hubbard model far from equilibrium," Phys. Rev. A **88**, 043635.

Plenio, M. B., and P. L. Knight, 1998, "The quantum-jump approach to dissipative dynamics in quantum optics," Rev. Mod. Phys. **70**, 101–144.

Preskill, John, 2018, "Quantum computing in the NISQ era and beyond," Quantum **2**, 79.

Preskill, John, 2020, "Lecture notes on quantum computation and information," http://theory.caltech.edu/~preskill/ph229/.

Prosen, Tomaž, 2008, "Third quantization: A general method to solve master equations for quadratic open Fermi systems," New J. Phys. **10**, 043026.

Prosen, Tomaž, 2011a, "Exact Nonequilibrium Steady State of a Strongly Driven Open XXZ Chain," Phys. Rev. Lett. **107**, 137201.

Prosen, Tomaž, 2011b, "Open *XXZ* Spin Chain: Nonequilibrium Steady State and a Strict Bound on Ballistic Transport," Phys. Rev. Lett. **106**, 217206.

Rader, Michael, and Andreas M. Läuchli, 2018, "Finite Correlation Length Scaling in Lorentz-Invariant Gapless iPEPS Wave Functions," Phys. Rev. X **8**, 031030.

Raghunandan, Meghana, Jörg Wrachtrup, and Hendrik Weimer, 2018, "High-Density Quantum Sensing with Dissipative First Order Transitions," Phys. Rev. Lett. **120**, 150501.

Raitzsch, U., R. Heidemann, H. Weimer, B. Butscher, P. Kollmann, R. Löw, H. P. Büchler, and T. Pfau, 2009, "Investigation of dephasing rates in an interacting Rydberg gas," New J. Phys. **11**, 055014.

Rao, D. D. Bhaktavatsala, and Klaus Mølmer, 2013, "Dark Entangled Steady States of Interacting Rydberg Atoms," Phys. Rev. Lett. **111**, 033606.

Reiter, Florentin, and Anders S. Sørensen, 2012, "Effective operator formalism for open quantum systems," Phys. Rev. A **85**, 032111.

Requist, Ryan, 2012, "Hamiltonian formulation of nonequilibrium quantum dynamics: Geometric structure of the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy," Phys. Rev. A **86**, 022117.

Robledo, L., L. Childress, H. Bernien, B. Hensen, P. F. A. Alkemade, and R. Hanson, 2011, "High-fidelity projective read-out of a solid-state spin quantum register," Nature (London) **477**, 574–578.

Rota, R., F. Storme, N. Bartolo, R. Fazio, and C. Ciuti, 2017, "Critical behavior of dissipative two-dimensional spin lattices," Phys. Rev. B **95**, 134431.

Rota, Riccardo, Fabrizio Minganti, Cristiano Ciuti, and Vincenzo Savona, 2019, "Quantum Critical Regime in a Quadratically Driven Nonlinear Photonic Lattice," Phys. Rev. Lett. **122**, 110405.

Saffman, M., T. G. Walker, and K. Mølmer, 2010, "Quantum information with Rydberg atoms," Rev. Mod. Phys. **82**, 2313–2363.

Schachenmayer, J., A. Pikovski, and A. M. Rey, 2015a, "Dynamics of correlations in two-dimensional quantum spin models with long-range interactions: A phase-space Monte-Carlo study," New J. Phys. **17**, 065009.

Schachenmayer, J., A. Pikovski, and A. M. Rey, 2015b, "Many-Body Quantum Spin Dynamics with Monte Carlo Trajectories on a Discrete Phase Space," Phys. Rev. X **5**, 011022.

Schlosshauer, Maximilian, 2005, "Decoherence, the measurement problem, and interpretations of quantum mechanics," Rev. Mod. Phys. **76**, 1267–1305.

Schollwöck, U., 2005, "The density-matrix renormalization group," Rev. Mod. Phys. **77**, 259–315.

Schollwöck, Ulrich, 2011, "The density-matrix renormalization group in the age of matrix product states," Ann. Phys. (Amsterdam) **326**, 96–192.

Schuch, Norbert, Michael M. Wolf, Frank Verstraete, and J. Ignacio Cirac, 2007, "Computational Complexity of Projected Entangled Pair States," Phys. Rev. Lett. **98**, 140506.

Schwabl, Franz, 2010, *Quantum Mechanics* (Springer, Berlin).

Shi, Y.-Y., L.-M. Duan, and G. Vidal, 2006, "Classical simulation of quantum many-body systems with a tree tensor network," Phys. Rev. A **74**, 022320.

Sieberer, L. M., M. Buchhold, and S. Diehl, 2016, "Keldysh field theory for driven open quantum systems," Rep. Prog. Phys. **79**, 096001.

Sieberer, L. M., S. D. Huber, E. Altman, and S. Diehl, 2013, "Dynamical Critical Phenomena in Driven-Dissipative Systems," Phys. Rev. Lett. **110**, 195301.

Somoza, Alejandro D., Oliver Marty, James Lim, Susana F. Huelga, and Martin B. Plenio, 2019, "Dissipation-Assisted Matrix Product Factorization," Phys. Rev. Lett. **123**, 100502.

Spohn, Herbert, 1976, "Approach to equilibrium for completely positive dynamical semigroups of *N*-level systems," Rep. Math. Phys. **10**, 189–194.

Tang, Baoming, Ehsan Khatami, and Marcos Rigol, 2013, "A short introduction to numerical linked-cluster expansions," Comput. Phys. Commun. **184**, 557–564.

Terhal, B. M., 2004, "Is entanglement monogamous?," IBM J. Res. Dev. **48**, 71–78.

Titvinidze, Irakli, Antonius Dorda, Wolfgang von der Linden, and Enrico Arrigoni, 2015, "Transport through a correlated interface: Auxiliary master equation approach," Phys. Rev. B **92**, 245125.

Titvinidze, Irakli, Antonius Dorda, Wolfgang von der Linden, and Enrico Arrigoni, 2016, "Resonance effects in correlated multilayer heterostructures," Phys. Rev. B **94**, 245142.

Tomadin, A., V. Giovannetti, R. Fazio, D. Gerace, I. Carusotto, H. E. Türeci, and A. Imamoglu, 2010, "Signatures of the superfluid-insulator phase transition in laser-driven dissipative nonlinear cavity arrays," Phys. Rev. A **81**, 061801.

Transchel, F. W. G., A. Milsted, and T. J. Osborne, 2014, "A Monte Carlo time-dependent variational principle," arXiv:1411.5546.

Troyer, Matthias, and Uwe-Jens Wiese, 2005, "Computational Complexity and Fundamental Limitations to Fermionic Quantum Monte Carlo Simulations," Phys. Rev. Lett. **94**, 170201.

Verstraete, F., J. J. García-Ripoll, and J. I. Cirac, 2004, "Matrix Product Density Operators: Simulation of Finite-Temperature and Dissipative Systems," Phys. Rev. Lett. **93**, 207204.

Verstraete, F., V. Murg, and J. I. Cirac, 2008, "Matrix product states, projected entangled pair states, and variational renormalization

group methods for quantum spin systems," Adv. Phys. **57**, 143–224.

Verstraete, Frank, Michael M. Wolf, and J. Ignacio Cirac, 2009, "Quantum computation and quantum-state engineering driven by dissipation," Nat. Phys. **5**, 633–636.

Vicentini, Filippo, Alberto Biella, Nicolas Regnault, and Cristiano Ciuti, 2019, "Variational Neural-Network Ansatz for Steady States in Open Quantum Systems," Phys. Rev. Lett. **122**, 250503.

Vicentini, Filippo, Fabrizio Minganti, Alberto Biella, Giuliano Orso, and Cristiano Ciuti, 2019, "Optimal stochastic unraveling of disordered open quantum systems: Application to driven-dissipative photonic lattices," Phys. Rev. A **99**, 032115.

Vicentini, Filippo, Fabrizio Minganti, Riccardo Rota, Giuliano Orso, and Cristiano Ciuti, 2018, "Critical slowing down in driven-dissipative Bose-Hubbard lattices," Phys. Rev. A **97**, 013853.

Vidal, G., 2004, "Efficient Simulation of One-Dimensional Quantum Many-Body Systems," Phys. Rev. Lett. **93**, 040502.

Vidal, G., 2007, "Classical Simulation of Infinite-Size Quantum Lattice Systems in One Spatial Dimension," Phys. Rev. Lett. **98**, 070201.

Vidal, Guifré, 2003, "Efficient Classical Simulation of Slightly Entangled Quantum Computations," Phys. Rev. Lett. **91**, 147902.

Vinjanampathy, Sai, and Janet Anders, 2016, "Quantum thermodynamics," Contemp. Phys. **57**, 545–579.

Weimer, H., M. Müller, I. Lesanovsky, P. Zoller, and H. P. Büchler, 2010, "A Rydberg quantum simulator," Nat. Phys. **6**, 382–388.

Weimer, Hendrik, 2015a, "Variational analysis of driven-dissipative Rydberg gases," Phys. Rev. A **91**, 063401.

Weimer, Hendrik, 2015b, "Variational Principle for Steady States of Dissipative Quantum Many-Body Systems," Phys. Rev. Lett. **114**, 040402.

Weimer, Hendrik, 2017, "Tailored jump operators for purely dissipative quantum magnetism," J. Phys. B **50**, 024001.

Weimer, Hendrik, Robert Löw, Tilman Pfau, and Hans Peter Büchler, 2008, "Quantum Critical Behavior in Strongly Interacting Rydberg Gases," Phys. Rev. Lett. **101**, 250601.

Werner, A. H., D. Jaschke, P. Silvi, M. Kliesch, T. Calarco, J. Eisert, and S. Montangero, 2016, "Positive Tensor Network Approach for Simulating Open Quantum Many-Body Systems," Phys. Rev. Lett. **116**, 237201.

White, Steven R., 1992, "Density Matrix Formulation for Quantum Renormalization Groups," Phys. Rev. Lett. **69**, 2863–2866.

White, Steven R., 1993, "Density-matrix algorithms for quantum renormalization groups," Phys. Rev. B **48**, 10345–10356.

Wichterich, Hannu, Markus J. Henrich, Heinz-Peter Breuer, Jochen Gemmer, and Mathias Michel, 2007, "Modeling heat transport through completely positive maps," Phys. Rev. E **76**, 031115.

Xu, Xiansong, Juzar Thingna, Chu Guo, and Dario Poletti, 2019, "Many-body open quantum systems beyond Lindblad master equations," Phys. Rev. A **99**, 012106.

Yoshioka, Nobuyuki, and Ryusuke Hamazaki, 2019, "Constructing neural stationary states for open quantum many-body systems," Phys. Rev. B **99**, 214306.

Zwolak, Michael, and Guifré Vidal, 2004, "Mixed-State Dynamics in One-Dimensional Quantum Lattice Systems: A Time-Dependent Superoperator Renormalization Algorithm," Phys. Rev. Lett. **93**, 207205.