Dissipative generation of highly entangled states of light and matter

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We investigate the full quantum evolution of ultracold interacting bosonic atoms confined to a chain geometry and coupled to the field of an optical cavity. Extending the time-dependent matrix product state techniques to capture the global coupling to the cavity mode and the open nature of the cavity, we examine the long time behavior of the system beyond the mean-field elimination of the cavity field. We find that in a wide range of parameters a highly entangled photon-atom state forms and investigate its properties. We show that in the self-organized phase the steady state consists in a mixture of the mean-field predicted density wave states and coherent states with lower photon number. For large dissipation strengths we develop a variant of the many-body adiabatic elimination technique and obtain a steady state with a high photon-atom entanglement and a fully mixed atomic sector. We observe numerically the crossover from the density wave state towards this mixed state.

I. INTRODUCTION

Experimental progress to achieve strong coupling of quantum matter to quantum light has opened exciting possibilities. Realizations of such systems nowadays exist both with ultracold atomic gases strongly coupled to optical cavities [1–3] or the electron gas in solids coupled to THz cavities [4–6]. In particular, these realizations have allowed to study self-organization phenomena and stabilize exotic phases by the interaction with the quantum light [3, 7, 8]. Beside the interest in the novel self-organized steady states, advantages of the coupling of quantum matter to quantum light is the fast self-organization dynamics due to the presence of the cavity induced long range interactions and the stabilization of complex states via the dissipative attractor dynamics typically present in these setups. The cavity induced long-range interaction has been observed in atomic gases with external optical lattice potentials, where an extended Bose-Hubbard model with long-range interactions has been experimentally realized [9–11] and the effect of the long-range interactions on the superfluid to insulator transition [12–22] and the out-of-equilibrium dynamics [23] have been analyzed.

Theoretical proposals use the attractor dynamics to stabilize complex quantum phases [24–27], including topologically non-trivial phases [28–35]. Together with the recent achievements regarding the coupling of the cavity field to the internal spin degrees of freedom of atoms [36–38], it has opened the possibilities of the realization of dissipaton-induced instabilities [39, 40] and dynamical spin-orbit coupling [41, 42].

The previous theoretical description of coupled atomic cavity systems was to a large extent performed using a mean field decoupling of the cavity field and the atomic degrees of freedom to describe the self-organization process [3, 15, 43]. This approach assumes the cavity field to be in a coherent state and the atoms to be in the ground state of an effective model and can therefore not take the atom-photon entanglement correctly into account. Above a certain threshold of the coupling strength between the cavity and the atoms, the cavity field has a finite value and the atoms self-organize into a non-trivial state.

So far the entanglement between the atomic and photonic states has been included only for small systems of one or two atoms, or two sites [44–49], or in closed systems [50]. In this work, we go beyond the mean field approximation and investigate the combined atom-cavity system using quasi-exact numerical simulations based on matrix product states and a many body adiabatic elimination valid for large photon losses. In particular, both methods gives access to the light-atom entanglement. These methods enable us to show that even starting with a disentangled state of atoms and photons, a high entanglement between the atoms and the quantum light is generated by a dissipative attractor dynamics. This self-organization of the entanglement makes it particularly stable against perturbations. We investigate the dependence of the atom-photon entanglement for a wide range of parameters. A strong coupling can be reached even for the limit of very lossy cavity mirrors.

II. MODEL

In the following we consider interacting bosons confined to a one-dimensional chain coupled to a single cavity mode and transversely pumped with a standing-wave laser beam (see Fig. 1). We describe the dynamics of the coupled cavity-atom system by a Lindblad equation for the density operator $\rho$ given by [3, 15, 51, 52]

$$\frac{\partial}{\partial t} \rho = -\frac{i}{\hbar} [H, \rho] + \frac{\Gamma}{2} (2a_\rho a^\dagger - a^\dagger a_\rho - a_\rho a^\dagger) .$$

(1)

where the bosonic operators $a$ and $a^\dagger$ are the annihilation and creation operators for the photon mode of the cavity and $\Gamma$ the dissipation strength. The second term on the right hand side of this equation takes into account the losses from the cavity due to the imperfections of the
FIG. 1. Sketch of the setup. The bosonic atoms in an optical cavity are confined in a one-dimensional chain. The atoms tune with the amplitude \(J\) and have an on-site interaction of strength \(U\). The coupling of the atoms to the cavity is realized with a retroreflected transversal pump beam. As the lattice spacing is commensurate with half of the wavelength of the cavity mode, the cavity field is coupled to the total imbalance between the odd and even sites of the chain. The strength of the coupling is controlled by the pump amplitude \(\Omega\). The cavity is losing photons with the dissipation strength \(\Gamma\), due to the imperfections of the mirrors.

The first term represents the unitary evolution in which the excited internal state of the atoms is adiabatically eliminated. The corresponding Hamiltonian is given by \[3, 15, 43\]

\[
H = H_c + H_{\text{kin}} + H_{\text{int}} + H_{\text{ac}} \tag{2}
\]

\[
H_c = \hbar \delta a^\dagger a
\]

\[
H_{\text{kin}} = -J \sum_{j=1}^{L-1} (b_j b_{j+1}^\dagger + b_{j+1} b_j^\dagger)
\]

\[
H_{\text{int}} = \frac{U}{2} \sum_{j=1}^{L} n_j (n_j - 1)
\]

\[
H_{\text{ac}} = -\hbar \Omega (a + a^\dagger) \Delta, \quad \Delta = \sum_{j=1}^{L} (-1)^j n_j.
\]

The term \(H_c\) describes the cavity mode with a detuning between the cavity mode and the transverse pump beam \(\delta = \omega_c - \omega_p\), in the rotating frame of the pump beam. The operators \(b_j\) and \(b_j^\dagger\) are the bosonic annihilation and creation operators of the atoms on site \(j\) and \(n_j = b_j^\dagger b_j\). \(L\) denotes the number of sites of the bosonic chain and the total number of bosons is \(N\). \(H_{\text{kin}}\) describes the tunneling processes of the atoms along the chain with the tunneling amplitude \(J\) and the term \(H_{\text{int}}\) represents the repulsive on-site interaction of strength \(U > 0\). The coupling between the atoms and the cavity field is described by \(H_{\text{ac}}\). Due to the assumed commensurability of the cavity mode with twice the periodicity of the lattice spacing within the chain, the cavity field is coupled to the total imbalance between the odd and even sites of the chain, \(\Delta\), with the effective pump amplitude \(\Omega\). In the following we use the scaled coupling strength \(\Omega\sqrt{N}\), in order to make our results independent on the particle number. Whereas typically already to determine the time-evolution of the Bose-Hubbard model alone is very involved, here an additional complication is due to the large and, in principle, unlimited dimension of the Hilbert space of the photonic mode.

This challenge is typically circumvented by adiabatically eliminating the cavity field and using a mean-field decoupling for the atoms and the cavity mode \[3\]. Within this crude approximation one finds, that above a certain threshold \(\Omega_{\text{MF},c} \sqrt{N}\) of the pump power \(\Omega \sqrt{N}\) the cavity field \(\langle a\rangle\) takes a finite value, either \(\pm \alpha\), and the atoms self-organize into a density modulated pattern either on the odd or even sites of the chain, depending on the sign of \(\alpha\). The corresponding density matrix is a pure state

\[
\rho_{\text{MF}} = |\alpha(\Delta_{\text{eff}}), \Delta_{\text{eff}}\rangle \langle \alpha(\Delta_{\text{eff}}), \Delta_{\text{eff}}|, \tag{3}
\]

with \(\alpha(\Delta) = -\frac{\Omega}{\sqrt{2} \Delta} \Delta_{\text{eff}}\) and \(\Delta_{\text{eff}}\) is the expectation value of the odd-even imbalance obtained by solving an effective atomic model with a self-consistency equation (see APPENDIX A). For large \(\Omega \sqrt{N}\), the imbalance tends towards its maximal value \(\Delta = N\). For later comparison, we mention that within the mean-field theory, the sudden onset of the cavity field is also reflected in the behavior of the photon number \(n_{\text{MF}}\), since \(n_{\text{MF}} = |\langle a\rangle|^2 = \frac{\Omega^2}{\sqrt{2} \Omega_{\text{MF},c} \Delta_{\text{eff}}^2}\) (blue line in Fig. 2 (a)).

The appearance of two steady states with \(\pm \alpha\) within the mean-field analysis is due to spontaneous breaking of the \(\mathbb{Z}_2\) symmetry of the Hamiltonian, Eq. (2) associated with the inversion of the sign of the cavity field, \(a\), and the atomic odd-even imbalance, \(\Delta\). However, the \(\mathbb{Z}_2\) symmetry is only a weak symmetry of the Liouvillian \[53, 54\], since the transformation does not commute with the jump operator \(a\) of the Lindblad equation, Eq. (1).

Thus, a zero expectation value for the cavity field is expected in the steady state of the system \[44, 45, 48, 55\]. In order to capture this within the mean field analysis, one can generalize the mean field result for the steady state to a mixture of two states from each \(\mathbb{Z}_2\) sector \[47, 48\],

\[
\rho_{\pm \alpha} = \frac{1}{2} [\alpha(|\Delta_{\text{eff}}|), |\Delta_{\text{eff}}\rangle \langle \alpha(|\Delta_{\text{eff}}|), |\Delta_{\text{eff}}|] \tag{4}
\]

\[
+ \frac{1}{2} [\alpha(|\Delta_{\text{eff}}|), -|\Delta_{\text{eff}}\rangle \langle \alpha(|\Delta_{\text{eff}}|), -|\Delta_{\text{eff}}|].
\]

In contrast to the mean-field result, one can see that this state has an entanglement entropy \(S_N = \log(2)\) between the atomic degrees of freedom and the photons.

### III. METHODS

We develop here two novel approaches taking the atom-cavity entanglement into account going beyond the mean-field approach described above.
A. Analytical method: Many-body adiabatic elimination

As the first approach, we develop a variant of the many-body adiabatic elimination technique [69, 70] including the photonic mode. This approach allows us to get analytical insights into the nature of the steady state in the limit of large dissipation, i.e. \( h \Gamma \gg h \Omega, h \delta \gg J \). For finite interaction we find that in this limit the steady state is given by

\[
\rho_{\text{mix}} = \frac{1}{N} \sum_{\{n_i\}} |\alpha(\Delta), \Delta \rangle \langle \alpha(\Delta), \Delta | \tag{5}
\]

(see APPENDIX B). The sum runs over all possible density configurations \( \{n_i\} \), where the odd-even imbalance \( \Delta \) determines the coherent state of the photons \( \alpha(\Delta) = \sqrt{\frac{1}{\Omega}} e^{i \delta \Delta} \). This state, \( \rho_{\text{mix}} \), is very distinct from the mean-field state which only allows a certain value of the photon occupation and the corresponding imbalance \( \Delta \). \( \rho_{\text{mix}} \) is characterized by high entanglement between the cavity mode and the atoms. By tracing out the photonic degrees of freedom we obtain a fully mixed atomic sector. Each density configuration has the same weight \( 1/N \) in the sum, with \( N = (L + N - 1) \), the total number of atomic configurations. The number of states with a certain imbalance \( \Delta \) is given by

\[
c_\Delta = \left( \frac{1}{2} (L + N + \Delta) - 1 \right) \left( \frac{1}{2} (L + N - \Delta) - 1 \right) \left( \frac{1}{2} (N + \Delta) \right) \left( \frac{1}{2} (N - \Delta) \right) \tag{6}
\]

The entanglement entropy between the cavity field and the bosonic atoms is

\[
S_{\text{cN}} = - \sum_\Delta (c_\Delta / N) \log(c_\Delta / N). \tag{7}
\]

For example, the entanglement entropy of \( \rho_{\text{mix}} \) for \( L = 10 \) sites and \( N = 5 \) particles is \( S_{\text{cN}} \approx 1.66 \), larger than the \( \log(2) \) value given by the mean-field density matrix \( \rho_{\pm \alpha} \).

B. Numerical tMPS method

We will show using our second approach, the numerical matrix product state (MPS) approach, how the nature of the steady state changes drastically for different parameters with the two extreme limits being a state close in nature to either the mixture of the two mean-field states \( \rho_{\pm \alpha} \), or to the fully mixed state \( \rho_{\text{mix}} \).

The second approach is a numerically exact treatment of the time-evolution following the dissipative master equation using the Monte-Carlo wave function method [56, 57] combined with the matrix product state methods. This combined approach has been applied for several atomic models recently [58–60]. Within this approach...
one important step is the determination of the time-evolution following an effective non-hermitian Hamiltonian which is typically solved using a Trotter-Suzuki decomposition for even and odd sites of the time-evolution operator. Here additional challenge is the presence of the globally coupled photon mode. We overcome this challenge with a variant of the quasi-exact time-dependent variational matrix product state (tMPS) [61–63] based on the Trotter-Suzuki decomposition of the time evolution propagator which separates off the parts in which the photonic mode occurs. Additionally, a dynamical deformation of the MPS structure using swap gates [63–65] needs to be applied. Such a variant of the MPS time-evolution had been applied previously in the context of spin-boson models [65, 66], which have no interaction between the spins. We implement this newly developed combination, for the first time for interacting bosons coupled to a cavity mode, efficiently using the ITensor library [67] taking good quantum numbers into account. Details on the numerical method and the parameters used in the simulations can be found in APPENDIX C and APPENDIX D. The results shown are typically taken at relatively long times, where we expect that most of the quantities are already close to their steady state values (see APPENDIX D).

IV. LARGE COUPLING REGIME: MIXTURE OF DENSITY WAVE STATES

We start by analyzing the behavior of the photon number [68] in the cavity as a function of the pump strength $\Omega \sqrt{N}$ (see Fig. 2) in a regime favourable for the mean-field treatment. In our numerical results (red symbols in Fig. 2 (a)) we observe a smooth increase in the photon number across the self-organization threshold predicted by the mean-field treatment. The smooth increase is expected for the system of finite size. However, the values of our numerical results remain a bit below $n_{\text{MF}}$ which points towards deviations from the mean-field state. We will show later that this has its origin in the admixture of states with a reduced photon number. In order to get more insight into the obtained state, we study the phase space distribution of the cavity field, represented by the Q-function $Q(\alpha) = \text{tr} (|\alpha\rangle \rho |\alpha\rangle)$, where $|\alpha\rangle$ is a photonic coherent state. We can observe in Fig. 2(b), that for $\hbar \Omega \sqrt{N} = 1.12 J$ which is below the mean-field threshold $\Omega_{\text{MF,c}} \sqrt{N}$, the Q-function $Q(\alpha)$ has a maximum at $\alpha = 0$ which resembles a coherent state with zero photons. In contrast, above the threshold ($\Omega \sqrt{N} > \Omega_{\text{MF,c}} \sqrt{N}$) the Q-function develops two maxima, as seen in Fig. 2(c) and if we increase $\Omega \sqrt{N}$ the Q-function indicates the photonic state of two coherent states with a small overlap (Fig. 2(d)). This state has a dominant contribution which resembles the mixture of the predicted mean-field states. However, if we increase the pump power even further (see Fig. 2(e)), we observe that both peaks in $Q(\alpha)$ deviate from the circular shape and states with a lower photon number are populated.

The atomic part of the steady state which corresponds to the photonic states well above the mean-field threshold, shows the characteristic staggered density-wave in the density-density correlations. In Fig. 3(a) we quantify this staggering, by computing the average contrast between the maxima and the minima $\frac{1}{N} \sum_j (\langle n_j n_{j+2} \rangle - \langle n_j n_{j+1} \rangle)$ as a function of $\Omega \sqrt{N}$. For comparison, the blue line represents $S_{\text{vN}} = \log(2)$ and the purple line $S_{\text{vN}} = 1.66$.

FIG. 3. (a) The averaged contrast of the density-density correlation, $\frac{1}{N} \sum_j (\langle n_j n_{j+2} \rangle - \langle n_j n_{j+1} \rangle)$ as a function of $\hbar \Omega \sqrt{N}/J$. Symbols and parameters as described in Fig.2(a). (b) The von Neumann entanglement entropy, $S_{\text{vN}}$, computed from the approximate steady state density matrix as a function of $\Omega \sqrt{N}$. For comparison, the blue line represents $S_{\text{vN}} = \log(2)$ and the purple line $S_{\text{vN}} = 1.66$. 
In order to analyze this admixture, we consider the single quantum trajectories sampled in the Monte Carlo wave function approach. We observe that the trajectories stabilize at two different photon numbers. Thus, we implemented a conditional averaging process, depending on the final photon number. The obtained photon number distributions are plotted in Fig. 4(a), where the two distributions are weighted with the probability of each class of trajectories averaged separately depending on the final photon number. In (a) the continuous lines for the separate averages correspond to the Poisson distributions expected for coherent states with the same average photon number as the numerical data. The errors bars represent the standard deviation of the Monte Carlo average. The numerical parameters used in the tMPS method are the same as in Fig.2.

The rise of the expectation value of the photon number of the average of the first class of trajectories averaged separately depending on the final photon number. The obtained photon number distribution resembles a coherent state. Thus, we attribute the second class of trajectories to states which have an additional defect due to the tunneling of an atom. In the limit of large pump strength, the state resembles a good charge density wave in the first class of trajectories. [Fig. 4(b)]. Thus, the state resembles a good charge density wave in the first class of trajectories.

In contrast, we attribute the second class of trajectories to states which have an additional defect due to the tunneling of an atom. In the limit of large pump strength and perfect imbalance with $\Delta_{\text{eff}} = N$ these states would have only one atom at the "wrong" site. More generally, we show in Fig. 2(a) that the reduced average value of the photon number can be well explained assuming that the imbalance is reduced as $\Delta \approx \Delta_{\text{eff}} - 2$. The mean-field prediction which we obtain using this reduced value of $\Delta$ follows nicely the numerically obtained average. The photon number distribution resembles a coherent state with this lower photon number [Fig. 4(a)].
tion is further supported by the results for the staggering of the density-density correlations which is also smaller in this case (see Fig. 3(a) and Fig. 4(b)).

In certain trajectories we observe transitions between the two states, characterized by the tunneling process of an atom, correlated with a sudden increase, or decrease, of the photon number. However, due to the suppression of the tunneling in the self-organized phase and the small overlap of the two corresponding photonic states for large $\Omega\sqrt{N}$ these processes become very rare. For the parameters of Fig. 4 we observe such transitions in the time interval $30 < tJ/\hbar < 50$ in 22 trajectories out of 600. We further note that we can distinguish between the two distributions only for $\hbar\Omega\sqrt{N}/J \geq 2.68$, as for lower pump strengths the individual quantum trajectories are too noisy due to the low photon number.

The presence of the trajectories belonging to two states different in nature, strongly suggests that the numerically observed steady state is a mixture of these two dominant contributions. Therefore, a crucial deviation from the mean-field predictions is identified. From the single trajectories we can infer the weight of these contributions and thus construct an approximate steady state density matrix. With this approach we can estimate the von Neumann entanglement entropy between the photon and the atoms, as represented in Fig. 3(b). We observe that value of the entanglement entropy, $S_{\text{VN}}$, is larger than $\log(2)$, indicating a stronger light-matter entanglement. The entanglement for the considered parameters is larger than in the mean-field state $\rho_{\text{MF}}$, but at the same time $S_{\text{VN}}$ is bounded from above by the corresponding value for the state, $\rho_{\text{mix}}$. For larger $\Omega\sqrt{N}$ the entanglement is increasing, as the trajectories with a lower photon number have a larger contribution to the mixture [Fig. 3(b)]. More contributions might be present with a low weight and therefore might not be identified in the presented numerics.

V. STRONG DISSIPATION LIMIT: HIGH PHOTON-ATOM ENTANGLEMENT

The deviations from the mean field predictions become even more prominent in the regime of strong dissipation. We attribute this to the admixture of states which correspond to more and more defects until in the limit of very large dissipation $\Gamma$ the state $\rho_{\text{mix}}$ is reached. Due to the larger number of states that are admixed into the steady state, a strong entanglement between the atoms and the photons builds up.

We can observe that for large $\Gamma$ the photon number does no longer agree with the mean-field value, but matches fairly well with the value computed for the adiabatic elimination steady state, for $\hbar\Gamma/J \gtrsim 7$ (see Fig. 5(a)). In particular, whereas the mean-field approach predicts that above $\hbar\Gamma/J \approx 11.6$ the system has a transition back to the normal phase, the photon number remains finite in the numerical results (see APPENDIX D). Also in the distribution of the photon number, the agreement with the adiabatic elimination results becomes very good [Fig. 5(b)-(c)]. Where at $\hbar\Gamma/J = 7.5$ still small deviations are present at low number states, the distribution for $\hbar\Gamma/J = 10$ agrees almost perfectly. The Q-function no longer has two maxima at large $\Gamma$ (insets of Figs. 5(b)-(c)), but only one maximum at $\alpha = 0$ and a squeezed profile deviating drastically from the mean-field result. The same approach of our numerical results to the adiabatic elimination results can be seen in the contrast of the density-density correlations. In the state $\rho_{\text{mix}}$ the density-density correlations as a function of distance exhibit a flat profile and the contrast in the staggering would vanish. Increasing $\Gamma$, we see that the contrast approaches zero [Fig. 5(a)]. Thus, at large values of the photon losses, the self-organized steady state no longer resembles a staggered density wave state. It is a state with a contribution from many atomic and photonic states, but with a large entanglement between the photonic and atomic sector.

VI. CONCLUSIONS

In summary, we performed the full quantum time-evolution towards the steady state of a chain of interacting bosonic atoms coupled to an optical cavity. We showed that by including the entanglement between the atomic degrees of freedom and the photonic field one finds important deviations from the mean-field approach of eliminating the cavity field. We saw that when the dissipation strength is comparable with the other energy scales in our system, the system is in a mixture where the largest contribution given by a density wave state. Other states without density ordering become more prominent in the mixture as we increase the dissipation strength, such that in the large $\Gamma$ limit the atomic sector is fully mixed, but with a strong entanglement between the atomic and the photonic sector.

In an experimental realization similar to the setups considered in Refs. [9–11, 37] one could trap the atoms in an array of independent one-dimensional tubes and see the predicted deviations from the mean-field results towards the totally mixed states. By having access to the photon number distributions via the photons leaking out of the cavity one could observe the deviations. In particular, for $\rho_{\text{mix}}$ the second order correlation function, $g^{(2)}(0)$, has large values, $g^{(2)}(0) > 2$, showing the importance of fluctuations in this regime.

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CRC 1238 project number 277146847 - projects C05, and Einzelantrag) and the ERC (Grant Number 648166).

APPENDIX A. MEAN-FIELD SOLUTIONS

In this section we derive the effective model for the bosonic atoms which gives the mean-field solutions, employing the adiabatic elimination of the cavity field [3]. Within this approximation the cavity photons are assumed to be in a coherent state with the cavity field given by its steady-state value, $\partial_t \langle a \rangle = 0$. Using Eqs. (1) and (2), this condition becomes

$$i\hbar \partial_t \langle a \rangle = -\Omega \langle \Delta \rangle + (\delta - i\Gamma/2) \langle a \rangle = 0.$$  \hspace{1cm} (A.1)

which relates the expectation value of the odd-even imbalance to the value of the cavity field by

$$\alpha = \langle a \rangle = -\frac{\Omega}{\delta - i\Gamma/2} \langle \Delta \rangle.$$ \hspace{1cm} (A.2)

The equations of motion for the bosonic operators read

$$i\hbar \partial_t \langle b_j \rangle = -J(b_{j+1} + b_{j-1}) - U(b_j(1 - n_j)) - \hbar \Omega(a + a^\dagger)(-1)^j \langle b_j \rangle.$$ \hspace{1cm} (A.3)

After substituting the expectation value for the cavity field, Eq. A.2, into the equations of motion of the bosonic operators, Eq. A.3, we obtain an effective Hamiltonian for the atoms

$$H_{\text{eff}} = H_{\text{kin}} + H_{\text{int}} + H_{\text{imb}}$$ \hspace{1cm} (A.4)

$$H_{\text{kin}} = -J \sum_{j=1}^{L-1} (b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j)$$

$$H_{\text{int}} = \frac{U}{2} \sum_{j=1}^{L} n_j(n_j - 1)$$

$$H_{\text{imb}} = -J_2 \Delta.$$  

Thus the steady state of the equations of motion is computed as the ground state of this effective model. The parameter $J_2$ has to be determined self-consistently as it depends on the expectation value of $\langle \Delta \rangle$, $J_2 = \frac{2\hbar\Omega^2\delta}{\delta^2 + \Gamma^2/4} \langle \Delta \rangle$.

The effective imbalance $\Delta_{\text{eff}}$ is defined as the expectation value of the odd-even imbalance in the ground state of the effective Hamiltonian, Eq. A.4.

APPENDIX B. MANY BODY ADIABATIC ELIMINATION FORMALISM

In order to understand the long-time behavior of our system in the strongly dissipative regime, we employ the many-body adiabatic elimination method [69, 70]. We assume that the effect of kinetic energy, $H_{\text{kin}}$ in the dynamic of the system is weak ($\hbar \Gamma \gg \hbar \Omega, \hbar \delta \gg J$) compared to the other terms in the Liouvillian $L_0 = -\frac{1}{\hbar} [H, H_{\text{int}} + H_{\text{imb}}] + \mathcal{D}(\cdot)$. This approach will give an insight into the effective dynamics of the density matrix in the decoherence free subspace of $L_0$, i.e. the space formed by all density matrices $\rho_0$ which are eigenstates of the superoperator $L_0$ with vanishing real part of the eigenvalue. The other spaces corresponding to non-zero real part of the eigenvalue are only considered within perturbation theory.

Since the eigenvalue equation belonging to $L_0$ is already complex, we show that states of the form

$$\rho = |\alpha(\Delta), \Delta, u\rangle \langle \alpha(\Delta'), \Delta', u'|$$ \hspace{1cm} (B.1)

are right eigenstates of the superoperator $L_0$. Here we do not assure that these states are physical density matrices. The atomic part is characterized by the odd-even imbalance $\Delta = \sum_j (-1)^j n_j$ and by its total interaction energy, $u = \frac{U}{2} \sum_j n_j(n_j - 1)$. Photons are in a coherent state which depends on the atomic imbalance

$$\alpha(\Delta) = -\frac{\Omega}{\delta - i\Gamma/2} \Delta.$$ \hspace{1cm} (B.2)

The corresponding eigenvalues for right eigenvectors in Eq. B.1 are given by

$$\lambda = -\frac{1}{2} \frac{\Omega^2\Gamma}{\delta^2 + \Gamma^2/4} (\Delta - \Delta')^2$$

$$+ i \left\{ \frac{\Omega^2\delta}{\delta^2 + \Gamma^2/4} (\Delta^2 - \Delta'^2) - (u - u') \right\}.$$ \hspace{1cm} (B.3)

For $\Delta = \Delta'$ the real part of the eigenvalues is zero. Thus, the states in Eq. B.1 with $\Delta = \Delta'$ lie in the decoherence free subspace of $L_0$. Interestingly, the states with $\Delta = \Delta'$, but with different interaction energies $u \neq u'$ have purely imaginary eigenvalues.

The subspace which can be accessed via a hopping event is given for the states in which $\Delta = \Delta' \pm 2$. If we consider only contributions from this subspace the effective dynamics in the decoherence free subspace is given by [70, 71]

$$\frac{d}{dt} \rho^0 = \lambda_0 \rho^0 + \frac{1}{\hbar^2} P_0 \left[ H_{\text{kin}}, L_0^{-1} P_1 \left[ H_{\text{kin}}, \rho^0 \right] \right],$$  \hspace{1cm} (B.4)

where $\rho^0$ lies in the decoherence free subspace of $L_0$ and $P_0$ and $P_1$ are the projectors to the decoherence free subspace and the excited subspace, respectively.

By explicitly writing the equations of motion, Eq. B.4 for the elements of the decoherence free subspace for the general case of $N$ particles in $L$ sites one can show that the mixed state given by

$$\rho_{\text{mix}} = \frac{1}{\mathcal{N}} \sum_{\{n_j\}} |\alpha(\Delta); n_1, \ldots, n_L\rangle \langle \alpha(\Delta); n_1, \ldots, n_L| $$ \hspace{1cm} (B.5)

is a steady state of the system. Here $\mathcal{N}$ is the number of ways one can arrange $N$ identical particles in $L$ sites.
Note that this state has a high entanglement between the atomic and the photonic degrees of freedom.

In Ref. [23] the authors consider the same model, but they eliminate the cavity field and analyze the obtained effective Liouvillian in the atomic sector. As in their case the effective jump operators are Hermitian, it follows directly that the fully mixed state is a steady state. In contrast, in our analysis we consider the full Liouvillian (Eqs. (1) and (2)), including the photonic degrees of freedom, and because the jump operator (annihilation operator of the cavity mode $a$) is not Hermitian we need to perform the complicated many-body adiabatic elimination in order to obtain insights into the nature of the steady state.

APPENDIX C. TIME-DEPENDENT MATRIX PRODUCT STATE (tMPS) METHOD FOR COMBINED ATOM-CAVITY SYSTEMS

The considered dissipative system of ultracold atoms coupled to an optical cavity poses several challenges. The first is the implementation of the cavity field, the second is the dissipative nature of the system. The cavity field can have arbitrarily high occupation and has a global coupling to the atoms, both properties which are not standard in the MPS implementations. In the following we will describe how our implementation overcomes all these difficulties.

In order to perform the time evolution within the MPS formalism, we represent the wave function of each trajectory as a matrix product state (MPS) [63], with initially the first site corresponding to the cavity mode and the rest to the atomic lattice using a Fock basis for each site (see Fig. 6(a)). The cutoff for the dimension of the local Hilbert space of the photonic site is set depending on the physical parameters of the model.

The global range coupling between the cavity mode and all the atomic sites makes the use of the usual tMPS implementation for short-range Hamiltonians impossible. Thus, we develop a variant of tMPS based on the dynamical deformation of the MPS structure, such that the order of the sites can be altered as needed. This is realized using swap gates [63–65]. Previous variants of the MPS time-evolution with swap gates dealt with short-range interaction two dimensional models [64], or spin-boson models [65]. This is to our knowledge the first implementation that can efficiently deal with interacting bosonic models globally coupled to a field with an arbitrarily large Hilbert space in the presence of dissipation.

In the following, we will describe the exact procedure for performing one time step in our method. It is based on the Trotter-Suzuki decomposition of the time evolution propagator. The terms are split in order to separate the terms containing the cavity field operators and the remaining terms:

$$e^{-rac{i}{\hbar}H} \approx$$

$$e^{-\frac{i}{\hbar}(H_{\text{kin}}+H_{\text{int}})}e^{-\frac{i}{\hbar}(H_{\text{ac}}+H_c)}e^{-\frac{i}{\hbar}(H_{\text{kin}}+H_{\text{int}})},$$

FIG. 6. The graphical representation of (a) the MPS structure, with the first (red) site corresponding to the cavity mode. To be noted that the cavity mode index marked with a red line has a large local dimension. (b) The time evolution operator $e^{-\frac{i}{\hbar}(H_{\text{ac}}+H_c)}$ corresponding to the cavity and the cavity-atoms coupling terms in the Hamiltonian. (c) The two site gates for the atomic terms. (d) The two site gates for the coupling terms.

FIG. 7. The graphical representation of one time step based on the Trotter-Suzuki decomposition described in the text, Eq. C.1. The meaning of the graphical symbols used can be found in Fig. 6.

This decomposition is valid to the order $O(dt^3)$. The evolution given by the operator $e^{-\frac{i}{\hbar}(H_{\text{kin}}+H_{\text{int}})}$ which
The swap gates are constructed from two Kronecker swap gate acts on two MPS sites and changes their or-
index for the bosonic atoms. In Fig. 8 we sketch how the operator acts on two sites—even though distant
ones—and renaming the indices (s, σ, σ′, s′).

This means that we need to apply two-site operators where the two sites are not neighbors in the initial
MPS representation. In order to solve this problem, we adapt the structure of the MPS while applying the
time-evolution method with an error of the order O(Ldt^3) for each time step, after multiple
time steps are performed.

To improve the performance of our tMPS algorithm we take good quantum numbers into account, by noting that
our system preserves the total number of bosonic atoms. In the rest of this section we present how the dissi-
pative aspect of the considered model is included in the numerical method. For the simulation of the dissipative
many body quantum systems the time-evolution of the
density matrix following the Lindblad equations needs
delta functions, each between indices of the same nature, but different sites, i.e. in Fig. 8(a) we have a Kronecker
delta from the cavity index s at the first site to the cavity index s′ at the second site (red curve) and a Kronecker
delta from the atomic index σ at the second site to the atomic index σ′ at the first site. The next step consists
in the application of the swap gate onto the MPS wavefunction and obtaining a two-site tensor with swapped
indices [Fig. 8(b)]. Finally an SVD decomposition is performed to restore the MPS structure. No additional error
is introduced by the swap gates, except the SVD truncation error. Thus, using the swap gates we can apply the
operator $e^{-i\frac{dt}{\hbar}(H_{ac}+H_c)}$ onto the wavefunction as a series of two-site gates, as depicted in Fig. 9.

The implemented time-evolution method has an error of the order O(Ldt^3) for each time step, after multiple
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The implemented time-evolution method has an error of the order O(Ldt^3) for each time step, after multiple
time steps are performed.
to be determined. State of the art are two different routes: the first is the purification approach which relies on the rewriting of the density matrix with a larger dimension \[72\]. The second is the stochastic unravelling of the master equation using quantum trajectories \[56, 57\]. This approach has the advantage of the simulation of the time-evolution of states instead of density matrices at the disadvantage of a stochastic sampling. Since in the combined atom-cavity system, the cavity photon can have a huge Hilbert space, we have chosen to employ the stochastic unravelling of the master equation in order to keep the dimension of the Hilbert space treatable. The combination of the stochastic unravelling of the master equation with the matrix product state methods has been relatively recent and only few groups have efficient implementations (see e.g. \[58-60, 65, 73-75\]).

The method implies performing the time evolution of wave functions with a non-hermitian effective Hamiltonian \( \tilde{\mathcal{H}} = H - \frac{i}{\hbar} \Gamma a^\dagger a \) and the application in a stochastic manner of the jump operator \( a \). The non-hermitian Hamiltonian does not raise any additional challenge to the time-evolution method described above, as we already have included all the relevant operators and only have to modify the following prefactor \( \hbar a^\dagger a \rightarrow \hbar \left( \delta - \frac{1}{2} \Gamma \right) a^\dagger a \).

The stochastic unravelling procedure consists first in performing the time evolution with a non-unitary operator, corresponding to the effective Hamiltonian. This leads to the decay of the norm of the evolved state, where the decrease of the norm is related to the probability of a stochastic jump to occur. The non-unitary deterministic time evolution is performed until the norm is smaller than a threshold \( \delta \) posed by a random number, which is sampled from an uniform distribution on the interval \([0, 1]\). Afterwards, the quantum jump is performed by applying the jump operator \( a \) onto the wavefunction, the state is normalized and the non-unitary time evolution continued until the next jump. One can show \[56, 57\] that the described time evolution reproduces the Lindblad dynamics correctly for the Monte Carlo average. The numerical parameters used in the tMPS method are the following: the time step \( dt \), the cut-off of the local dimension for the photon mode of 40 for (c) and (e), and 750 trajectories for (c), (d) and (f).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{image}
\caption{The dependence of the photon number on the parameters which control the accuracy of the numerical method, the cut-off of the photonic Hilbert space, \( N_{\text{pho}} \), the truncation error (c)-(d) and the time step (e)-(f). We present the behavior for two parameter sets, \( L = 10 \) sites, \( N = 5 \) particles, \( \hbar \delta / J = 2, \hbar \Omega / \sqrt{N} / J = 3.35, \hbar \Gamma / J = 1 \) (a), (c), (e) and \( \hbar \Omega / \sqrt{N} / J = 4.47, \hbar \Gamma / J = 10 \) (b), (d), (f). The error bars represent the standard deviation of the Monte Carlo average. The numerical parameters used in the tMPS method are the following: the time step \( dt \), the cut-off of the local dimension for the photon mode of 40 for (c) and (e), and 750 trajectories for (c), (d) and (f).}
\end{figure}

\section*{APPENDIX D. tMPS METHOD - NUMERICAL CONVERGENCE}

The convergence of the Monte Carlo average is controlled by the number of quantum trajectories included in the average and we can estimate the error computing its standard deviation. For the numerical data presented in the main text we average over at least 500 trajectories, which ensures that the relative error in the expectation value of the photon number is smaller than 3%. For the case where the photon number is smaller than 1 we average over 750 trajectories to obtain the same relative error, as the fluctuations have a greater influence.

The accuracy of the simulation of the time evolution with the tMPS method is controlled by the time step, \( dt \), bond dimension and truncation error. The bond dimension in the results presented in the main article was chosen such that the truncation error \( \varepsilon \) of the singular value decomposition performed in the time evolution gates and swap gate is at most \( 10^{-12} \). In Fig. 10(c)-(d) we show that close to this value, the results only weakly depend on the value of the maximal truncation error \( \varepsilon \) and is of the order to the statistical error. The dependence of the results on the value of the time-step is shown in Fig. 10(e)-(f). It is approximately quadratic and we have chosen for the results presented in the main paper a time-step of \( dt \) = 0.0125 for the parameter sets with \( h \Gamma / J = 1 \) and \( dt \) = 0.01 for larger values of the dissipation strength.
FIG. 11. The scaled photon number, $\langle a^\dagger a \rangle / N$, as a function of (a) the scaled atoms-cavity coupling $\hbar \sqrt{N}/J$ for the parameter sets, $L \in \{10, 12, 14\}$ sites, $N = L/2$ particles, $\hbar \delta / J = 2$, $U/J = 2$, $\hbar \Gamma / J = 1$; (b) the dissipation strength $\Gamma$ for the parameter sets, $L \in \{10, 12, 14\}$ sites, $N = L/2$ particles, $\hbar \delta / J = 2$, $U/J = 2$, $\hbar \Omega / \sqrt{N}/J = 4.47$. We compare our numerical results with the mean-field (MF) and many-body adiabatic elimination (AE). The dashed vertical line marks the self-organization threshold as obtained from the mean-field approach for $L = 10$ sites. The numerical parameters used in the tMPS method are the following: the time step $(a) \ dt J / \hbar = 0.0125$, $(b) \ dt J / h = 0.01$, the truncation error $10^{-12}$ for $L = 10$ and $10^{-10}$ for $L > 10$, and the cut-off of the local dimension for the photon mode is between 10 and 25, adapted to the average photon number. The Monte-Carlo average contains at least 500 trajectories.

In this regime of values for $dt$ the resulting inaccuracies are again of the order to the statistical uncertainty.

The dimension of the local Hilbert space for the photon can be infinite and thus a cut-off for its dimension is needed in the numerical implementation. For a given set of parameters we observe that above a certain value of the cut-off $N_{\text{pho}}$ the average value of the photon number is varying with increasing the cut-off only within the error bars of the Monte Carlo averaging. Examples are shown in Fig. 10(a)-(b). However, since the required cut-off changes very much with the considered parameters, we used very different values in order to produce the results presented in the main text. Additionally, since we consider bosonic atoms, the maximal local dimension is the total atom number. However, we checked that for the parameter sets with not too large values of the dissipation strength, with $\hbar \Gamma / J = 1$, a maximal local dimension of four bosons per site is sufficient.

In order to evaluate the finite size effects we analyze how the transition from the normal state to the self-organized state takes place for different system sizes. In Fig. 11(a) we scale the photon number and the atoms-cavity coupling with the number of particles. For a comparison we show both the mean field and the numerically exact tMPS method results. Both show only small deviations with increasing the system size. In particular, in the mean field results the transition to the self-organized phase starts later and becomes steeper with increasing system size. In the tMPS results, the rise of the photon number also seems to occur for a bit larger scaled pump strength. However, the effect are very small which leads us to the expectation that our main findings will re-
main valid for large systems. To further support this, in Fig. 11(b) the scaled photon number is plotted as a function of the dissipation strength. The numerical results are compared with the many-body adiabatic elimination results. The dependence on the system length for both is very weak and only a slight lowering of the photon number is seen.

Since we are interested in the steady states of the system, the results shown in the main text are typically taken at times where the considered quantities are almost constant in time. Typically, such a regime is reached at \( tJ/h = 49.75 \) as shown in Fig.12(a), where the photon number has reached a plateau. For many of the considered parameters, the average photon number is reaching the steady state faster than the density-density correlations in the atomic sector. As one can see from Fig.12(b) the density-density correlations, \( \langle n_2 n_2^+ \rangle \), at even distances are still slowly evolving at the times considered. It seems that these correlations still perform oscillations around an average value which leads to an uncertainty in the determination of the steady state value. However, even considering this additional uncertainty, the staggering in the density-density correlations is clearly pronounced. Therefore, we expect that the presented values in the main article give a very good approximation of the steady state values.

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