Generalized mean-field approach to simulate large dissipative spin ensembles with long range interactions

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Abstract

We simulate the collective dynamics in spin lattices with long range interactions and collective decay in one, two and three dimensions. Starting from a dynamical mean-field approach derived by local factorization of the density operator we improve the numerical approximation of the full master equation by including pair correlations at any distance. This truncations enable us to drastically increase the number of spins in our numerical simulations from about ten spins in case of the full quantum model to several ten-thousands in the mean-field approximation and a few hundreds if pair correlations are included. Extensive numerical tests help us identify interaction strengths and geometric configurations where these approximations perform well and allow us to state fairly simple error estimates. By simulating systems of increasing size we show that in one and two dimensions we can include as many spins as needed to capture the properties of infinite size systems with high accuracy, while in 3D the method does not converge to desired accuracy within the system sizes we can currently implement. Our approach is well suited to give error estimates of magic wavelength optical lattices for atomic clock applications and corresponding super radiant lasers.
I. INTRODUCTION

Ensembles of interacting spins in various geometries are at the heart of quantum statistical physics since first models on magnetism \[1\]. As the spin-spin interaction is nonlinear and the corresponding Hilbert space grows exponentially with the number of spins, exact analytic as well as full numeric solutions are only possible in very special cases and geometries \[2-4\] or small spin numbers. As a very successful approximate numerical approach based on factorization of single site expectation values, dynamical mean-field was developed for efficient treatment of larger systems \[5\]. One the one hand it allowed analytical results in the large dimensions limit \[6\] and on the other hand soon proved very useful for numerical treatment in low dimensions. The general idea of the method subsequently was also successfully applied to wide range of solid state physics models in the very low temperature quantum domain \[7\]. Recently, this approach also proved useful in the description of ultra-cold particle dynamics in optical lattices \[8, 9\].

The present work is motivated by another, more recent implementation of spin lattices based on ultra-cold atoms or molecules trapped in an optical lattice, which nowadays can almost routinely be prepared in the laboratory with well defined filling and close to zero temperature \[10, 11\]. When excited on an optical or infrared transition the trapped particles will interact via dipole-dipole energy exchange forming collective excitations \[12, 13\]. Optical transitions intrinsically also exhibit dissipation via spontaneous decay, which in such a lattice becomes a collective effect leading to super- or sub-radiance \[14\]. To consistently treat such an open system, one has to start from a master equation instead of the Schroedinger equation after tracing over the electromagnetic vacuum modes \[15\].

Besides using polar molecules which can possess relatively strong dipole moments \[16\], another interesting implementation is based on using long lived atomic clock transitions in a differential light shift free magic wavelength lattice \[17, 18\]. Here, one gets extremely well controllable and precisely measurable systems to study even weak spin interactions \[19\] and collective decay via dipole-dipole energy exchange \[14\]. For sufficient densities the particles effective transition frequency and spontaneous decay is modified by dipole-dipole interaction \[20\], which in turn also will influence performance of a corresponding clock or super-radiant laser \[21\].

While the extremely small dipole moment of a clock transition keeps these interactions small, even tiny shifts and broadenings ultimately influence clock accuracy and precision. Hence reliable and converging numerical models are required to estimate these effects to many digits,
in particular as one tries to work with as large as possible ensembles to reduce measurement time and projection noise. For rather small atom numbers, up to about 10, a numerical solution of the master equation is still possible [20] and showed that shift and broadening can be non-negligible. For larger ensembles at low densities a so called cluster approach based on statistical average of important small particle number configurations has already produced first estimates of their scaling with system size [22]. Here, we focus on a more generally valid approach, namely the above mentioned mean-field plus pair-correlation method (MPC) to tackle large systems at high density, i.e. up to unit filling. The long range nature of the dipole coupling is here accounted for by adding higher order corrections to the standard local factorization approach. In particular for cavity mediated dipole interactions or coupling via nano-fibers even infinite range interactions have to be considered [23]. The focus of this work is put on developing the appropriate general numerical framework to treat such extended open spin lattices in various configurations and test their accuracy and convergence properties at the example of collective decay of a highly excited spin state. This should be the basis of future more specific work on concrete implementations of lattice clock Ramsey spectroscopy [21] and super-radiant laser setups [21, 25].

This work is organized as follows. First we give a short description of the system of coupled spins and introduce the corresponding master equation governing their time evolution including decay. Using generalized factorization assumptions for the density operator of the system we derive two approximate and numerically advantageous methods to calculate its time evolution. In the subsequent section we perform an extensive numerical analysis to characterize the magnitude and scaling of the error of these two approximations depending on the geometry and choice of initial state. Finally, we use this method to simulate systems of increasing size to study to which extend a finite sized sample can capture the dynamics of larger or even infinite systems.

II. INTERACTING SPIN DYNAMICS

We consider a system consisting of $N$ two-level systems with transition frequency $\omega_0$ and decay rate $\gamma$ in arbitrary spatial configuration as shown in fig. 1. Each particle couples to the modes of the free electro-magnetic field and therefore all particles are indirectly coupled to one another. Mathematically, this problem can be simplified by treating the electro-magnetic modes
as a single bath and introducing effective particle-particle interactions and effective decay of particle excitations into this bath, according to [12]. The time evolution of the $N$ spins in a rotating frame corresponding to $\sum_i \omega_0 \sigma_i^z$ is then governed by a master equation

$$\dot{\rho} = -\frac{i}{\hbar} [H, \rho] + \mathcal{L}[\rho]$$

with Hamiltonian

$$H = \sum_{i,j; i \neq j} \hbar \Omega_{ij} \sigma_i^+ \sigma_j^-$$

and Lindblad-term

$$\mathcal{L}[\rho] = \frac{1}{2} \sum_{i,j} \Gamma_{ij}(2\sigma_i^- \rho \sigma_j^+ - \sigma_i^+ \sigma_j^- \rho - \rho \sigma_i^+ \sigma_j^-).$$

The dipole-dipole interaction $\Omega_{ij} = \frac{3}{4} \gamma G(k_0 r_{ij})$ and the collective decay $\Gamma_{ij} = \frac{3}{2} \gamma F(k_0 r_{ij})$ can be derived to be

$$F(\xi) = \left(1 - \cos^2 \theta\right) \frac{\sin \xi}{\xi} + \left(1 - 3 \cos^2 \theta\right) \left(\frac{\cos \xi}{\xi^2} - \frac{\sin \xi}{\xi^3}\right)$$

and

$$G(\xi) = -\left(1 - \cos^2 \theta\right) \frac{\cos \xi}{\xi} + \left(1 - 3 \cos^2 \theta\right) \left(\frac{\sin \xi}{\xi^2} + \frac{\cos \xi}{\xi^3}\right),$$

where $k_0$ is related to the transition frequency of the two-level systems and $\theta$ is the angle between the line connecting the two considered particles and the polarization axis.

While for systems consisting of only very few particles we can study the time evolution by directly integrating the master equation, the exponential scaling of the dimension of the Hilbert space soon defeats any numerical abilities. To be able to represent the state of such a high particle number system in a computer one has to utilize simplifying assumptions on the form of the density matrix. In our following calculations we will truncate correlations between the

![FIG. 1. Collectively interacting and decaying spins.](image-url)
particles at a certain order which greatly reduces the space needed to store the state of the system in memory and allows to treat larger particle numbers.

A. Mean-field method: product state assumption

In the first nontrivial approximation we neglect correlations altogether and assume that the system is at all times in a product state of the subsystems at each site. The density matrix here is approximated by $\rho = \bigotimes_k \rho^{(k)}$, which is also called mean-field approximation. The time evolution of the system is then governed by the local on site density matrices, which for two-level systems can be obtained from complete set of expectation values for each spin, i.e. the expectation values of the Pauli operators $\langle \sigma_x \rangle$, $\langle \sigma_y \rangle$ and $\langle \sigma_z \rangle$ for a spin $1/2$ system. Using this Pauli representation we need three real numbers to characterize the state of each of the two-level sub-systems at a certain point in time. The resulting equations for the local spin allows for an intuitive understanding of the corresponding physics. Explicitly we get:

$$\langle \dot{\sigma}_x^k \rangle = \sum_{i:i \neq k} \Omega_{ki} \langle \sigma_i^y \sigma_k^z \rangle - \frac{1}{2} \gamma \langle \sigma_k^x \rangle - \frac{1}{2} \sum_{i:i \neq k} \Gamma_{ki} \langle \sigma_i^x \sigma_k^z \rangle$$

$$\langle \dot{\sigma}_y^k \rangle = -\sum_{i:i \neq k} \Omega_{ki} \langle \sigma_i^x \sigma_k^z \rangle - \frac{1}{2} \gamma \langle \sigma_k^y \rangle - \frac{1}{2} \sum_{i:i \neq k} \Gamma_{ki} \langle \sigma_i^y \sigma_k^z \rangle$$

$$\langle \dot{\sigma}_z^k \rangle = -i \sum_{i:i \neq k} \Omega_{ki} \left( \langle \sigma_k^x \sigma_i^y \rangle - \langle \sigma_i^x \sigma_k^y \rangle \right) + \gamma \left(1 - \langle \sigma_k^z \rangle \right) + \frac{1}{2} \sum_{i:i \neq k} \Gamma_{ki} \left( \langle \sigma_k^x \sigma_i^x \rangle + \langle \sigma_i^y \sigma_k^y \rangle \right)$$

These equations still contain two-particle expectation values of the form $\langle \sigma_i^\alpha \sigma_j^\beta \rangle$, which according to our above assumption can factorized, i.e. $\langle \sigma_i^\alpha \sigma_j^\beta \rangle \approx \langle \sigma_i^\alpha \rangle \langle \sigma_j^\beta \rangle$. As we will see in the next section for weak inter-particle interactions this gives a surprisingly good approximation to the interaction induced shifts and can also account for spatial inhomogeneities of the system.

B. Extended mean-field method including pair-correlations corrections (MPC)

As next order correction to the above mean-field approach we now include also pair-correlations but still neglect all higher-order correlations. To this end the density matrix can be approximated by $\rho = \bigotimes_i \rho^{(i)} + \sum_{j<k} \left( \rho^{(j,k)} \otimes \bigotimes_{i \neq j,k} \rho^{(i)} \right)$, where the first term is the previously used product state and the correlations are captured in the operators $\rho^{(j,k)}$. The correlations thus have to be chosen to generate vanishing single particle expectation values,
i.e. $\text{Tr} \{ \sigma_i^\alpha \rho^{(j,k)} \} = 0$. Deriving the equations of motion in terms of expectation values of Pauli operators leads to the same equations as in the mean-field case \(^8\). The two-particle expectation values then are determined via a set of additional equations for the expectation values of all two-particle Pauli operator pairs of the type $\langle \sigma_i^\alpha \sigma_j^\beta \rangle$. In principle there are nine such quantities for any pair of particles $\rho^{(j,k)}$. For symmetry reasons three of them are trivially obtained from the others. Similarly to the mean-field in the equations for these two-particle correlations higher order three-particle correlations appear, which based on our assumption of the form of the density operator again are approximated by

$$
\langle \sigma_i^\alpha \sigma_j^\beta \sigma_k^\gamma \rangle \approx -2\langle \sigma_i^\alpha \rangle \langle \sigma_j^\beta \rangle \langle \sigma_k^\gamma \rangle + \langle \sigma_i^\alpha \rangle \langle \sigma_j^\beta \rangle + \langle \sigma_j^\beta \rangle \langle \sigma_k^\gamma \rangle + \langle \sigma_k^\gamma \rangle \langle \sigma_i^\alpha \rangle.
$$

(9)

Although the resulting equations of motions for the two-particle correlations are bulky, we want to explicitly display them as an essential basis of our work.

$$
\langle \sigma_k^x \sigma_l^x \rangle = \sum_{j:j \neq k,l} \Omega_{kj} \langle \sigma_k^x \sigma_j^x \rangle - \frac{1}{2} \sum_{j:j \neq k,l} \Gamma_{kj} \langle \sigma_k^x \sigma_j^x \rangle - \frac{1}{2} \sum_{j:j \neq k,l} \Gamma_{lj} \langle \sigma_l^x \sigma_j^x \rangle
$$

(10)

$$
\langle \sigma_k^y \sigma_l^y \rangle = -\sum_{j:j \neq k,l} \Omega_{kj} \langle \sigma_k^y \sigma_j^y \rangle - \frac{1}{2} \sum_{j:j \neq k,l} \Gamma_{kj} \langle \sigma_k^y \sigma_j^y \rangle - \frac{1}{2} \sum_{j:j \neq k,l} \Gamma_{lj} \langle \sigma_l^y \sigma_j^y \rangle
$$

(11)

$$
\langle \sigma_k^z \sigma_l^z \rangle = \sum_{j:j \neq k,l} \Omega_{kj} \left( \langle \sigma_k^z \sigma_j^z \rangle - \langle \sigma_k^x \sigma_j^x \rangle \right) + \frac{1}{2} \sum_{j:j \neq k,l} \Omega_{lj} \left( \langle \sigma_l^z \sigma_j^z \rangle - \langle \sigma_l^x \sigma_j^x \rangle \right)
$$

(12)

$$
\langle \sigma_k^\alpha \sigma_l^\beta \rangle = \Omega_{kl} \left( \langle \sigma_k^\alpha \rangle - \langle \sigma_l^\beta \rangle \right) + \sum_{j:j \neq k,l} \Omega_{kj} \langle \sigma_k^\alpha \sigma_j^\beta \rangle - \sum_{j:j \neq k,l} \Omega_{lj} \langle \sigma_l^\alpha \sigma_j^\beta \rangle
$$

(13)

$$
\langle \sigma_k^\alpha \sigma_l^\beta \rangle = \Omega_{kl} \langle \sigma_k^\alpha \rangle + \sum_{j:j \neq k,l} \Omega_{kj} \langle \sigma_k^\alpha \sigma_j^\beta \rangle + \sum_{j:j \neq k,l} \Omega_{lj} \left( \langle \sigma_l^\alpha \sigma_j^\beta \rangle - \langle \sigma_l^\alpha \sigma_j^\beta \rangle \right)
$$

(14)
\[
\langle \sigma_k^y \sigma_l^z \rangle = -\Omega_{kl} \langle \sigma_i^z \rangle - \sum_{j \neq k, l} \Omega_{kj} \langle \sigma_k^z \sigma_l^z \sigma_j^x \rangle + \sum_{j \neq k, l} \Omega_{ij} \left( \langle \sigma_k^y \sigma_l^y \sigma_j^x \rangle - \langle \sigma_k^y \sigma_l^z \sigma_j^y \rangle \right) \\
- \frac{3}{2} \gamma \langle \sigma_k^y \sigma_l^z \rangle + \gamma \langle \sigma_k^y \rangle - \Gamma_{kl} \left( \langle \sigma_k^x \sigma_l^y \rangle - \frac{1}{2} \langle \sigma_l^y \rangle \right) \\
- \frac{1}{2} \sum_{j \neq k, l} \Gamma_{kj} \langle \sigma_k^z \sigma_l^z \sigma_j^y \rangle + \frac{1}{2} \sum_{j \neq k, l} \Gamma_{ij} \left( \langle \sigma_k^y \sigma_l^x \sigma_j^x \rangle + \langle \sigma_k^y \sigma_l^y \sigma_j^y \rangle \right)
\]

Note that the number of equations to be solved increases quadratically with the number of particles, as we include all possible two-particle combinations. This is exponentially slower as the growth of the corresponding Hilbert space. In many cases one might even be able to restrict this to only nearest neighbors couplings, but for long range dipole interactions or cavity mediated interactions as we are interested here no such truncations can be safely made. In principle the method, which in many respect resembles the known cumulant expansion method \cite{26}, can be extended towards higher order. However, as we will see below, it is already very accurate for our purposes so that we will not continue this task here.

III. NUMERICAL ACCURACY OF MEAN-FIELD METHOD AND SECOND ORDER CORRECTIONS

In the previous section we presented two numerical approaches to approximate the master equation (eq. 1) by neglecting higher-order quantum correlations. To examine for which conditions these assumptions lead to accurate solutions, we compare this approximations with the numerical solution of the full master equation for different spatial arrangements, number of particles and initial states. Additionally we also calculate the case of independent particles which allows us to identify examples, where the error of the approximations is only small due to negligible influence of the dipole dipole interaction and the collective decay.

1. Spin dynamics

To obtain a first intuitive understanding for the quality of the different methods we compare the time evolution of the expectation values of the Pauli operators for three different geometries, i.e. a chain \cite{2} a square lattice \cite{3} and a cube \cite{4}. As a generic physical situation we start with a product state of all spins pointing in x-direction. This is the state prepared in the first step of a typical Ramsey spectroscopy procedure. It is fully superradiant, when all particles are confined
in a very small spatial volume. Clearly the dynamics of all three cases is significantly different,

![Graphs showing time evolution of expectation values for different cases.]

FIG. 2. Time evolution of the expectation values of the Pauli operators $\sigma_x$, $\sigma_y$ and $\sigma_z$ of the middle spin in a chain consisting of 7 spins with spin-spin distance $d = 0.15\lambda_0$. The system is simulated using independent spins (red), mean-field method (blue), MPC (green) and by solving the whole master equation (black dashed). The dipole is orientated orthogonal to the chain.

![Graphs showing time evolution of expectation values for different cases in a 2D-square lattice.]

FIG. 3. Time evolution of the expectation values of the Pauli operators $\sigma_x$, $\sigma_y$ and $\sigma_z$ of the middle spin in a 2D-square lattice consisting of 3x3 spins with nearest spin-spin distance $d = 0.5\lambda_0$. The system is simulated using independent spins (red), mean-field method (blue), MPC (green) and by solving the whole master equation (black dashed). The dipole is orientated orthogonal to the plane.

but they all share certain features. First, the solution of the full master equation deviates drastically from the independent particle case, which means that the effect of the collective interaction is significant. This deviation is almost perfectly captured by the second order MPC solution, which is, at least visually, almost identical to the full solution of the master equation. Surprisingly already the mean-field solution is showing a qualitatively very similar behavior, although it is clearly not as accurate. Its accuracy gets the better the higher the dimension. Note that for that case of the cube both methods also well predict the subradiance of initial spin state [24]. Lets now turn from a visual to a more accurate numerical error estimation.
FIG. 4. Time evolution of the expectation values of the Pauli operators $\sigma_x$, $\sigma_y$ and $\sigma_z$ of a single spin in a cube configuration with nearest spin-spin distance $d = 0.6\lambda_0$. The system is simulated using independent spins (red), mean-field method (blue), MPC (green) and by solving the whole master equation (black dashed). The dipole is orientated orthogonal to an arbitrary face of the cube.

2. Systematic accuracy analysis

In the following we will perform a more rigorous, quantitative analysis for a large range of parameters, but to do this effectively we need a simple measure of accuracy of the different methods. An especially in quantum information frequently used tool is the trace distance which is defined as $\mathcal{T}(\rho, \sigma) = \frac{1}{2}||\lambda_i||$ where the $\lambda_i$ are the eigenvalues of the matrix representation of $\rho - \sigma$. For qubits this measure has a very intuitive interpretation, it is just half of the geometric distance of the two states on the Bloch sphere. In fig. 5 we use this trace distance between the solution of the master equation and the previously presented numerical methods at equal points in time to characterize the error of the different approximations. In all our examples

FIG. 5. Trace distance between the density operators calculated by master equation and density operators calculated by independent spins (red), mean-field (blue) and MPC (green) for the previously discussed chain configuration (a), 3x3 square lattice configuration and cube configuration (c).
we start initially in a product state, which means that the error at \( t = 0 \) is always zero and since no additional pumping is included the system decays for all numerical methods to the ground state and the trace distance in the long time limit will vanish. Instead of inspecting the variation of the trace distance over time we will use the time-maximum of the trace distance as characterization of the error.

### A. Geometry dependence

In this section we study the geometry dependence of the error of the numerical methods measured by the previously introduced time maximum of the trace distance. We distinguish between systems of different dimensionality, a 1D chain consisting of 8 particles (fig. 6), a 3x3 section of a 2D square lattice (fig. 7) and a cube as 3D representative (fig. 8). For each of these examples we calculate the dependence of the error on the distance between the particles. Further on we vary the initial state and the orientation of the polarization vector and show here three typical results. Several interesting features stand out immediately. The bigger the distance between the particles is, the smaller the error of neglecting higher-order correlations. As can be seen from the trace distance between the solution of the master equation and the independently decaying case this is to some degree an artifact of decreasing strength of the dipole-dipole interaction which in the far field limit has a \( \frac{1}{r} \) dependency but at least for MPC the error decreases much faster. In nearly all cases also the mean-field approach yields a noticeable

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**FIG. 6.** Distance dependency of the time-maximum of the trace distance between results of the master equation and results of independent evolution (red), mean-field (blue) and MPC (green) for a chain consisting of 8 spins for different initial states and dipole orientations. (a) \( \Theta = \pi/2, \ e_{\text{dipole}} = e_z \). (b) \( \Theta = \pi, e_{\text{dipole}} = e_z \). (c) \( \Theta = \pi/2, e_{\text{dipole}} = e_x \).
Trace distance $d/\lambda$

FIG. 7. Distance dependency of the time-maximum of the trace distance between results of the master equation and results of independent evolution (red), mean-field (blue) and MPC (green) for a square lattice consisting of 3x3 spins for different initial states and dipole orientations. (a) $\Theta = \pi/2$, $e_{dipole} = e_z$. (b) $\Theta = \pi$, $e_{dipole} = e_z$. (c) $\Theta = \pi/2$, $e_{dipole} = e_x$.

FIG. 8. Distance dependency of the time-maximum of the trace distance between results of the master equation and results of independent evolution (red), mean-field (blue) and MPC (green) for 8 spins in a cube configuration for different initial states and dipole orientations. (a) $\Theta = \pi/2$, $e_{dipole} = e_z$. (b) $\Theta = \pi$, $e_{dipole} = e_z$. (c) $\Theta = \pi/2$, $e_{dipole} = (e_x + e_y + e_z)$.

improvement - only when all spins start initially in the excited state it only reproduces the results of independent particles. In fact, as one can show from the mean-field equations, in this case the time evolution is completely identical, so mean-field gives no improvement over simply ignoring the collective effects.

**B. Initial state dependence**

To further analyze the dependence of the error on the initial state we consider a chain of six particles with three different particle distances. Initially the system is in a product state
where all single particles are in the same Bloch state. For simplicity we only consider pure states and since the time evolution is invariant under global rotation around the z-axis the only remaining variable is the azimuthal angle $\Theta$. In fig. 9 the dependence of the error on this azimuthal angle is shown. For $\Theta = 0$ the system is in the ground state and the error vanishes. For small excitation the mean-field method gives a substantial improvement compared to the independently decaying system but for a nearly totally excited state the advantage disappears more and more. In contrast, MPC performs for all initial states convincingly.

FIG. 9. Dependence of the time-maximum of the trace distance between results of the master equation and results of independent evolution (red), mean-field (blue) and MPC(green) on the initial Bloch state characterized through $\Theta$ for a chain consisting of 6 spins with spin-spin distance $d = 0.5\lambda_0$ (a), $d = 1.0\lambda_0$(b) and $d = 10.0\lambda_0$ (c).

C. Spin-number dependence

Finally, we investigate the dependence of the error on the number of particles in the system, i.e. a chain consisting of $N$ particles. The result of this analysis is shown in fig. 10a. In this double logarithmic plot the error appears to be nearly linear but slightly shifted for varying particle number which leads us to following estimate for the error

$$\text{err}(N, d) = C_N * d^{k_N}. \quad (16)$$

The exponent $k_N$ and the factor $C_N$ can be determined by from this error plot and are shown in fig. 10b and fig. 10c respectively. The error exponent turns out to be independent from the number of particles and is -1 for independently decaying spins which is not surprising since the collective interaction in the far field drops with $\frac{1}{r}$. However, increasing the distances doesn’t
improve the mean-field results whereas MPC has an error exponent of -2 and gains drastically on accuracy.

FIG. 10. Analysis of the time-maximum trace distance between results of the master equation and results of independent evolution (red), mean-field (blue) and MPC (green) on the spin distance of a chain consisting of $N = 3 \ldots 9$ spins. Higher spin numbers correspond to slightly increased trace distances (a). Approximation of the trace distances by $C_N \cdot d^{k_N}$ results in the spin-number dependency of the error-exponent $k_N$ (b) and the error-factor $C_N$ (c).

IV. APPROXIMATION OF VERY LARGE (INFINITE) SYSTEMS

Recent research on the effect of geometry onto the perturbation of the spin dynamics by collective interactions was mostly limited to systems consisting of only very few atoms. In lack of better alternatives one might be tempted to extrapolate results obtained from these small-sized systems to larger ensembles but in general this attempt might fail miserably. Prepared with the knowledge about the accuracy of the mean-field and MPC methods and their ability to simulate moderately large systems we can use them to investigate how many particles are needed to make satisfying statements about infinite systems. More precisely we want to know how collective spin quantities of the type $\frac{1}{N} \sum_i \langle \sigma_i^\alpha \rangle$ change for different numbers of particles. Of course it’s a priori not clear if these expectation values converge at all. To answer this question we will study two different examples.

A. Linear equidistant chain

We consider a $N$-particle spin chain with particle distance $d$ and calculate the dynamics of the whole system where initially all spins are in the $\langle \sigma_z \rangle = 1$ state. Tracing out all but
the innermost spin allows us to compare the dynamics of this single spin for varying amount of enclosing particles. The result of this analysis for a certain distance $d$ after an integration time of $2\gamma^{-1}$ is shown in fig. [11]. Fortunately, all methods yield more or less the same outcome and differ significantly from the independently decaying case, meaning that the variation for small particle numbers and the ultimately convergence for large systems is not a numerical artifact. This result gives hope that a suitable choice of number of particles indeed gives a usable approximation of big systems. To solidify this claim we perform a more extensive and quantitative test. What we actually would like to test is how much the time evolution of the single central spin in a chain consisting of $N$ particles differs compared to the time evolution of a spin in an infinite chain. However, we are not aware of a method to solve the infinite chain exactly which leaves us only the option to compare the central spin of a $N$ particle chain with a chain containing as many spins as numerically possible to simulate and hope that this already is close enough to an actually infinite chain. In fig. [12] and fig. [13] where the dynamics of a 20001 particle mean-field simulation and a 401 particle MPC simulation are respectively used as best possible approximation of the infinite chain for three different spin-spin distances. In most cases the addition of further spins affects the central spin less and less and is approximately linear in this double logarithmic plot, i.e. the trace distance between the infinite chain and the $N$-particle chain for a certain distance can be estimated by $T(N,\text{inf}) = C_d N_d^k$. By fitting this function to the numerical result we can determine the exponent $k_d$ and the factor $C_d$ depending on the distance which is plotted in fig. [14]. For nearly all distances both the mean-field method

FIG. 11. Expectation values of the Pauli operators $\langle \sigma_x \rangle$, $\langle \sigma_y \rangle$ and $\langle \sigma_z \rangle$ of the middle spin in a chain consisting of $N$ spins with distance $d = 0.9\lambda_0$ after a time evolution for $2\gamma^{-1}$. Initially all spins are in the state $\langle \sigma_x \rangle = 1$ and the system is solved for independent spins (red), using mean-field (blue), MPC (green) and the master-equation (black dashed).
FIG. 12. Time-maximum of the trace-distance between the reduced density matrix of the middle state in a chain consisting of $N$ spins compared to the chain consisting of $N_{\text{meanfield}}^{\text{max}} = 20001$ (blue) where both quantities are results of mean-field simulations. Approximation of this trace-distance by $C_d \ast N^{k_d}$ (yellow dashed) for different spin-spin distances $d = 0.7\lambda_0$(a), $d = 1.0\lambda_0$(b) and $d = 3.7\lambda_0$(c).

FIG. 13. Time-maximum of the trace-distance between the reduced density matrix of the central spin in a chain consisting of $N$ spins compared to the chain consisting of $N_{\text{MPC}}^{\text{max}} = 401$ (blue) where both quantities are results of MPC simulations for different spin-spin distances $d = 0.7\lambda_0$(a), $d = 1.0\lambda_0$(b) and $d = 3.7\lambda_0$(c). Approximation of this trace-distance by $C_d \ast N^{k_d}$ (yellow dashed).

as well as the MPC method predict that adding further particles only has an effect proportional to $\frac{1}{N}$ allowing us to easily estimate the number of particles needed to approximate the infinite chain dynamics to a desired accuracy. However, when the spin-spin distance is close to a multiple of the transition wavelength $\lambda_0$ the dynamics of the infinite chain seems to be never captured by a finite size approximation.
FIG. 14. Error exponent $k_d$ and Error factor $C_d$ dependence on the spin-spin distance determined in the previous fits $C_d \propto N^{k_d}$ using mean-field (blue) and MPC (green).

B. Hexagonal lattice

With these very encouraging results for a 1D chain, let us see now if this holds true for higher dimensional geometries as well. Unfortunately we failed to obtain convincing results for 3D cubic lattices, since the number of particles needed for convergence of the numerical result turns out to far exceed the possibility of MPC and even of the mean-field method. For 2D geometries at least the mean-field method delivers some meaningful, albeit by far not as beautiful results. We will only show the example of a hexagonal lattice here. Fig. [15] shows the numerically obtained approximations for the error exponent and the error factor for the case of a hexagonal lattice, where additional particles were added in rings around the central spin. The outcome looks rather noisy, probably due to a too small choice for the number of particles used as approximation of the infinite lattice. Unsurprisingly it turns out that compared to the chain a lot more particles are needed to reliably approximate an infinite hexagonal lattice, i.e. the influence of additional particles reduces the error with approximately $N^{-0.3}$, where this exponent is a rather rough estimate.

V. NUMERICAL COMPLEXITY OF THE DIFFERENT METHODS

Finally we want to add some considerations on the memory and CPU requirements of the different methods and show that our implementations behave as expected in this respect. When
solving the master equation the state of the system is captured as density matrix of dimension $2^{2N}$. The time evolution according to a master equation is equivalent to a matrix-matrix multiplication and therefore has a time complexity of $O(2^{3N})$. In case of mean-field a state can be characterized by $3N$ real numbers and according to [8] the time complexity is then approximately $O(N^2)$. For the MPC method the state consists of one mean-field state and nine correlation matrices of the form $C_{ij}^{\alpha\beta} = \langle \sigma_i^{\alpha} \sigma_j^{\beta} \rangle$. Using the relation $C_{ij}^{\alpha\beta} = C_{ji}^{\alpha\beta}$ means we need roughly $\frac{9N^2}{2}$ real numbers to represent one MPC state. The time complexity is, according to [15] approximately $O(N^3)$.

VI. CONCLUSIONS AND OUTLOOK

We have demonstrated that an effective mean-field method with added pair corrections constitutes a numerical efficient and surprisingly accurate method to simulate open spin systems with general non local spin-spin interaction and collective decay up to moderately high particle numbers and significant interaction strength. Specializing to dipole-dipole interaction and collective spontaneous decay allows us to establish a numerical estimate of the accuracy and scaling properties of our methods. Furthermore we can show for 1D chains that tractable system size already approaches the behavior of infinite systems allowing to estimate the magnitude of the error due to truncation of the system. For 2D systems the lowest order mean-field approach still allows to reach adequate system sizes to approximate infinite systems, whereas the scaling

FIG. 15. Error exponent $k_d$ and error factor $C_d$ dependence on the spin-spin distance determined in the previous fits $C_d \ast N^{k_d}$ using mean-field.
FIG. 16. Time needed to integrate a spin chain consisting of $N$ spins from 0 to $\gamma^{-1}$ on a single CPU. The solid lines are the result of the benchmarks for master (black), MPC (green) and mean-field (blue), the dashed lines are the corresponding theoretical predictions.

is unfavorable to accurately approximate infinite 3D systems. In the future work we plan to apply these methods to study collectively enhanced as well as suppressed decay in magic wavelength lattices for clock atoms. The simulations should also provide us with predictions of geometries and excitation schemes to minimize dipole-dipole induced shifts in order to improve the accuracy of atomic clocks. Possible approaches would be to analyze different geometries, use initial phase spread rotations and spin squeezing. As interesting extension of this model we also want to embed such spin systems inside a cavity and derive corresponding mean-field and MPC equations for the corresponding infinite range interactions. This should give us a basis to simulate super-radiant lasers for larger ensembles including interaction. Note that as we are simulating an open system anyway, including a finite bath temperature will hardly change the complexity of these calculations and could be used to identify temperature dependent phase transitions in the system.
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