Dynamical Pruning of the Non-Equilibrium Quantum Dynamics of Trapped Ultracold Bosons

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The investigation of the nonequilibrium quantum dynamics of bosonic many-body systems is very challenging due to the excessively growing Hilbert space and poses a major problem for their theoretical description and simulation. We present a novel dynamical pruning approach in the framework of the multi-configuration time-dependent Hartree method for bosons (MCTDHB) to tackle this issue by dynamically detecting the most relevant number states of the underlying physical system and modifying the many-body Hamiltonian accordingly. We discuss two different number state selection criteria as well as two different ways to modify the Hamiltonian. Our scheme regularly re-evaluates the number state selection in order to dynamically adapt to the time evolution of the system. To benchmark our methodology, we study the nonequilibrium dynamics of bosonic particles confined in either an optical lattice or in a double well potential. It is shown that our approach reproduces the unpruned MCTDHB results accurately while yielding a significant reduction of the simulation time. The speedup is particularly pronounced in the case of the optical lattice.

I. INTRODUCTION

Ever since the first realizations of Bose-Einstein condensates (BECs) [1–3], ultracold atomic gases attracted a lot of interest both from the experimental and the theoretical side. Their tunability and almost perfect isolation from the environment renders such systems ideal candidates to simulate a variety of quantum many-body systems [4–6]. Due to experimental advancements ensembles of ultracold atoms with a controlled number of particles [7, 8] can be realized in arbitrarily shaped confining potentials [9] such as optical lattices [10, 11], harmonic [12] or ring traps [13]. By varying the confinement the crossover from three-dimensional [14, 15] to two-dimensional [16, 17] to one-dimensional [18, 19] traps can be tuned. Feshbach [20, 21] and confinement-induced resonances [22–25] offer fine-grained control of the inter-particle interaction. Recent studies within the realm of ultracold atoms provide close links to solid-state systems [26, 27], electronic structure of molecules [28], light-matter interaction [29], topological matter [30, 31] and black-hole analogs [32]. The increasing progress of the experimental control of these many-body systems demands appropriate theoretical and numerical methods to describe them and to calculate their properties as well as their dynamical behavior. Exactly solvable models are rare while usually relying on more or less crude approximations or focusing on certain limiting cases.

Let us discuss the state of the art of analytically solvable models and numerical approaches. The time-dependent Schrödinger equation of two bosons in a parabolic and spherically symmetric trapping potential is exactly solvable [33]. However, the applicability of such a small system is very limited. Larger particle numbers can be studied using the Lieb-Liniger model [34, 35] for spinless bosons with contact interactions [36] assuming periodic boundary conditions. Yet, this approach is not capable of taking external trapping potentials into account and cannot directly describe the dynamical response of the system. The Tonks-Girardeau [37, 38] model on the other hand grants access to the full many-body spectrum and nonequilibrium solutions by mapping bosons to non-interacting fermions. However, this model is only valid in the limit of infinitely strong interactions and in one spatial dimension. Beyond these limitations of analytical approaches powerful computational methods are needed to study ensembles of ultracold atoms.

A very useful approach is the Gross-Pitaevskii equation (GPE) [39, 40] which represents a non-linear Schrödinger equation for a bosonic many-body ensemble in the presence of an external trap with contact inter-particle interaction in the thermodynamic limit. It assumes the Hartree-Fock approximation [41, 42] to the many-body wave function, leading to an effective, mean-field description. The GPE is a partial differential equation which can be solved efficiently using the typical finite element and finite difference methods [43–49]. This mean-field treatment allows for the study of setups containing large particle numbers and enables the description of a multitude of non-linear wave structures such as dark and bright solitons [50, 51]. In some cases, when potential and interaction energy dominate the kinetic energy, the calculation can be further simplified by ignoring the kinetic term of the Schrödinger equation leading to the Thomas-Fermi [52] approximation. In general however, these mean-field descriptions do not provide an adequate description of the system dynamics as they cannot account for quantum correlations. A prominent example where
the GPE fails to capture the correct physical behavior is the bosonic Josephson junction [53, 54]. For weakly depleted condensates Bogoliubov theory [55–57] can be applied. For the investigation of few- to many-body systems with substantial correlations and correlated dynamics, however, ab initio beyond-mean-field methods are necessary.

One of the most fundamental of such methods is the exact diagonalization treatment of the many-body Hamiltonian [58–60] which grants access to the spectrum and the eigenstates of the physical system. However, this approach is limited to a small number of particles due to the computational complexity of diagonalization algorithms. Furthermore, the choice of an appropriate basis can prove difficult so that a large number of basis functions may be required, thereby further enlarging the numerical effort. This computational challenge calls for more efficient numerical approaches.

Many computational approaches focus on the investigation of optical lattices as these setups are of major interest in the research of ultracold neutral atoms due to the condensed matter counterparts (crystals). Often the Bose-Hubbard model [10, 61] is employed to describe bosonic atoms loaded into the lowest band of a sufficiently deep lattice. In this model, the bosonic field operator is expanded into Wannier states yielding an effective theoretical model, where the kinetic term as well as the trapping potential are reduced to a hopping between lattice sites and the interaction term to an on-site interaction. This model has been studied using a plethora of different methods [62] including density matrix renormalization group (DMRG) [63, 64] and Quantum Monte Carlo (QMC) [65, 66]. However, other approaches are required to describe physical systems and effects beyond the applicability of a Hubbard model, covering in particular their out-of-equilibrium dynamics.

The multi-configuration time-dependent Hartree (MCTDH) [67, 68] is such a method and has proven to be a powerful and versatile tool to ab initio solve the time-dependent Schrödinger equation for correlated many-body systems of distinguishable degrees of freedom ab initio. MCTDH has been extended to study fermionic ensembles using the multi-configuration time-dependent Hartree-Fock (MCTDHF) method [69, 70] and for bosonic systems using the MCTDHB [71, 72] rendering the treatment of ultracold atoms possible. Further extensions [73–75] employing a multi-layer approach also allow for the treatment of Bose-Bose mixtures and more recently Bose-Fermi and Fermi-Fermi mixtures further increasing the usefulness and applicability of this family of methods. The power of this class of methods stems from the usage of a variationally optimized, time-dependent set of basis functions that allows for a compact representation of the many-body wave function and yields a beyond-mean-field description that takes all correlations into account.

As all numerical approaches however, MCTDHB faces the problem of an exponentially growing Hilbert space when studying large many-body systems. In particular, when increasing either the number of particles or the size of the single-particle function (SPF) basis used to describe such an atomic ensemble, the number of possible number states or configurations respectively grows rapidly rendering the treatment of systems typically with particle numbers larger than one hundred (in other superfluid regime) challenging if not computationally prohibitive. To tackle this issue within the family of MCTDH methods, different approaches have been proposed in the literature. For instance, the configuration selection schemes for MCTDH [76–78] or the restricted-active-space (RAS) schemes for MCTDHF [79, 80] and MCTDHB [81] perform a static selection of the most relevant Hartree products/Slater determinants for the physical system and exploit this partitioning to reduce the required numerical effort. However, these methods cannot dynamically adapt to the evolution of the system and require a priori knowledge such as the choice of an excitation scheme in the case of RAS. Such static truncation schemes of the Hilbert space can impose artificial constraints on the physical system if important many-body states are removed. Therefore the development of dynamical, self-adapting approaches is required in order to enable a more general treatment of dynamical many-body systems.

Referring to the investigation of distinguishable degrees of freedom, dynamical procedures have been applied successfully within the framework of MCTD. E.g. by pruning the primitive basis/grid [82, 83] or the coefficients of the wave function [83] the runtime of the simulations can be greatly reduced. Unfortunately however, the pruning of the grid is not very lucrative in calculations with ultracold atoms as these ensembles are usually confined using an external potential so that there rarely exist unoccupied regions of real space. Furthermore, the coefficient based pruning approach presented in Ref. [83] cannot be applied as the proposed neighborhood criteria for the coefficients cannot be easily transferred to the number states of indistinguishable particles. Therefore the development of new dynamical methods for the treatment of indistinguishable particles is necessary.

In the present work, we develop a general method that automatically detects the important number states of bosonic many-body systems when studying the nonequilibrium dynamics using MCTDHB. This selection procedure dynamically adapts during the time evolution of the system. In Section II we start by briefly reviewing the MCTDHB theory in order to introduce the key concepts of this method and motivate our pruning algorithm. In Section III we show two different ways to modify the MCTDHB equations of motion (EoMs) in order to reduce the numerical effort. To achieve this, we introduce a pruning threshold and a selection criterion for determining the importance of each number state. In Section IV we present two different criteria for the selection of the number states relying on the overlap with the many-body wave function and the total energy of the system. To
showcase the usefulness of our approach, we benchmark it using two different physical scenarios in Section V. We focus both on the performance benefits as well as the accuracy when compared to a regular MCTDHB simulation. Finally, we summarize our findings in Section VI and discuss future perspectives of our approach. In Appendix A we comment on the convergence of our numerical results.

II. KEY ASPECTS OF THE MULTI-CONFIGURATION TIME-DEPENDENT HARTREE METHOD FOR BOSONS

MCTDHB allows to describe the correlated quantum dynamics of ensemble of $N$ interacting bosons. It employs a variationally optimal, time-dependent basis \{$\varphi_i(t)$\}$_{i=1}^m$ of $m$ single-particle functions (SPFs) also called orbitals. Compared to other methods that employ a stationary basis, significantly fewer basis functions are required to achieve the same level of description of correlations. The many-body wave function is expanded as a superposition

$$|\Psi(t)\rangle = \sum_{n \in \mathcal{V}} C_n(t) |n; t\rangle$$

of all $N_V = \binom{N+m-1}{N}$ time-dependent permanents \{$|n; t\rangle\}_{n \in \mathcal{V}}$ that retain the total number of particles $N$ using time-dependent coefficients \{$C_n(t)$\}$_{n \in \mathcal{V}}$.

Each vector $n = (n_1 \ n_2 \ \cdots \ n_m)^T$ resembles one way of distributing $N$ particles in $m$ orbitals and is called a configuration. The $i$th component $n_i$ of such a vector specifies the number of particles in the orbital $\varphi_i(t)$ for the given configuration. $\mathcal{V} = \{ n \in \mathbb{N}_0^m : \|n\|_1 = N \}$ is the set of all such configurations that with the total number of particles $N$.

The permanents are given by

$$|n; t\rangle = \left( \prod_{i=1}^m \frac{a_i^\dagger(t)^{n_i}}{\sqrt{n_i!}} \right) |0\rangle$$

in terms of the bosonic creation operators \{$a_i^\dagger(t)$\}$_{i=1}^m$ with respect to the instantaneous basis.

MCTDHB solves the time-dependent Schrödinger equation \(i\hbar \partial_t \Psi(t) = \hat{H}(t) \Psi(t)\) as an initial value problem by propagating an initial wave function $|\Psi(0)\rangle$ in time according to a, potentially time-dependent, Hamiltonian operator $\hat{H}(t)$. In this work we limit ourselves to Hamiltonians of the form

$$\hat{H}(t, \{x_i\}) = \sum_{i=1}^N \hat{h}(t, x_i) + \sum_{i<j} \hat{W}(t, x_i, x_j),$$

containing only one-body ($\hat{h}$) and two-body ($\hat{W}$) terms. By employing the Lagrangian [84], Dirac-Frenkel [85, 86] or McLachlan [87] variational principle, one can derive the corresponding MCTDHB EoMs [71, 72, 88] which are integrodifferential equations describing the time evolution of the coefficients \{$C_n(t)$\}$_{n \in \mathcal{V}}$ and the SPFs \{$\varphi_i(t)$\}$_{i=1}^m$.

The SPF EoM describes a rotation of the orbitals in such a way that they represent the state of the physical system optimally. For details on this equation we refer the reader to Ref. [72] as the precise structure is irrelevant for the pruning approach that we describe herein. The time evolution of the time-dependent coefficients \{$C_n(t)$\}$_{n \in \mathcal{V}}$ is governed by

$$i\hbar \partial_t C_n(t) = \sum_{m \in \mathcal{V}} \left( \langle n| \hat{H}(t) |m\rangle C_m(t) \right)$$

which is coupled to the EoMs of the orbitals via the configurations $|n; t\rangle$.

III. PRUNED EQUATIONS OF MOTION

The number of possible configurations $N_V$ grows rapidly with the number of particles $N$ and orbitals $m$. This scaling behavior renders the treatment of large systems challenging if not infeasible as the number of matrix elements grows quadratically with $N_V$ causing the integration of Equations (4) to become very costly and the dominant contribution to the simulation runtime.

From intuition and experience we know that not all configurations are of equal importance for the corresponding physical systems under consideration. In the present work, we establish measures to automatically detect configurations of lesser importance and leverage this knowledge to reduce the numerical effort of the integration of the coefficient EoMs. Our approach is dynamical and regularly reevaluates the importance of all configurations, in particular also those that have been deemed negligible previously.

In order to derive our pruning approach, we start by defining a measure $f : \mathcal{V} \times \mathbb{R} \rightarrow \mathbb{R}$ that determines the importance of each configuration $n$ at time $t$. We divide the set $\mathcal{V}$ of all configurations into the subset of unpruned (i.e. active) configurations

$$\mathcal{P}(t) = \{ n : f(n, t) > \gamma \}$$

and the subset of pruned (i.e. inactive) configurations

$$\mathcal{Q}(t) = \{ n : f(n, t) \leq \gamma \}$$

by introducing a pruning threshold $\gamma \in \mathbb{R}$. Additionally, we introduce the operators

$$\hat{P}(t) = \sum_{m \in \mathcal{P}(t)} |m; t\rangle \langle m; t|$$

and

$$\hat{Q}(t) = \sum_{m \in \mathcal{Q}(t)} |m; t\rangle \langle m; t|$$

in Section V.
that project onto the configuration subsets $\mathcal{P}(t)$ and $\mathcal{Q}(t)$. In the following, we drop the explicit notation of the time-dependence of the sets and the projection operators for the sake of readability. The many-body Hamiltonian can be rewritten in terms of $\hat{P}$ and $\hat{Q}$ as
\[
\hat{H} = \hat{P}\hat{H}\hat{P} + \hat{Q}\hat{H}\hat{Q} + \hat{P}\hat{H}\hat{Q} + \hat{Q}\hat{H}\hat{P},
\]
where we exploited the property $\hat{P} + \hat{Q} = 1$.

The idea of the pruning approach is to neglect terms in this representation, thus defining a new, truncated Hamiltonian which replaces the original in Equation (4). In order to make an adequate choice for the pruning, it is essential to consider the meaning of each term of Eq. (9) within the context of the coefficient EoMs (4), see also Figure 1. The term $\hat{Q}\hat{H}\hat{Q}$ mediates between number states belonging to configurations from $\mathcal{Q}$, i.e. configurations that we consider negligible. Therefore, the most apparent modification is to neglect this part of the Hamiltonian yielding
\[
\hat{H}_1 = \hat{H}\hat{P} + \hat{P}\hat{H}\hat{Q}.
\]

We note that $\hat{H}_1$ is Hermitian. When inserting this Hamiltonian into Equation (4), the resulting modified EoM reads
\[
i\partial_t C_n(t) = \sum_{m \in \mathcal{P}(t)} \langle n; t | \hat{H}(t) | m; t \rangle C_m(t) + \sum_{m \in \mathcal{Q}(t)} \langle n; t | \hat{H}(t) | m; t \rangle C_m(t),
\]
where the second term is only present for coefficients associated with configurations from $\mathcal{P}$. However, we note that only the right-hand side of the EoMs is modified while the total number of EoMs remains unchanged such that all coefficients $\{C_n(t)\}_{n \in \mathcal{V}}$ are propagated in time. This is a key element of our approach as it allows coefficients corresponding to inactive configurations (from the set $\mathcal{Q}$) to evolve such that they could be activated again should they transcend the pruning threshold.

In the present work, we also investigate a second type of pruned Hamiltonian
\[
H'_2 = \hat{H}\hat{P}
\]
that we obtain by also neglecting the term $\hat{P}\hat{H}\hat{Q}$ which mediates scattering from the negligible configurations $\mathcal{Q}$ to the active configurations $\mathcal{P}$. However, this operator is non-Hermitian but our numerical results in Sec. V suggest that this weak non-hermiticity may still be acceptable in the sense that the many-body dynamics can still be described to some accuracy (see Section V). The corresponding EoM reads
\[
i\partial_t C_n(t) = \sum_{m \in \mathcal{P}(t)} \langle n; t | \hat{H}(t) | m; t \rangle C_m(t).
\]

In the standard MCTDHB algorithm, an initial wave function $|\Psi(t_0)\rangle$ is propagated from the initial time $t_0$ to a final time $t_f$ using some time step $\Delta t$ at which the wave function is to be computed. The interval $\Delta t$ is usually divided further due to the usage of an adaptive integrator [89–91]. Algorithm 1 shows how we integrate the pruning approach into this existing procedure. We introduce an additional timescale $\tau$ that determines when the pruning criterion is to be evaluated. The resulting selection of active configurations is kept constant for the time $\tau$. Initially, all configurations are marked as active as can be seen in Line 4 and 5. The initial wave function is then propagated until the target time $t_f$ is reached (see Lines 6–19). Whenever the time $\tau$ has passed, the pruning criterion is reevaluated and the selection of active configurations is updated (see Lines 9–13).

Algorithm 1 Propagation procedure for pruned MCTDHB simulations

1: procedure PRUNED_PROPAGATION($|\Psi(t_0)\rangle$, $t_0$, $t_f$, $\Delta t$, $\tau$, $\gamma$)
2: $\quad t_{\text{next}} \leftarrow t_0 + \Delta t$
3: $\quad t_{\text{pruning}} \leftarrow t_0 + \tau$
4: $\quad \mathcal{P} \leftarrow \mathcal{V}$
5: $\quad \mathcal{Q} \leftarrow \{\}$
6: while $t < t_f$ do
7: $\quad t' \leftarrow \min\{t_{\text{next}}, t_{\text{pruning}}\}$
8: $\quad |\psi(t')\rangle \leftarrow$ propagate($t, t', |\psi(t)\rangle$, $\mathcal{P}$, $\mathcal{Q}$)
9: if $t' = t_{\text{pruning}}$ then
10: $\quad \mathcal{P} \leftarrow \{n : f(n, t) > \gamma\}$
11: $\quad \mathcal{Q} \leftarrow \{n : f(n, t) \leq \gamma\}$
12: $\quad t_{\text{pruning}} \leftarrow t_{\text{pruning}} + \tau$
13: end if
14: if $t' = t_{\text{next}}$ then
15: $\quad$ write $|\Psi(t)\rangle$, evaluate observables, etc.
16: $\quad t_{\text{next}} \leftarrow t_{\text{next}} + \Delta t$
17: end if
18: $\quad t \leftarrow t'$
19: end while
20: end procedure

Both the pruning time $\tau$ and the threshold $\gamma$ impact the dynamical pruning algorithm. Choosing small values of $\gamma$ reduces the ratio of configurations that can be disabled on the right-hand side of each EoM (see Equation (11) and (13)) and thus the speedup that can be achieved. In the case $\gamma = 0$, all configurations are taken into account and the dynamical pruning approach
is equivalent to the original MCTDHB. However, choosing γ very large may lead to incorrect results as important number states might be neglected. As the pruning time τ determines how often the pruning criterion is evaluated, this parameter has to be chosen appropriately depending on the timescales of the physical system. Small values of τ lead to very frequent reevaluations of the pruning criterion which can negate any performance gain due to neglecting the configuration n, i.e. setting C_n(t) to 0. Consequently, an estimate of the absolute, energetic contribution of the configuration n is given by

\[ E_n(t) = E_V(t) - E_{V\setminus\{n\}}(t) = \frac{\partial E_V(t)}{\partial C_n^*(t)} C_n^*(t). \]  \hspace{1cm} (17)

We normalize this quantity by dividing by the total energy and taking the absolute value

\[ f(n, t) = \Delta E_n(t) = \left| \frac{E_n(t)}{E_V(t)} \right| = \left| \frac{1}{E_V(t)} \frac{\partial E_V(t)}{\partial C_n^*(t)} C_n^*(t) \right| \]  \hspace{1cm} (18)

in order to obtain a real number \( f(n, t) \in [0, 1] \) which can be interpreted as the relative energy contribution.

### IV. PRUNING CRITERIA

In Section III we outlined our pruning approach and introduced the function \( f(n, t) \) without further specifying it. In the following, we present two different pruning criteria that we use for the applications in Section V. We base our choices on the norm of the wave function and the total energy as these quantities are easily accessible and interpretable.

#### A. Magnitude Criterion

The most obvious way to assess the importance of a configuration is to project the many-body wave function onto the corresponding number state and compute the magnitude of the overlap

\[ f(n, t) = |\langle \Psi(t)|n; t \rangle|^2 = |C_n(t)|^2. \]  \hspace{1cm} (14)

This criterion, which we refer to as the magnitude criterion (MC) in the following, is intuitive as we can compute a real number \( f(n, t) \in [0, 1] \) that determines the importance of the configuration n. A value of 0 means that the configuration does not contribute at all to the many-body wave function whereas a value of 1 implies that the wave function is given solely by the corresponding number state.

#### B. Energy Criterion

In order to investigate the impact of the pruning criterion on the numerical results, we study a second possible choice. For the so-called energy criterion (EC) we determine the contribution of a configuration to the total energy. The energy of a MCTDHB wave function is given by

\[ E(t) = E_V(t) = \sum_{n,m \in V} C_n^*(t) C_m(t) H_{n,m}(t) \]  \hspace{1cm} (15)

and depends solely on the time-dependent coefficients \{C_n(t)\}. In order to estimate the energetic contribution of a single, specific configuration n we expand \( E_V(t) \) as a Taylor polynomial of first order with respect to the corresponding coefficient

\[ E_V(t) \approx E_{V\setminus\{n\}}(t) + \frac{\partial E_V(t)}{\partial C_n^*(t)} C_n^*(t), \]  \hspace{1cm} (16)

where \( E_{V\setminus\{n\}}(t) \) is the energy of the system when neglecting the configuration n, i.e. setting \( C_n(t) \) to 0. Consequently, an estimate of the absolute, energetic contribution of the configuration n is given by

\[ E_n(t) = E_V(t) - E_{V\setminus\{n\}}(t) = \frac{\partial E_V(t)}{\partial C_n^*(t)} C_n^*(t). \]  \hspace{1cm} (17)

V. APPLICATION TO THE QUANTUM DYNAMICS OF TRAPPED ULTRACOLD BOSONIC ENSEMBLES

In the following, we consider a one-dimensional system of N identical bosons confined in an external potential \( V(x) \). Note that within the ultracold regime s-wave scattering is the dominant interaction process \[36, 92\] such that we consider contact interactions between the particles. The many-body Hamiltonian of such a system is given by

\[ \hat{H}(\{x_i\}) = \sum_{i=1}^{N} \left( -\frac{\hbar}{2m} \partial^2 \partial x_i + V(x_i) \right) + \sum_{i<j} g \delta(x_i - x_j). \]  \hspace{1cm} (19)

Starting from the ground state of the non-interacting system (i.e. \( g = 0 \)) we compute the many-body ground state of the interacting ensemble by imaginary time propagation leading to energy relaxation \[68, 93\] or via the improved relaxation algorithm \[94\]. The resulting initial ground state wave function is then propagated in time with respect to a quenched Hamiltonian which involves an instantaneous change in one of the system parameters \[6, 14, 95\]. The propagation of the wave function is performed using the usual, unpruned MCTDHB as well as the pruned variants introduced in Sec. III. To determine the benefits of pruning we measure the CPU time of all simulations and also monitor the number of configurations that are pruned at each time step. In order
to quantify the amount of deactivated configurations we define the quantity

$$\beta(t) = \frac{|\mathcal{Q}(t)|}{|\mathcal{V}(t)|}$$  \hspace{1cm} (20)$$
as the ratio between the number of inactive configurations (the cardinality of the set \(\mathcal{Q}(t)\), see Equation (6)) and the total number of configurations (the cardinality of the set \(\mathcal{V}\), see Section II). Additionally, we compare different physical quantities between the pruned and unpruned MCTDHB data in order to assess the accuracy of our pruning approach.

MCTDHB provides the full many-body wave function at each time step of the evolution and thus grants access to a plethora of different observables that allow us to analyze and understand the physical system. One of the most general of such quantities is the reduced \(p\)-body density matrix \([96]\)

$$\rho_p(x_1, \ldots, x_p, x'_1, \ldots, x'_p, t) = \frac{N!}{(N-p)!} \int \Psi(x_1, \ldots, x_N, t)\Psi^*(x'_1, \ldots, x'_p, x_{p+1}, \ldots, x_N, t)dx_{p+1} \ldots dx_N$$  \hspace{1cm} (21)$$

that can be used to calculate particle densities as well as correlation functions. The reduced one-body density matrix (i.e. \(p = 1\)) is of special interest as its diagonal \(\rho_1(x, x) = \rho_1(x, x' = x, t)\) is the one-body density matrix which describes the spatial distribution of particles. The spectral representation of the reduced one-body density matrix

$$\rho_1(x, x', t) = \sum_{\alpha=1}^{m} \lambda_{\alpha}(t)\phi_{\alpha}(x, t)\phi_{\alpha}^*(x', t)$$  \hspace{1cm} (22)$$
is given by the eigenvectors \(\{\phi_{\alpha}(t)\}\), the so-called natural orbitals, and the decreasingly ordered eigenvalues \(\lambda_{\alpha}(t) \in [0,1]\), the so-called natural populations. The natural populations fulfill \(\sum_{\alpha=1}^{m} \lambda_{\alpha}(t) = 1\) and determine the degree of inter-particle correlations within the ensemble. A system with \(\lambda_1 = 1 \land \lambda_{\alpha > 1} = 0\) is called condensed, is accurately described in a mean-field treatment using a single orbital and does not exhibit inter-particle correlations. In order to quantify the impact of the pruning approach on the natural populations, we compute the absolute difference between the natural population \(\lambda_{i}(t)\) obtained by a regular MCTDHB calculation and the corresponding natural population \(\lambda'_{i}(t)\) from a pruned simulation

$$\varepsilon_{\lambda_i}(t) = |\lambda'_{i}(t) - \lambda_i(t)|.$$  \hspace{1cm} (23)$$

Moreover, we study the reduced two-body density operator which can be used to calculate second order correlation functions and two-particle densities. For the sake of brevity we only report results on the diagonal \(\rho_2(x, x) = \rho_2(x_1 = x, x_2 = x, x'_1 = x, x'_2 = x, t)\) that can be interpreted as the probability distribution to find two particles at the same position.

Furthermore, the pruning might affect the total energy of the system due to the modifications of the many-body Hamiltonian. In order to quantify any such effects, we introduce the relative deviation

$$\varepsilon_E(t) = \left| \frac{E'(t)}{E(t)} - 1 \right|.$$  \hspace{1cm} (24)$$

between the energy \(E'(t)\) of a pruned calculation and \(E(t)\) of a regular MCTDHB calculation.

The MCTDHB algorithm conserves the norm of the wave function, the orthonormality of the SPFs and, if the Hamiltonian is time-independent, the energy. The dynamical pruning might introduce inaccuracies that lead to violations of these properties which we investigate by defining appropriate error quantities. The norm of the wave function should always have the value 1. By computing the absolute difference

$$\varepsilon_{\|\Psi\|^2}(t) = \left| (\Psi(t)|\Psi(t))^2 - 1 \right|$$  \hspace{1cm} (25)$$
from this target value we can quantify the violation of the norm conservation at each time \(t\). In Sections V A and V B we study the dynamics after a sudden change of the Hamiltonian at time \(t = 0\). However, we keep the Hamiltonian \(H(t \geq 0)\) constant such that the energy should be conserved throughout the simulation. In order to measure violations of this conservation law, we compute the relative difference

$$\varepsilon_E(t) = \left| \frac{E(t)}{E(0)} - 1 \right|$$  \hspace{1cm} (26)$$
of the momentary total energy \(E(t)\) with respect to the initial energy \(E(0)\). During the propagation of a many-body wave function using MCTDHB the SPF basis should remain orthonormal. To quantify deviations from this property at time \(t\) we introduce the quantity

$$\varepsilon_{\perp}(t) = \left| \langle \varphi_i(t)|\varphi_j(t) \rangle - \delta_{ij} \right|.$$  \hspace{1cm} (27)$$
However, we do not discuss this property in detail in the following sections as we find that it does not seem to be affected by the pruning approach. The value of this quantity is always comparable to the unpruned MCTDHB calculation and is bounded by \(\varepsilon_{\perp}(t) < 10^{-10}\).

In the following, we discuss two physical scenarios by choosing different potentials and quench procedures to showcase the performance of the pruning approach. To ensure comparability, all numerical simulations where performed on an AMD® Ryzen™ Threadripper™ 1950X 16-core processor using a single, dedicated core.
A. Quench Dynamics in an Optical Lattice

We investigate the nonequilibrium dynamics of repulsively interacting bosons trapped in an optical lattice [10] following a sudden change of the interaction strength. This quench procedure is experimentally accessible through Feshbach resonances [20, 21] or changes of the transversal confinement frequency [23–25]. Similar setups have been investigated using MCTDHB in several previous works [97–104] so that this setup serves as an ideal testbed for new methodological advancements.

We parameterize the lattice potential as

\[ V(x) = \begin{cases} V_0 \sin^2 \left( \frac{\pi x}{L} \right) & -\frac{L}{2} \leq x \leq \frac{L}{2} \\ \infty & \text{otherwise} \end{cases} \] (28)

with an odd number of wells \( p \), the barrier height \( V_0 \) and the system size \( L \). Based on these lattice parameters we use the recoil energy [105] \( E_R = \hbar^2 \pi^2 p^2 / 2mL^2 \) as the natural energy unit of the system and choose a barrier height of \( V_0/E_R = 4 \) for the lattice in the following. Starting from the ground state of the system with \( \tilde{g} = \pi g \gamma L/E_R = 0.1 \), we study the dynamics following a quench to \( \tilde{g} = 0.4 \) and \( \tilde{g} = 0.8 \). According to the convergence checks that we performed (see Appendix A) it proves sufficient to restrict the SPF basis to \( m = 5 \) orbitals.

Figure 2 shows the evolution of the one-body density after the aforementioned quench protocol for the case of \( N = 20 \) particles and a quench to \( \tilde{g} = 0.4 \) which has been computed using a regular MCTDHB simulation. The quench excites intrawell breathing dynamics which is visible as a periodic expansion and contraction of the atomic cloud around the center of each well. Additionally, over-barrier transport between the wells [97] is induced which can be identified by the finite particle density between the wells. In Figure 2 we show the propagation up to a final time \( t_f \approx 15 \hbar / E_R \). In the further analysis we investigate the different pruning approaches for a varying number of particles and post-quench interaction strengths leading to a large number of independent simulations. As the simulation times can become large, especially when treating larger numbers of particles, we simplify the analysis by only studying the dynamics up to a final time \( t_f = 2 \hbar / E_R \) as indicated by the dotted white line in Figure 2. In order to ensure that our pruning approach also captures the correct long-term behavior of the physical system, we also performed calculations up to a time \( t = 10 \hbar / E_R \) for a selection of these simulations, the results of which we do not present for the sake of brevity.

We apply the various pruning methods described in Sections III and IV to this lattice setup and choose a pruning threshold of \( \gamma = 10^{-8} \) and a pruning time \( \tau = 10^{-2} \hbar / E_R \). Figure 3 shows the reduction of the simulation time in comparison with the regular MCTDHB for different numbers of particles. The initial state can be described using only a few configurations such that for small times almost all configurations can be marked as disabled. Over time this number reduces as can be seen in the inset of Figure 3. This fact can be explained with scattering from the few initially important configurations to the lesser important ones as mediated by the term \( \hat{Q} \hat{H} \hat{P} \) in Equations (10) and (12). However, the number of inactive configurations remains large throughout the simulation such that a significant speedup compared to the regular MCTDHB calculation is achieved. The performance benefit depends on the pruned Hamiltonian that is used as well as the number of particles \( N \) (see Figure 3). The evaluation of the pruning criterion introduces computational overhead. When propagating wave functions containing only few configurations, e.g. when studying small particle numbers \( (N \approx 5) \), only a small speedup can be achieved. However, for larger systems \( (N = 20) \) a considerably larger speedup by a factor of more than seven can be reached. The EoMs based on the Hamiltonian \( \hat{H} \hat{P} \) yield higher performance gains than the ones based on \( \hat{Q} \hat{H} \hat{P} \). This is to be expected as the first variant incorporates less of the original matrix elements while the pruning ratios did not differ substantially. Furthermore, the stronger quench requires a higher number of configurations and thus leads to a smaller speedup.

Moreover, comparing the MCTDHB and the pruned one- and two-body density (see Figure 4) no difference is noticeable throughout the evolution. Thereby, we can infer that both quantities are reproduced accurately in the pruned simulations. When applying the EC in conjunction with the Hermitian Hamiltonian (10) for \( N = 20 \) bosons and a post-quench interaction of \( \tilde{g} = 0.4 \), the corresponding, maximal absolute deviation is 0.016 and 0.13 for the one- and two-body density respectively over the evolution.

The approximation via the pruning procedure introduces deviations in the energy of the system as well as the natural populations when comparing to the usual MCTDHB. The results for the energetic error \( \varepsilon_E(t) \) (see Equa-
Figure 3. Speedup of the pruned compared to the unpruned simulations for the five well lattice. The solid lines are affiliated with the weak interaction quench to \( \tilde{g} = 0.4 \) while the dotted lines indicate the strong interaction quench to \( \tilde{g} = 0.8 \). The different colors indicate the number state selection criteria (Equation (14) or (18)) and the modified Hamiltonian (Equation (10) or (12)) is used. The inset shows the ratio of the pruned configurations at each time step \( \beta(t) \) (see Equation (20)) for the case \( N = 20 \) using the energy criterion and the Hamiltonian \( \bar{H}P \) after a weak interaction quench to \( \tilde{g} = 0.4 \). A pruning threshold \( \gamma = 10^{-8} \) and pruning time \( \tau = 10^{-2} h/E_R \) was employed.

Figure 4. One-body density \( \rho_1(x,t) \) (a)-(c) and diagonal of the reduced two-body density matrix \( \rho_2(x,x,t) \) (d)-(f) at selected time instants (see legends) for \( N = 20 \) particles in the five well lattice following an interaction quench from \( \tilde{g} = 0.1 \) to \( \tilde{g} = 0.4 \). The solid blue lines correspond to the regular MCTDHB and the dashed orange lines to a pruned calculation using the energy criterion with the Hamiltonian \( \bar{H}P + \bar{P}Q \). However, due to the good agreement of the unpruned and pruned calculation, these lines lie on top of each other. A pruning threshold \( \gamma = 10^{-8} \) and pruning time \( \tau = 10^{-2} h/E_R \) was employed.

Figure 5. Maximal energetic error (see Equation (24)) between the unpruned and pruned simulations for the five well lattice. The solid lines correspond to a quench to \( \tilde{g} = 0.4 \) and the dashed lines to \( \tilde{g} = 0.8 \). The inset shows the exemplary evolution of the error over time for \( \tilde{g} = 0.4 \) and \( N = 20 \). A pruning threshold \( \gamma = 10^{-8} \) and pruning time of \( \tau = 10^{-2} h/E_R \) was employed.

The different colors indicate the number state selection criteria (Equation (14) or (18)) and the modified Hamiltonian (Equation (10) or (12)) is used. The inset shows the ratio of the pruned configurations at each time step \( \beta(t) \) (see Equation (20)) for the case \( N = 20 \) using the energy criterion and the Hamiltonian \( \bar{H}P \) after a weak interaction quench to \( \tilde{g} = 0.4 \). A pruning threshold \( \gamma = 10^{-8} \) and pruning time \( \tau = 10^{-2} h/E_R \) was employed.

The different colors indicate the number state selection criteria (Equation (14) or (18)) and the modified Hamiltonian (Equation (10) or (12)) is used. The inset shows the ratio of the pruned configurations at each time step \( \beta(t) \) (see Equation (20)) for the case \( N = 20 \) using the energy criterion and the Hamiltonian \( \bar{H}P \) after a weak interaction quench to \( \tilde{g} = 0.4 \). A pruning threshold \( \gamma = 10^{-8} \) and pruning time \( \tau = 10^{-2} h/E_R \) was employed.

Similarly, the depletion for a quench to \( \tilde{g} = 0.8 \) exhibits a maximum value of \( \max \lambda_1(t) = 0.16 \) for \( N = 20 \) particles.

In Figure 6 we also compare the maximal depletion of the natural populations \( \max \lambda_1(t) \) (see Equation (23)) between the pruned and the unpruned simulations over time. We exemplarily present the results for the dominant, first orbital. Over time \( \varepsilon_{\lambda_1}(t) \), shows an oscillatory behavior around a central value so that we compute the standard deviation of this quantity to quantify these fluctuations (see error bars in Figure 6). For the natural population error, the pruning criterion has a larger impact than the type of EoM being used. The energy criterion (blue and orange line) shows slightly better results than the magnitude criterion (green and red line) but stays in
the same order of magnitude. As the energetic error, the error increases with the system size but stays of the order of $10^{-4}$ for a post-quench interaction of $\tilde{g} = 0.4$ and of the order of $10^{-3}$ for $\tilde{g} = 0.8$.

![Figure 6](image6.png)

Figure 6. Maximum error of the first natural population as given by Equation (23) for various numbers of bosons in a five well lattice. The solid lines illustrate a post-quench interaction strength of $\tilde{g} = 0.4$ while the dashed lines represent $\tilde{g} = 0.8$. The error bars indicate the standard deviation of the error. The inset shows the evolution of all 5 natural populations for the case $N = 20$ after a weak quench to $\tilde{g} = 0.4$ and using the regular MCTDHB. A pruning threshold of $\tau = 10^{-8}$ and pruning time of $\tau = 10^{-2} \hbar/E_R$ was employed.

The post-quench Hamiltonian is time-independent and therefore the energy should be conserved in addition to the norm of the wave function. Figure 7 shows the maximum violation of these constraints over time. The norm conservation as quantified by $\xi_{||\Psi||^2}(t)$ (see Equation (25)) shows a drastic difference between the two kinds of EoMs. Overall however, this error is small and acceptable.

![Figure 7](image7.png)

Figure 7. Maximal violation of the conservation of (a) the norm (see Equation (25)) and (b) the energy (see Equation (26)) during the propagation of the five well lattice system for an increasing number of particles $N$.

### B. Nonequilibrium Dynamics in a Double Well

Our second physical example system is an ensemble of interacting bosons confined in a double well that is created from a harmonic trap with an additional Gaussian-shaped barrier at the center, also known as a dimple trap in the literature [106],

$$V(x) = \frac{1}{2} m \omega x^2 + V_0 \exp\left(-\frac{x^2}{2\sigma^2}\right).$$

Here, $\sigma$ is the standard deviation of the Gaussian and $V_0$ is the height of the barrier. We use the harmonic oscillator length $l_H = \sqrt{\hbar m / \omega}$ as the natural length scale of the system with $\omega$ being the angular frequency of the harmonic potential. The energy units are given by $\hbar \omega$ and the time units by $1/\omega$. In order to induce the nonequilibrium dynamics in this setup we prepare the ground state of the system without a barrier (i.e. for $V_0 = 0$) and then quench the barrier height to $V_0/\hbar \omega = 4$. A similar scheme, where the central barrier was continuously ramped up was investigated in [71].

We study setups with $N = 5, 10, 15, 20, 25, 30$ particles using $m = 10, 9, 7, 6, 5, 5$ orbitals respectively and ensure convergence with respect to $m$ (see Appendix A). The interaction strength is chosen to be $g/\hbar \omega l_H = 0.1$ and the width of the barrier to be $\sigma = l_H$. We also choose a pruning threshold of $\gamma = 10^{-10}$. The dynamics of the system takes place on a larger timescale compared to the lattice system from Section V A so that we use a pruning time of $\tau \omega = 5 \cdot 10^{-2}$.

The evolution of the single-particle density of the system is showcased in Figure 8. By quenching to a finite height of the central barrier, the initial Gaussian distribution of the bosons is split into two branches veering away from each other with opposite momenta. With the given parameters, the two clouds possess enough energy to overcome the hump after being reflected by the harmonic trap and collide in the trap center $x = 0$ at a
time $t\omega \approx 4$. Afterwards, these density branches separate again each one moving in one of the wells of the double well and subsequently collide at $x = 0$ again. This motion is repeated almost periodically throughout the evolution. Our main focus is the performance of the pruning approach in this scenario, i.e. we do not analyze the overall dynamics in further detail.

Figure 8. Time evolution of the one-body density $\rho_1(x, t)$ of $N = 15$ bosons in a double well trap after a quench of the central Gaussian barrier to a finite height obtained with a regular MCTDHB calculation.

Figure 9 shows the speedup of the pruned versus the unpruned simulations. In comparison to the lattice system, the benefits of the pruning approach are smaller yielding a speedup between 1.4 and 2 depending on the system size. This can be explained by a smaller pruning ratio as it can be seen in the inset. The ratio of inactive configurations quickly drops from almost 1 to around 0.5 where it saturates, suggesting that a higher amount of configurations is required to describe the physical system accurately.

Figure 9. Speedup of the various pruned simulations compared to regular MCTDHB in the double well setup for varying particle numbers. The inset shows the ratio of inactive configurations $\beta(t)$ (see (20)) over time for $N = 15$ particles using the energy criterion and the Hamiltonian $\hat{H}\hat{P}$. We used a pruning threshold of $\gamma = 10^{-10}$ and a pruning time of $\tau\omega = 5 \cdot 10^{-2}$.

Even though the pruning approach does not speed up the simulation as much as in the case of an optical lattice, the evolution of the system is still reproduced accurately. We show the good agreement of the one-body (see Figure 10) and the two-body (see Figure 11) densities between a regular MCTDHB and a pruned simulation using the EC in conjunction with the Hermitian Hamiltonian (10). The corresponding maximal, absolute deviation of the order of $10^{-3}$ for the one-body and $0.0012$ for the two-body density.

The energetic error $\varepsilon_E$ (see Equation (24)) between the pruned and the unpruned MCTDHB calculation is depicted in Figure 12. In contrast to the lattice system, the difference between the two types of EoMs (11) and (13) is only minor and the error does not increase with the number of particles. Using the pruning approach, the unpruned MCTDHB energy is reproduced up to a relative deviation of the order of $10^{-4}$. The inset of Figure 12 shows that the energetic error grows in a similar fashion as in the lattice system over the simulated time and that it does saturate within the given time range.

Again, we also investigate the impact of the pruning on the natural orbitals. The maximal absolute error of the first, dominant natural population $\max_t \varepsilon_{\lambda_1}(t)$ (see Equation (23)) is shown in Figure 13. We observe that it is at most of the order of $10^{-3}$ verifying that the first natural population is reproduced accurately. As in the lattice system, the depletion of the system increases with the number of particles. For $N = 30$ particles we achieve a maximal depletion of $\max (1 - \lambda_1(t)) = 0.125$ so that the given parameters lead to beyond-mean-field dynamics. The evolution of the natural populations with time is visualized in the inset of Figure 13.

In Figure 14 (a) we show the violation of the norm...
VI. CONCLUSIONS AND OUTLOOK

Studying the nonequilibrium quantum dynamics of large many-body systems poses a great challenge for numerical methods due to the excessively growing number of configurations. We have presented an intuitive, novel approach to address this issue in the framework of multi-configuration time-dependent Hartree method for bosons (MCTDHB). Our scheme dynamically classifies number states according to their importance for the physical sys-
tem under consideration employing pruning criteria that can be controlled using tunable accuracy parameters. We have derived two such criteria based on understandable quantities that can be computed efficiently. Our approach is dynamical and can adapt the number state selection during the evolution of the system to ensure an accurate description. The resulting, time-dependent selection of important configurations can be exploited by modifying the MCTDHB EoMs. Our algorithm cannot overcome the exponential growth of the Hilbert space but can greatly reduce the numerical effort by purposefully neglecting terms of the Hamiltonian.

We have benchmarked our scheme using the quench dynamics of two typical systems from the field of ultra-cold atoms, namely an optical lattice and a double well. The dynamical pruning approach is able to accurately reproduce the results of the unpruned MCTDHB, while often reducing the computation time significantly. The speedup was particularly large for the lattice systems because a large number of coefficients are of small importance.

Based on these results, we can conclude that our scheme captures the important aspects of the physical system correctly while reducing the numerical effort, making it an attractive candidate for future investigations. A promising prospect in doing so is the realization of extrapolation studies. By studying a physical system both with unpruned and pruned MCTDHB up to a certain, feasible size one can ensure the agreement of both approaches and that the parameters $\gamma$ and $\tau$ are chosen appropriately. Afterwards, larger system sizes, that are not achievable using unpruned MCTDHB, could be investigated using the pruning approach while extrapolating the quantities that have been used to compare to the regular MCTDHB for the smaller sizes. Furthermore, the method we presented in this work may be further refined by employing alternative pruning criteria or by modifying the EoMs in a different manner. Another promising direction for further studies is the application of the dynamical pruning scheme to other methods from the family of MCTDH such as the MCTDHF [69, 70] for fermionic systems. Due to the strong interest that developed in the investigation of binary mixtures using multi-configuration time-dependent Hartree method for mixtures (ML-MCTDHX) [73–75] in recent years, the implementation of a dynamical pruning scheme for this method could be very helpful in order to reduce the numerical effort of these time-consuming simulations. One possible way is to apply the pruning approach presented in this article on a per-species basis.

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Appendix A: Convergence of the MCTDHB Calculations

The SPFs used by MCTDHB are variationally optimal, however the number of these orbitals has to be sufficiently large to ensure the numerical exactness of the method. In order to ensure the convergence with respect to the number of orbitals, we performed calculations with varying number of orbitals. By comparing the results for different basis sizes, we ensure that the employed observables such as the particle densities do not change up to a certain degree when using more orbitals than the numbers we presented in the main text. Additionally, the natural populations are important when discussing the convergence of MCTDHB. In a converged calculation, the natural populations should show a rapidly decreasing hierarchy and orbitals that are neglected should only be weakly occupied.

We use $m = 5$ orbitals for the investigations of the lattice system in Section V A. The least occupied orbital shows a maximal natural population of $\max_{t} \lambda_{5}(t) = O(10^{-3})$ for all particle numbers and post-quench interaction strengths throughout the time evolution. Any orbitals added to the simulation are only weakly occupied. We observe a clear drop in the natural populations as already the next orbital shows an occupation of $\max_{t} \lambda_{6}(t) = O(10^{-5})$ and further natural populations are even smaller. In general, the occupation of the last orbital increases with the number of particles and is larger for the stronger quench to $\tilde{g} = 0.8$ but only slightly. Overall, we consider $m = 5$ orbitals to be sufficient due to the clear drop in natural populations and the observation that the evolution of the one- and two-body densities does not change qualitatively. Furthermore, the energy of the final state of the propagation is converged to a precision of at least $O(10^{-5})$.

For the setup with the double well presented in Section V B, we used different numbers of orbitals depending on the number of particles. We ensure that the least occupied orbital that is taken into account is occupied with a natural population of $\max_{t} \lambda_{m}(t) = O(10^{-4})$. Further orbitals added do not change the behavior of the system qualitatively and the corresponding natural populations decay rapidly. Additionally, the energy of the final state is converged to at least $O(10^{-4})$ such that we consider the used number of orbitals to be sufficient.
