Mode folding in systems with local interaction: unitary and non-unitary transformations using tensor states

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Abstract
An approach to the simulation of locally interacting systems is demonstrated and assayed. The proposal is built upon the concept of folding of bosonic modes previously introduced in the context of linear dynamics and can be seen as an alternative to Trotter–Susuki expansion in studies of quantum propagation based on tensor states. It is shown that evolution as well as ground state computations can be implemented and that test simulations deliver comparatively accurate results. The whole analysis provides insight into the way well-known quantum structures affect mean values and fluctuations in realistic setups. The proposed method can be used to study a variety of systems and phenomena arising in optical lattice experiments such as superfluid or Mott insulator regimes, quantum phase transitions, soliton propagation in Bose–Einstein condensates or Bose mixtures and elementary vortex excitations.

Keywords: boson systems, renormalization group methods, computational techniques

1. Introduction

The study of numerical methods of quantum mechanics has become an exciting and increasingly active field of research, not only because numerical methods are extremely important as simulation instruments, but also because they help understand the underlying functioning of the quantum theory. Such is the case of density matrix renormalization group (DMRG) [1], which has played an important role as a calculation tool since its inception. Time evolving block decimation (TEBD) [2] has appeared more recently and integrates elements of DMRG with concepts of quantum computation. Both DMRG and TEBD have inspired a number of variants such as tDMRG [3], iTEBD [4], MERA [5], to mention just a
few [6, 7]. However, there exist instances where the lack of efficient simulation protocols is yet an issue. Here, a proposal in this direction is explored, namely, a method that can be used to simulate real as well as imaginary quantum evolution under more relaxed conditions than those encountered in standard TEBD applications. This paper expands on the themes first addressed in reference [8], and can be seen as its continuation, especially in what concerns the inclusion of interaction and the treatment of non-unitary transformations.

Many of the efforts devoted during recent times to the study of efficient simulation options have been motivated by the remarkable advancement in cold atom experiments and the possibility of probing fundamental theoretical models in the laboratory [9]. As a result, applications of numerical methods based on tensor states are getting increasingly common in descriptions of quantum gases in optical lattices [10–15]. Tensor states display an assortment of properties that can be exploited to absorb symmetries and implement transformations selectively rather that on the whole Hilbert space [16–19]. As described in [20], a symmetric tensor network can be decomposed as a product of two types of tensors. The first type accounts for all the degrees of freedom and the second type is determined by the symmetry. The implementation of symmetries in tensor network algorithms has proved successful in reducing simulation times and memory consumption while keeping tolerable errors. Here, an attempt is made to establish a way of using all this knowledge to effectively simulate quantum evolution and find ground states by looking at the way the evolution operator can be decomposed as a product of two-site operations. The aim of this proposal is to provide an alternative way to proceed in cases where the Trotter–Susuki expansion (TSE) becomes less efficient or impractical.

Let us introduce the Bose–Hubbard Hamiltonian in one dimension as follows

\[
\hat{H} = \sum_{j=1}^{N} \left( U \hat{n}_j (\hat{n}_j - 1) - J (\hat{a}_j^\dagger \hat{a}_{j+1} + \hat{a}_j^\dagger \hat{a}_{j+1}^\dagger) \right) + \mu \hat{n}_j,
\]

so that \( \hat{n}_j = \hat{a}_j^\dagger \hat{a}_j \), while \( \hat{a}_j \) and \( \hat{a}_k^\dagger \) satisfy \( [\hat{a}_j, \hat{a}_k^\dagger] = \delta_{jk} \) and \( [\hat{a}_j, \hat{a}_k] = 0 \) for \( j, k = 1, 2, \ldots, N \). Operators \( \hat{a}_j \) and \( \hat{a}_j^\dagger \) represent the \( j \)-th mode. If these modes are associated to Wannier functions with no significant (but finite) overlap in position [21, 22], as it is normally the case in applications of the Bose–Hubbard model, then \( j \) numbers a site in a quantum chain. In order to allow for benchmarking against TEBD, open boundary conditions are embraced, \( \hat{a}_{N+1} = 0 \), yet the validity of the central arguments here is not tied to such a specific kind of boundary conditions. Moreover, periodic boundary conditions were used in [8]. The Bose–Hubbard model undergoes a continuous phase transition from Mott insulator to superfluid and its phase diagram as well as its phenomenology has been worked out in various contributions [23–25].

The standard version of TEBD makes use of the TSE [26–28] to decompose the evolution operator as a product of transformations involving only nearest neighbor sites. This is done by splitting the evolution operator in two sub-evolutions, each generated by a part of the Hamiltonian grouping neighboring terms in Hamiltonian (1). The approach is efficacious and theoretically robust, but a number of issues might arise when dealing with long range couplings or periodic boundary conditions [29, 30]. Here it is proposed to separate the Hamiltonian into single-particle and many-particle operators, such as they are understood from a second-quantization perspective, and then write the evolution operator as a composition of infinitesimal evolutions for each part. A second order split can thus be considered as follows

\[
e^{-it\hat{H}} = e^{-it\hat{H}_{\text{MP}}} e^{-it\hat{H}_{\text{SP}}} e^{-it\hat{H}_{\text{MP}}} + \mathcal{O}(t^3),
\]
knowing that

\[ \hat{H}_{SP} = \sum_{j=1}^{N} \left( -\frac{U}{2} + \mu_j \right) \hat{a}_j - J \left( \hat{a}^+_j \hat{a}_{j+1} + \hat{a}^+_{j+1} \hat{a}_j \right), \]  

\[ \hat{H}_{MP} = \sum_{j=1}^{N} \frac{U}{2} \hat{n}_j^2. \]  

The only request being that the terms appearing in \( \hat{H}_{MP} \), i.e., the interaction, must be local, but \( \hat{H}_{SP} \) can take any form as long as it remains single-body. This means that \( \hat{H}_{SP} \) could include couplings of arbitrary scope, e.g., \( \hat{a}^+_j \hat{a}_{j+2} \), \( \hat{a}^+_j \hat{a}_{j+3} \), etc.

Independently of the formulation of the exponential split, the simulation protocols that have relevance in this study employ the tensorial representation and the updating routines for one- and two-site transformations on a quantum chain that were first introduced in [31]. The protocol include a tensorial representation written in canonical form using singular value decompositions. In coherence to this, the cost of a given computation is reported by the variable \( \chi \), which establishes, in the shape of a polynomial, the maximum number of arithmetic operations necessary to calculate the action of an operator on at most two consecutive sites of the chain. In the current proposal, tensor states such as singular value decompositions are used to implement numerically the folding schemes that are the focus of this work, and as such, there is no attempt to propose or refine updating protocols of matrix product state formulations.

In the next section the fundamentals of the technique, here referred to in general as mode folding, are explained. Then it is seen how interaction is incorporated and how the whole proposal performs against characteristic parameters and in comparison to TSE. Subsequently, it is shown how to work with the imaginary-time evolution operator and the particularities found in the calculation of ground states. It is pointed out that different versions of the proposal can be used together in cases where ground state and evolution are both required, such as in studies of quench dynamics. Alternative approaches and conclusions are presented in the last part.

2. Mode folding

A solution of the Schrödinger equation for a system of identical particles is given by

\[ |\psi(t)\rangle = \prod_{q=1}^{N} \left( \hat{a}^+_q(t) \right)^{n_q} |0\rangle, \]  

where

\[ \hat{a}^+_q(t) = e^{-\imath H t} \hat{a}^+_q e^{\imath H t} (\hbar = 1). \]  

\( N \) is the number of modes and \( M = \sum_{q=1}^{N} n_q \) is the total number of particles. It follows from equation (5) that \( |\psi(0)\rangle = \prod_{q=1}^{N} |n_q\rangle \). Differentiation of equation (6) leads to

\[ \frac{d\hat{a}^+_q}{dt} = \imath e^{-\imath H t} \left[ \hat{a}^+_q, \hat{H} \right] e^{\imath H t}, \]  

for \( q = 1, 2, \ldots, N \). In this way, a system of differential equations is generated. Such a system is usually unsolvable. However, if many body terms are neglected (\( \hat{H}_{MP} = 0 \), the
system is complete and can be written as

\[
\begin{pmatrix}
\hat{a}_1^+ \\
\hat{a}_2^+ \\
\vdots \\
\hat{a}_N^+
\end{pmatrix}
= i
\begin{pmatrix}
\frac{U}{2} - \mu_1 & J & 0 & \cdots & 0 \\
J & \frac{U}{2} - \mu_2 & J & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & \cdots & J & \frac{U}{2} - \mu_{N-1} & J \\
0 & \cdots & 0 & J & \frac{U}{2} - \mu_N
\end{pmatrix}
\begin{pmatrix}
\hat{a}_1 \\
\hat{a}_2 \\
\vdots \\
\hat{a}_{N-1} \\
\hat{a}_N
\end{pmatrix}.
\tag{8}
\]

A solution can be obtained using standard results from linear theory and considering \(\hat{a}_q^+(0) = \hat{a}_q^+\). Therefore, an evolved mode acquires the form

\[
\hat{a}_q^+(t) = c_{1,q}(t)\hat{a}_1^+ + c_{2,q}(t)\hat{a}_2^+ + \cdots + c_{N,q}(t)\hat{a}_N^+.
\tag{9}
\]

Since the matrix that generates the transformation in (8) is Hermitian, the coefficients of equation (9) are effectively governed by a unitary operation and thus they obey

\[
\sum_{j=1}^{N} c_{j,q}^*(t)c_{j,p}(t) = \delta_{q}^p.
\tag{10}
\]

In this sense it can be said that the evolved modes remain orthonormal. This result holds only in absence of many-body terms and as long as the original transformation is unitary.

On the other hand, unitary operations on \(|\psi(t)\rangle\) can be seen as transformations that act simultaneously on every \(\hat{a}_q^+\):

\[
e^{-i\theta} \prod_{q=1}^{N} \frac{(\hat{a}_q^+)^{n_q}}{\sqrt{n_q!}} |0\rangle = \prod_{q=1}^{N} \frac{\left( e^{-i\theta}\hat{a}_q^+ e^{i\theta} \right)^{n_q}}{\sqrt{n_q!}} |0\rangle,
\tag{11}
\]

where \(J\) can be any Hermitian operator. There are two types of such transformations that have applications in the folding method. The first one affects mode operators individually and is used to make the coefficients real. Such an effect is achieved by implementing the inverse of

\[
\hat{R}_l^{(l)}(t) = e^{i\phi_l(t)\hat{a}_l^+ \hat{a}_l}, \quad \phi_l(t) = \arg c_{l,k}(t),
\tag{12}
\]

getting as a result \(c_{l,k} \hat{a}_l^+ \rightarrow |c_{l,k}| \hat{a}_l^+\). When this is done consecutively for \(l = 1, 2, \ldots, N\) only real coefficients are left in the equivalent of equation (9) with \(q = k\). The \(c_{l,k}\)s can then be redefined as the absolute values of the original coefficients. This does not mean that the phase information has been lost, instead, it has been stored in the description of the \(\hat{R}_l^{(l)}\)s. The other type of transformation involves pairs of modes and is given by the inverse of

\[
\hat{R}_k^{(j+l)}(t) = e^{i\theta_{j+l}(t)\hat{a}_j^+ \hat{a}_l},
\tag{13}
\]
The transformation is essentially a rotation since its generator is a genuine quantum angular momentum. The procedure yields

\[
\hat{R}_k^{[j+1,j]} = \hat{R}_k^{[j+1,j]} (c_{j+1,q} \hat{a}^\dagger_{j+1} + c_{j,q} \hat{a}^\dagger_j),
\]

\[
= c'_{j+1,q} \hat{a}^\dagger_{j+1} + c'_{j,q} \hat{a}^\dagger_j,
\]

\[
c'_{j+1,q} = c_{j+1,q} \cos \left( \frac{\theta_{j,k}}{2} \right) - c_{j,q} \sin \left( \frac{\theta_{j,k}}{2} \right),
\]

\[
c'_{j,q} = c_{j+1,q} \sin \left( \frac{\theta_{j,k}}{2} \right) + c_{j,q} \cos \left( \frac{\theta_{j,k}}{2} \right).
\]

The fact that the change on the coefficients is unitary is pivotal to the ensuing discussion. After making \( c'_{j+1,q} = 0 \) it follows

\[
\tan \left( \frac{\theta_{j,q}}{2} \right) = \frac{c_{j+1,q}}{c_{j,q}}.
\]

As a result, operator \( \hat{a}_{j+1}^\dagger \) is neutralized in \( \hat{a}_q^\dagger \). In order to see the complete action of these operations, let us propose a view in which the evolved modes appear stacked as shown by Equation (19). Transformations affect all the coefficients vertically aligned. In the first part of the proposed protocol, all the coefficients in the first row of the stack, i.e., those belonging to \( \hat{a}_1^\dagger \), are stripped from their complex phases employing transformations of the first kind. Notice that once this has been completed, all the coefficients in the stack have most likely changed, not just the ones in the first row. The next step consists in making \( \hat{a}_N^\dagger \) disappear from the first row by operating on the two columns at the left of the stack, as indicated in (19), and then making \( c'_{N,1} = 0 \). This cancellation technique is repeated systematically, advancing toward the right, until all the operators except \( \hat{a}_1^\dagger \) are eliminated from the first row, as indicated by (20) and (21). It is worth noticing that the last of these operations entails the cancellation of all but the top \( \hat{a}_1^\dagger \) in the column at the right extreme of the stack, by virtue of the unitarity of all previous transformations and the fact that the modes are orthonormal. At the end of this first series (or layer) of changes, the first mode has been folded and the stack of operators appears just like (22). The second layer of operations is aimed at folding the second mode and has a very similar structure, but it is carried without reaching the first mode, lest it unfolds. The scheme goes on in an orderly manner until the stack is left with a different operator in every level. At this point, it can be argued that the system has been returned to its initial state \((t = 0)\) independently of the distribution of \( n_q \) in equation (5)
Having determined the set of transformations required by this folding mechanism, it is possible to reassemble the evolved state implementing the sequence in reverse order. All of this can be mathematically synthesized as

\[ \prod \prod \prod \psi = \prod c_{N-1,N}^{\dagger} \hat{a}^\dagger_{N-1} + c_{N-2,N}^{\dagger} \hat{a}^\dagger_{N-2} + \ldots + c_{1,1} \hat{a}^\dagger_{1}. \]  

However, equation (23) is not the only possibility. In particular, if the stack is folded starting by \( \hat{a}^\dagger_N \), it is found instead

\[ \prod \prod \prod \psi = \prod c_{2,1}^{\dagger} \hat{a}^\dagger_2 + c_{1,1} \hat{a}^\dagger_1. \]  

In this expression the operators \( \hat{a}^\dagger_1 \) and \( \hat{a}^\dagger_2 \) are different from the ones that appear in equation (23) because the transformation angles do not necessarily coincide. Henceforth this latter approach will be referred to as inverse mode folding, in order to differentiate it from the former scheme, or ‘normal’ mode folding. Although both forms are in principle equivalent, it will be seen that their numerics might display different accuracy due to limitations arising from machine arithmetic precision.

3. The inclusion of interaction and the case of rapidly decaying coefficients

As it was introduced in the previous section, mode folding can be used to calculate the effect of an evolution operator generated by a non-interacting Hamiltonian on a Fock state. The procedure consists in first finding the effect that the evolution operator has on the creation operators, similar to equation (9), so that each evolved operator has a place in the stack shown in (19). At this stage all the coefficients that appear in the stack must be known. Then the
stack is folded following the recipe given above. This allows to know the angles underlying
every folding transformation. Since such transformations involve at most two neighbor sites
of the chain, they can be efficiently implemented in terms of tensor states protocols whenever
the amount of entanglement in the system is moderate. Consequently, to get the evolved
quantum state the inverses of the original folding operations are executed in reverse order
over the initial state, such as it is indicated in equations (23) and (24). Since
\[ \psi_0 \]
in
\[ \text{equations (23) and (24)} \]
can be any Fock state, it is possible to extend the formalism by
writing an arbitrary initial state as a superposition of Fock states and then using the fact that
the quantum evolution operator acts linearly on such a superposition. In order to incorporate
interaction effects, the evolution operator is split, as in equation (2), into single-particle and
many-particle step evolutions. The tensorial representation of the state is obtained applying
the unitary transformations related to mode folding, which account for the single-particle step,
as well as the many-particle step using the updating protocols demonstrated in [31]. Fur-
thermore, because the interaction terms are assumed to be local, the latter step does not alter
\( \chi \), i.e., it does not produce immediate changes in the size of the tensorial representation. In order to test
the proposal, the obtained tensorial representation in canonical form is passed to the Fock
basis and then compared to benchmark results found from the diagonalization of the corre-
sponding Hamiltonian in the Fock basis. In order to manage the error incurred by splitting the
evolution operator, \( t_r \) must be made small compared to the eigenvalues of the Hamiltonian. As
a consequence, the distribution of coefficients in (19) is highly sparse, with most of the
coefficients falling below machine accuracy. The exception being diagonal elements, which
remain close to one, and their neighbors. As small coefficients can be a source of numerical
errors, it is convenient to simply drop them and fold what is left of the stack. This leads to a
slightly different version of equation (23), namely
\[
|\psi(t + t_r)\rangle = \prod_{k=N}^{1} \left( \prod_{l=k}^{k+N} \hat{R}_l^{[j]} \prod_{j=k+1}^{j+N-1} \hat{R}_j^{[j+1,j]} \right) |\psi(t)\rangle,
\]
where \( \eta \) is the largest number of non-vanishing coefficients on either side of the stack
diagonal. In order to measure the difference between the results delivered by mode folding
and other reference results, the following error measure is introduced
\[ \Delta = 1 - |\langle \psi' | \psi \rangle|^2, \]  

(26)

where \( |\psi' \rangle \) comes from a tensorial representation and \( |\psi \rangle \) from standard diagonalization. It can be seen in figure 1(a) that different versions of mode folding produce results with distinct accuracies. It can also be seen that the best estimation is given by the inverse mode folding, although the difference with the next best estimation is rather marginal. The observed optimal parameter is \( \eta = 2 \), but in general the appropriate \( \eta \) depends on the distribution of coefficients in (19). For small values of \( t_s \) the distribution is tight and the optimal \( \eta \) is short. Likewise, \( \eta \) should grow with increasing \( t_s \). It is empirically seen that the best performance is achieved when the smallest considered coefficient is approximately of the same order of magnitude than the square root of machine accuracy. The reduction in correctness observed when more coefficients are included occurs because substantial error is transmitted to some folding angles calculated using coefficients with an insufficient number of significant figures at the beginning of each layer of calculations. Contrariwise, no such a tendency is observed in the inverse scheme since, even though poorly estimated coefficients are retained, the folding routine starts by the biggest coefficients on each layer. This makes inverse mode folding reliable, although it requires the inclusion of all the folding operations. Normal folding taking less coefficients is numerically more efficient, but a little bit less exact. Figures 1(b) and (c) show the characteristic behavior of the error as a function of time for different values of the time slice. For relatively large \( t_s \), \( \Delta \)'s growth is essentially polynomial. As \( t_s \) diminishes, the corresponding error curves scale down until for an optimal time slice the error starts showing saturation. As \( t_s \) diminishes further, the error scales up but the saturation profile remains. It can therefore be argued that while the theoretical error is gradually suppressed with decreasing \( t_s \), the computing error caused by division by small numbers augments. Similarly, the optimal value \( \chi = 105 \) seems to be independent of the values given to \( \eta \) and \( t_s \). However, the error dependence with respect to \( \chi \) is rather characteristic. Making \( \chi \) slightly smaller than its optimal value produces exponentially growing deviations from the actual state at very early times. This contrasts with the behavior of \( \Delta \) in simulations where although the time slice has been chosen well above its optimal value, \( \chi \) has remained at or above its equilibrium value. In such cases the error growth is polynomial and the simulation can be sustained for quite longer intervals. In this sense it can be said that a right estimation of \( \chi \) is more important for numerics than the chosen \( t_s \). This feature is encountered in both mode folding and TSE simulations. The comparative graphs depicted in figures 1(d) and (e) suggest that the difference in terms of deviations from the correct state between mode folding and TSE is minimal over a wide range of values of the ratio \( U/J \). Since it has been shown in [8] that folding alone delivers results with a tolerance of the order of machine accuracy, it follows that the observed error is mostly due to the splitting of the evolution operator into single- and many-particle parts and that such an error is comparable to the one produced by TSE. In terms of efficiency, because both approaches seem to require the same \( \chi \), the determining factor is the number of transformations effectuated on pairs of modes per loop in a computer routine, i.e., the number of updates of the tensorial representation necessary to advance the state a time \( t_s \). In a second order version such a number is approximately \( 3N/2 \) for TSE and \( N\eta - \eta(\eta + 1)/2 \) for mode folding. The difference can be understood in terms of the cost associated to the inclusion of more hopping terms in mode folding, in contrast to the less-strict neighbor approach dictated by TSE.
4. Non-unitary transformations and the calculation of ground states

Ground states play a prominent role in the study of quantum systems and it is known that they usually display less entanglement than dynamical states. As a consequence, the associated simulation cost in terms of tensor states is manageable to a great extent. Simulation protocols that rely on tensorial representations can be formulated as variational methods. This is the case for DMRG, where the ground state is found as the network that minimizes the energy. Another approach is to realize the limit

$$\lim_{t\to\infty} e^{-i\hat{H}t} \left| \psi_0 \right\rangle = \left| \psi_G \right\rangle,$$

(27)
as an iteration of an infinitesimal imaginary-time evolution of length $\tau_s$. Such is the strategy followed in the context of TEBD and it is also the approach adopted here. The crux of the problem is that imaginary-time evolutions are not unitary, ergo the foundation of the updating protocols of the tensorial representation [32] and the folding technique is compromised. To deal with the issue it is important, on the one hand, to use a sufficiently small 'imaginary' time slice $\tau_s$, so that the corresponding advancement is close enough to unitary and the updating protocols work. On the other hand, it is necessary to find a folding protocol that is not as heavily dependent on the unitariety of the evolution operation. Moreover, the protocol itself must integrate genuine non-unitary transformations so as to account for the non-unitariety of the whole transformation. In accordance with these premises, let us introduce

$$\hat{Q}^{j+1,j} = e^{i\hat{J}^{(j+1,j)}},$$

(28)where

$$\hat{J}^{[j+1,j]}_z = \cos \varphi_j \hat{J}^{[j+1,j]}_x + \sin \varphi_j \hat{J}^{[j+1,j]}_z,$$

(29)$$\hat{J}^{[j+1,j]}_x = \frac{1}{2} \left( \hat{a}_{j+1}^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_{j+1} \right),$$

(30)$$\hat{J}^{[j+1,j]}_z = \frac{1}{2} \left( \hat{a}_{j+1}^\dagger \hat{a}_{j+1} - \hat{a}_j^\dagger \hat{a}_j \right).$$

(31)Transformation (28) depends on $\epsilon_j$, which is chosen to be real and small, and also on $\varphi_j$, which can take any value in $[0, 2\pi]$. The operation is defined in terms of the quantum angular momenta $\hat{J}_z$ and $\hat{J}_x$ but it is not strictly a rotation. In fact, it can be seen instead as a boost. The action is confined to the modes $j$ and $j+1$ and the effect of the inverse on the coefficients of the $q$th row is

$$c_{j+1,q}' = -c_{j,q} \cos \varphi_j \sinh \left( \frac{\epsilon_j}{2} \right)$$

$$+ c_{j+1,q} \left( \cosh \left( \frac{\epsilon_j}{2} \right) - \sin \varphi_j \sinh \left( \frac{\epsilon_j}{2} \right) \right),$$

(32)$$c_{j,q}' = -c_{j+1,q} \cos \varphi_j \sinh \left( \frac{\epsilon_j}{2} \right)$$

$$+ c_{j,q} \left( \cosh \left( \frac{\epsilon_j}{2} \right) + \sin \varphi_j \sinh \left( \frac{\epsilon_j}{2} \right) \right).$$

(33)
Demanding that both $c_{j+1,q} = 0$ and $c_{j,q+1} = 0$, it results
\[
\tan \varphi_j = \frac{c_{j+1,q}c_{j+1,q+1} - c_{j,q}c_{j,q+1}}{2c_{j+1,q}c_{j,q+1}},
\]
\[
\tanh \left( \frac{\varphi_j}{2} \right) = \frac{c_{j+1,q}}{c_{j+1,q} \sin \varphi_j + c_{j,q} \cos \varphi_j}.
\]

It can be seen that the hyperbolic tangent is well defined as long as $|c_{j+1,q}| \ll |c_{j,q}|$ and $|c_{j,q+1}| \ll |c_{j+1,q+1}|$, except if $c_{j+1,q} = 0$ or $c_{j,q+1} = 0$. These consistency conditions are met if $\tau_s$ is sufficiently short but non-vanishing. In particular, $\tau_s$ can be set to a value for which $\eta = 1$, yielding the operator stack shown in (36). In this context the coefficients are most likely real and positive. If they are not, they can be adjusted using unitary operations as previously discussed. A two-mode transformation is applied on the right-extreme of the stack, resulting in the simultaneous cancellation of $\hat{a}_{1}^\dagger$ in the first row and $\hat{a}_{1}^\dagger$ in the second row, leaving the stack as indicated in (37). The lack of unitarity of this transform means coefficient $c_{1,1}^\prime$ can hardly be equal to one, hence it is normalized using the inverse of $\hat{Q}^{(1,1)} = e^{\varphi_j} \hat{a}_{1}^\dagger$, with $\varphi_j = \log c_{j,j}$, when $j = 1$. Thereafter the first mode has been folded and the cancellation-and-normalization sequence starts over again as depicted by (37) and (38).

\[
\begin{bmatrix}
1 & c_{1,1}^\prime & c_{1,2}^\prime & c_{1,3}^\prime & \ldots \\
0 & c_{2,1}^\prime & c_{2,2}^\prime & c_{2,3}^\prime & \ldots \\
0 & 0 & c_{3,2}^\prime & c_{3,3}^\prime & \ldots \\
0 & 0 & 0 & c_{4,3}^\prime & \ldots \\
0 & 0 & 0 & 0 & c_{5,4}^\prime \\
0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\]

\textsuperscript{1} In addition, this operation turns on $\hat{a}_{1}^\dagger$ in the third row, but with a coefficient that is below machine accuracy.
Gathering all the involved steps and putting them in reverse order, the advanced state can be written as

\[
\Psi(\tau + \tau_c) = \left( \prod_{k=N-1}^{1} \hat{Q}^{[k+1,k]} \hat{q}^{[k]} \right) \hat{q}^{[N]} |\Psi(\tau)\rangle.
\]

Furthermore, interaction mechanisms can be incorporated using the split-operator method, analogously to the case of normal evolution. Beginning with a state that has an overlap with the ground state, the whole set of operations is applied systematically until a convergence criterion is satisfied. Figure 1(f) depicts the convergence behavior as captured by measuring the fidelity to the actual ground state as a function of \(\tau\). For the cases studied, convergence is steady but tolerance depends on \(\tau\). As seen for real time calculations, there exists an optimal slice that minimizes the simulation error. The test simulations displayed in figure 2 show a system of interacting bosons subject to a confining potential under the regimes of Mott insulator (top) and superfluid (bottom). Both phases can be realized in experiments of cold atoms in optical lattices with the parameters used in the plots of figure 2. These outcomes coincide qualitatively with the results obtained in [33] using TSE in chains with the same set of parameters and size. Of relevance is the fact that, as long as \(\chi\) is optimal, the symmetry of the state is correctly reproduced by the folding method in spite of the relatively large number of operations correlating modes that are distant. All this reaffirms that little error is generated by the folding process alone, even in the presence of interaction. One advantage of mode folding is that real- and imaginary-time versions can be used in conjunction to simulate quench dynamics where the initial state is set to the ground state of a Hamiltonian with dominant interaction. This is especially useful when the evolution is governed by a single-particle Hamiltonian. Figure 3 exemplify this approach using the ground states featured in figure 2 as initial states. After interaction and confining potential have been switched off, atoms evolve freely toward a fluctuation-dominated phase. In the time span considered, the atom cloud does not expand significantly beyond its initial domain, instead, there is an increase in hopping across the whole extent of the cloud. As longer times are addressed, the simulation cost soars.
The techniques introduced in this work make use of the basic idea of folding of modes to develop numerical routines that calculate the quantum state. Although each application is different, the essence of every method is the same. Certainly, the folding idea is potentially versatile and may give rise to additional simulation protocols. To give an example of another application, let us conceive the dynamical modes as a superposition of the Hamiltonian eigenvectors as follows

\[
\begin{pmatrix}
\alpha_1^\dagger(t_1) \\
\alpha_2^\dagger(t_2) \\
\alpha_3^\dagger(t_3) \\
\vdots
\end{pmatrix} = \hat{b}_1^\dagger e^{-\imath \mu \xi} \begin{pmatrix} E_{11} \\
E_{21} \\
E_{31} \\
\vdots
\end{pmatrix} + \hat{b}_2^\dagger e^{-\imath \nu \xi} \begin{pmatrix} E_{12} \\
E_{22} \\
E_{32} \\
\vdots
\end{pmatrix} + \ldots
\]  

(40)

Figure 3. Mean number of particles and fluctuations after a quench. Once interaction and trapping have been shut down, \( U = \mu = 0 \), the dynamics is generated only by the kinetic term \( J = 0.14 \). The simulation constant is \( \chi = \mathcal{O}(10^3) \). The corresponding states at \( t = 0 \) are shown in figure 2. Mean values do not change much, rather, it is fluctuations that capture the state evolution.

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E_{22} \\
E_{32} \\
\vdots
\end{pmatrix} + \ldots
\]  

(40)
so that
\[ \hat{b}_q^\dagger = \hat{a}_{1q}^\dagger E_{1q} + \hat{a}_{2q}^\dagger E_{2q} + \hat{a}_{3q}^\dagger E_{3q} + \ldots \] (41)

Initially, making \( t_i = 0 \), the superposition lacks the exponential terms. Therefrom, the first move is to fold \( \hat{b}_1^\dagger \) using unitary transformations until only \( \hat{a}_1^\dagger \) remains. Without further action, \( \hat{a}_1^\dagger \) is automatically expelled from the updated versions of all the other \( \hat{b}_s \). Next, the single-particle operation \( e^{-i\hat{E}_1 t_i} \) is applied. The inverses of the transformations employed to fold \( \hat{b}_1^\dagger \) are then executed in reverse order. This brings \( \hat{b}_1^\dagger \) back into the superposition, but accompanied by the term \( e^{-i\hat{E}_1 t_i} \), leaving the other \( \hat{b}_s \) as they were at the beginning. An analogous sequence is then applied, focusing this time on \( \hat{b}_2^\dagger \), in order to incorporate \( e^{-i\hat{E}_2 t_i} \). The rest of the protocol ensues in a logical manner until all the exponentials are introduced. The transformations are then collected and put together to assemble an evolution operator that can be implemented in terms of tensor states. A very similar scheme can be formulated to handle non-unitary transformations, although stability is limited due to the recurrent folding-refolding sequence. Additional folding schemes will be reported in future contributions.

5. Conclusions

Numerical techniques with applications to interacting systems have been introduced and probed. The proposals are developed in the context of local interactions and are based on the idea of mode folding and on the efficient use of tensor states. Real as well as imaginary time implementations of the evolution operator are discussed, elaborating on the handling of each particular case. The method compares well with Trotter–Suzuki expansion in terms of accuracy and simulation time. However, its potential mainly resides, on the one hand, in the possibility of managing hopping of arbitrary scope, and on the other hand, in the perspective that it offers about the role of single-body and many-body structures in the calculation of a quantum state. Mode folding can be applied to study a variety of problems where the Hamiltonian is written in terms of bosonic modes and the interaction is local in the Fock basis. This kind of configurations are frequent in descriptions of cold atom experiments. Some direct fields of application include: studies of weakly interacting Bose–Einstein condensates or Bose mixtures, superfluid to Mott insulator transitions in optical lattices and in helium, formation and expansion of dark or bright solitons, and the formation and dynamics of vortices. As an extension, it would be interesting to consider the prospects of folding of fermionic modes. As it is known, fermion ladder operators display non-local properties. It remains to be seen whether the alternative path taken by mode folding somehow allows to circumvent the adverse effects of fermion algebra for a useful subset of Hamiltonians.

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