Electron-light interaction in nonequilibrium – exact diagonalization for time dependent Hubbard Hamiltonians

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Abstract. We present a straightforward implementation scheme for solving the time dependent Schrödinger equation for systems described by the Hubbard Hamiltonian with time dependent hoppings. The computations can be performed for clusters of up to 14 sites with in principle general geometry. For the time evolution, we use the exponential midpoint rule, where the exponentials are computed via a Krylov subspace method, which only uses matrix-vector multiplication. The presented implementation uses standard libraries for constructing sparse matrices and for linear algebra therefore the approach is easy to use on both desktop computer and computational cluster. We apply the method to calculate time evolution of double occupation and nonequilibrium spectral function of a photo-excited Mott-insulator. The results show that not only the double occupancy increases due to creation of electron-hole pairs but also the Mott gap becomes partially filled.

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1 Introduction

Photo-induced states of matter gain increasing attention for their exotic properties [1, 2, 3] and possible applications, e.g. in the context of energy conversion [4]. The description of these states necessitates nonequilibrium approaches, which are particularly demanding in cases where light brings a strongly correlated electronic system out of equilibrium. The approximate theoretical approaches to correlated systems are being successfully adapted to treat systems out-of-equilibrium (e.g. non-equilibrium dynamical mean-field theory (DMFT) [5], dynamical cluster approximation [6], auxiliary master equation approach [7], GW [8]). The numerically exact approaches, exact diagonalization (ED) [9], or density-matrix renormalization group [10, 11], where the error can be systematically controlled, are still limited to relatively small system sizes. They are however invaluable for benchmarking sophisticated approximate methods. The purpose of this paper is to present a straightforward implementation of the ED method using well-known data formats and algorithms in order to employ highly-optimized libraries. The method allows currently for calculations with up to 14 sites.

We specifically focus on the application of the method to calculate electronic properties of a system that is described by a time-dependent Hubbard Hamiltonian. The time dependence is introduced by coupling of the electronic system to the electromagnetic (EM) field pulse. The EM field is treated classically and enters the hoppings via Peierls’ substitution. We apply the method to study the time evolution of a Mott-insulator after interaction with a light-pulse. By calculating double occupancy and the nonequilibrium spectral function, we show photo-doping of the original Mott-insulator [12] as well as filling of the Mott gap [4, 13].
Figure 1: Example geometry of a two-dimensional six-site lattice with lexicographical ordering of the sites. The energies $v_{ii}$ describe an additional on-site potential, $v_{ij}$ describe the hoppings between sites $i$ and $j$.

The paper is organized as follows. In Sec. 2 we introduce the Hamiltonian of the Hubbard model with Peierls’ substitution, the observables that we present later, as well as notation and units. In Sec. 3 we give a detailed description of data formats and the time stepping algorithm as well as how observables are practically calculated. In Sec. 4 we present the time evolution of double occupancy and non-equilibrium spectral function to illustrate the application of the method. In Sec. 5 we give a short summary and outlook.

2 Model

2.1 Hubbard model

We focus on the paradigm model for strongly correlated electrons, the Hubbard model [14], given by the following Hamiltonian:

$$\hat{H}_{\text{Hubbard}} = -\sum_{i,j,\sigma} v_{ji} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

where $v_{ji}$ describes the relative probability amplitude of an electron hopping from site $j$ to $i$ without change of spin; $U > 0$ is the on-site Coulomb repulsion between two electrons if they reside at the same site (with opposite spins); $\hat{c}_{i\sigma}^{\dagger}$ ($\hat{c}_{i\sigma}$) denote the fermionic creation (annihilation) operators at site $i$ with spin $\sigma$ and $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^{\dagger} \hat{c}_{i\sigma}$ is the occupation number operator (for details on second quantization formalism c.f. [15]).

In the following we restrict our considerations to finite size systems of $N_s \in \mathbb{N}$ sites with hoppings explicitly given by a hopping matrix $v = (v_{ij})_{i,j=1}^{N_s}$. The hopping matrix can be arbitrary, i.e. we can allow for finite hoppings between any two sites. This is where the geometry of the studied system is encoded and where also periodic boundary conditions can be introduced. Lattices of arbitrary dimension and shape can be studied with this approach. Additionally, we can introduce on-site potentials, which can be added as diagonal elements $v_{ii}$ of the hopping matrix. Figure 1 illustrates a $2 \times 3$ box geometry with open boundary conditions.

2.2 Time dependent electron-light interaction

The interaction of electrons with light puts the system out of equilibrium. Here, the light is modeled as a classical electric field pulse

$$\mathbf{E}(t) = E_0 \sin(\omega(t - t_p)) e^{-\frac{(t-t_p)^2}{\sigma^2}}$$

of width $\sigma$, peaked around the time $t_p$ with frequency $\omega$. We set the units of frequency equal to the units of energy ($\hbar \equiv 1$) and the unit of time is then the inverse of the unit of energy. The EM field is
Any state in \( H \) by the state vector \(|\psi\rangle\). Allowing for at most two electrons (with different spins) per site, a state of the system can be represented \(|\psi\rangle\) results presented the NN hoppings will be set to have equal absolute value and this value is used as the unit of energy, i.e., \( |\psi\rangle \). The parameter \( a \) describes the strength of the EM field, whereas \( b \) can be used to set the initial phase factor of the hoppings to 1. Please note, that the Peierls’ substitution introduces only a phase factor to the hoppings and does not change their absolute value. For all the results presented the NN hoppings will be set to have equal absolute value and this value is used as the unit of energy, i.e., \( |v_{ij}| = 1 \).

2.3 Symmetries of the Hamiltonian

Allowing for at most two electrons (with different spins) per site, a state of the system can be represented by the state vector \(|\psi\rangle = |n_{1\uparrow}n_{1\downarrow}n_{2\uparrow} \ldots n_{N_{\downarrow}}\rangle\), where \( n_{i\sigma} \in \{0, 1\} \) is the number of electrons with spin \( \sigma \) at site \( i \). All states of this form are orthonormal and form an abstract Hilbert space which we denote by \( \mathcal{H}(N_s) \). The subspace of all states with \( n_t \) electrons with spin up and \( n_d \) electrons with spin down is denoted by \( \mathcal{H}_{n_t}^n(N_s) \). It is easy to see that there holds (with \( \oplus \) being the direct sum)

\[
\mathcal{H}(N_s) = \bigoplus_{0 \leq n_t, n_d \leq N_s} \mathcal{H}_{n_t}^{n_d}(N_s).
\]

Any state in \( \mathcal{H}(N_s) \) can be seen as excitation of the vacuum state:

\[
(\hat{c}^\dagger_1)^{n_1\uparrow} \cdot (\hat{c}^\dagger_{i\downarrow})^{n_{i\downarrow}} \cdot \ldots \cdot (\hat{c}^\dagger_{N_s\downarrow})^{n_{N_s\downarrow}} |00\ldots0\rangle = |n_{1\uparrow}n_{1\downarrow} \ldots n_{N\downarrow}\rangle,
\]

where the action of fermionic creation and annihilation operators \( \hat{c}^\dagger \) and \( \hat{c} \) on a particular state is given by

\[
\hat{c}^\dagger_{i\sigma}|n_{1\uparrow} \ldots n_{i\sigma} \ldots n_{N\downarrow}\rangle = \delta_{n_{i\sigma}, 0} \sqrt{n_{i\sigma} + 1} |n_{1\uparrow} \ldots (n_{i\sigma} + 1) \ldots n_{N\downarrow}\rangle,
\]

\[
\hat{c}_{i\sigma}|n_{1\uparrow} \ldots n_{i\sigma} \ldots n_{N\downarrow}\rangle = \delta_{n_{i\sigma}, 1} \sqrt{n_{i\sigma}} |n_{1\uparrow} \ldots (n_{i\sigma} - 1) \ldots n_{N\downarrow}\rangle,
\]

respectively. Due to the fermionic anticommutator relations, switching the order of two adjacent operators results in an additional negative sign. Note that the definition (6) is not consistent throughout literature. Finally, the action of the number operator \( \hat{n}_{i\sigma} = \hat{c}^\dagger_{i\sigma} \hat{c}_{i\sigma} \) is given by the equation

\[
\hat{n}_{i\sigma}|n_{1\uparrow}n_{1\downarrow} \ldots n_{N\downarrow}\rangle = n_{i\sigma}|n_{1\uparrow}n_{1\downarrow} \ldots n_{N\downarrow}\rangle,
\]

i.e., this operator counts how many electrons exist on site \( i \) with spin \( \sigma \).

Because the Hubbard Hamiltonian commutes with the occupation number and spin operators, the number of electrons of spin \( \sigma \) in the system \( \sum_i \hat{n}_{i\sigma} \) is invariant under the Hamiltonian (1). This means that in the basis of all states in the Hilbert space \( \mathcal{H}(N_s) \) the Hamiltonian takes a block-diagonal form, according to the direct sum in equation (5). We examine the Hamiltonian in a subspace \( \mathcal{H}_{n_t}^{n_d}(N_s) \) with a fixed number of electrons. Since we are interested in Mott-insulators, we take the system to be half-filled, i.e., \( n_t = n_d = N_s/2 \) and the total spin is zero. For the spectral function calculations, however, we also need the subspace with one electron less (or more).
2.4 Time evolution and observables

The Hubbard Hamiltonian with time-dependent hoppings is a time-dependent Hermitian operator that describes the evolution of a state $|ψ_0⟩ ∈ ℋ(Ns)$ in terms of the Schroedinger equation ($ℏ = 1$)

$$i∂t|ψ(t)⟩ = ˆH(t)|ψ(t)⟩, \quad |ψ(0)⟩ = |ψ_0⟩. \tag{10}$$

Exact diagonalization means that (10) is solved over the finite dimensional Hilbert space $ℋ(Ns)$, which yields a large system of ordinary differential equations. The exact solution is given by

$$|ψ(t)⟩ = ℋ e^{-i \int_{0}^{t} H(τ) dτ} |ψ_0⟩,$$ \tag{11}

where $ℋ$ is the time ordering operator $[15]$. From the solution we can calculate the observables of interest. Specifically, we are interested in the (time-dependent) average double occupation per site

$$⟨d(t)⟩ = \frac{1}{Ns} \sum_{i=1}^{Ns} (⟨ψ(t)|d_i|ψ(t)⟩), \tag{12}$$

with $d_i = ˆn_i↑ ˆn_i↓$, and the average energy per site

$$E(t) = ⟨ ˆH(t)⟩ = \frac{1}{Ns} ⟨ψ(t)| ˆH(t)|ψ(t)⟩. \tag{13}$$

In the following, we drop the explicit time dependencies if it is clear from context. To numerically obtain these quantities of interest, one must assemble a matrix representation of $H$, compute the ground state and then carry out a time stepping before building the expectation values. These tasks are computationally not trivial, since the number of independent variables grows exponentially in the number of sites $Ns$. Note, however, that one can still treat the subspaces $ℋ_{σ}^S(Ns)$ separately, because the time-dependent Hamiltonian $ ˆH(t)$ commutes with $∑_i ˆn_iσ$ (i.e., it preserves the number of electrons).

2.5 Non-equilibrium spectral function

The time-stepping algorithm allows also for calculation of double-time correlation functions. For example the non-equilibrium Green’s functions $G^<$ and $G^>$ are obtained through [5]

$$G^<_{ijσ}(t, t') = i⟨ψ(t)|  ˆc_{jσ}^† ℋ e^{-i \int_{0}^{t'} H(τ) dτ}  ˆc_{iσ} |ψ(t')⟩,$$

$$G^>_ {ijσ}(t, t') = i⟨ψ(t)|  ˆc_{iσ} ℋ e^{-i \int_{0}^{t'} H(τ) dτ}  ˆc_{jσ}^† |ψ(t')⟩, \tag{14}$$

where $ℋ$ is the time ordering operator $|ψ(t)⟩$ is the solution of (10). In order to obtain the correlation functions in (14), we further need to act on $|ψ(t)⟩$ with the annihilation (creation) operator $ ˆc_{iσ}$ $( ˆc_{jσ}^†)$ and then time-evolve the resulting state according to (10) in the subspace with one electron less (more), then act again with $ ˆc_{jσ}^†$ $( ˆc_{iσ})$ and finally build the expectation value.

The non-equilibrium spectral function $[5] A(ω, t) = \frac{1}{π} (A^<(ω, t) + A^>(ω, t))$ can then be obtained after performing a forward Fourier transform of $G^>(t, t')$:

$$A^>(ω, t) = \pm \frac{1}{π} \text{Im} \int e^{iωt_{rel}} G^>(t, t') dt_{rel} \tag{15}$$

with $t_{rel} = t' - t$ (we omitted spin and site indices for simplicity).
Lehmann representation  In equilibrium, the spectral function must remain time independent and can be benchmarked against the Lehmann representation. The site-averaged spectral function is then given by

$$A(\omega) = \frac{1}{N_s} \sum_{i, \sigma} \sum_{|\phi\rangle} (|\langle \phi | c_{i\sigma}^\dagger \psi_0 \rangle|^2 \delta(\omega - E_{|\phi\rangle} + E_0) + |\langle \phi | c_{i\sigma} \psi_0 \rangle|^2 \delta(\omega + E_{|\phi\rangle} - E_0))$$  \hspace{1cm} (16)

Here, \{|\phi\rangle\} is an eigenbasis of \(\mathcal{H}(N_s)\) with respective energy eigenvalues \(E_{|\phi\rangle}\), and \(|\psi_0\rangle\) is the ground state of \(\hat{H}\) with energy \(E_0\).

3 Implementation

The aim of the present paper is to provide efficient data structures and algorithms for assembling matrix representations of Hubbard-Hamiltonians for arbitrary problems of the type that was introduced above, as well as a simple time-stepping algorithm for solving the arising time-dependent Schrödinger equation (10). In the following, the key points of the implementation are discussed. For linear algebra subroutines, existing libraries such as Intel’s MKL, and LAPACK / BLAS were used, as well as the matrix exponentiation library Expokit [17], which was used in the time-stepping algorithm.

3.1 State generation

The matrix representation of the Hamiltonian depends on the chosen basis of \(\mathcal{H}(N_s)\). We now turn to the task of creating a basis for all subspaces \(\mathcal{H}_{n_\uparrow n_\downarrow}^{n_\uparrow n_\downarrow}(N_s)\).

Number of states  Due to spin-up and spin-down electrons being independent, \(\mathcal{H}_{n_\uparrow n_\downarrow}^{n_\uparrow n_\downarrow}(N_s)\) can be identified with the tensor-product space \(\mathcal{H}_{n_\uparrow}^{n_\uparrow}(N_s) \otimes \mathcal{H}_{n_\downarrow}^{n_\downarrow}(N_s)\). The problem of how to place \(n_\uparrow \) \(n_\downarrow\) electrons on \(N_s\) sites is well known in combinatorics. This leads to

$$N_\psi(n_\uparrow, n_\downarrow) = \dim \left( \mathcal{H}_{n_\uparrow}^{n_\uparrow}(N_s) \right) = \dim \left( \mathcal{H}_{n_\downarrow}^{n_\downarrow}(N_s) \right) = \binom{N_s}{n_\uparrow} \binom{N_s}{n_\downarrow}.$$  \hspace{1cm} (17)

Note that \(N_\psi = N_\psi(n_\uparrow, n_\downarrow)\) takes a maximum for \(n_\uparrow = n_\downarrow = N_s/2\). For the number of all states there holds

$$\dim(\mathcal{H}(N_s)) = 2^{2N_s} = 4^{N_s},$$  \hspace{1cm} (18)

since there are \(2N_\psi\) vacancies in the lattice that can be occupied by an electron, or not. This suggests that the general computational effort for assembling a Hamiltonian and for time-stepping on a system with \(N_s\) sites scales at least like \(O(4^{N_s})\). This is shown in Table 1.

Multi-indices  On a computer, the state vectors can be stored internally as integers of sufficient size, with the last \(2N_s\) bits of their binary representation acting as the state. All actions like hopping, creation, and annihilation of electrons can then be implemented as bitwise operations.

To obtain all states that constitute a basis \(\mathcal{B}\) of \(\mathcal{H}_{n_\uparrow}^{n_\uparrow}(N_s)\) for fixed numbers \(n_\uparrow, n_\downarrow,\) and \(N_s\), the hopping of electrons is emulated. Starting from an initial state with the right number of electrons in leftmost position (consistent with Pauli’s principle), all other states can be obtained by repeated hopping (flipping two bits). Due to the independence of spin-up and spin-down electrons, we can treat \(\mathcal{H}_{n_\uparrow}^{n_\uparrow}(N_s)\) and \(\mathcal{H}_{n_\downarrow}^{n_\downarrow}(N_s)\) separately and get all states from building the tensor-product of the respective bases \(\mathcal{B}_\uparrow\) and \(\mathcal{B}_\downarrow\). Therefore, we restrict the presentation to the case of spin-up electrons in the following.
A multi-index $\alpha \in \{1, \ldots, N_s\}^{\{1, \ldots, n\}}$ can be used to represent the (ordered) positions of electrons on the sites, i.e., $\alpha_i = j$ means that the $i$-th electron resides at site $j$. From Pauli’s principle we see that

$$1 \leq \alpha_1 < \ldots < \alpha_n \leq N_s. \quad (19)$$

For such multi-indices one can define a total ordering by

$$\alpha < (>) \hat{\alpha} \quad \iff \quad \alpha_j < (>) \hat{\alpha}_j \quad \text{with} \quad j = \arg \min \{ \alpha_i \neq \hat{\alpha}_i \mid i = 1, \ldots, n \}. \quad (20)$$

This gives a natural meaning to increasing $\alpha$ by one. From (19) we see further that the smallest admissible multi-index satisfies $\alpha_i = i$ and the largest satisfies $\alpha_i = N_s - n_i - i$ for all $i = 1, \ldots, n$. By iterating over all multi-indices yielding to the limitation (19), one obtains all possible permutations of electrons. This is shown in pseudo-code in Algorithm 1.

**Algorithm 1 Generating states with only spin-up excitations**

**Input:** $n_\uparrow, N_s$

**Output:** $\mathcal{B}_\uparrow$

1: $\mathcal{B}_\uparrow = \emptyset$
2: $\alpha_i = \text{for } i = 1, \ldots, n_\uparrow$
3: $|\psi_{\text{init}}\rangle = |11\ldots0\rangle$ /* ones up to the $n_\uparrow$-th position */
4: while $\alpha$ can be further increased do
5: $|\psi\rangle = |\psi_{\text{init}}\rangle$
6: for $i = 1$ to $n_\uparrow$ do
7: /* hop from $i$-th to $\alpha_i$-th position in $|\psi\rangle$ */
8: $\psi[i] = 0, \psi[\alpha_i] = 1$
9: end for
10: $\mathcal{B}_\uparrow = \mathcal{B}_\uparrow \cup |\psi\rangle$
11: increase $\alpha$ by one
12: end while

### 3.2 Assembly of the Hamiltonian

Because of (18), even for small numbers of sites the matrix representation of the Hamiltonian for most electron configurations would require vast amounts of memory if implemented as double-precision complex matrix. Due to the limited overlap of states, many elements of the matrix representation are zero. Utilizing this fact allows for using a well-known sparse matrix format, resulting in a much more memory efficient implementation.

**CSR-format** The most suitable storage format for sparse matrices in the context of the present paper is the so-called Compressed-Sparse-Row (CSR) format [18]. This format stores only the non-zero elements and their positions within the matrix. For a matrix $A \in \mathbb{C}^{N \times N}$ with $N_{nz}$ non-zero elements it consists of three arrays:

- $V \in \mathbb{C}^{N_{nz}}$ consists of all non-zero elements of $A$ in the order they appear in $A$ in a row-wise fashion.
- $J \in \mathbb{N}^{N_{nz}}$ consists of the column indices of all non-zero elements in the same order as in $V$.
- $I \in \mathbb{N}^{N+1}$ stores where the rows in $J$ are. Its $k$-th element refers to the position in $J$ where the $k$-th row begins and the $(k-1)$-th ends.

If $A_{ij}$ is the $k$-th non-zero element of $A$, it can thus be accessed via $V_k$, and there holds $j = J_k$ as well as $I_k \leq k < I_{k+1}$. Due to the Hamiltonian being Hermitian, its matrix representation satisfies $A^\dagger = A$, hence only the upper triangular part needs to be stored explicitly, i.e., $A_{ij}$ for all $i \leq j$. For all other
The memory consumption of storing the Hamiltonian can be estimated by

\[ O(N_{\psi}) \]

Note that (22) is only a worst-case result. If some of the coefficients \( U_i \), \( v_{ij} \), or combinations thereof are zero, this further reduces the number of non-trivial entries of the Hamiltonian’s matrix representation. For the case of half-filling, we get \( N_{na} = N_{\psi} \left( 1 + \frac{1}{2} n_\uparrow (N_s - n_\uparrow) + \frac{1}{2} n_\downarrow (N_s - n_\downarrow) \right) \). Together with the observation that \( N_{\psi} = O(4^N) \), the memory consumption of storing the Hamiltonian can be estimated by \( O(N_{\psi} \ln^2(N_{\psi})) \), which is nearly linear, as opposed to quadratic memory \( O(N_{\psi}^2) \) for dense matrices.

| \( N_s \) | 2 | 4 | 6 | 8 | 10 | 12 | 14 | 16 |
|---|---|---|---|---|---|---|---|---|
| \( N_{\psi} \) | 4.0E+0 | 3.6E+1 | 4.0E+2 | 4.9E+3 | 6.4E+4 | 8.5E+5 | 1.2E+7 | 1.7E+8 |
| \( N_{na} \) | 8.0E+0 | 1.8E+2 | 4.0E+3 | 8.3E+4 | 1.7E+6 | 3.2E+7 | 5.9E+8 | 1.1E+10 |
| \( N_{mem} \) [GB] | 5.5E-7 | 1.2E-5 | 2.6E-4 | 5.3E-3 | 1.1E-2 | 2.0E+0 | 3.7E+1 | 6.8E+2 |

Table 1: Number of states \( N_{\psi} \), maximum number of non-zero elements of the Hubbard-Hamiltonian \( N_{na} \), and estimated memory consumption \( N_{mem} \) in gigabyte for a system with \( N_s \) sites and \( n_\uparrow = n_\downarrow = N_s/2 \). Note that \( N_{na} \) and hence also \( N_{mem} \) are just upper bounds, the real memory consumption may be much lower.

Non-zero elements

For implementing the assembly of the Hamiltonian it is advantageous to know the number of non-zero elements \( N_{nz} \) beforehand, so that the arrays the sparse representation of the Hamiltonian is composed of only need to be allocated once. We now compute this number for a general setting.

Consider fixed numbers \( N_s \), \( n_\uparrow \), and \( n_\downarrow \). Conservation of electron numbers implies that two states can only differ by an even number of entries. Two states differing by an odd number of entries cannot have the same number of electrons and thus do not belong to the same subspace \( H_{nz}^{\uparrow}(N_s) \). Furthermore, a difference of more than two implies that hopping occurs between more than two sites, which is not accounted for by the Hubbard Hamiltonian (1). This leaves only two cases that give an non-zero contribution.

First, a state differs from itself by zero entries, which gives a contribution on the diagonal of the Hamiltonian. Second, one of the \( n_\uparrow \) \( (n_\downarrow) \) spin up (spin down) electrons can hop to one of the \( N_s - n_\uparrow \) \( (N_s - n_\downarrow) \) unoccupied sites, creating a state differing in exactly two entries. There are \( n_\uparrow (N_s - n_\uparrow) + n_\downarrow (N_s - n_\downarrow) \) possibilities for that process, each giving an off-diagonal non-zero contribution to the Hamiltonian. Taking into account that due to the hermiticity of the Hamiltonian, the CSR-format only stores the upper triangle of a matrix, which consists of the diagonal and half of all off-diagonal non-zero elements, the number of non-zero elements evaluates to

\[ N_{nz} = N_{\psi}(1 + \frac{1}{2} n_\uparrow (N_s - n_\uparrow) + \frac{1}{2} n_\downarrow (N_s - n_\downarrow)). \]  

(22)

Only the upper triangular part of \( A \) are considered and the non-zero elements are stored. Note that due to row 3 having no non-zero element above the diagonal, there holds \( I_3 = I_4 = 6 \).

A comparison of memory requirement between naive and sparse (CSR) implementation of the Hamiltonian matrix for the worst case (half-filling) is shown in Table 1. Due to the small number of elements that have to be stored, the addition of matrices with the same sparsity structure can be carried out efficiently by adding the \( V \) arrays of both matrices. Furthermore, because of the row-wise storage of the matrix, the CSR format is predestined for matrix-vector multiplication. Both of which can be done in \( O(N_{nz}) \) operations. The drawbacks of this format, however, lie in element-access for which a linear search of the \( V \) array must be carried out, and in changing the sparsity structure (i.e. set a former zero element to a value other than zero), in which case all three arrays must be altered and possibly reallocated.

The \( \psi \) elements there holds \( A_{ji} = A_{ij}^\dagger \). The following example illustrates this concept:

\[
A = \begin{pmatrix}
1 & 0 & 1 & i & 0 & 1 & 1 & 0 & 1 \\
0 & 2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
-i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}, \quad V = [1, 1, i, 2, 1, 4, 5], \quad F = [1, 3, 4, 2, 5, 4, 5], \quad J = [1, 4, 6, 6, 7, 8].
\]  

(21)

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Time dependent Hamiltonian  We assume the hopping amplitudes to be time dependent in the following way: We consider a Hermitian matrix \( v^{\text{Re}} \in \mathbb{C}^{N_x \times N_x} \) and an Anti-Hermitian matrix \( v^{\text{Im}} \in \mathbb{C}^{N_x \times N_x} \), as well as a phase factor \( f(t) \in \mathbb{C} \) which vanishes for large times, i.e., \( |f(t)| = 1 \) and \( f(t) \to 1 \) as \( t \to \infty \). For each hopping pair \((i, j)\), we can decide if the corresponding hopping amplitude should explicitly depend on time or not. Then, the time dependent hopping amplitudes read

\[
v_{ij}(t) = \begin{cases} v_{ij}^{\text{Re}}(f(t)) + iv_{ij}^{\text{Im}}(f(t)) & \text{if hopping is time dependent,} \\ v_{ij}^{\text{Re}} & \text{else.} \end{cases}
\]

(23)

Note that this definition renders the matrix \( v \) time dependent. By separating time dependent and time independent parts of the Hamiltonian according to (23), the full time dependent matrix representation can be written as

\[
H(t) = H^{(\text{stat})} + \text{Re}(f(t))H^{(\text{Re})} + i\text{Im}(f(t))H^{(\text{Im})}.
\]

(24)

Here, the matrix \( H^{(\text{stat})} \) includes all time independent contributions to the Hamiltonian. These are the Coulomb interaction \( U \) and hopping amplitudes \( v_{ij}^{\text{Re}} \) if hopping between sites \( i \) and \( j \) is modeled as time independent. The matrices \( H^{(\text{Re})} \) and \( H^{(\text{Im})} \) include all hopping amplitudes \( v_{ij}^{\text{Re}} \) and \( v_{ij}^{\text{Im}} \), respectively, which are modeled as time dependent. Due to the function \( f(t) \) converging to one at large times \( t \), the Hamiltonian for such \( t \) is \( H(t) = H^{(\text{stat})} + H^{(\text{Re})} \), which describes the system in equilibrium.

Due to the addition of CSR-matrices being most efficient if all of them have the same structure, we suppose that \( H^{(\text{full})} \), \( H^{(\text{stat})} \), \( H^{(\text{Re})} \), and \( H^{(\text{Im})} \) can be described by only one pair of index arrays \( I \) and \( J \). The assembly of this structure is shown in Algorithm 2. This costs \( \mathcal{O}(N^2) \) operations and is the only operation in our code that has quadratic complexity. However, the assembly is done without knowledge of either \( U \) or \( v \), so the structure is independent of the interaction between sites and hence of the geometry. Therefore, the structure for a specific set of \( N_x, n^*, \) and \( n_s \) only needs to be computed once (which can be done in parallel) and stored as arrays of indices \( I \) and \( J \), hence this step is in general not a bottleneck for repeated simulations (e.g., parameters studies).

**Algorithm 2** Computing the structure of the Hamiltonian

**Input:** \( N_x, B \)

**Output:** \( I, J \)

1. allocate arrays \( I \in \mathbb{N}^{N_x + 1} \) and \( J \in \mathbb{N}^{N_x} \)
2. \( k = 1 \)
3. for \( i = 1 \) to \( N_x \) do
   4. \( I_i = k \)
   5. for \( j = i \) to \( N_x \) do
      6. if \( |\psi_i\rangle \) and \( |\psi_j\rangle \) differ by 2 entries or less then
         7. \( J_k = j \)
         8. \( k = k + 1 \)
      end if
   end for
4. \( I_{N_x + 1} = k + 1 \)

Pre-assembling the structure allows for fast assembly of the Hamiltonian for specific coefficients \( U \) and \( v \), which is shown in Algorithm 3. Note that the first entry in each row of the sparse representation of the Hamiltonian lies on the diagonal, thus line 4 adds a diagonal contribution. Furthermore, as noted in Section 2.3, applying \( \hat{c}^\dagger_{ix} \hat{c}_{j\sigma} \) to a state where hopping from \( j\sigma \) to \( i\sigma \) is possible results in a factor \((-1)^{\delta(i,j,\sigma)}\). Here, \( \delta(i, j, \sigma) \) is given by

\[
\delta(i, j, \sigma) = \text{the number of electrons that lie between the } i\sigma \text{ and } j\sigma \text{ entry.}
\]

This explains the signs in lines 8 and 10.
To further reduce the memory consumption and computational effort for the time-stepping, one can carry out the assignments in lines 6–12 only if at least one of the contributions that would be assigned is non-vanishing. Afterwards, the structure can be updated to only account for the actual non-vanishing elements of the Hamiltonian.

It is apparent that the cost of Algorithm 3 is $O(N_{nz})$ and that the memory consumption of the Hamiltonian is proportional to $N_{nz}$ (the column indices and values) plus a small offset (the row-index pointer array $I$). Upper bounds for the memory consumption for certain parameters $N_s$, $n^\uparrow$, and $n^\downarrow$ are shown in Table 1.

Algorithm 3 Assembling all parts of the Hamiltonian

**Input:** $N_\psi, B, U, v, \text{ precomputed } I, J$

**Output:** $H^{(\text{stat})}, H^{(\text{Re})}, H^{(\text{Im})}$

1: allocate arrays $H^{(\text{stat})}, H^{(\text{Re})}, H^{(\text{Im})} = 0 \in \mathbb{C}^{N_{nz}}$

2: $k = 1$

3: for $i = 1$ to $N_\psi$ do

4: $H^{(\text{stat})}_k = U \sum_{i=1}^{N_s} \langle \psi_i | \hat{d}_i | \psi_i \rangle$

5: for $j = I_i$ to $I_i + 1$ do

6: determine sites $\alpha$ and $\beta$ between which the hopping $| \psi_J \rangle \rightarrow | \psi_i \rangle$ happens

7: if hopping between sites $\alpha$ and $\beta$ is time-dependent then

8: $H^{(\text{Re})}_k = (-1)^{\delta(\alpha,\beta,\sigma)} v^{(\text{Re})}_{\alpha\beta}, H^{(\text{Im})}_k = (-1)^{\delta(\alpha,\beta,\sigma)} v^{(\text{Im})}_{\alpha\beta}$

9: else

10: $H^{(\text{stat})}_k = H^{(\text{stat})}_k + (-1)^{\delta(\alpha,\beta,\sigma)} v^{(\text{Re})}_{\alpha\beta}$

11: end if

12: $k = k + 1$

13: end for

14: end for

3.3 Time-stepping algorithm

Each state in $\mathcal{H}^{n^\uparrow n^\downarrow}_s(N_s)$ can be uniquely represented by a vector $v \in \mathbb{R}^{N_\psi}$. Hence, we can write the ODE system resulting from the time dependent Schrödinger equation (10) as

$$
\frac{d}{dt} \mathbf{v}(t) = \hat{H}(t) \mathbf{v}(t), \quad \mathbf{v}(0) = \mathbf{v}_0,
$$

where $\hat{H} \in \mathbb{C}^{N_\psi \times N_\psi}$ is the matrix representation of $\hat{H}$ and $\mathbf{v}_0$ is the vector representing the ground state of the system. We now discuss how to solve (25) numerically.

**Ground state** In order to obtain the initial state for the time-stepping, we consider the system described by (10) to be in thermal equilibrium. Then, the ground state $\psi_0 \in \mathcal{H}^{n^\uparrow n^\downarrow}_s(N_s)$ is defined as the eigenstate corresponding to the smallest eigenvalue of $\hat{H}$:

$$
\hat{H} | \psi_0 \rangle = E_0 | \psi_0 \rangle, \quad E_0 = \min \left\{ E \mid E \text{ is an eigenvalue of } \hat{H} \right\}.
$$

Numerically, we obtain a representation $(E_0, \mathbf{v}_0)$ of the eigenpair $(E_0, \psi_0)$ by a variant of the so-called power iteration method (see e.g. [19]).

The power iteration method iteratively computes the eigenvalue $\lambda$ of largest absolute value and the corresponding eigenvector $\mathbf{v}$ of a Hermitian matrix $M \in \mathbb{C}^{N \times N}$ by the recursive formulae

$$
\mathbf{v}^{(n)} = \frac{M \mathbf{v}^{(n-1)}}{\| M \mathbf{v}^{(n-1)} \|}, \quad \lambda^{(n)} = (\mathbf{v}^{(n-1)})^\dagger M \mathbf{v}^{(n-1)},
$$

(27)
starting with an arbitrary vector \(v^{(0)}\) not orthogonal to the desired vector. The iteration stops if \(\lambda^{(n)}\) and \(v^{(n)}\) are sufficiently near to the real values, which is determined by an a-posteriori error estimate. This is shown in Algorithm 4.

Applying the power iteration to \(H\) gives an approximate eigenpair \((E, v)\). If \(E\) is negative, we have already found the smallest eigenvalue of \(H\) and we can set \(E_0 = E\), and \(v_0 = v\). Else, if \(E \geq 0\) and hence is the largest eigenvalue of \(H\), we apply the power iteration once again to the shifted matrix \(H - EI\), obtaining an approximate eigenpair \((E', v')\). Since \(H - EI\) has only non-positive eigenvalues, \(E'\) approximates its smallest eigenvalue. Then, we set \(E_0' = E + E'\) and \(v_0 = v'\), as they approximate the smallest eigenvalue of \(H\) and the corresponding eigenvector, respectively. This is shown in Algorithm 5.

**Algorithm 4** Power iteration method

**Input:** Hermitian matrix \(M \in \mathbb{C}^{N \times N}\), maximum number of iterations \(N_{\text{max}}\), \(\text{tol}\)

**Output:** approximate eigenpair \((\lambda, v)\) of \(M\)

1. initialize \(v^{(0)}\) randomly and normalize, \(\lambda^{(0)} = 0\)
2. for \(i = 1\) to \(N_{\text{max}}\) do
3. \(v^{(i)} = Hv^{(i-1)}\)
4. \(\lambda^{(i)} = \langle v^{(i)} | v^{(i-1)} \rangle\)
5. \(v^{(i)} = v^{(i)} / \|v^{(i)}\|\)
6. if \(|\lambda^{(i)} - \lambda^{(i-1)}| \leq \text{tol} |\lambda^{(i-1)}| \) and \(\|v^{(i)} - v^{(i-1)}\| \leq \text{tol} \|v^{(i-1)}\|\) then
7. break
8. end if
9. end for
10. \(\lambda = \lambda^{(i)}, v = v^{(i+1)}\)

**Algorithm 5** Computing the ground state

**Input:** matrix representation \(H\) of hamiltonian, \(N_{\text{max}}\), \(\text{tol}\)

**Output:** approximate groundstate \((E, v)\) of \(H\)

1. obtain \((E, v)\) from applying Algorithm 4 to \((H, N_{\text{max}}), \text{tol}\)
2. if \(E < 0\) then
3. \(v_0 = v, E_0 = E\)
4. return
5. end if
6. obtain \((E', v')\) from applying Algorithm 4 to \((H - EI, N_{\text{max}}, \text{tol})\)
7. \(v_0 = v', E_0 = E + E'\)

**Exponential midpoint rule and Krylov subspace method** The continuous evolution solving (25) is the discrete analog of (11). For small times \(t\), it can be approximated with sufficient accuracy by a Magnus-expansion of order zero [20], which gives

\[
\mathbf{v}(t) \approx \exp \left( -i \int_0^t H(\tau) \, d\tau \right) \mathbf{v}_0. \tag{28}
\]

By approximating the integral in the exponent via the midpoint rule

\[
\int_a^b f(t) \, dt \approx (b - a) f \left( \frac{b + a}{2} \right), \tag{29}
\]

the approximation (28) can be further simplified. Considering consecutive intervals of length \(\tau\) for which the midpoint rule and the Magnus-expansion are sufficient approximations, yields a sequence of vectors defined by

\[
\mathbf{v}^{(n+1)} = \exp ( -iH(n\tau + \tau/2) ) \mathbf{v}^{(n)}, \quad \mathbf{v}^{(0)} = \mathbf{v}_0, \tag{30}
\]

that approximate the solution at times \(n\tau\): \(\mathbf{v}^{(n)} \approx \mathbf{v}(n\tau)\). Note that these approximations are of lowest order and thus the time stepping cannot, in general, be expected to surpass first-order convergence.
The main difficulty in (30) is evaluating the exponential of the large anti-Hermitian sparse matrix \(-iH\tau\). To this end we employ a so called Krylov subspace method as described in [17] and references therein. For a matrix \(H\) and a vector \(v\), the \(m\)-th Krylov subspace is defined as
\[
K_m(H, v) = \text{span}\{v, Hv, \ldots, H^{m-1}v\}.
\]  
(31)

The space \(K_m(H, v)\) is thus spanned by vectors obtained by (sparse) matrix-vector multiplication only, which can be carried out efficiently in the CSR-format. Let \(V \in \mathbb{C}^{N_x \times m}\) be a projection to an orthonormal basis of \(K_m(H, v)\). Then, by projection, we can approximate \(H\) by a lower dimensional matrix \(h \in \mathbb{C}^{m \times m}:
\[
H \approx VhV^\dagger.
\]  
(32)

Hermiticity of \(H\) implies hermiticity of \(h\) and basic orthogonality properties of a Krylov space (c.f. [17]) cause \(h\) to be Hessenberg, i.e. \(h_{i,j} = 0\) for \(i > j + 1\). Together, we can infer \(h\) to be tridiagonal, hence the orthonormal basis \(V\) as well as \(h\) can be computed via a Lanczos-algorithm in \(O(mN_v)\) operations, as is done in Algorithm 6.

Algorithm 6 Computing a time-step by the Krylov subspace method

\[\begin{align*}
\text{Input: } & H, v, \tau, N_{\text{max}}, \text{tol} \\
\text{Output: approximation to } & \exp(-iH\tau)v
\end{align*}\]

1: \(\alpha = \|H\|, \beta = \|v\|
2: V_1 = v, y^{(0)} = 0
3: for \(j = 1 \text{ to } N_{\text{max}} \text{ do}
4: \quad w = HV_{j,i} - h_{j-1,i}V_{j-1,i}
5: \quad h_{j,j} = V_{j,i}^Tw
6: \quad w = w - h_{j,j}V_{j,j}
7: \quad h_{j+1,j} = \|w\|, h_{j,j+1} = h_{j,j+1}^*
8: \quad V_{j+1,i} = w/h_{j,j+1}
9: \quad y^{(j)} = \exp(-i\tau h_{j,j})(1,0,\ldots,0)^T
10: \text{* \text{a-posteriori error \text{*}}}
11: \quad \delta = \|y^{(j)} - y^{(j-1)}\|/\|y^{(j)}\|
12: \text{if } \delta < 1 \text{ then}
13: \quad \varepsilon = \min(1 + \|y^{(j)}\|, \frac{\alpha}{1-\tau})\|y^{(j)}\|
14: \text{else}
15: \quad \varepsilon = 1 + \|y^{(j)}\|
16: \text{end if}
17: \text{if } \varepsilon < \text{tol or } |h_{j+1,j}| < \alpha \text{ tol then}
18: \quad \text{return } \beta y^{(j)}
19: \text{end if}
20: \text{end for}
\]

For the exponentiation of a small \(m\)-by-\(m\) tridiagonal matrix, numerically stable and efficient methods are implemented in the library Expokit [17]. In total, this steps requires \(O(m^3)\) operations. Together, this leads to an approximation of the exponential in (30):
\[
\exp(-iH\tau)v \approx \sum_n \frac{1}{n!}(-iVhV^\dagger\tau)^n v = V \exp(-iH\tau)V^\dagger v.
\]

The the dimension \(m\) of the Krylov subspace should be chosen sufficiently large to ensure small approximation errors, but small enough to limit the computational effort. In Algorithm 6, the dimension is chosen adaptively in each step via an a-posteriori error estimate, because the difficulty of computing a time-step can vary, according to \(H(t)\). We use a method suggested in [21], which uses the norm of the difference of two consecutive approximations of the solution in \(K_{m-1}(H, v)\) and \(K_m(H, v)\). The validity of this error estimate is shown in Figure 2. Although the error estimator underestimates the error by nearly an order of magnitude, its convergence has the same rate as the error, rendering the estimate a good indicator of convergence.
Algorithm 6 shows one time step as presented above. For sake of brevity, $V_{:,j}$ denotes the $j$-th column of $V$, and $h_{j,j}$ denotes the restriction of $h$ to the first $j$ rows and columns. The whole time stepping algorithm to solve (25) consists of applying Algorithm 6 iteratively.

### 3.4 Observables

To compute the discrete analog of the expectation value $\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle$ of an observable $\hat{A}$ with respect to a state $\psi \in H_{n_s}^n(N_{\psi})$, we need to discretize the action of $\hat{A}$ on $\psi$. For the energy $\langle \hat{H}(t) \rangle$, this is already achieved by the discrete Hamiltonian $H(t)$.

For the double occupation, a discretization must mimic the evaluation $\hat{d} | \psi \rangle = d | \psi \rangle$. This is done by computing a weight vector $w_{d} \in \mathbb{N}^{N_{\psi}}$. The $k$-th element of $w_{d}$ is the number of double occupations in the $k$-th state of the considered basis, i.e., $(w_{d})_k = \langle \psi_k | \hat{d} | \psi_k \rangle$. The desired expectation value can then be obtained by

$$\langle \hat{d} \rangle = v^\dagger (w_{d} \circ v),$$  \hspace{1cm} (33)$$

where $\circ$ denotes element-wise multiplication of vectors. For other observables like double occupation at a specific site, or electron occupation, one can compute the corresponding weight vector and proceed analogously.

### 3.5 Equilibrium spectral function

The implemented tools can also be used to compute the spectral function of the system from the Lehmann representation. Formula (16) is not suitable for implementation, because of the $\delta$-distributions. Approx-
imating these by Lorentzians with width $\epsilon > 0$, this leads to

$$A(\omega) = \sum_{i,\sigma} \sum_{|\phi\rangle} \left( \frac{\epsilon |\langle \phi| \hat{c}^\dagger_i \sigma |\psi_0 \rangle|^2}{(\omega - E_\phi + E_0)^2 + \epsilon^2} + \frac{\epsilon |\langle \phi| \hat{c}_i \sigma |\psi_0 \rangle|^2}{(\omega + E_\phi - E_0)^2 + \epsilon^2} \right). \tag{34}$$

This approximation preserves relative values of spectral weights.

To compute (34), note that, e.g., the creation operator $\hat{c}^\dagger_i$ maps $H_n^{\uparrow \downarrow}(N_s)$ to $H_{n+1}^{\uparrow \downarrow}(N_s)$. Then, from (5) it is clear that only an eigenbasis of $H_{n+1}^{\uparrow \downarrow}(N_s)$ needs to be considered, which can be obtained by assembling the Hamiltonian in this subspace and applying an eigendecomposition. For the evaluation of $\hat{c}^\dagger_i |\psi_0\rangle$ the relation between states in $H_n^{\uparrow \downarrow}(N_s)$ and $H_{n+1}^{\uparrow \downarrow}(N_s)$ introduced by $\hat{c}^\dagger_i$ must be known. This relation can be found by a linear search on the states of $H_{n+1}^{\uparrow \downarrow}(N_s)$, or, more efficiently, via hash-maps (see the following subsection). Here, the anti-commutator relations for creation and annihilation operators have to be taken into account.

These computations can be carried out analogously for the corresponding term with annihilation operators and for the spin-down case (which can be omitted for systems with spin symmetry).

### 3.6 Non-equilibrium spectral function

In order to evaluate Eq. (14), the action of a creation (annihilation) operator $\hat{c}_i^{\dagger \sigma}$ ($\hat{c}_i^{\sigma}$) on a state vector $|\psi\rangle$ is implemented following the definition in Eq. (7).

**Algorithm 7 Operator $\hat{c}_i^{\sigma}$**

**Input:** Basis-state $|\varphi_k\rangle$, $N_s$, site-orbital index $i=\{\sigma\}$  
**Output:** $c_{i\sigma} = \delta_{n_{i\sigma}, n_{i\sigma} + 1}$

1: if $n_{i\sigma} \neq 0$ then  
2: $c_{i\sigma} = 0$  
3: else  
4: $c_{i\sigma} = 1$  
5: for $\{j\sigma\} < \{i\sigma\}$ do  
6: if $n_j \neq 0$ then  
7: $c_{i\sigma} = c_{i\sigma} \cdot (-1)$  
8: end if  
9: end for  
10: end if

Since a general state $|\psi\rangle$ is represented as a linear combination of basis states $|\varphi_k\rangle$

$$|\psi\rangle = \sum_{k=1}^{N_{\psi}} w(k) |\varphi_k\rangle \equiv w \cdot |\varphi\rangle, \tag{35}$$

it remains only to determine the ordering of states in the subspace with one added or one removed electron. It is not identical to the ordering of the states obtained from $\hat{c}_i^{\dagger \sigma} |\psi\rangle$ or $\hat{c}_i^{\sigma} |\psi\rangle$. Hence, after applying e.g. $\hat{c}_i^{\dagger \uparrow}$ we have to find the index of the resulting state in the subspace $H_{n+1}^{\uparrow \downarrow}(N_s)$. A simple linear search and match are very inefficient. To this aim we apply a fermionic hashing function from Ref. [22] given by

$$I = \sum_{i=1}^{N_s} \left( \frac{p_i}{i} \right), \tag{36}$$

13
where $I$ is the hashing index, $p_i$ is the spin-site that the particle $i$ occupies and \( \binom{m}{n} = 0 \) if $n > m$. This function provides a unique mapping of a state-vector (in its binary representation as an integer) to an integer in the range $0 \leq I < N_{\text{states}}$, which also directly corresponds to the ordering of the states. Thus, if the action of a creation (annihilation) operator on a given state-vector is non-zero, the corresponding hashing index will be calculated in order for it to be correctly assigned.

The Fourier transform in equation (15) is performed as post-processing. As in case of equation (34) we also use broadening to numerically represent the delta-distributions occurring for a finite system. This is achieved by modifying the Fourier transform in (15) by adding the factor $e^{-\varepsilon t_{\text{rel}}}$:

$$A^\omega(\omega, t) = \pm \frac{1}{\pi} \text{Im} \int e^{-\varepsilon t_{\text{rel}}} e^{i\omega t_{\text{rel}}} G^\omega(t, t') \, dt_{\text{rel}}.$$  

(37)

### 3.7 Numerical cost and limitations

The method presented in this paper can handle computations of up to 14 sites. For more than 14 sites, some issues must be resolved. First, indexing with a 32-bit integer format is no longer possible. Possible remedies include using long integer indexing or splitting the arrays.

Furthermore, computation time may be an issue. The computation necessary for obtaining double occupancies for a 14-site chain (presented in Fig. 6) took about seven hours on a single node on the VSC-3 computer cluster, which is equipped with a 16-core Intel Xeon processor and 256 GB of RAM. Multi-node computing may accelerate simulations, e.g., by outsourcing computations of expectation values. As seen in Sec. 3.2, the time needed for the time-stepping rises with $\mathcal{O}(N^2 \ln^2(N \psi))$. Moreover, Algorithm 2 may become the bottleneck. Although it only needs to be executed once for a specific electron-configuration, the number of operations scales with $\mathcal{O}(N^2 \psi^2)$. For 14 sites and half-filling, this takes about one day to compute on 16 cores in parallel. To overcome this issue, one needs to implement a more efficient way of state generation. If the states are created in an order that for a given state the task of finding all states that give a non-zero contribution to the Hamiltonian can be done in less than linear time, the effect of the bottleneck can be significantly reduced.

Also virtual memory can be an issue for more than 14 sites, as can be seen from Table 1. For 16 sites, the upper bound for the memory needed to store the Hamiltonian is 680 GB. However, for typical geometries, many elements of $v$ are zero so that the effective memory consumption is about one fourth of the upper bound.

### 3.8 Benchmarking

For certain values of the parameters $U$ and $v_{ij}$, the eigenvalues of the Hamiltonian (1) can be computed analytically. They were compared to the numerically obtained values, and agreement within machine precision was found. Also the eigenvalues of Hamiltonians that emanate from different geometries for which the physics should be the same were compared. Again, no significant deviation was found.

For the time-stepping algorithm we tested if stationary systems are described correctly. Figure 3 shows double occupancy and its error as well as the error of calculating the energy (difference between expected and obtained values) as a function of time for a time independent Hamiltonian. The time evolution was started from a ground state. From Fig. 3 we can infer that the ground state is indeed an eigenstate and that the time evolution of such a state can be correctly integrated by our algorithm. The computation of the Green’s function was benchmarked against an analytical computation for a two-site system.
4 Results

In the following we present results obtained for chain and box geometries with nearest neighbour hopping and open boundary conditions. We always start the time evolution from the ground state of the system and choose it to be a Mott-insulator with $n_\uparrow = n_\downarrow = N_s/2$. The time step in the time-stepping algorithm is set to $\tau = 0.005$, with the unit of time being $1/\text{energy}$. The unit of energy (as already introduced in Sec. 2) is the absolute value of the NN hopping $|v_{ij}| = 1$.

4.1 Time evolution of double occupation

The effect of the light pulse described by $f(t)$ given in Eq. (4) on the electronic system mainly depends on the relation between the pulse frequency $\omega$ and the size of the gap. In Fig. 4 we show the time evolution of average double occupation and energy per site for an 8-site chain with $U = 4$ for different pulse frequencies. The size of a gap for $U = 4$ is approximately equal to 2 (it can be seen in Fig. 5, where we show the equilibrium spectral functions obtained from Lehmann representation for the same chain and different values of $U$). For frequencies that are significantly lower or higher than $\omega = 2$ the electrons cannot be excited across the Mott gap and thus the system cannot absorb energy. Almost no electron-hole pairs are generated and the double occupancy and energy stay the same after the pulse. Only during the pulse energy is absorbed for $\omega = 11$ (there is still some spectral weight in the tails of the Hubbard bands, see Fig. 5), but this energy is returned to the pulse (similar effects are seen in [13]).

For frequencies $3.5 - 8.5$ we observe an increase of double occupancy during the pulse and the increase is the strongest for $\omega = 3.5$ which approximately matches the distance between the centra of the Hubbard bands. The energy is absorbed and transformed into potential energy by creating doubly occupied sites (electrons in the upper Hubbard band and holes in the lower Hubbard band). For $\omega = 8.5$ only the
lowest energy electrons can be excited to the range of the upper Hubbard band, where they occupy the high-energy part. Thus only a few electrons are excited but with high energies. This causes the double occupation to barely rise, whereas the energy rises by a moderate amount.

We see that, as a function of time, the double occupation oscillates with two different frequencies. This is even more visible when we look at the site resolved double occupation as presented in Fig. 6 for a 14-site chain. The high frequency oscillation is equal to the light pulse frequency and is typically compensated by another site where the oscillation is in opposite phase. The lower frequency is found to be inversely proportional to the length of the chain (not shown here). It can be viewed to originate from doublon and holon movements through the chain, leaving the overall number of doublons nearly constant. The site-averaged double occupancy is almost constant in time after the pulse. We see only a slight oscillation (with the lower frequency), almost not visible in Fig. 6. In Fig. 7 we also show the values of double
Figure 6: Time evolution of double occupation for a 14-site chain with $U = 3.5, v_{ij} = 1.0$, and pulse frequency $\omega = \frac{7}{4} \pi, t_p = 6, \sigma = 2$ and $\alpha = 0.8$. Here the colored lines represent the double occupation of the separate sites, the black line represents the average value. Sites that have the same distance from the center of the chain have the same color. The vertical dashed lines represent times, at which snapshots are shown in figure 7. The first snapshot is taken at a phase of steepest ascend. The second and third snapshots are taken at a local maximum and minimum, respectively, of the total double occupation after the pulse.

occupancy along the chain for three different times: $t = 6.1$ during the pulse, $t = 17.2$ after the pulse at a local maximum of total double occupancy and $t = 18.9$, at a local minimum.

4.2 Nonequilibrium spectral function

In Fig. 8 we show the imaginary part of the lesser Green’s function, as defined in Eq. (14), for different times after the pulse. At $t = 0$ we start from the ground state where $A^<$ does not have any spectral weight above $\omega = 0$. For later times we observe photo-induced generation of electrons in the upper Hubbard band with a simultaneous reduction of spectral weight in the lower Hubbard band. This effect, known as photo-doping, has already been found with other methods – nonequilibrium DMFT [12] and also with quantum Boltzmann equation [13]. At later times, there is also an additional spectral weight shift inside the upper Hubbard band, which corresponds to the first step of thermalisation [13].
Figure 7: Snapshots of the time evolution depicted in Figure 6 at different times. The darkest lines mark the value of the double occupation at the specified time $t = 6.1, 17.2, 18.9$, the other lines are the values of the three previous time steps with $\Delta t = 0.05$, increasing in saturation and darkness with time, creating the effect of the values leaving a trace.

Figure 8: Local, site averaged, $A^< (\omega, t)$ for $t = 8, 12, 20$ and the equilibrium spectral function from Lehmann representation (grey) for an 8-site chain with $U = 6$ and open boundary conditions at half-filling. The parameters of the pulse are $a = 0.8, \omega = 9, t_p = 8$ and $\sigma = 2$.

In Fig. 9 we show the full spectral function $A(\omega, t)$ for the same parameters and times as in Fig. 8. We additionally see that the spectral weight shifts also into the Mott-gap causing a gap reduction (photomelting). This effect is also seen in the nonequilibrium DMFT study [12], but is missed by the quantum
Boltzmann approach [13]. The gap filling is even stronger in case we choose a smaller pulse frequency \( \omega = 6 \) (as compared to \( \omega = 9 \) for the earlier plots), which allows to initially pump more energy into the system. At \( t = 8 \), during the pulse, the gap is smallest and then the energy is reabsorbed into the pulse which leads to a slightly increased gap at later times.

![Graph](image)

Figure 9: Local, site averaged, nonequilibrium spectral function \( A(\omega,t) \) for \( t = 8, 12, 20 \) and the equilibrium spectral function from Lehmann representation (grey) for the same parameters as in Fig. 8

![Graph](image)

Figure 10: Local, site averaged, nonequilibrium spectral function \( A(\omega,t) \) for \( t = 8, 12, 20 \) and the equilibrium spectral function from Lehmann representation (grey) for the same parameters as in Fig. 8 but for the pulse frequency \( \omega = 6 \)

For the box geometry, which we illustrate in Fig. 11 for the same parameters as in Fig. 10, but for \( 2 \times 4 \) arrangement of sites, we observe very similar behaviour of the spectral weight transfers as for the chain.
5 Summary and outlook

We have presented a simple implementation scheme for solving the time dependent Schrödinger equation for systems described by the Hubbard Hamiltonian with time dependent hoppings. As example application we study the photo-induced doping and gap filing of a Mott-insulator. We also show a detailed time dependence of double occupation after applying a light pulse for a 14-site system with open boundary conditions.

Larger cluster sizes can become possible when the matrix elements are generated during computation and not stored explicitly. The presented implementation allows for this change, since only matrix-vector multiplications are needed. These can be replaced by operators that directly change the vector, without storing them in the matrix form.

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