Calculating Floquet states of large quantum systems: A parallelization strategy and its cluster implementation

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Abstract

We present a numerical approach to calculate non-equilibrium eigenstates of a periodically time-modulated quantum system. The approach is based on the use of a chain of single-step time-independent propagating operators. Each operator is time-specific and constructed by combining the Magnus expansion of the time-dependent system Hamiltonian with the Chebyshev expansion of an operator exponent. A construction of a unitary matrix of the Floquet operator, which evolves a system state over the full modulation period, is performed by propagating the identity matrix over the period. The independence of the evolutions of basis vectors makes the propagation stage suitable for implementation on a parallel cluster. Once the propagation stage is completed, a routine diagonalization of the Floquet matrix is performed. Finally, an additional propagation round, now with the eigenvectors as the initial states, allows to resolve the time-dependence of the Floquet states and calculate their characteristics. We demonstrate the accuracy and scalability of the algorithm by applying it to calculate the Floquet states of two quantum models, namely (i) a synthesized random-matrix Hamiltonian and (ii) a many-body Bose-Hubbard dimer, both of the size up to $10^5$ states.

Keywords: Many-body quantum systems, Floquet theory, Magnus expansion, Scalability analysis, High performance computing

1. Introduction

Fast progress in manipulations with cold and ultra-cold atoms, quantum optics and nanoscale fabrication techniques has brought quantum physics in touch with technology \cite{1,2,3}. It is natural then that computational quantum physics plays an ever increasing role in explaining and guiding current experiments and suggesting new \cite{4}. From the computational point of view, the complete resolution of a coherent, i.e., an isolated from the environment, quantum system means the solution of the eigenvalue problem for the system Hamiltonian $H$. When the Hamiltonian is time-independent, this task can be executed by performing full diagonalization of the Hamiltonian matrix. When the system becomes large then the size of the matrix does not allow for the full diagonalization. The task, however, could be restricted to finding lowest energy eigenstate(s) which can be accomplished by using the Lanczos algorithm \cite{5} or more sophisticated tools, such as the Density-Matrix Renormalization Group (DMRG) methods \cite{6}. In cases that the system is periodically modulated in time, its Hamiltonian becomes a time-periodic matrix $H(t + T) = H(t + 2\pi/\omega) = H(t)$. Then, the dynamics of the system is governed by the set of so termed Floquet eigenstates \cite{7,8}. These states are not eigenvectors of the Hamiltonian $H(t)$ but instead of the unitary Floquet operator

$$U_T = T \exp \left[ -i \frac{\hbar}{T} \int_0^T H(\tau) d\tau \right], \quad (1)$$

where $T$ is Dyson’s time-ordering operator. This operator propagates the system over the one full period $T$ of modulation, while the corresponding time-periodic Floquet states (see below) at equal times $t = t'$ \cite{9,10} form a time-periodic orthogonal basis spanning the system Hilbert space and evolving under the action of the time-dependent Hamiltonian. The structure of the unitary Floquet matrix, and thus properties of the Floquet states, depend on the modulation protocols and parameters. This is a key feature of periodically driven quantum systems which makes them so attractive to the theoreticians and experimentalists working in the filed of quantum optics, optomechanics and solid state physics \cite{9,10,11,12,13}. Strong modulations can sculpt a set of non-equilibrium eigenstates which may drastically differ from the states exhibited by the system in the unmodulated, time-independent limit. Modulations allow to grasp novel phenomena and effects which are out of reach within time-independent Hamiltonians; they can be used to create topological insulators in semiconductor wells \cite{14}, synthesize Majorana fermions in quantum wires \cite{15}, and engineer gauge fields for spinless neutral atoms \cite{16}. The calculation of Floquet states of a large quantum system constitutes a challenge. The key step is a construction of the corresponding unitary Floquet matrix, Eq. (1) (its final diagonalization is such a routine as, for example, the diagonalization...
of stationary Hamiltonian matrices). The most straightforward way to obtain $U_T$ is to numerically propagate the identity matrix over the time period $T$. However, the propagation with a time-dependent Hamiltonian operator is an issue itself, to be addressed in the next section. There are two ways to do so.

The first option is to use piecewise-constant modulation functions. This allows to reduce the computational task to the diagonalization of time-independent Hamiltonians, one for every time interval, and the expansion of eigenvectors of a preceding Hamiltonian in the basis of the consecutive one. Such modulations were used to investigate connections between integrability and thermalization [17, 18, 19], and to explore disorder-induced localization [20] in periodically driven many-body systems. With respect to the thermalization it was found that the modulations heat the system to the infinite temperature so that the system Floquet states are near uniformly smeared over the eigenbasis of the system in the absence of driving [17, 18, 19]. An important question that immediately arises is whether this is a universal phenomenon or it is related to the non-differentiability of the modulation function (which property induces the presence of all multiple frequencies $k\omega$, $k = 1, 2, ...$, in the spectrum of the modulations function). Evidently, this question cannot be answered without going beyond the piecewise setup. In addition, in the view of possible experimental realizations, smooth continuous modulations are also more preferable.

An alternative option is to expand the time-dependent Hamiltonian into a Fourier series and, and then truncating it, by keeping $2F + 1$ harmonics $k\omega$, $k = -F, ..., 0, ..., F$ only, to reduce the problem to the diagonalization of a time-independent super-Hamiltonian [8, 21]. This is a reliable method to obtain Floquet spectrum of a system of a size up to a hundred of states. For larger systems, this strategy leads to a computational problem: The size of the super-Hamiltonian scales as $N \times (2F + 1)$, where $N$ is the dimension of the system’s Hilbert space. Computational diagonalization efforts increase as $[N \times (2F + 1)]^3$, while the known diagonalization algorithms are poorly scalable. For a system of the size $N = 10^4$, already $F = 50$ harmonics is too much; a full diagonalization of a $10^6 \times 10^6$ matrix is unfeasible.

At the same time, this large number of harmonics is seemingly not enough to resolve faithfully the Floquet spectrum of the system.

Therefore, in order to calculate the Floquet state of a system with $N \geq 10^3$ states, the propagation stage has to be included into an algorithm. A propagation method should guarantee a high accuracy with respect not only to the unitarity of the time evolution but also with respect to the phases of complex vectors. That is because Floquet states appear as superpositions of basis vectors used to write system’s Hamiltonian. Accumulated phase errors will destroy the interference and lead to an incorrect set of Floquet states. As we show in Section 4 quantum interference effects, together with some facts from the quantum chaos theory, can be used to benchmark the accuracy of an algorithm.

Because of the trade-off between the accuracy and system size, the time of sequential vector propagation grows super-linearly with $N$. Faithful calculations of Floquet spectra of non-integrable systems (that are systems whose Hilbert space cannot be decomposed into several non-interacting low-dimensional manifolds [22]), with tens of thousands of states, can only be performed with scalable algorithms.

This paper presents an algorithm to calculate the Floquet spectra of strongly-modulated quantum systems with $N \geq 10^4$ states and its implementation on a parallel supercomputer. The propagation part of the algorithm is based on the combination of the Magnus expansion of time-dependent linear operators [23] and the Chebyshev expansion of operator exponents [24]. This combination has been proposed in [25], where its particular numerical realization, implementing a commutator-free Magnus scheme, was tested. We illustrate the accuracy and scalability of the algorithm by using two quantum models, with a synthesized random-matrix Hamiltonian and a many-body non-integrable bosonic dimer. The size of model system is limited by the diagonalization routine only, so the algorithm can be used to calculate Floquet states of systems of the size up to $N \sim 50\,000$ states.

The rest of the paper is organized as follows: Section 2 outlines the theoretical background and introduces the Magnus and Chebyshev expansions; Section 3 describes the algorithm; in Section 4 we introduce model systems, apply the cluster implementation to calculate their Floquet states in Section 5, and analyze the results in Section 6. Finally we summarized our findings and outline further perspectives in Section 8.

2. Theoretical background

Floquet states. We consider quantum systems whose dynamics is determined by the time-dependent Schrödinger equation

$$i\hbar \partial_t |\psi(t)\rangle = H(t)|\psi(t)\rangle,$$

where the Hamiltonian $H(t)$ denotes a time-periodic Hermitian operator, $H(t + T) = H(t)$. We assume that the system evolves in a finite-dimensional Hilbert space spanned by $N$ basis vectors. The time evolution of the system is fully determined by a unitary operator $U(t_0, t)$, being the solution of the equation

$$i\hbar \partial_t U(t_0, t) = H(t)U(t_0, t),$$

for the initial condition in the form of the identity matrix, $U(t_0, t_0) = I$. This provides the propagator of the system, i.e., a unitary operator which evolves any system state from a time $t_0$ to time $t$, $U(t_0, t)|\psi(t_0)\rangle = |\psi(t)\rangle$. A time $t_0 \in [0, T]$ specifies the state of the Hamiltonian operator at the initial time, when, for example, the driving was switched on. This starting time can be absorbed into the Hamiltonian as a parameter, $H(t, t_0) = H(t + t_0)$ (the propagator $U(t_0, t)$ can be obtained from $U(0, t)$ as $U(t_0, t) = U^\dagger(0, t_0)U(0, t + t_0)$), so for later convenience, we set $t_0 = 0$ in Eq. (3) and denote $U(0, t)$ by $U$. Eigenvectors $|\varphi_\mu\rangle$ of the normal matrix $U_T$, $U_T|\varphi_\mu\rangle = e^{-i\omega_\mu t}|\varphi_\mu\rangle$, $\mu = 1, \ldots, N$, (4)
form an orthonormal basis in the system Hilbert space. These vectors could also be taken as snapshots of time-dependent vectors \( |\varphi_n(t)\rangle \) at the time instant \( t = T \), \( U(T)|\varphi_n(0)\rangle = e^{-i\mathbf{h}T/\hbar}|\varphi_n(0)\rangle \), with \( \varphi_n = \mathbf{h} \partial_\varphi/T \). The exponents \( \epsilon_n \) have the dimension of energy and are termed quasienergies. Quasienergies can be determined up to multiples of \( \hbar \). The Floquet states \( |\phi\rangle \) can be constructed to obtain a time independent Hamiltonian operator \( \mathbf{H} \), and the system initial state \( |\psi(0)\rangle \), one can calculate the state of the system at any instant of time \( t > 0 \),

\[
|\psi(t)\rangle = \sum_n c_n e^{-i\epsilon_n t/\hbar}|\varphi_n(t)\rangle, \quad c_n = \langle\psi(0)|\varphi_n(0)\rangle. \tag{6}
\]

**Magnus expansion.** The idea of the Magnus expansion \([24]\) is to construct a time independent Hamiltonian operator \( \Omega(t_1, t_2) \), parameterized by the two times, \( t_1 \) and \( t_2 \), such that

\[
U(t_1, t_2) = \exp \left[ -i \hbar \Omega(t_1, t_2) \right]. \tag{7}
\]

The operator is given by an infinite series involving nested commutators \([23]\):

\[
\Omega(t_1, t_2) = \int_{t_1}^{t_2} \mathbf{H}(t_1) \; dt_1 + \frac{1}{2} \int_{t_1}^{t_2} \int_{t_1}^{t_2} \{ \mathbf{H}(t_1), \mathbf{H}(t_2) \} \; dt_2 + \frac{1}{6} \int_{t_1}^{t_2} \int_{t_1}^{t_2} \int_{t_1}^{t_2} \{ \{ \mathbf{H}(t_1), \mathbf{H}(t_2) \}, \mathbf{H}(t_3) \} \; dt_3 + \ldots. \tag{8}
\]

An implementation of the expansion \([8]\) assumes a truncation of the infinite series, summation of the finite series into an operator \( \Omega(t_1, t_2) \), and use of the latter as the propagator \( U(t_1, t_2) \). The Floquet operator \( U_T \) can be approximated as a chain

\[
U_T = U(0, t_1)U(t_1, t_2) \ldots U(t_{M-1}, t_M) \approx e^{-i\Omega(0, t_1)/\hbar} e^{-i\Omega(t_1, t_2)/\hbar} \ldots e^{-i\Omega(t_{M-1}, t_M)/\hbar}, \tag{9}
\]

where \( t_k = k\hbar = kT/M, \) \( k = 0, \ldots, M \). Since all terms on the rhs of Eq. \([8]\) are Hermitian, the truncated operator \( \Omega(t_1, t_2) \) is Hermitian, and an approximation of any order preserves the unitary time evolution. The truncated operator in the form \([8]\) is not very suitable for computations. It is more convenient to approximate \( \Omega(t_1, t_2) \) with lower-order commutator series, calculated by using values of \( \mathbf{H}(t_{j/2}) \) at the midpoints \( t_{j/2} = (t_j + t_{j+1})/2 \) (this is our choice, see Section \([4]\) for more details), or with a commutator-free linear combination of \( \mathbf{H}(t_j) \), calculated at different times \( t_j \in [t_1, t_2] \) \([23]\).

**Chebyshev expansion.** The exponentiation of an operator is a computationally expensive operation \([27]\). In order to propagate vector \( |\psi(t_1)\rangle \) to time \( t_2 \), the knowledge of the unitary operator \( \exp(-i\Omega(t_1, t_2)/\hbar) \) is redundant: we need only the result of its action on the vector, \( |\psi(t_2)\rangle = \exp(-i\Omega(t_1, t_2)/\hbar)|\psi(t_1)\rangle \). This can be calculated by implementing the Chebyshev polynomial expansion of the operator exponent, which is based on a recursive iteration scheme \([24]\),

\[
|\psi_{t+1}(t_2)\rangle = -i\hbar \Omega(t_1, t_2)|\psi_{t}(t_2)\rangle + |\psi_{t-1}(t_2)\rangle \tag{10}
\]

with the initial conditions \( |\psi_{0}(t_2)\rangle = |\psi(t_2)\rangle \) and \( |\psi_{1}(t_2)\rangle = -i\mathbf{h}(t_1, t_2)|\psi_{0}(t_2)\rangle \). Here \( \Omega(t_1, t_2) \) is a shifted and rescaled operator,

\[
\tilde{\Omega}(t_1, t_2) = \frac{\Omega(t_1, t_2) - \langle l | \mathbf{H} | E_{\min} \rangle}{\Delta E}, \tag{11}
\]

which has all its eigenvalues restricted to the interval \([-1, 1] \([24]\). The spectral half-span \( \Delta E = (E_{\max} - E_{\min})/2 \) should be estimated from the extreme eigenvalues \( E_{\min} \) and \( E_{\max} \) of \( \Omega(t_1, t_2) \) operator beforehand.

Finally, the new vector can be obtained as

\[
|\psi(t_2)\rangle = e^{-i\hat{\mathbf{h}}t_2/\hbar} \sum_{l=0}^{N} a_l |\psi_l(t_2)\rangle, \tag{12}
\]

where \( \beta = \Delta E + E_{\min} \) and \( h = t_2 - t_1 \). The expansion coefficients \( a_l = 2J_l(R) \) and \( a_0 = J_0(R) \), where \( J_l(R) \) are the Bessel functions of the first kind and \( R = h\Delta E/h \). Parameters \( L \) sets the order of the Chebyshev approximation by truncating the series \([12]\). Strictly speaking, this scheme does not preserve the unitary time evolution. However, its convergence with the increase of \( L \) is fast so that \( L \) can be chosen such that the deviation from unitarity is dominated by the round-off error \([24]\). We have found that it is enough to take \( L < 100 \) for \( N \lesssim 10^4 \) and the further increase of \( L \) does not improve the accuracy of calculations.

### 3. The algorithm

We restrict the consideration to Hamiltonians of the form

\[
H(t) = H_0 + f(t) \cdot H_{\text{mod}}, \quad f(t + T) = f(t), \tag{13}
\]

where \( f(t) \) is a scalar function and \( H_0, H_{\text{mod}} \) are time-independent Hermitian operators. Most of the currently used models, including the ones discussed in Section \([4]\), belongs to this class. Equation \([13]\) is the simplest nontrivial case of a general situation, \( H(t) = H_0 + \sum_{s} f_s(t) \cdot H^{(s)}_{\text{mod}} \), with \( s \leq N^2 \). Our results can be generalized to the case \( s > 1 \) in a straightforward manner.

Next we specify the method to approximate \( \Omega(t_1, t_2) \). As we discussed in the previous section, there exist a variety of schemes \([23]\). Our choice is conditioned by the form of the Hamiltonian, Eq. \( [13] \), and the intention to realize the algorithm on a parallel cluster. More specific on the last point, we are not concerned about the number of commutators needed to be calculated (and then stored) as long as they are all time-independent and do not have to be recalculated in course of the propagation. Here we use the midpoint approximation of the Magnus expansion with three commutators \([23, 28] \):

\[
\Omega = \alpha_1 + \frac{1}{12} \alpha_3 + \frac{1}{240} [-20\alpha_1 - \alpha_3 + C_1, \alpha_2 + C_2], \tag{14}
\]
so that \( \Omega = \Omega + \mathcal{O}(\hbar^7) \). Specifically,

\[
\alpha_j = \frac{\hbar^l}{(j - 1)!} \frac{d^{j-1} H(t_{1/2})}{dt^{j-1}}, \quad C_1 = [\alpha_1, \alpha_2], \quad C_2 = -\frac{1}{60} [\alpha_1, 2\alpha_3 + C_1].
\]

The original formulation demands the calculation of \( \alpha_j \) on every time step. This task, for the specific choice given by Eq. (13), reduces to calculations of midpoint values of the scalar functions \( f(t), f'(t), \) and \( f''(t) \). These values have to be weighted with time-independent commutators of the forms \( [H_0, H_{\text{mod}}], [H_0, [H_0, H_{\text{mod}}]], \) etc. There are nine commutators for the chosen scheme, Eq. (14), but they have to be calculated only once, when initiating the algorithm.

The choice of the operational basis to write operators \( H_0 \) and \( H_{\text{mod}} \) constitutes an important point. We use the eigenbasis of the operator \( H_0 \) without going into the interaction picture (see a relevant discussion in Ref. [25]). In this basis equation (13) assumes the form

\[
\hat{h}\hbar \hat{\psi}(t) = \text{diag} E_i + f(t) \cdot \tilde{H}_{\text{mod}} \hat{\psi}(t),
\]

where \( \text{diag} E_i \) is a diagonal matrix consisting of the eigenvalues \( \{E_i\} \) of \( H_0 \), and \( \tilde{H}_{\text{mod}} \) is the matrix representation of the operator in the eigenbasis of \( H_0 \). In numerical experiments with different periodically-driven nonlinear potentials, we found that this choice of the basis guarantees stable performance for \( N > 10^3 \). Because of the diagonal form of the matrix \( H_0 \), it also simplifies calculation of the nested commutators.

The algorithm can be described as the propagation of the \( N \times N \) identity (in the eigenbasis of \( H_0 \)) matrix over the time interval \( T \). The propagation is realized with a chain of \( L \) Chebyshev iterations (cf. Eqs. (9), (12)) with the rescaled operator \( \tilde{\Omega}(t_{l-1}, t_l), k = 1, \ldots, L \). Eq. (14). Note, that in order to apply the rescaling procedure (11), \( \Omega \mapsto \tilde{\Omega} \), one has to estimate the extreme eigenvalues \( E_{\text{min}} \) and \( E_{\text{max}} \) beforehand.

We diagonalize the matrix \( \tilde{\Omega} \) at five equidistant time instants \( t_j \in [0, T] \), and use the maximal and minimal values from the collected eigenvalue set as \( E_{\text{min}} \) and \( E_{\text{max}} \). Once the propagation stage is completed, the result, i.e. the \( N \times N \) unitary matrix \( U_T \) is diagonalized and its eigenvalues \( \{E_i\} \) and eigenvectors \( \{\phi_i(0)\} \), are written into the output file. An additional propagation round can be performed, now with eigenvectors \( \{\phi_i(0)\} \) as initial vectors, in order to calculate relevant characteristics of the Floquet states. For example, it can be the expectation value of a relevant operator \( A(t) \), averaged over the one period

\[
\langle A(\nu) \rangle_T = \frac{1}{T} \int_0^T \langle \phi_\nu(t)|A(t)|\phi_\nu(t) \rangle \, dt.
\]

4. Models

To test the algorithm, we employed two specific physical cases for the Hamiltonians entering the setup given by equation (13).

The first system is a synthesized model, with the Hamiltonians \( H_0 \) and \( H_{\text{mod}} \) being members of a Gaussian orthogonal ensemble \( \text{GOE}(N) \) of a variance \( \sigma \), that is a parameter of the system. Random matrix theory and the corresponding models remain at the center of research in many areas of quantum physics [24], but it is only very recently that these two hitherto disentangled research fields started to interact [18, 19].

Our second test model consists of a driven \( N \)-particle Bose-Hubbard dimer [35], with the Hamiltonians

\[
\begin{align*}
H_0 &= -\nu(\hat{a}^\dagger_1 \hat{a}_2 + \hat{a}^\dagger_2 \hat{a}_1) + \frac{U}{2} (\hat{n}_1 - \hat{n}_2)^2, \\
H_{\text{mod}} &= (\hat{n}_2 - \hat{n}_1),
\end{align*}
\]

where \( \hat{a}^\dagger \) (\( \hat{a} \)) and \( \hat{n}_j = \hat{a}^\dagger \hat{a} \) are the bosonic creation (annihilation) and particle number operators for the \( j \)-th site, respectively. Parameters \( \nu \) and \( U \) are the hopping rate and one-site interaction strength. In the Fock basis the Hamiltonian \( H_0 \) acquires a tridiagonal structure, while \( H_{\text{mod}} \) becomes a diagonal matrix. This model is extensively used in many-body quantum physics, both in theoretical and experimental domains; e.g., see Ref. [35].

5. Implementation of the algorithm on a cluster

We now describe a program realization of the algorithm and its subsequent realization on a high-performance cluster. Our C code employs Intel® Parallel Studio XE package [29]. The main data structures are complex double-precision matrices. Computational load is distributed among cluster nodes by the standard Message Passing Interface (MPI). On each node computationally intensive operations are implemented by calling BLAS functions from Intel® Math Kernel Library (Intel MKL), in shared-memory parallel mode [30].

The code consists of three main steps (they are summarized in the pseudocode shown in Algorithm [1]). In the first step, the
program initializes MPI, allocates memory, reads the seed data and parameters from configuration files, and makes necessary pre-calculations before launching the main cycle: calculates the eigenbasis of the Hamiltonian $H_0$ and auxiliary matrices $\text{diag}E_i, \tilde{H}_{\text{mod}}$ (see Eq. (16)), the Bessel functions $J_l(R), R = R(h), l = 0, ..., L$, needed for the Chebyshev series (see Eq. (12)), and nine commutators needed for the Magnus expansion (see Eq. (14)). These computations are performed on each cluster node. It is important to choose appropriate operational presentation of the $N \times N$ matrices, starting from the initial identity matrix $I$. The most straightforward solution is to split $I$ into $N$ vectors, store the vectors as independent arrays, and then propagate them independently and in parallel. A more efficient solution is to form sub-matrices of initial vectors that allows for parallel propagation and then make use of the third-level BLAS operations, in particular, matrix-matrix product, instead of a series of matrix-vector products. As a result, the memory hierarchy would be used in a more efficient way and a substantial decrease of the computation time would be achieved.

The second step involves the propagation of the initial matrix $I$ over one period $T$. Because the process is iterative, a parallelization in time is not possible. However, a data parallelization is feasible. The initial identity matrix can be split into $P$ sub-matrices $X_i, i = 1, ..., P$, each consisting of $N/P$ basis vectors, which are then distributed among $P$ cluster nodes. Therefore, the first $N/P$ rows are propagated on the first node, the next $N/P$ rows on the second node, etc. (according to the C row-major order, initial vectors are written as rows). This idea is sketched in Fig. 1. The scheme possesses a potential minor drawback that could be encountered in the case of a large number of processing units, when splitting could cause a strong imbalance in this might affect the performance of the mathematical kernels, which were not developed to handle “thin” matrices consisting of a few rows and thus limits number of processing units that could be used to accelerate the propagation. The major advantage of the scheme, however, is a next to uniform distribution of the workload among the nodes. Together with a constant number of operations on each step, this allows to estimate the scaling of the overall computing time with $P$.

A single propagation step realizes the recipe given at the end of Section 5. By employing MKL functions, we calculate the matrix $\Omega(t_{k-1}, t_k)$ following the Magnus expansion (14). It is computed independently on each cluster node, as the small computing time does not justify parallelization on a distributed memory.

The computationally intensive part of the algorithm is the approximation of the action of the matrix exponent by Chebyshev’s iterations, Eqs. (10,12), and the further updating of propagated sub-matrices on each cluster node. The mathematical core of this step is the multiplication of complex double-precision dense matrices (it is realized with zgemm routine [32]). This part of the algorithm is fully parallel.

During the final, third step the program assembles sub-matrices into the Floquet matrix and diagonalizes the latter by using a multi-threaded Intel MKL implementation (we use zgeev routine [32]). For the matrix size $N \sim 10^4$, a multi-core implementation is sufficient. Finally, the results of the diagonalization are written to the output files, the memory is deallocated, and MPI is finalized.

### 6. Program performance and scalability analysis

In this section we present the performance analysis of the code. Test runs were performed on the “Lobachevsky” supercomputer at the Lobachevsky State University of Nizhni Novgorod [37]. We employed up to 64 computational nodes, with the following configuration per node: 2× Intel Xeon E5 − 2660 CPU (8 cores, 2.2 GHz), 64 GB RAM, OS Windows HPC Server 2008. We use Intel MKL, Intel C/C ++ Compiler, and Intel MPI from Intel Parallel Studio XE [29]. All parallel versions of computationally intensive routines from MKL utilized 16 cores on each node.

To test the performance of the program we use the synthesized random-matrix model as a benchmark (see Section 4). In this case, Hamiltonians $H_0$ and $\tilde{H}_{\text{mod}}$ in Eq. (16) were generated randomly from the GOE($N$) ensemble of the unit variance.
σ = 1 \[38\]. The driving function is \( f(t) = \cos(\omega t) \) with \( \omega = \pi \) \[39\].

**Single-node performance.** To test a single-node performance, we use \( L = 50 \) Chebyshev iterations on every step. The number of steps per period, \( M = 10^2 \), was used for testing the program. The execution time for larger values of \( M \) can be easily extrapolated: due to the linear increase of operations number with iterations in time, it is sufficient to find and appropriately scale execution time of the core part of the code, and add execution time of the other parts, which are independent of \( M \). Table 1 presents the dependence of the execution time on the size of the model system. The last column of Table 1 presents estimates for the case when the number of steps is increased 100-fold, i.e. for \( M = 10^4 \).

To gain a further insight, we analyze a single-node performance in some more detail. We consider two metrics, both normalized by the number of operations, \( OC_N \), required to make calculations for a system of a size \( N \). Namely, we calculate the operation rate \( R_N \) that is the number of operations per unit time, and take the value obtained for \( N = 256 \) as a unit measure. The first metrics reads \( R_N = (OC_N/OC_{256})/(TIME_{N}/TIME_{256}) \), where \( TIME_N \) is the execution time of the code for the system of size \( N \). Further, we consider a similar quantity, \( P_N \), where the number of operations is estimated by \( N^3 \), according to the scaling of the most computationally intensive and most frequently called MKL subroutine \( zgemm \). Table 2 presents \( R_N \) and \( P_N \) as functions of \( N \).

The number of operations is calculated by Intel® VTune™ Amplifier profiler \[40\] and returned to CPU performance counter SIMD_FP_256.PACKED_DOUBLE \[41\]. This variable contains the number of issued Advanced Vector Extensions (AVX) instructions for processing double precision values \[42\]. The choice of this counter is based on the fact that almost all computations in our code occur in Intel MKL BLAS routines. Note, however, that this estimate of the number of operations is not exact. It is well known that for the current architectures the profiler tends to oversize this number, since it counts the number of instructions issued but retired. Nevertheless, this estimate is reliable for CPU-bound processes.

The behavior of \( R \) and \( P \) as functions of \( N \) are presented in two last columns of Table 2. The efficiency increases with the size of the model system, doubling for \( N = 5 \) 120 as compared to \( N = 256 \). That is because of the increasing efficiency in evaluation of larger matrices of the BLAS computational kernels in the parallel regime. While the efficiency grows with the system size, the execution time also increases, mainly because the increase of the number of steps per period needed, and for \( N = 5 \) 120 the estimated calculation time is about 22 days. Therefore, a multi-node parallelization is required to decrease the calculation time to more realistic time scales.

**Strong scalability of the algorithm.** We next analyze the performance of the algorithm on a cluster. To benchmark the code, we use the random-matrix model of the size \( N = 5 \) 120 and launch the code on \( P = \{1, 2, \ldots, 2^i, \ldots, 2^5\} \) cluster nodes, using the multi-threaded implementation on each node as before. The results are summarized in Table 3. Let us note that the time needed for the diagonalization of \( N = 5 \) 120 matrix is 242.1 sec and does not depend on \( P \) (see column vi in Table 1). Therefore, it is omitted from the further analysis.

For \( M = 10^2 \) the code accelerates as the number of nodes increases to 64 (1 024 computational cores in total), though the efficiency of parallelization, defined as the ratio between the speed up and the number of nodes, drops to 35%. That is be-

### Table 1: Single-node performance: Execution times (in sec) as a function of system size \( N \). Multi-threaded version of the code employs all 16 node’s cores on shared memory. Columns ii-iv and vi present data obtained for \( M = 10^2 \) time steps per period and \( L = 50 \) Chebyshev iterations on every step. To get an estimate for \( M = 10^4 \), the time needed to calculate \( \Omega \) and perform Chebyshev iterations were extrapolated (last column), see text for more details.

| System size, \( N \) | Auxiliary computations time | Time of \( \Omega \) calculation | Chebyshev iterations time | Diagonalization time | Total time \( M = 10^2 \) | Total time \( M = 10^4 \), extrapolation |
|---------------------|-----------------------------|-------------------------------|--------------------------|--------------------|--------------------------|----------------------------------|
| 256                 | 0.2                         | 0.4                           | 4.3                      | 0.2                | 5.1                      | 470.4                            |
| 512                 | 0.4                         | 1.8                           | 25.3                     | 0.6                | 28.1                     | 2 711.0                          |
| 768                 | 1.3                         | 3.2                           | 79.9                     | 1.4                | 85.8                     | 8 312.7                          |
| 1 024               | 1.8                         | 8.3                           | 177.5                    | 2.6                | 190.0                    | 18 564.4                         |
| 1 536               | 4.3                         | 18.9                          | 559.1                    | 7.3                | 589.6                    | 57 811.6                         |
| 2 048               | 8.6                         | 33.2                          | 1 296.6                  | 16.0               | 1 354.4                  | 133 004.6                        |
| 3 072               | 23.5                        | 72.1                          | 4 179.2                  | 51.0               | 4 325.8                  | 425 204.5                        |
| 4 096               | 49.2                        | 126.0                         | 9 730.5                  | 117.5              | 10 023.2                 | 985 816.7                        |
| 5 120               | 100.5                       | 184.3                         | 18 667.2                 | 242.1              | 19 194.1                 | 1 885 492.6                     |
| 10 240              | 755.3                       | 919.7                         | 181 722.3                | 1 857.7            | 185 254.9                | 18 266 809.4                    |

### Table 2: Single-node performance. Computational intensity and efficiency measures, \( R_N \) and \( P_N \), as functions of the model system size \( N \). Multi-threaded implementation of the algorithm on a single cluster node (16 cores on shared memory) was used. The number of steps per period is \( M = 10^2 \) with \( L = 50 \) Chebyshev iterations on every step.

| System size, \( N \) | Total time, \( TIME_N \) in sec | Operations count, \( OC_N \) in mln | \( R_N \) | \( P_N \) |
|---------------------|---------------------------------|-----------------------------------|--------|--------|
| 256                 | 5.1                             | 173 612                           | 1.00   | 1.00   |
| 512                 | 28.1                            | 1 365 642                         | 1.43   | 1.45   |
| 768                 | 85.8                            | 4 594 916                         | 1.57   | 1.60   |
| 1 024               | 190.0                           | 10 875 688                        | 1.68   | 1.72   |
| 1 536               | 589.6                           | 36 655 208                        | 1.83   | 1.87   |
| 2 048               | 1 354.4                         | 86 961 706                        | 1.89   | 1.93   |
| 3 072               | 4 325.8                         | 292 683 840                      | 1.99   | 2.04   |
| 4 096               | 10 023.2                        | 693 473 512                      | 2.03   | 2.08   |
| 5 120               | 19 194.1                        | 1 354 053 950                    | 2.07   | 2.13   |
For the dimer model, Eq. (18), we use parameters above.

7. Applications

In this section we test the accuracy of the algorithm by using two physical model systems which we described in Section 6 above.

The random-matrix model was already specified in Section 6. For the dimer model, Eq. (18), we use parameters \( \nu = 1 \) and \( U = U' \cdot N = 2 \). The one-site interaction is scaled with the number of bosons, \( N - 1 \), to match in the limit \( N \to \infty \) the classical mean-field Hamiltonian \[ H_{\text{cl}}(z, \nu) = \frac{U'}{2} z^2 - 2\nu \sqrt{1 - z^2} \cos(\nu) + 2z \cdot f(t). \] (19)

The mean-field variables \( z \) and \( \nu \) measure the population imbalance and relative phase between the dimer sites, respectively. The driving function \( f(t) = f_{\text{dc}} + f_{\text{ac}} \cos(\omega t) \) consists of two components, a constant dc-bias \( f_{\text{dc}} = 2.7 \) and single-harmonic term \( f_{\text{ac}} \cos(\omega t) \), with the amplitude \( f_{\text{ac}} = 2.5 \) and frequency \( \omega = 3 \). We use the phase space of the mean-field system, Eq. (19) together with the semi-classical eigenfunction hypothesis [43] and the concept of \"hierarchical eigenstates\" [45], for a \"quantum\" benchmarking of the program.

Once the diagonalization of \( U_T \) is completed, the program initiates an additional round of \( T \)-propagation to calculate the average energies of the Floquet states with \( A(t) = H(t) \) in Eq. (17). Finally, the Floquet states are sorted in ascending order according to their average energies. To quantify the accuracy, we adapt the idea of overlap phase error [24] and modified it to account for the periodicity of the Floquet states,

\[
\Sigma_p = |\langle \phi_{\mu}(0)|U_T|\tilde{\phi}_{\mu}(0)\rangle|.
\] (20)

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\] (20)

where \( \tilde{\phi}_{\mu}(0) \) is the Floquet state calculated with the time step \( \hbar = h/2 \). Note that the error is state-specific.

Figure 3 presents the error \( \Sigma_p \) as a function of number of steps per period \( M \) and number of system states \( N \). A linear dependence of \( \log_{10} \Sigma_p \) on \( \log_{10} M \) observed for the random-matrix model is typical for stepwise integrators. The error convergence with the number of steps does not saturate up to largest value \( M = 10^{240} \). In the case of the dimer, however, the error does not reveal the power-law scaling and demonstrate a noticeable saturation. The difference in the scalings can be attributed to the differences in the spectral properties of the matrices \( H_0 \) and \( H_{\text{mol}} \) while in case of the random-matrix model the level spacings of the Hamiltonians are characterized by a probability density function (pdf) with a gap near zero, the level spacings in the energy spectrum of the integrable dimer Hamiltonian are characterized by a gapless Poisson pdf [46]. The Floquet groundstate \( |\phi_{\mu}\rangle \) turns to be the most sensitive to the discretization of the unitary evolution (see Fig. 3(a)). We use this state to test state dependence of the error on the size of the model system. Figure 3(b) shows that the scaling of \( \Sigma_p \) with \( N \) is qualitatively similar for both models.

Now we turn to the quantum benchmarking of the algorithm with the dimer model. Following the semi-classical eigenfunction hypothesis [44, 45], the Floquet states of the model in the limit \( N \gg 1 \) can be sorted according to the location of the

| Number of nodes, \( P \) | Auxiliary computations time (sec) | Time of \( \Omega \) calculation (sec) | Chebyshev iterations | Chebyshev iterations speed up | Total time \( M = 10^2 \) (sec) | Speed up | Total time \( M = 10^4 \) (sec) | Speed up |
|-----------------|----------------|----------------|----------------|----------------|----------------|--------|----------------|--------|
| 1               | 100.5          | 184.3          | 18 667.2       | 1.0            | 19 194.1       | 1.0    | 1 885 457.9    | 1.0    |
| 2               | 186.4          | 181.5          | 9 406.9        | 2.0            | 10 017.8       | 1.9    | 959 150.8      | 2.0    |
| 4               | 195.3          | 180.2          | 4 670.7        | 4.0            | 5 288.8        | 3.6    | 485 400.8      | 3.9    |
| 8               | 173.6          | 178.7          | 2 341.2        | 8.0            | 2 935.8        | 6.5    | 252 305.2      | 7.5    |
| 16              | 137.1          | 178.4          | 1 187.2        | 15.7           | 1 744.7        | 11.0   | 136 882.6      | 13.8   |
| 32              | 103.9          | 178.7          | 628.0          | 29.7           | 1 152.6        | 16.7   | 81 006.1       | 23.3   |
| 64              | 98.9           | 178.6          | 338.3          | 55.2           | 858.6          | 22.4   | 52 053.6       | 36.2   |

Figure 2: (color online) Computational efficiency as a function of number of cluster nodes \( P \). Results are shown for two values of number of steps per period, \( M = 10^2 \) and \( M = 10^4 \). The parameters are \( N = 5 \times 120 \) and \( L = 50 \).
Hierarchical states are exceptional in the sense that their absolute number increases sub-linearly with the number of states, $N_{\text{hier}} \sim N^\chi$, $\chi < 1$, so that their relative fraction $N_{\text{hier}}/N$ goes to zero in the limit $N \to \infty$. These states must be carefully selected from the complete set of $N$ Floquet states.

Hierarchical states are coherent superpositions of many basis vectors and therefore sensitive to the phase errors. Even a small mismatch in vector phases blurs the interference pattern and causes the flooding of the state’s Husimi distribution into the island. The high coherence of the superpositions is also a trait of the regular Floquet states but there is an important difference: Quasienergies $\epsilon_q$ of the hierarchical states are randomly distributed over the interval $[-\hbar \omega/2, \hbar \omega/2]$ while the quasienergies of regular and chaotic states tend to cluster in different regions. Because of that, phases of hierarchical states are most vulnerable to the error produced by the numerical propagation. We selected several hierarchical states for the dimer model with $N = 249$ bosons and inspect their Husimi distributions [7], see Figs. 4 (a,b,d). The offshore localization and absence of the flooding [see zoomed distribution on Fig. 4 (d)] are clearly visible.

8. Summary and Outlook

We have put forward a method to calculate Floquet states of periodically-modulated quantum system with $N \geq 10^5$ states. Our method is advantageous in that it is scalable and therefore well suited for its implementation on parallel computers. Our study uses massively parallel clusters as efficient devices to explore complex quantum systems far from equilibrium, thus answering the need of several, actively developing, research fields involving quantum physics [12, 13, 14, 15, 16, 17, 18, 19, 20].

We use the definition of the Husimi distribution for the dimer given in Refs. [48]. The expression involves summation over the series of square roots of binomial coefficients of the order $N$. We did not find an alternative expression which allows to avoid term-by-term summation. Although we calculated the Floquet states for the dimer with $10^5$ bosons, we were not able to go beyond the limit $N = 2500$ when calculating Husimi distributions.
Figure 4: (color online) Husimi distributions for hierarchical, chaotic and regular Floquet states of the dimer model with \( N = 2\,499 \) bosons. Dots show the Poincaré section for the mean-field Hamiltonian, Eq. (19). Circle-like formations correspond to the KAM tori [47], the solutions of the mean-field system inside regular islands. (a,b,d,) Hierarchical Floquet states of the quantum system: \( \mu = 118 \) (a), \( \mu = 1\,024 \) (b), \( \mu = 101 \) (d, zoom). (c) Chaotic Floquet state, \( \mu = 1002 \). (f,g) Two regular Floquet states: \( \mu = 30 \) (f) and \( \mu = 55 \) (g).

The method particularly allows for improvements, such as the increase of the order of the Magnus expansion [28] or the use of commutator-free Magnus approximations [25]. With respect to further acceleration of the code for systems with \( N \leq 10^4 \) states, there is a promising perspective related to the fact that the main contribution to the computation time stems from the BLAS operations. These operations fit GPU and Intel Xeon Phi architectures very well. By our estimates, even a straightforward implementation of the most computationally intensive Chebyshev iteration stage on a heterogeneous CPU+GPU configuration will result in a three-fold speedup. A yet further speed-up can be obtained by using multiple accelerators.

There are several interesting research directions for which the proposed algorithm may serve as a useful starting point. For example, there is the perspective to resolve Floquet states of even larger systems by applying the spectral transformation Lanczos algorithm [49] to the corresponding time-independent super-Hamiltonians, to name but a few. Because the super-Hamiltonian elements can be generated on the fly, this idea potentially would allow to calculate Floquet states of a system with \( N \sim 10^5 \) states for \( F \sim 10^4 \) Fourier harmonics, by employing massively parallel exact diagonalization schemes [50]. Note, however, that the eigenvalues of the Hamiltonian supermatrix (as well as the respective quasienergies) are merely phase factors and are not directly related with the properties of the corresponding Floquet states (average energy, etc.). Therefore, some targeting of the algorithm to the low-energy states is required. Our method can be used to locate the relevant Floquet eigenvectors in the quasi-energy spectrum of a system with a smaller number of states; combining this with a knowledge of the spectrum scaling with \( N \), one can target the Lanczos algorithm.

Another direction relates to the computational physics of open periodically-modulated quantum systems that interact with a large environment (heat bath). Asymptotic states of such systems are affected by the combined effects of modulation and the decoherence induced by the environment [51]. Due to linearity of the model equations describing the evolution of the density matrices of the systems, the corresponding asymptotic states are specified by time-periodic density matrices, which can be called “quantum attractors”. There is presently limited knowledge about the theme of quantum attractors beyond the limit of the rotating-wave approximation [52]. In the Floquet framework, the attractor’s density matrix is a zero-eigenvector of the corresponding non-unitary Floquet super-operator, which acts in the space of \( N \times N \) Hermitian matrices. This super-operator can be constructed by propagating the identity opera-
tor – but now in the space of $N \times N$ matrices. The propagation stage can be realized by using Padé approximation [27] or with Newton or Faber polynomial schemes [53], while the question whether there exists a possibility to generalize the Magnus expansion to dissipative quantum evolution equations remains open. As the number of the basis matrices scales as $N^2$, the scalability of non-unitary propagation algorithms then presents an even more demanding task.

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