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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 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. The construction of the unitary 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 evolution of basis vectors makes the propagation stage suitable for realization 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 involving 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 10^4 states.

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 [1–3]. It is then natural that computational quantum physics plays an ever increasing role in explaining and guiding current experiments and suggesting new ones [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 too large the size of the matrix may not allow any longer for its full diagonalization. The task, however, could be restricted to finding lowest energy eigenstate(s) which can be accomplished by using the Lanczos algorithm [5] or more sophisticated tools, such as the Density-Matrix Renormalization Group (DMRG) methods [6]. In cases that the system is periodically modulated in time, its Hamiltonian becomes a time-periodic operator $H(t+T) = H(t+2\pi/\omega) = H(t)$. The dynamics of the system is accordingly then governed by the set of so termed *Floquet states* [7,8]. These states are not eigenvectors of the Hamiltonian $H(t)$ but instead of the unitary Floquet operator

$$U_T = \mathcal{T} \exp\left[-\frac{i}{\hbar}\int_0^T H(t')dt'\right], \tag{1}$$

where $\mathcal{T}$ is Dyson's time-ordering operator. This operator propagates the system over the period T of modulations, while the corresponding time-periodic Floquet states form a time-periodic orthogonal basis spanning the system Hilbert space [9,10]. The structure of the unitary Floquet matrix, and thus the properties of the Floquet states, depend on the modulation protocols and parameters. This is a key feature of periodically driven quantum systems

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which makes them so attractive to the theoreticians and experimentalists working in the field of quantum optics, optomechanics and solid state physics [9–13]. Strong modulations can sculpt a set of non-equilibrium eigenstates which may drastically differ from the states exhibited by the system in the unmodulated, stationary limit. Thus, 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 [14], synthesize Majorana fermions in quantum wires [15], and engineer gauge fields for spinless neutral atoms [16].

The calculation of Floquet states of a large quantum system constitutes a challenge. The key step is a construction of the unitary Floquet matrix, Eq. (1) (its final diagonalization computationally similar to 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 presents an issue of its own. 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 [17–19], and to explore disorder-induced localization [20] in periodically driven many-body systems. With respect to the thermalization it was found that the temporal modulations heat the system to infinite temperature so that the system Floquet states are near uniformly smeared over the eigenbasis of the system in the absence of driving [17–19]. 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 (whose property induces the presence of all multiple frequencies $k\omega$, $k = 1, 2, \ldots$, in the spectrum of the modulations function). Evidently, this question cannot be answered without going beyond the piecewise setup. In addition, in 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 $k\omega$, $k = -F, \ldots, 0, \ldots, F$ 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 far too much; a full diagonalization of a $10^6 \times 10^6$ matrix becomes unfeasible. At the same time, this large number of harmonics is not enough to resolve faithfully the Floquet spectrum of the system.[1]

Therefore, in order to calculate the Floquet state of a system with $N \geqslant 10^3$ 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 unitary time evolution, but as well 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 7, quantum interference effects, together with some results from quantum chaos theory [22], 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 superlinearly with N. Faithful calculations of Floquet spectra of non-integrable systems (whose Hilbert space cannot be decomposed into several non-interacting low-dimensional manifolds [23]), 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 $N \geqslant 10^4$ quantum 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 [24] and the Chebyshev expansion of operator exponents [25]. This combination has been proposed in [26], where its particular numerical realization, implementing a commutator-free Magnus scheme, was tested. We demonstrate here 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 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 7. Finally we summarize 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

$$i\hbar\partial_t|\psi(t)\rangle = H(t)|\psi(t)\rangle, \tag{2}$$

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

$$i\hbar\partial_t U(t_0, t) = H(t)U(t_0, t) \tag{3}$$

for the initial condition in the form of the identity matrix, $U(t_0, t_0) = \mathbb{1}$. This provides the *propagator* of the system, i.e. a unitary operator, which evolves any system state from a time t_0 to time $t_0 + t$, $U(t_0, t)|\psi(t_0)\rangle = |\psi(t_0 + t)\rangle$. A time $t_0 \in [0, T]$ specifies the state of the Hamiltonian operator at the initial time, when, for example, the driving is 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_t. Eigenvectors $\{|\phi_\mu(0)\rangle\}$ of the unitary matrix U_T,

$$U_T|\phi_\mu(0)\rangle = e^{-i\theta_\mu}|\phi_\mu(0)\rangle, \quad \mu = 1, \ldots, N, \tag{4}$$

form a time-periodic full orthonormal basis in the system Hilbert space[2] [7–9,15,16,18,20]

$$|\phi_\mu(t + T)\rangle = |\phi_\mu(t)\rangle. \tag{5}$$

[1] The eigenvalue spectrum of the super-Hamiltonian can be resolved with the accuracy $2\pi/(2F + 1)$ at best. This is not enough taking into account that the actual mean spacing between the eigenvalues is π/N.

[2] When the notion of the Floquet states was introduced in quantum physics, the following convention has originally been employed: The set $\{\varphi_\mu(t) =$