Quantum computing Floquet band structures

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Quantum systems can be dynamically controlled using time-periodic external fields, leading to the concept of Floquet engineering, with promising technological applications. Computing Floquet band structures is harder than only computing ground state properties or single time-dependent trajectories, and scales exponentially with the Hilbert space dimension. Especially for strongly correlated systems in the low frequency limit, classical approaches based on truncation break down. Here, we present two quantum algorithms to determine effective Floquet modes and band structures. We combine the defining properties of Floquet modes in time and frequency domains with the expressiveness of parameterized quantum circuits to overcome the limitations of classical approaches. We benchmark our algorithms and provide an analysis of the key properties relevant for near-term quantum hardware.

1 Introduction

The interaction between the electromagnetic field and matter is one of the basic principles, which is used to probe and manipulate electronic and magnetic degrees of freedom. Quantum systems that are subjected to time-periodic irradiation show intriguing phenomena such as light-induced surface states [1], topological phases of matter [2, 3], high harmonic generation [4] and light-induced superconductivity [5]. With advances in high-power ultra-fast spectroscopy, non-linear phenomena, including multi-photon processes, have opened up new prospects of dynamically controlling quantum dynamics, engineering atomic [6], molecular [7–9] and solid-state [10, 11] properties on demand. On the theoretical side the study of non-equilibrium dynamics in highly entangled many-body systems is at the forefront of current research [12–20]. Light-driven quantum systems are described by time-dependent Hamiltonians $H(t)$, which include the interaction between the external electromagnetic field and the electronic or magnetic degrees of freedom.

If the field is periodic in time, i.e., $H(t) = H(t + T)$ for some period $T$, one can use the concept of Floquet engineering to control the microscopic degrees of freedom [21]. Floquet engineering is based on the Floquet theorem [22, 23], which states that there exists a complete and orthogonal set of solutions $|\Psi(t)\rangle$ to the time-dependent Schrödinger equation

$$i \frac{d}{dt} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle,$$

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Figure 1: Graphical representation of both algorithms for the determination of Floquet eigenstates and energies. (a) Algorithm Fauseweh-Zhu-1. The parameterized ansatz circuit $U_\Theta |0\rangle$ is time evolved over a full period and the overlap to its starting state is calculated. Once the overlap is maximized, we compute the Floquet quasi-energy using iterative quantum phase estimation. (b) Algorithm Fauseweh-Zhu-2. The Hilbert space is extended by Fourier expansion of the Hamiltonian. A parameterized quantum circuit approximates the combined Floquet state described by both physical and Fourier quantum numbers. Excited state VQE is used to determine Floquet states and energies.

which have the form

$$|\Psi_\alpha(t)\rangle = |\Phi_\alpha(t)\rangle e^{-i\epsilon_\alpha t}, |\Phi_\alpha(t+T)\rangle = |\Phi_\alpha(t)\rangle.$$  \hspace{1cm} (2)\

Here we have chosen the reduced Planck constant $\hbar = 1$, $|\Phi_\alpha(t)\rangle$ is the Bloch amplitude periodic in time, and $\epsilon_\alpha$ denotes the Floquet quasi-energy. The quasi-energies depend on the eigenstates of the non-driven system as well as the specific form of the driving field. They are uniquely defined up to the fundamental frequency $\Omega = 2\pi/T$. Changing the modulation of the driving field, such as shape, intensity and frequency allows to modify the $\epsilon_\alpha$’s and thereby the quasi-energy or Floquet band structure, inducing novel topological phases not present in equilibrium [24].

While the Floquet theorem is a strong statement, computing the quasi-energy band structure explicitly, depending on the microscopic degrees of freedom and the time-dependence of the external field, remains a difficult problem due to the exponentially scaling Hilbert space. Various classical techniques, such as time-dependent dynamical mean-field theory (t-DMFT) [25–28], time-dependent density matrix renormalization group (t-DMRG) [29], kinetic equations [30, 31], perturbative high-frequency expansions [32–38] and exact diagonalization [39–41] have been employed, but unfortunately most are either not universally applicable or scale exponentially in system size. Especially the computation of the whole quasi-energy band structure requires more than a simple time-evolution.

Another problem in Floquet-engineering comes from the limited theoretical modeling, in which only a few band model is considered and the perturbative infinite frequency expansion can be applied. In real materials however the situation is more difficult, as higher bands become important once the frequency is sufficiently large to induce optical transitions.

In this work, we propose to use quantum computers to overcome the limitations of previous classical approaches. We present two algorithms that in principle can calculate all Floquet eigenstates and quasi-energies. Our quantum-classical hybrid approach takes the limitations of modern Noisy Intermediate-Scale Quantum (NISQ) hardware [42] into account and allows to either improve accuracy by increasing the number of auxiliary qubits or by deepening the quantum circuits. Both algorithms make use of the enhanced expressiveness [43] of parameterized quantum circuits to find approximate Floquet eigenstates and compute the corresponding quasi-energies. While the first algorithm works in the original Hilbert space of the time-dependent problem, the second algorithm makes use of
the extended Floquet Hilbert space in frequency domain. After a detailed explanation of the basic principles, we evaluate the performance of both algorithms by investigating the simplest system that is not analytically solvable: a spin-$\frac{1}{2}$ in a linear polarized periodic magnetic field.

2 First Algorithm

In the first algorithm, Fauseweh-Zhu-1, we use a parameterized quantum circuit $U_\Theta$, with variational parameters $\Theta$, in combination with the defining properties of the time evolution operator

$$\left( H(t) - i \frac{d}{dt} \right) U(t, t_0) = 0, \quad U(t_0, t_0) = 1,$$

(3)

to determine a good approximation for Floquet eigenstates. Without loss of generality, we set $t_0 = 0$ and denote $U_t = U(t, 0)$. The Floquet theorem implies that for a full time period $t = T$ the time evolution operator has complex eigenvalues of the form

$$U_T |\Psi_\alpha(0)\rangle = |\Psi_\alpha(T)\rangle = e^{-i\epsilon_\alpha T} |\Psi_\alpha(0)\rangle,$$

(4)

We represent the Floquet eigenstate $|\Psi_\alpha(0)\rangle$ using a parameterized quantum circuit

$$|\Psi_\alpha(0)\rangle \approx U_\Theta |0\rangle,$$

(5)

where $|0\rangle$ is the initial state of the quantum computer. If $U_\Theta |0\rangle$ is a Floquet eigenstate, then

$$\left| \langle 0 | U_\Theta^\dagger U_T U_\Theta |0\rangle \right|^2 = 1,$$

(6)

holds for the overlap between the time-evolved state and the initial state. Note that overlaps of the form $|\langle 0 | U_\Theta^\dagger V |0\rangle|^2$ can be efficiently computed on a quantum computer by interpreting them as the measurement of the computational initial state projector

$$|\langle 0 | U_\Theta^\dagger V |0\rangle|^2 = \langle 0 | V^\dagger U |0\rangle \langle 0 | U^\dagger V |0\rangle.$$  (7)

Thus we devise a hybrid algorithm that maximizes the overlap to determine a Floquet eigenstate. An optimal solution $\Theta_\alpha$ has a maximal overlap of 1. To obtain the complete set of eigenstates, we modify the target function using a Lagrange multiplier $\lambda > 0$ to project out solutions $\Theta_\beta$ that have previously been computed:

$$L(\Theta) = \left| \langle 0 | U_\Theta^\dagger U_T U_\Theta |0\rangle \right|^2 - \lambda \sum_\beta \left| \langle 0 | U_\Theta^\dagger U_\Theta |0\rangle \right|^2.$$

(8)

Here $\lambda$ has to be chosen sufficiently large for the algorithm to find a new solution, see also [44]. Once a Floquet eigenstate has been determined, we use iterative quantum phase estimation (IQPE) [45–47] to compute the complex phase $e^{-i\epsilon_\alpha T}$ of $U_T$ upon application to the eigenstate. The algorithm is sketched in Fig. 1 a).

We turn to a high-level analysis of the algorithm and its requirements. The basis for the algorithm is the optimization of a parameterized quantum circuit. Thus one of the fundamental requirements is that the manifold spanned by all the possible quantum circuits within the ansatz [48] contains the Floquet eigenstates or is at least close to it. Thus carefully choosing a circuit ansatz is important for the applicability of our algorithm,
Algorithm 1 Fauseweh-Zhu-1

Require:
- parameterized quantum circuit $U_{\Theta}$
- previous solutions $\Theta_\beta$
- periodic Hamiltonian $\mathcal{H}(t)$

1: procedure Optimize($U_{\Theta}$) 
2: Choose initial parameters $\Theta$
3: while Maximize $\mathcal{L}(\Theta) = \left|\langle 0 U_{\Theta}^\dagger U_{\Theta} | 0 \rangle \right|^2 - \lambda \sum_{\beta} \left| \langle 0 U_{\Theta_{\beta}}^\dagger U_{\Theta_{\beta}} | 0 \rangle \right|^2$ do 
4: Evaluate circuit $U_{\Theta}^\dagger U_{\Theta} | 0 \rangle$
5: Evaluate circuits $U_{\Theta_{\beta}}^\dagger U_{\Theta_{\beta}} | 0 \rangle$
6: Update parameters $\Theta$ to increase target $\mathcal{L}(\Theta)$
7: Iterative quantum phase estimation on optimized state $U_{\Theta_{\alpha}} | 0 \rangle$ for 
8: return $\epsilon_{\alpha}, \Theta_{\alpha}$

and is currently a subject of intensive research [49–54]. Note that the target function $\mathcal{L}(\Theta)$ allows for a gradient-based optimization using parameter shift rules [55].

The algorithm optimizes a global observable and is therefore, in principle subject to the problem of barren plateaus [56]. This can be avoided by replacing the global observable with a local observable with identical extremum, see also [57].

We do not specify how the time evolution in the first part of the algorithm is performed. Trotterization is in principle applicable to $k$-local Hamiltonians [58] and is the most accurate. However, it is disadvantageous with respect to circuit depth [59–61]. Hence it is best applied if $T$ is the smallest time scale, i.e., in the large frequency limit. Various other methods have been developed [62–66] that make use of shallower circuits, including approaches that work directly within the variational manifold [67, 57, 68]. All of these methods can be combined with our algorithm, as long as they keep track of the global phase alignment.

The final part of the algorithm uses a single ancillary qubit to perform IQPE. It applies controlled $(U_T)^{2^n}$ gates to compute the $n$-th bit of the phase $2\pi \phi = \epsilon_{\alpha} T$. The iteration depths $n_{\text{max}}$ of IQPE determines the phase resolution and thereby desired precision of the quasi-energies. Unless powers of $U_T^2$ can be obtained within the same circuit depth, e.g., with variational time evolution, IQPE leads to an increasing circuit depth requirement for increasing precision.

3 Second algorithm

The second algorithm, Fauseweh-Zhu-2, uses Fourier analysis to map the problem onto an extended Hilbert space that is then solved using variational quantum eigensolver approaches. From the definition of the Floquet modes in (2) one can derive that the Hermitian operator $\mathcal{H}(t) = H(t) - i \frac{d}{dt}$ has eigenvalues

$$\mathcal{H}(t) | \Phi_{\alpha}(t) \rangle = \epsilon_{\alpha} | \Phi_{\alpha}(t) \rangle .$$  

(9)
Applying a Fourier expansion we can map the time-dependent evolution problem to a time-independent eigenvalue problem

\[ H(t) = \sum_j e^{-ij\Omega t} H_j, \quad |\Phi_\alpha(t)\rangle = \sum_j e^{-ij\Omega t} |\Phi_j^\alpha\rangle \]

\[ \Rightarrow \sum_j (H_{j-k} - j\Omega \delta_{j,k}) |\Phi_j^\alpha\rangle = \epsilon_\alpha |\Phi_\alpha\rangle. \]

Note that the state \(|\Phi_k^\alpha\rangle\) is part of an extended Hilbert space \(\mathcal{R} \otimes \mathcal{T}\) containing the original Hilbert space \(\mathcal{R}\) onto which \(H(t)\) acts and the Hilbert space \(\mathcal{T}\) of square-integrable periodic functions of period \(T\). This extended Hilbert space is not physical, but it has a clear connection to the original Hilbert space: the eigenvalues of the time-independent problem are identical to the original time-dependent problem, up to multiples of \(j\Omega\). A graphical interpretation of this procedure is shown in Fig. 1 b), as the original system is expanded into infinitely many copies. The Hamiltonian \(H_0\) acts within the plane, while \(H_{\pm\gamma}, \gamma > 0\) introduces hopping in the \(j\) direction. In the literature, this is understood as extending the system in a new dimension [21]. This is certainly true for non-interacting systems, but not in the strict many-body sense, as with each additional layer in the quantum number \(j\) the Hilbert space dimension increases by \(\text{dim}(\mathcal{R})\), but in a many-body system it would be multiplied by \(\text{dim}(\mathcal{R})\).

The eigenvalue problem in (11) is the starting point for our second algorithm. We parameterize the Floquet eigenstates \(|\Phi_k^\alpha\rangle\) using a parameterized quantum circuit

\[ |\Phi_k^\alpha\rangle \approx U_\Theta |0\rangle_\mathcal{T} |0\rangle_\mathcal{R}. \]

Notice that we used the notation \(|0\rangle_\mathcal{T} |0\rangle_\mathcal{R}\) to mark the extended Hilbert space computational basis. Here the first number marks the quantum number \(j\) of the \(\mathcal{T}\) Hilbert space part, while the second number refers to the original Hilbert space \(\mathcal{R}\). In the following we neglect the indices \(\mathcal{T}\) and \(\mathcal{R}\) of the states. We define the effective Hamiltonian

\[ H_{\text{eff}}^{ik} = H_{j-k} - j\Omega \delta_{j,k}. \]

Now we want to compute the eigenstates of \(H_{\text{eff}}\) to obtain the Floquet band structure. We use the variational principle to optimize the parameters \(\Theta\). As the extended Hilbert space is infinite dimensional, we truncate \(H_{\text{eff}}\) at \(\pm j_{\text{max}}\). This truncation introduces finite size errors in our calculation. We expect that finite size errors are smallest in the center of the band structure. We therefore minimize \(H_{\text{eff}}^2\) instead of \(H_{\text{eff}}\), giving us the squared eigenvalues \(\epsilon_\alpha^2\). The sign of the eigenvalues can then be determined after optimization by measuring the expectation value of \(H_{\text{eff}}\). As in the first algorithm we define our target function using a Lagrange multiplier \(\lambda > 0\) to project out solutions \(\Theta_\beta\) that have previously been computed

\[ \mathcal{L}(\Theta) = |\langle 0 | \langle 0 | U_\Theta^\dagger H_{\text{eff}}^2 U_\Theta |0\rangle |0\rangle - \lambda \sum_\beta |\langle 0 | \langle 0 | U_\Theta^\dagger U_\Theta U_\Theta |0\rangle |0\rangle|^2, \]

which corresponds to an excited state variational quantum eigensolver [44] for the squared effective Hamiltonian. An overview of the Algorithm is sketched in Fig. 1 b).

By analyzing the second algorithm in comparison to the first algorithm, we immediately identify the increased auxiliary qubits that are required due to the extension of the Hilbert space. While this increases the width of the quantum circuit, its depth now depends
**Algorithm 2** Fauseweh-Zhu-2

**Require:**
- parameterized quantum circuit $U_\Theta$ in extended Hilbert space $\mathcal{R} \otimes T$
- previous solutions $\Theta_i$
- Fourier expansion of Hamiltonian $H_{\text{eff}} = H_{j-k} - j\Omega \delta_{j,k}$
- Truncation value $j_{\text{max}}$

1: **procedure** OPTIMIZE($U_\Theta$)

2: Choose initial parameters $\Theta$

3: while Maximize $L(\Theta) = \langle 0 \vert \langle 0 \vert U^{\dagger}_\Theta H_{\text{eff}}^2 U_\Theta \vert 0 \rangle \vert 0 \rangle - \lambda \sum_\beta \vert \langle 0 \vert \langle 0 \vert U^{\dagger}_\Theta \beta \vert U_\Theta \vert 0 \rangle \vert 0 \rangle \vert^2$

4: Evaluate observable $\langle 0 \vert \langle 0 \vert U^{\dagger}_\Theta H_{\text{eff}}^2 U_\Theta \vert 0 \rangle \vert 0 \rangle$

5: Evaluate circuits $U^{\dagger}_\Theta \beta U_\Theta \vert 0 \rangle \vert 0 \rangle$

6: Update parameters $\Theta$ to increase target $L(\Theta)$

7: Compute $\epsilon_\alpha \pm j\Omega = \langle 0 \vert \langle 0 \vert U^{\dagger}_\Theta H_{\text{eff}} U_\Theta \vert 0 \rangle \vert 0 \rangle$

8: **return** $\epsilon_\alpha \pm j\Omega, \Theta_\alpha$

purely on the depth of the ansatz. This is in striking contrast to the first algorithm, where the maximum depth is determined by the IQPE part of the algorithm, and hence by the required quasi-energy resolution. The second algorithm also has the property of benefiting from a mixed qudit-qubit architecture, as the truncated $T$ part of the Hilbert space naturally leads to states such as $\vert \pm j \rangle \vert \phi \rangle$, with $\vert \phi \rangle$ being a state in the $\mathcal{R}$ Hilbert space. This could be useful for quantum computer architectures that have access to more than two states per fundamental quantum building block. The accuracy of the approach also directly depends on the maximum truncation $j_{\text{max}}$, that needs to be determined, depending on the driving and the original Hamiltonian.

4 **Benchmark**

To evaluate the performance of both algorithms, we investigate one of the simplest systems that remains not analytically solvable, the linear driven spin-$\frac{1}{2}$,

$$H(t) = -\frac{\Delta}{2} \sigma_z + \frac{A}{2} \cos(\Omega t) \sigma_x .$$

(15)

Here $\sigma_i$ are the Pauli matrices. We fix the energy spacing $\Delta = 1$ and the driving frequency $\Omega = 2.5$, and investigate the Floquet band structure as a function of the amplitude $A$.

4.1 **Algorithm Fauseweh-Zhu-1**

We use the $U3$ gate as a generic single qubit rotation for the parameterized quantum circuit:

$$U3(\theta, \phi, \nu) = \begin{pmatrix} \cos(\frac{\theta}{2}) & -e^{i\nu} \sin(\frac{\theta}{2}) \\ e^{i\phi} \sin(\frac{\theta}{2}) & e^{i(\phi+\nu)} \cos(\frac{\theta}{2}) \end{pmatrix}$$

(16)

The time evolution $U_T = \mathcal{T} \exp(-i \int dt H(t))$ is performed using Trotterization with 100 time steps. Optimization is performed using conjugate gradient descent on a quantum computer simulator using the IBM qiskit package [69]. The eigenstates are optimized with $10^4$ samples, while the IQPE uses 100 samples with 5 iterations. Results for the Floquet
band structure are shown in Fig. 2. We see a very good agreement between the simulated results and the exact quasi-energy band structure. The error bars are the result of the limited iteration depth in the IQPE.

4.2 Algorithm Fauseweh-Zhu-2

As the second algorithm uses the extended Hilbert basis we transfer the problem in (15) to frequency space with a truncation value of $j_{\text{max}} = \pm 1$

$$H_{\text{eff}} = \frac{\Delta}{2} \sigma_z \otimes 1 + \frac{A}{2} \sigma_x \otimes S_x,$$

(17)

where the matrix $S_x$ is defined in the appendix A. To account for this, we must also enlarge the ansatz in the parameterized quantum circuit and cannot use a single qubit gate. We use a variational Hamiltonian approach [50] to effectively reach the target states,

$$U_{\Theta} = \prod_l \exp(-iK_l \Theta_l).$$

(18)

We specify the hermitian generators $K_l$ in the appendix A. The parameters are optimized using the conjugate gradient descent method. We used $10^4$ samples for optimization and evaluation of observables on a quantum computing simulator. For comparison we also computed the exact eigenvalues of the Floquet matrix. The results are shown in Fig. 3. We see a very good agreement between the simulated results and the exact quasi-energy structure of the truncated Hamiltonian. Naturally the truncation leads to an increasing error with amplitude $A$ and only qualitatively captures the exact quasi-energy band structure to a certain point.
Figure 3: Simulation results for the Floquet energies of the driven spin-$\frac{1}{2}$ system using algorithm Fauseweh-Zhu-2 with $\lambda = 5$ and $j_{\text{max}} = 1$. Straight lines show the exact result, dashed lines show the exact eigenstates of the truncated Hamiltonian in the extended Hilbert space. Errorbars are from $10^4$ samples.

5 Discussion

In this paper we have presented two quantum algorithms, Fauseweh-Zhu-1 and Fauseweh-Zhu-2, to compute Floquet eigenstates and quasi-energies. Both algorithms use parameterized quantum circuits in combination with a quantum-classical hybrid approach to find solutions to the defining Floquet properties in time- and frequency-domain, respectively. While the precision of the first algorithm depends on the depth of the quantum circuit due to the IQPE application, the precision of the second algorithm mainly depends on the frequency truncation $j_{\text{max}}$ and thereby on the width of the parameterized quantum circuit. There are no fundamental hurdles in applying both algorithms on NISQ devices, with the advantage of complementary requirements in circuit depth and width for increasing system size. We tested both algorithms on a quantum computer simulator for the linear driven spin-$\frac{1}{2}$ problem and showed the principal applicability of our approach. As with other variational hybrid algorithms, the ansatz for the parameterized quantum circuit is fundamental for the success of the approach. In this context, the qudit-qubit structure of the second algorithm calls for novel schemes that have so far not been explored. It will be interesting to explore more complicated driving schemes with our approach and to test the performance on real devices using advanced error mitigation methods [59] in the near future.

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A Generators for variational Hamiltonian ansatz

To find an efficient variational ansatz for the Fauseweh-Zhu-2 algorithm we first separate the gates required for the $T$ and the $R$ part of the Hilbert space. For $j_{\text{max}} = \pm 1$ the qudit space is 3 dimensional. A general unitary matrix in SU(3) can be parameterized using the Gell-Mann matrices, which span the corresponding Lie-Algebra. For our particular case we find, that a much more limited set is sufficient to find all Floquet eigenstates. For $R$ a simple Ry gate is sufficient. Naturally for nonzero $A$ the Floquet eigenstates do not separate into the two Hilbert spaces anymore and we need an entangling gate to account for this. We use the matrices

$$S_4 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad S_5 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$S_x = \frac{1}{2} (S_5 + S_4),$$

(19)

to define our variational Hamiltonian ansatz

$$U_\Theta = e^{i\Theta_1 \sigma_y} e^{i\Theta_2 S_4} e^{i\Theta_3 S_5} e^{i\Theta_4 S_x \sigma_z} e^{i\Theta_5 \sigma_y} e^{i\Theta_6 S_4} e^{i\Theta_7 S_5},$$

(20)

where $e^{i\Theta_4 S_x \sigma_z}$ is the aforementioned entangling gate.