$\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\text{¡}\mathcal{N}$: a Python Package for Dynamics and Exact Diagonalisation of Quantum Many Body Systems
part I: spin chains

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Abstract

We present a new open-source Python package for quantum dynamics of spin chains based on exact diagonalisation, called $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\text{¡}\mathcal{N}$. The package is well-suited to study, among others, quantum quenches at finite and infinite times, the Eigenstate Thermalisation hypothesis, many-body localisation and other dynamical phase transitions, periodically-driven (Floquet) systems, adiabatic and counter-diabatic ramps, and spin-photon interactions. Moreover, $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\text{¡}\mathcal{N}$'s user-friendly interface can easily be used in combination with other Python packages which makes it amenable to a high-level customisation. We explain how to use $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\text{¡}\mathcal{N}$ using three detailed examples: (i) adiabatic ramping of parameters in the many-body localised XXZ model, (ii) heating in the periodically-driven transverse-field Ising model in a parallel field, and (iii) quantised light-atom interactions: recovering the periodically-driven atom in the semi-classical limit of a static Hamiltonian.

Contents

1 What Problems can I Solve with $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\text{¡}\mathcal{N}$?

The study of quantum many-body dynamics comprises a variety of problems, such as dynamical phase transitions (e.g. many-body localisation), thermalising long-time evolution, adiabatic change of parameters, periodically-driven systems, and many others. In contrast to the tremendous progress made in studying low-energy phenomena based on well-developed sophisticated techniques, such as Quantum Monte Carlo methods, Density Matrix Renormalisation Group, Matrix Product States, Dynamical Mean-Field Theory, etc., one of the most popular "cutting-edge" investigation technique for out-of-equilibrium quantum many-body problems is 'old school' exact diagonalisation (ED).

Over the last years, there appeared a positive tendency to develop and provide open source, freely accessible numerical packages and libraries which contribute to widespread the use of such numerical techniques among the condensed matter community: the Algorithms and Libraries for Physics Simulations (ALPS), the C++ library ITensor, as well as the Quantum Toolbox in Python (QuTiP) are among the most common available and freely accessible tools. In this paper, we report on a newly developed optimised open-source Python package for dynamics and exact diagonalisation of quantum many-body spin systems, called $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\text{¡}\mathcal{N}$.

In $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\text{¡}\mathcal{N}$, quantum many-body operators are represented as matrices, the computation of which is done through custom code written in Cython. Cython is an optimizing static compiler which takes code written in a syntax similar to Python, and compiles it into a highly efficient C/C++ code. This code is then automatically interfaced with Python, but can run orders of magnitude faster than pure Python codes do. The quantum operators are stored as memory efficient SciPy sparse matrices. This allows $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\text{¡}\mathcal{N}$ to easily interface with mature Python packages, such as NumPy and SciPy, or any other Python package. These packages provide reliable state-of-the-art tools for scientific computation as well as support from the Python community to regularly improve and update them. Moreover, we have included specific functionality in $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\text{¡}\mathcal{N}$ which uses NumPy and SciPy to do many desired calculations common to ED studies, while making sure the user only has to call a few NumPy or SciPy functions directly. Last but not least, $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\text{¡}\mathcal{N}$ has been especially designed to construct particularly short and efficient ED codes (typically less than 200 lines, as we explicitly demonstrate in Sec. 2 and App. B). This greatly reduces the amount of time required to start a new study; it also allows users with little-to-no programming experience to do state of the art ED calculations. We, therefore, believe $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\text{¡}\mathcal{N}$ to be of particular interest to undergraduate and graduate students, post-doctoral researchers, and young professors who can use it to quickly test new exciting ideas, build up their intuition about quantum many-body problems, or even benefit from the code in a teaching process.

Let us be specific and give a short list of 'hot' topics that can successfully be studied with the help of $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\text{¡}\mathcal{N}$:

* quantum quenches and quantum dynamics at finite and infinite times

* adiabatic and counter-diabatic ramps
* periodically driven (Floquet) systems
* many-body localisation, Eigenstate Thermalisation hypothesis
* quantum information
* quantised photon-spin interactions and similar cavity QED related models
* dynamical phase transitions and critical phenomena
* machine learning with quantum many-body systems

This list is far from being complete, but it can serve as a useful guideline to the interested user. In Sec. 2, we illustrate in detail how to use $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{¡}\mathcal{N}$, addressing three exciting problems, which we believe cover a wide range of interesting topics, to exemplify some of the most common $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{¡}\mathcal{N}$ tools.

Before we close the introduction, let us describe some of the general features that make $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{¡}\mathcal{N}$ interesting and useful and which, we believe, can serve a countless number of different studies.

- A major representative feature of $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{¡}\mathcal{N}$ is the construction of spin Hamiltonians containing arbitrary (possibly non-local in space) many-body operators. One example is the four-spin operator $\mathcal{O} = \sum_j \sigma^z_j \sigma^+_{j+1} \sigma^-_{j+2} \sigma^z_{j+3} + \mathrm{h.c.}$. Such multi-spin operators are often times generated by the nested commutators typically appearing in higher-order terms of perturbative expansions, such as the Schrieffer-Wolff transformation[CITE] and the inverse-frequency expansion[CITE]. Sometimes they can appear in the study of exactly solvable engineered topological models.

- Another important feature is the availability to use symmetries which, if present in a given model, give rise to conservation laws leading to selection rules between the many-body states. As a result, the Hilbert space reduces to a tensor product of the Hilbert spaces corresponding to the underlying symmetry blocks. Consequently, the presence of symmetries effectively diminishes the relevant Hilbert space dimension which, in turn, allows one to study larger systems. Currently, $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{¡}\mathcal{N}$ supports the following spin chain symmetries:

  – total magnetisation (particle number in the case of hard-core bosons)
  – parity (i.e. reflection w.r.t. the middle of the chain)
  – spin inversion (on the entire chain but also individually for sublattices A and B)
  – the joint application of parity and spin inversion (present e.g. when studying staggered or linear external potentials)
  – translation symmetry
  – all physically meaningful combinations of the above

  As we shall see in Sec. 2, constructing Hamiltonians with given symmetries is done by specifying the desired symmetry block.

- As we mentioned above, as of present date ED methods represent one of the most reliable ways to safely study quantum dynamics in a secure, generic way. In this respect, it is important to emphasise that with $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{¡}\mathcal{N}$ the user can build arbitrary time-dependent Hamiltonians. The package contains built-in routines to calculate the real (and imaginary) time evolution of any quantum state under a user-defined time-dependent Hamiltonian based on SciPy's integration tool for ordinary differential equations[CITE].

- Besides spin chains, $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{¡}\mathcal{N}$ also allows the user to couple an arbitrary interacting spin chain to a single photon mode (i.e. quantum harmonic oscillator). In this case, the total magnetisation symmetry is replaced by the combined total photon and spin number conservation. Such an example is discussed in Sec. 2.3.

2 How do I use $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{¡}\mathcal{N}$?

One of the main advantages of $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{¡}\mathcal{N}$ is its user-friendly interface. To demonstrate how the package works, we shall guide the reader step by step through a short Python code, explaining all details of a proper usage of the package. In case the reader is unfamiliar with Python, we kindly invite them to accept the challenge of learning the Python basics, while enjoying the study of quantum many-body dynamics!

Installing $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{¡}\mathcal{N}$ is quick and efficient; just follow the steps outlined in App. A.

Below, we stick to the following general guidelines: first, we define the problem containing the physical quantities of interest and show their behaviour in a few figures. After that, we present the $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{¡}\mathcal{N}$ code used to generate them, broken up into its building blocks. We explain each step in great detail. The complete contiguous code, including the lines used to generate the figures shown below, is available in App. B. It is not our purpose in this paper to discuss in detail the interesting underlying physics of these systems; instead, we focus on setting up the Python code to study them with the help of $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{¡}\mathcal{N}$, and leave the interested reader figure out the details themselves.

2.1 Adiabatic Control of Parameters in Many-Body Localised Phases

Physics Setup—Strongly disordered many-body models have recently enjoyed a lot of attention in the theoretical condensed matter community. It has been shown that, beyond a critical disorder strength, these models undergo a dynamical phase transition from an delocalised ergodic (thermalising) phase to a many-body localised (MBL), i.e. non-conducting, non-thermalising phase[CITE], in which the system violates the Eigenstate Thermalisation hypothesis[CITE].

In our first $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{¡}\mathcal{N}$ example, we show how one can study the adiabatic control of model parameters in many-body localised phases. It was recently argued that the adiabatic theorem does not apply to disordered systems [CITE]. On the other hand, controlling the system parameters in MBL phases is of crucial experimental[CITE] significance. Thus, the question as to whether there exists an adiabatic window for some, possibly intermediate, ramp speeds (as is the case for periodically-driven systems[CITE]), is of particular and increasing importance.

Let us consider the XXZ open chain in a disordered z-field with the Hamiltonian

$$\begin{aligned} H(t) &= \sum_{j=0}^{L-2} \frac{J_{xy}}{2} \left(S^+_{j+1} S^-_j + \text{h.c.} \right) + J_{zz}(t) S^z_{j+1} S^z_j + \sum_{j=0}^{L-1} h_j S^z_j, \\ J_{zz}(t) &= (1/2 + vt) J_{zz}(0), \end{aligned} \tag{1}$$

where J_{xy} is the spin-spin interaction in the xy-plane, disorder is modelled by a uniformly distributed random field $h_j \in [-h_0, h_0]$ of strength h_0 along the z-direction, and the spin-spin interaction along the z-direction – $J_{zz}(t)$ – is the adiabatically-modulated (ramp) parameter. In the following, we set $J_{zz}(0) = 1$ as the energy units. Note that we enumerate the L sites of the chain by $j = 0, 1, \ldots, L-1$ to conform with Python's array indexing convention. It has been demonstrated that this model exhibits a transition to an MBL phase [CITE]. In particular, for $h_0 = h_{\text{MBL}} = 3.9$ the system is in a many-body localised phase, while for $h_0 = h_{\text{ETH}} = 0.1$ the system is in the ergodic (ETH) delocalised phase. We now choose the ramp protocol $J_{zz}(t) = (1/2 + vt) J_{zz}(0)$ with the ramp speed v, and evolve the system with the Hamiltonian $H(t)$ from $t_i = 0$ to[1] $t_f = (2v)^{-1}$. We choose the initial state $|\psi_i\rangle = |\psi(t_i)\rangle$ from the middle of the spectrum of $H(t_i)$ to ensure typicality; more specifically we choose $|\psi_i\rangle$ to be that eigenstate of $H(t_i)$ whose energy is closest to the rum of middle of the spectrum of $H(t_i)$, where the density of states, and thus the thermodynamic entropy, is largest.

To determine whether the system can adiabatically follow the ramp, we use two different indicators: (i) we evolve the state up to time t_f and project it onto the eigenstates of $H(t_f)$. The corresponding diagonal entropy density:

$$s_d = -\frac{1}{L} \text{tr} \left[\rho_d \log \rho_d \right], \qquad \rho_d = \sum_n |\langle n | \psi(t_f) \rangle|^2 |n\rangle\langle n| \tag{2}$$

in the basis $\{|n\rangle\}$ of $H(t_f)$ at small enough ramp speeds v, is a measure of the delocalisation of the time-evolved state $\psi(t_f)\rangle$ onto the energy eigenstates of $H(t_f)$. If, for instance, after the ramp the system still occupies a single eigenstate $|\tilde{n}\rangle$, then $s_d = 0$. Figure ??? shows the entropies vs. ramp speed data in the MBL and ETH phases.

The second measure of adiabaticity we use is (ii) the entanglement entropy density

$$s_{\text{ent}}(t_f) = -\frac{1}{|\text{A}|} \text{tr}_\text{A} \left[\rho_\text{A}(t_f) \log \rho_\text{A}(t_f) \right], \qquad \rho_\text{A}(t_f) = \text{tr}_{\text{A}^\text{c}} |\psi(t_f)\rangle\langle\psi(t_f)| \tag{3}$$

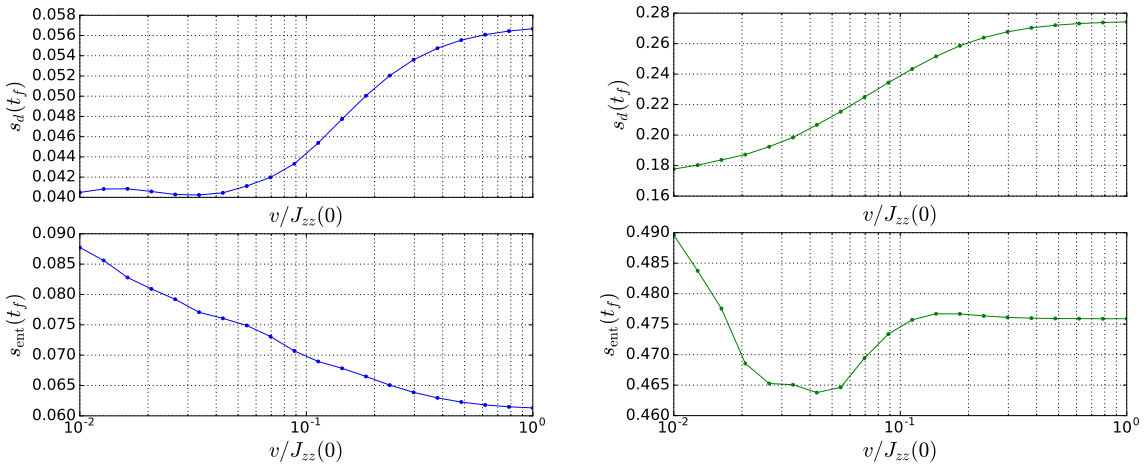
of subsystem A, defined to contain the left half of the chain and $|\text{A}| = L/2$. We denoted the reduced density matrix of subsystem A by ρ_A, and A^c is the complement of A.

The entropies are shown in Fig. 1.

Code Analysis—Let us now explain how one can study this problem numerically using $\mathcal{Q}^\text{u}\mathcal{S}\rho\text{¡}\mathcal{N}$. First, we load the required Python packages. Note that we adopt the commonly used abbreviation for NumPy, `np`.

```
from qspin.operators import hamiltonian # Hamiltonians and operators
from qspin.basis import spin_basis_1d # Hilbert space spin basis
from qspin.tools.measurements import ent_entropy, diag_ensemble # entropies
from numpy.random import ranf,seed # pseudo random numbers
from joblib import delayed,Parallel # parallelisation
import numpy as np # generic math functions
from time import time # timing package
```

[1] Notice that $t_f \to \infty$ as $v \to 0$ and thus, the total evolution time increases with decreasing the ramp speed v.



(a) ETH phase (b) MBL phase

Figure 1: Diagonal and entanglement entropy densities as a function of the ramp speed in the MBL and delocalised (ETH) phases of the ramped disordered XXZ model. The ramped protocol is chosen as $J_{zz}(t) = (1/2 + vt)J_{zz}(0)$. The parameters are $J_{xy}/J_{zz}(0) = 1.0$, $h_{\rm MBL}/J_{zz}(0) = 3.9$, $h_{\rm ETH}/J_{zz}(0) = 0.1$, and $L = 10$. Disorder averaging was performed over 1000 realisations.

Since we want to produce many realisations of the data and average over disorder, we specify the simulations parameters: `n_real` is the number of disorder realisations, while `n_jobs` is the `joblib` parallelisation parameter which determines how many Python processes to run simultaneously[2].

```
##### define simulation parameters #####
n_real=20 # number of disorder realisations
n_jobs=2 # number of spawned processes used for parallelisation
```

Next, we define the physical model parameters. In doing so it is advisable to use the floating point when the coupling is meant to be a non-integer real number, in order to avoid problems with division: for example, `1` is the integer 1 while `1.0` – the corresponding float. For instance, in Python 2.7 `0.5` is *not* equal to `1/2`, but rather to `1.0/2.0`.

```
##### define model parameters #####
L=10 # system size
Jxy=1.0 # xy interaction
Jzz_0=1.0 # zz interaction at time t=0
h_MBL=3.9 # MBL disorder strength
h_ETH=0.1 # delocalised disorder strength
vs=np.logspace(-2.0,0.0,num=20,base=10) # log_2-spaced vector of ramp speeds
```

The time-dependent disordered Hamiltonian consists of two parts: the time-dependent XXZ model which is disorder-free, and the disorder field whose values differ from one realisation to another. We focus on the XXZ part first. Let us code up the driving protocol $J_{zz}(t) = (1/2 + vt)J_{zz}(0)$. As already explained, our goal is to obtain the disorder-averaged entropies

[2] While one can spawn as many processes as one desires, it is optimal to spawn only about as many processes as there are available cores in the processor.

as a function of the ramp speed v. Hence, for each disorder realisation, we need to evolve the initial state many times, each corresponding to a different ramp speed. However, defining the Hamiltonian from the get-go every single time is not particularly efficient from the point of view of simulation runtime. We thus want to set up a family of Hamiltonians $\{v : H(t; v)\}$ at once, and we shall employ Python's features to do so. This will require that the drive speed `v` is *not* a parameter of the function `ramp`, see `line 29`, but is declared beforehand as a global variable. Once, `ramp` has been defined, reassigning `v` dynamically induces a change of `ramp` without the need to modify `ramp` itself. We shall comment on how this works later on in the code.

```
26 ##### set up Heisenberg Hamiltonian with linearly varying zz-interaction #####
27 # define linear ramp function
28 v = 1.0 # declare ramp speed variable
29 def ramp(t):
30     return (0.5 + v*t)
31 ramp_args=[]
```

To set up any Hamiltonian, we need to calculate the basis of the Hilbert space it is defined on. Since the Hamiltonian (1) conserves the total magnetisation, the overlap betweens states of different magnetisation sectors vanishes trivially, and we can reach larger system sizes by working in a fixed magnetisation sector. A natural choice is the zero-magnetisation sector which contains the ground state. All symmetries in $\mathcal{QuSpy}$ can be declared when the `basis` is being created. As shown below, the `basis` class has one required argument `L` – the system size. The user can declare a symmetry with the help of optional arguments: for instance, `Nup=L/2` defines the zero-magnetisation sector. In general, the magnetisation symmetry is defined by specifying the number of up spins in the chain. In Sec. 2.2 we shall show how to use two other symmetries – translation and parity (reflection). Last, since we work with spin operators here, it is required to pass the flag `pauli=False`; failure to do so will result in a Hamiltonian defined in terms of the Pauli spin matrices.

```
27 # compute basis in the 0-total magnetisation sector (requires L even)
28 basis = spin_basis_1d(L,Nup=L/2,pauli=False)
```

Setting up the spin-spin operators goes as follows. First, we need to define the site-coupling lists `J_zz` and `J_xy`. To uniquely specify a two-spin interaction, we need (i) the coupling, and (ii) – the labels of the sites the two operators act on. $\mathcal{QuSpy}$ uses Python's indexing convention meaning that the first lattice site is always $i = 0$, and the last one: $i = L - 1$. For example, for the zz-interaction, the coupling is `Jzz_0`, while the two sites are the nearest neighbours `i,i+1`. Hence, the tuple `[Jzz_0,i,i+1]` defines the bond operator $J_{zz}(0) \times S^\mu_i S^\mu_{i+1}$ (we specify μ in the next step). To define the total interaction energy $J_{zz}(0) \sum_{i=0}^{L-2} S^\mu_i S^\mu_{i+1}$, all we need is to loop over the $L - 2$ bonds of the open chain[3]. In the same way one can define boundary or single-site operators.

```
29 # define operators with OBC using site-coupling lists
30 J_zz = [[Jzz_0,i,i+1] for i in range(L-1)] # OBC
31 J_xy = [[Jxy/2.0,i,i+1] for i in range(L-1)] # OBC
```

The above lines of code specify the coupling but not yet which spin operators are being coupled. To do this, we need to create a `static` and/or `dynamic` operator list. As the name suggests, static lists define time-independent operators. Given the site-coupling list `J_xy` from above,

[3] The Python expression `range(L-1)` produces all integers between `0` and `L-2` including.

it is easy to set the operator $J_{xy}/2\sum_{i=0}^{L-2} S_i^+ S_{i+1}^-$ by specifying the spin operator type in the same order as the site indices appear in the corresponding site-coupling list: `[["+-",J_xy]]`. In other words, the order `"+-"` corresponds directly to the site-index order `"i,i+1"`. Similarly, one can set up the hermitian conjugate term $J_{xy}/2\sum_{i=0}^{L-2} S_i^- S_{i+1}^+$ as `[["-+",J_xy]]`. In the end, one can concatenate these operator lists to produce the static part of the Hamiltonian.

```
32 # static and dynamic lists
33 static = [["+-",J_xy],["-+",J_xy]]
```

The time-dependent part of the Hamiltonian is defined using `dynamic` lists. Similar to their static counterparts, one needs to define an operator string, say `"zz"` to declare the specific operator our of a site-coupling list. Apart from the site-coupling list `J_zz`, however, a dynamic list also requires a time-dependent function and its arguments. If one desires to define a time-independent Hamiltonian, then one should set an empty dynamic list, `dynamic=[]`. In the linearly driven XXZ-Hamiltonian we are setting up here, the function arguments `ramp_args` is an empty list. The careful reader might have noticed that there is a certain freedom in coding the coupling of the time-dependent term, $J_{zz}(t) = (1/2 + vt)J_{zz}(0)$: here we choose to include the constant `Jzz_0` in the `zz` site-coupling list and hence this factor is absent in the definition of the `ramp` function.

```
34 dynamic =[["zz",J_zz,ramp,ramp_args]]
```

Once the static and dynamic lists are set up, building up the corresponding Hamiltonian is a one-liner. In $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathcal{N}$, this is done using the `hamiltonian` class, see `line 36` below. The first required argument is the `static` list, while the second one – the `dynamic` list. These two arguments necessarily must appear in this order. Another required argument is the `basis`, which carries the necessary information about symmetries. Yet whether a given Hamiltonian has these symmetries or not, depends on the operators defined in the static and dynamic lists. The `hamiltonian` class performs an automatic check on the Hamiltonian for hermiticity and the presence of magnetisation conservations and other symmetries.

```
35 # compute the time-dependent Heisenberg Hamiltonian
36 H_XXZ = hamiltonian(static,dynamic,basis=basis,dtype=np.float64)
```

To produce the entropies vs. ramp speed data over many disorder realisations, we define the function `realization` which returns a two-element NumPy array, `np.array([S_d,Sent])` with the values of the diagonal entropy s_d in the first element, and the values of the entanglement entropy s_{ent} – in the second element. We now walk the reader step by step through the definition of `realization`. The first argument is the vector of ramp speeds, `vs`, required for the dynamics. The second argument is the time-dependent XXZ Hamiltonian `H_XXZ` to which we shall add a disordered z-field for each disorder realisation. The third argument is the spin `basis` which is required to calculate s_{ent}. The fourth (last) argument is the realisation number, which is only used to print a message about the duration of the single realisation run.

```
38 ##### calculate diagonal and entanglement entropies #####
39 def realization(vs,H_XXZ,basis,real):
40     """
41     This function computes the entropies for a single disorder realisation.
42     --- arguments ---
43     vs: vector of ramp speeds
44     H_XXZ: time-dep. Heisenberg Hamiltonian with driven zz-interactions
45     basis: spin_basis_1d object containing the spin basis
46     n_real: number of disorder realisations; used only for timing
```

```
47      """
```

In order to time each realisation simulation, we use the package `time`:

```
48      ti = time() # start timer
```

In order to properly be able to use $H_{\mathrm{XXZ}}(t;v)$ as a family of Hamiltonians in v (we shall see exactly how this works in a moment), we explicitly declare the variable `v` global.

```
50      global v # declare ramp speed v a global variable
```

Since the problem involves disorder, we have to generate multiple disorder realisations. In this case, it is recommended to reset the pseudo-random generator before any random numbers have been drawn. It is important that the seed is reset within each realisation, since we shall allow for the option to run realisations simultaneously.

```
52      seed() # the random number needs to be seeded for each parallel process
```

Next, we set up the full disordered time-dependent Hamiltonian of the problem $H(t) = H_{\mathrm{XXZ}}(t) + \sum_j h_j S^z_j$. The random field h_j differs from one realisation to another. Hence, it has to be defined inside the `realisation` function. Recall that we want to compare the localised with the delocalised regimes, corresponding to the disordered strengths h_{MBL} and h_{ETH}, respectively. To this end, we first, for each lattice site i, draw a random number `unscaled_fields[i]` uniformly in the interval $[-1,1]$, and store it in the vector `unscaled_fields`, see `line 55` below. Building the external z-field proceeds in exactly the same way as before: (i) we calculate the site-coupling list, `line 57`, (ii) we designate that the operator is along the z-axis by defining a static operator list, `line 59`, and (iii) we use the already computed spin basis to construct the operator matrix with the `hamiltonian` class, `lines 61-62`. $\mathcal{QuSpinN}$ has the option to disable the default checks on hermiticity, magnetisation (particle number) conservation, and symmetries using the auxiliary dictionary `no_checks` passed straight to `hamiltonian` as keyword arguments. This can allow the user to define non-hermitian operators. Last, in `lines 64-65`, we define the MBL and ETH time-dependent Hamiltonians, corresponding to the two disorder strengths h_{ETH} and h_{MBL}.

```
54      # draw random field uniformly from [-1.0,1.0] for each lattice site
55      unscaled_fields=-1+2*ranf((basis.L,))
56      # define z-field operator site-coupling list
57      h_z=[[unscaled_fields[i],i] for i in range(basis.L)]
58      # static list
59      disorder_field = [["z",h_z]]
60      # compute disordered z-field Hamiltonian
61      no_checks={"check_herm":False,"check_pcon":False,"check_symm":False}
62      Hz=hamiltonian(disorder_field,[],basis=basis,dtype=np.float64,**no_checks)
63      # compute the MBL and ETH Hamiltonians for the same disorder realisation
64      H_MBL=H_XXZ+h_MBL*Hz
65      H_ETH=H_XXZ+h_ETH*Hz
```

We choose to first focus on the MBL phase. Re-setting the ramp speed `v` to unity is required for calculating the correct eigensystem of the Hamiltonian at the end of the ramp, since v is a parameter of $H(t;v)$ (see `line 77`). We want the initial state to be as close as possible to an infinite-temperature state within the given symmetry sector. To this end, we can first calculate the minimum and maximum energy, `Emin` and `Emax` of the spectrum of $H_{\mathrm{MBL}}(t=0)$. This is achieved using the `hamiltonian` attribute method `eigsh`, see `lines 70-71`, which is a wrapper for `scipy.sparse.linalg.eigsh`, cf. App. C. Then, by taking the 'centre-of-mass'

we obtain a number, `E_inf_temp`, which is as represents the infinite-temperature energy up to finite-size effects, `line 72`. The initial state `psi_0` is then that eigenstate of $H_{\mathrm{MBL}}(t=0)$, whose energy is closest to `E_inf_temp`, cf. `lines 74-75`.

```
67      ### ramp in MBL phase ###
68      v=1.0 # reset ramp speed to unity
69      # calculate the energy at infinite temperature for initial MBL Hamiltonian
70      eigsh_args={"k":2,"which":"BE","maxiter":1E10,"return_eigenvectors":False}
71      Emin,Emax=H_MBL.eigsh(time=0.0,**eigsh_args)
72      E_inf_temp=(Emax+Emin)/2.0
73      # calculate nearest eigenstate to energy at infinite temperature
74      E,psi_0=H_MBL.eigsh(time=0.0,k=1,sigma=E_inf_temp,maxiter=1E10)
75      psi_0=psi_0.reshape((-1,))
```

The calculation of the diagonal entropy s_d requires the eigensystem of the Hamiltonian $H_{\mathrm{MBL}}(t_f)$ at the end of the ramp $t_f = (2v_f)^{-2}$. The entire spectrum and the corresponding eigenstates are obtained using the `hamiltonian` method `eigh`. For time-dependent Hamiltonians, `eigh` accepts the argument `time` to specify the time slice. Unless explicitly specified, `time=0.0` by default.

```
76      # calculate the eigensystem of the final MBL hamiltonian
77      E_final,V_final=H_MBL.eigh(time=(0.5/vs[-1]))
```

To calculate the entropies for each ramp speed, we define the helper function `_do_ramp`, which first evolves the initial state according to the v-dependent Hamiltonian $H_{\mathrm{MBL}}(t;v)$ for a fixed ramp speed v. In `line 78` we loop over the ramp speed greed `vs`. More importantly, however, the iteration index `v` carries the same name as the parameter in the drive function `ramp`. Thus, every time a new ramp speed is read off the vector `vs`, the external parameter `v` changes its value. Because `v` is a global variable, this change induces a change into the function `ramp` which, in turn, induces a change in the `dynamic` list. Thus, at the end of the day, a new member of the family of MBL Hamiltonians, $\{v : H_{\mathrm{MBL}}(t;v)\}$, is picked and parsed to `_do_ramp` to do the time evolution with. Hence, we end up with a convenient and automatic way of generating the whole family $\{v : H_{\mathrm{MBL}}(t;v)\}$, while having to calculate the operators in the Hamiltonian only once.

```
78      # evolve states and calculate entropies in MBL phase
79      run_MBL=[_do_ramp(psi_0,H_MBL,basis,v,E_final,V_final) for v in vs]
80      run_MBL=np.vstack(run_MBL).T
```

It remains to discuss the helper function `_do_ramp`. It evolves the initial state `psi_0` with the `hamiltonian` object `H` and calculates the entropies at the end of the ramp.

```
100 ##### evolve state and evaluate entropies #####
101 def _do_ramp(psi_0,H,basis,v,E_final,V_final):
102     """
103     Auxiliary function to evolve the state and calculate the entropies after the
104     ramp.
105     --- arguments ---
106     psi_0: initial state
107     H: time-dependent Hamiltonian
108     basis: spin_basis_1d object containing the spin basis (required for Sent)
109     E_final, V_final: eigensystem of H(t_f) at the end of the ramp t_f=1/(2v)
110     """
```

Given a ramp speed `v`, we first determine the total ramp time `t_f`. Evolving a quantum state under any Hamiltonian `H` is easily done with the `hamiltonian` method `evolve`, see `line 114`. `evolve` requires the initial state `psi_0`, the starting time – here `0.0`, and a vector of times to return the evolved state at, but since we are only interested in the state at the final time – we pass `t_f`. The `evolve` method has further interesting features which we discuss in Secs. 2.2 and 2.3.

```
111     # determine total ramp time
112     t_f = 0.5/v
113     # time-evolve state from time 0.0 to time t_f
114     psi = H.evolve(psi_0,0.0,t_f)
```

Once we have the state at the end of the ramp, we can obtain the entropies as follows. Calculating s_{ent} is done using the `measurements` function `ent_entropy` which we imported in `line 3`. It requires the quantum state (here the pure state `psi`), and the `basis` the state is stored in[4]. Optionally, one can specify the site indices which define the subsystem of interest using the argument `chain_subsys`. Note that `ent_entropy` returns a dictionary, in which the value of the entanglement entropy is stored under the key `"Sent"`. The function `ent_entropy` has a variety of interesting features, described in the documentation, see App. C.

```
115     # calculate entanglement entropy
116     subsys = range(basis.L/2) # define subsystem
117     Sent = ent_entropy(psi,basis,chain_subsys=subsys)["Sent"]
```

Similarly, there is a built-in function to calculate the diagonal entropy s_d of a state `psi` in a given basis (here `V_final`), called `diag_ensemble`. This function can calculate a variety of interesting quantities in the diagonal ensemble defined by the eigensystem arguments (here `E_final`, `V_final`). We again invite the interested reader to check out the documentation in App. C. This concludes the definition of `_do_ramp`.

```
118     # calculate diagonal entropy in the basis of H(t_f)
119     S_d = diag_ensemble(basis.L,psi,E_final,V_final,Sd_Renyi=True)["Sd_pure"]
```

Back to the function `realization`, we have already seen how to obtain the entropies in the MBL phase. We now do the same thing in the delocalised ETH phase. Once again, before we start, we have to re-set the parameter `v` to unity, see `line 83`. This is required since the iteration over the ramp speeds `vs` in `line 79` changes dynamically not only the Hamiltonian `H_MBL` but also `H_ETH`. Apart from this subtleties, the code is the same as the MBL one.

```
81      ###  ramp in ETH phase ###
82      v=1.0 # reset ramp speed to unity
83      # calculate the energy at infinite temperature for initial ETH hamiltonian
84      Emin,Emax=H_ETH.eigsh(time=0.0,**eigsh_args)
85      E_inf_temp=(Emax+Emin)/2.0
86      # calculate nearest eigenstate to energy at infinite temperature
87      E,psi_0=H_ETH.eigsh(time=0.0,k=1,sigma=E_inf_temp,maxiter=1E10)
88      psi_0=psi_0.reshape((-1,))
89      # calculate the eigensystem of the final ETH hamiltonian
90      E_final,V_final=H_ETH.eigh(time=(0.5/vs[-1]))
91      # evolve states and calculate entropies in ETH phase
92      run_ETH=[_do_ramp(psi_0,H_ETH,basis,v,E_final,V_final) for v in vs]
93      run_ETH=np.vstack(run_ETH).T # stack vertically elements of list run_ETH
```

[4] The `basis` is required since the subsystem may not share the same symmetries as the entire chain.

We can now display how long the single iteration took

```
95      # show time taken
96      print "realization {0}/{1} took {2:.2f} sec".format(real+1,n_real,time()-ti)
```

and conclude the definition of `realization`:

```
98      return run_MBL,run_ETH
```

Now that we have written the `realization` function, we can call it `n_real` times to produce the data. The easiest way of doing this is to loop over the disorder realisation, as shown in `lines 125-126`. However, a better way of doing this makes use of the `joblib` package which can distribute simultaneous function calls over `n_job` Python processes, see `line 128`. To learn more about how to do this, we invite the readers to check the documentation of `joblib`. Having produced and extracted the entropy vs. ramp speed data, we are ready to perform the disorder average by taking the mean over all realisations, `lines 130-132`.

```
123 ##### produce data for n_real disorder realisations #####
124 """
125 # alternative way without parallelisation
126 data = np.asarray([realization(vs,H_XXZ,basis,i) for i in xrange(n_real)])
127 """
128 data = np.asarray(Parallel(n_jobs=n_jobs)(delayed(realization)(vs,H_XXZ,basis,i) for
        i in xrange(n_real)))
129 run_MBL,run_ETH = zip(*data) # extract MBL and data
130 # average over disorder
131 mean_MBL = np.mean(run_MBL,axis=0)
132 mean_ETH = np.mean(run_ETH,axis=0)
```

The complete code including the lines that produce Fig. 1 is available in Fig. 1.

2.2 Heating in Periodically Driven Spin Chains

Physics Setup—As a second example, we now show how one can easily study heating in the periodically-driven transverse-field Ising model with a parallel field[CITE David, Tomaz]. This model is non-integrable even without the time-dependent driving protocol. The time-periodic Hamiltonian is defined as a two-step protocol as follows:

$$\begin{aligned} H(t) &= \left\{ \begin{array}{ll} J\sum_{j=0}^{L-1}\sigma_j^z\sigma_{j+1}^z + h\sum_{j=0}^{L-1}\sigma^z, & t\in[-T/4,\ T/4] \\ g\sum_{j=0}^{L-1}\sigma_j^x, & t\in[\ T/4, 3T/4] \end{array} \right\} \text{mod } T, \\ &= \sum_{j=0}^{L-1}\frac{1}{2}\left(J\sigma_j^z\sigma_{j+1}^z + h\sigma^z + g\sigma_j^x\right) + \frac{1}{2}\text{sgn}\left[\cos\Omega t\right]\left(J\sigma_j^z\sigma_{j+1}^z + h\sigma^z - g\sigma_j^x\right). \end{aligned} \quad (4)$$

Unlike the previous example, here we a closed spin chain with a periodic boundary (i.e. a ring). The spin-spin interaction strength is denoted by J, the transverse field – by g, and the parallel field – by h. The period of the drive is T and, although the periodic step protocol contains infinitely many Fourier harmonics, we shall refer to $\Omega = 2\pi/T$ as *the* frequency of the drive.

Since the Hamiltonian is periodic, $H(t+T) = H(t)$, Floquet's theorem applies and postulates that the dynamics of the system at times lT, integer multiple of the driving period

(a.k.a. stroboscopic times), is governed by the time-independent Floquet Hamiltonian[5] H_F. In other words, the evolution operator is stroboscopically given by

$$U(lT) = \mathcal{T}_t \exp\left(-i\int_0^{lT} H(t)\mathrm{d}t\right) = \exp(-ilTH_F). \tag{5}$$

While the Floquet Hamiltonian for this system cannot be calculated analytically, a suitable approximation can be found at high drive frequencies by means of the van Vleck inverse-frequency expansion[CITE]. However, this expansion is known to calculate the effective Floquet Hamiltonian H_{eff} in a different basis than the original stroboscopic one: $H_F = \exp[-iK_{\text{eff}}(0)]H_{\text{eff}}\exp[iK_{\text{eff}}(0)]$, which requires the additional calculation of the so-called Kick operator $K_{\text{eff}}(0)$ to 'rotate' to the original basis.

In the inverse-frequency expansion, we expand both H_{eff} and $K_{\text{eff}}(0)$ in powers of the inverse frequency. Let us label these approximate objects by the superscript $^{(n)}$, suggesting that the corresponding operators are of order $\mathcal{O}(\Omega^{-n})$:

$$\begin{aligned}
H_F &= H_F^{(0)} + H_F^{(1)} + H_F^{(2)} + H_F^{(3)} + \mathcal{O}(\Omega^{-4}) = H_F^{(0+1+2+3)} + \mathcal{O}(\Omega^{-4}),\\
H_{\text{eff}} &= H_{\text{eff}}^{(0)} + H_{\text{eff}}^{(1)} + H_{\text{eff}}^{(2)} + H_{\text{eff}}^{(3)} + \mathcal{O}(\Omega^{-4}),\\
K_{\text{eff}} &= K_{\text{eff}}^{(0)} + K_{\text{eff}}^{(1)} + K_{\text{eff}}^{(2)} + K_{\text{eff}}^{(3)} + \mathcal{O}(\Omega^{-4}),
\end{aligned}$$

Using the short-hand notation one can show that, for this problem, all odd-order terms in the van Vleck expansion vanish [see App. G of Ref.[CITE thesis]]

$$H_F^{(0+1+2+3)} = H_F^{(0+2)} \approx \mathrm{e}^{-iK_{\text{eff}}^{(2)}(0)}\left(H_{\text{eff}}^{(0)} + H_{\text{eff}}^{(2)}\right)\mathrm{e}^{+iK_{\text{eff}}^{(2)}(0)}, \tag{6}$$

while the first few even-order ones are given by

$$\begin{aligned}
H_{\text{eff}}^{(0)} &= \frac{1}{2}\sum_j J\sigma_j^z\sigma_{j+1}^z + h\sigma_j^z + g\sigma_j^x,\\
H_{\text{eff}}^{(2)} &= -\frac{\pi^2}{12\Omega^2}\sum_j J^2 g\sigma_{j-1}^z\sigma_j^x\sigma_{j+1}^z + Jgh(\sigma_j^x\sigma_{j+1}^z + \sigma_j^z\sigma_{j+1}^x) + Jg^2(\sigma_j^y\sigma_{j+1}^y - \sigma_j^z\sigma_{j+1}^z)\\
&\qquad + \left(J^2 g + \frac{1}{2}h^2 g\right)\sigma_j^x + \frac{1}{2}hg^2\sigma_j^z,\\
K_{\text{eff}}^{(0)} &= \mathbf{0},\\
K_{\text{eff}}^{(2)}(0) &= -\frac{\pi^2}{8\Omega^2}\sum_j Jg\left(\sigma_j^z\sigma_{j+1}^y + \sigma_j^y\sigma_{j+1}^z\right) + hg\sigma_j^y,
\end{aligned} \tag{7}$$

It was recently argued based on the aforementioned Floquet theorem[CITE] that, in a closed periodically driven system, stroboscopic dynamics is sufficient to completely quantify heating, and we shall make use of this fact in our little study here. We choose as the initial state the ground state of the approximate Hamiltonian $H_F^{(0+1+2+3)}$ and denote it by $|\psi_i\rangle$:

$$|\psi_i\rangle = |\mathrm{GS}(H_F^{(0+1+2+3)})\rangle. \tag{8}$$

[5] One has to be careful when using the term 'Hamiltonian', as H_F need not be a local operator. In such cases there does not exist a static physically meaningful system described by H_F.

Regimes of slow and fast heating can then be easily detected by looking at the energy density $\mathcal{E}$ absorbed by the system from the drive

$$\mathcal{E}(lT) = \frac{1}{L}\langle\psi_i|e^{ilTH_F}H_F^{(0+1+2)}e^{-ilTH_F}|\psi_i\rangle, \tag{9}$$

and the entanglement entropy of a subsystem. We call this subsystem A and define it to contain $L/2$ consecutive chain sites[6]:

$$s_{\rm ent}(lT) = -\frac{1}{L_{\rm A}}{\rm tr}_{\rm A}\left[\rho_{\rm A}(lT)\log\rho_{\rm A}(lT)\right], \quad \text{with} \quad \rho_{\rm A}(lT) = {\rm tr}_{\rm A^c}\left[e^{-ilTH_F}|\psi_i\rangle\langle\psi_i|e^{ilTH_F}\right], \tag{10}$$

where the partial trace in the definition of the reduced density matrix (DM) $\rho_{\rm A}$ is over the complement of A, denoted $\rm A^c$, and $L_{\rm A} = L/2$ denotes the length of subsystem A.

Since heating can be exponentially slow at high frequencies[CITE], one might be interested in calculating also the infinite-time quantities

$$\overline{\mathcal{E}} = \lim_{N\to\infty}\frac{1}{N}\sum_{l=0}^{N}\mathcal{E}(lT), \qquad \overline{s}_{\rm rdm} = -\frac{1}{L_{\rm A}}{\rm tr}_{\rm A}\left[\overline{\rho}_{\rm A}\log\overline{\rho}_{\rm A}\right], \qquad s_d^F = -\frac{1}{L}{\rm tr}\left[\rho_d^F\log\rho_d^F\right], \tag{11}$$

where $\overline{\rho}_{\rm A}$ is the infinite-time reduced DM of subsystem A, and ρ_d^F is the DM of the Diagonal ensemble in the exact Floquet basis $\{|n_F\rangle\colon H_F|n_F\rangle = E_F|n_F\rangle\}$ [CITE TD review]:

$$\overline{\rho}_{\rm A} = \lim_{N\to\infty}\frac{1}{N}\sum_{l=0}^{N}\rho_{\rm A}(lT) = {\rm tr}_{\rm A^c}\left[\rho_d^F\right], \qquad \rho_d^F = \sum_n |\langle\psi_i|n_F\rangle|^2|n_F\rangle\langle n_F|$$

We note in passing that in general $\overline{s}_{\rm rdm} \neq \lim_{N\to\infty} N^{-1}\sum_{l=0}^{N} s_{\rm ent}(lT)$ due to interference terms, although the two may happen to be close.

In Fig. 2 we show the time evolution of $\mathcal{E}(lT)$ and $s_{\rm ent}(lT)$ as a function of the number of driving cycle for a given drive frequency, together with their infinite-time values.

Code Analysis—Let us now discuss the $\mathcal{Q}^{\rm u}\mathcal{S}\rho\mathrm{i}\mathcal{N}$ code for this problem in detail. First we load the required classes, methods and functions required for the computation:

```
from qspin.operators import hamiltonian # Hamiltonians and operators
from qspin.basis import spin_basis_1d # Hilbert space spin basis
from qspin.tools.measurements import obs_vs_time, diag_ensemble # t_dep measurements
from qspin.tools.Floquet import Floquet, Floquet_t_vec # Floquet Hamiltonian
import numpy as np # generic math functions
```

After that, we define the model parameters as

```
L=14 # system size
J=1.0 # spin interaction
g=0.809 # transverse field
h=0.9045 # parallel field
Omega=4.5 # drive frequency
```

The time-periodic step drive can easily be incorporated through the following function:

[6] Since we use periodic boundaries, it does not matter which consecutive sites we choose. In fact, in $\mathcal{Q}^{\rm u}\mathcal{S}\rho\mathrm{i}\mathcal{N}$ the user can choose any (possibly disconnected) subsystem to calculate the entanglement entropy and the reduced DM, see Sec. C.

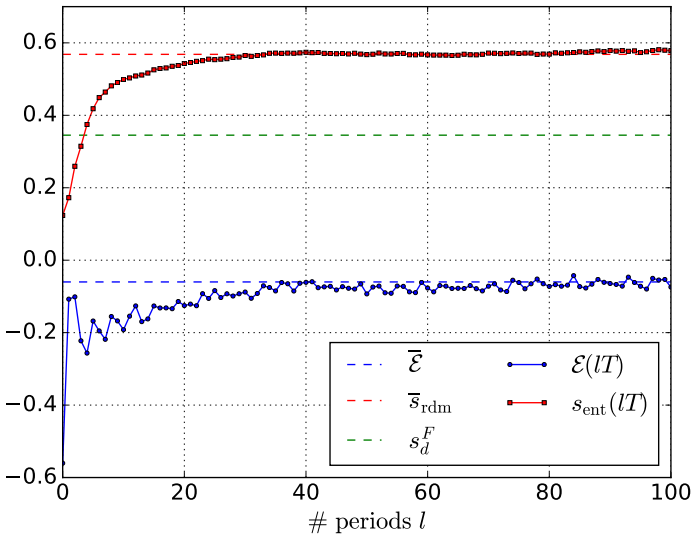


Figure 2: Stroboscopic dynamics of the energy density and entanglement entropy density (solid lines), together with their infinite-time values (dashed lines) in the periodically-driven TFIM in a parallel field. The parameters are $g/J = 0.809$, $h/J = 0.9045$, $\Omega/J = 4.5$, and $L = 14$.

```
15 # define time-reversal symmetric periodic step drive
16 def drive(t,Omega):
17     return np.sign(np.cos(Omega*t))
18 drive_args=[Omega]
```

Next, we define the basis, similar to the example in Sec. 2.1. One can convince oneself that the Hamiltonian in Eq. (4) possesses two symmetries at all times t which are, therefore, also inherited by the Floquet Hamiltonian. These are translation invariance and parity (i.e. reflection w.r.t. the centre of the chain). To incorporate them, one needs to specify the desired block for each symmetry: `kblock=int` selects the many-body states of total momentum $2\pi/L$`*int`, while `pblock=`± 1 sets the parity sector. For all total momenta different from 0 and π, the translation operator does not commute with parity, in which case semi-momentum states producing a *real* Hamiltonian are the natural choice [CITE Anders].

```
19 # compute basis in the 0-total momentum and +1-parity sector
20 basis=spin_basis_1d(L=L,kblock=0,pblock=1)
```

The definition of the site-coupling lists proceeds similarly to the MBL example above. It is interesting to note how the periodic boundary condition is encoded in `line 25` using the modulo operator `%`. Compared to open boundaries, the PBC `J_nn` list now also has a total of `L` elements, as many as there are sites and bonds on the ring.

```
21 # define PBC site-coupling lists for operators
22 x_field_pos=[[+g,i] for i in range(L)]
23 x_field_neg=[[-g,i] for i in range(L)]
24 z_field=[[h,i]      for i in range(L)]
25 J_nn=[[J,i,(i+1)%L] for i in range(L)] # PBC
```

To program the full Hamiltonian $H(t)$, we use the second line of Eq. (4). The time-independent part is defined using the static operator list. For the time-dependent part, we need to pass the function `drive` and its arguments `drive_args`, defined in `lines 15-18`, to all operators

the drive couples to. In fact, $\mathcal{Q}^{\text{u}}\mathcal{S}\rho\mathrm{i}\mathcal{N}$ is smart enough to automatically sum up all operators multiplied by the same time-dependent function in any dynamic list created. Note that since we are dealing with a Hamiltonian defined by Pauli matrices and not the spin-1/2 operators, we drop the optional argument `pauli` for the `hamiltonian` class, since by default it is set to `pauli=True`.

```
# static and dynamic lists
static=[["zz",J_nn],["z",z_field],["x",x_field_pos]]
dynamic=[["zz",J_nn,drive,drive_args],
         ["z",z_field,drive,drive_args],["x",x_field_neg,drive,drive_args]]
# compute Hamiltonians
H=0.5*hamiltonian(static,dynamic,dtype=np.float64,basis=basis)
```

The following lines define the approximate van Vleck Floquet Hamiltonian, cf. Eq. (7). Of particular interest is `line 37` where we define the site-coupling list for the three-spin operator `"zxz"`. Apart from the coupling `J**2*g`, we now need to specify the *three* site indices `i,(i+1)%L,(i+2)%L` for each of the operators `"zxz"`, respectively. In a similar fashion, one can define any multi-spin operator.

```
##### set up second-order van Vleck Floquet Hamiltonian #####
# zeroth-order term
Heff_0=0.5*hamiltonian(static,[],dtype=np.float64,basis=basis)
# second-order term: site-coupling lists
Heff2_term_1=[[+J**2*g,i,(i+1)%L,(i+2)%L] for i in range(L)] # PBC
Heff2_term_2=[[+J*g*h, i,(i+1)%L] for i in range(L)] # PBC
Heff2_term_3=[[-J*g**2,i,(i+1)%L] for i in range(L)] # PBC
Heff2_term_4=[[+J**2*g+0.5*h**2*g,i] for i in range(L)]
Heff2_term_5=[[0.5*h*g**2,        i] for i in range(L)]
# define static list
Heff_static=[["zxz",Heff2_term_1],
             ["xz",Heff2_term_2],["zx",Heff2_term_2],
             ["yy",Heff2_term_3],["zz",Heff2_term_2],
             ["x",Heff2_term_4],
             ["z",Heff2_term_5]                      ]
# compute van Vleck Hamiltonian
Heff_2=hamiltonian(Heff_static,[],dtype=np.float64,basis=basis)
Heff_2*=-np.pi**2/(12.0*Omega**2)
# zeroth + second order van Vleck Floquet Hamiltonian
Heff_02=Heff_0+Heff_2
```

In order to rotate the state from the van Vleck to the stroboscopic (Floquet-Magnus) picture, we also have to calculate the kick operator at time $t = 0$. While the procedure is the same as above, note that $K_{\text{eff}}(0)$ has imaginary matrix elements, whence the variable `dtype=np.complex128` is used (in fact this is the default `dtype` optional argument that the `hamiltonian` class assumes if one does not pass this argument explicitly). If the user tries to force define a real-valued Hamiltonian which, however, has complex matrix elements, $\mathcal{Q}^{\text{u}}\mathcal{S}\rho\mathrm{i}\mathcal{N}$ will raise an error.

```
##### set up second-order van Vleck Kick operator #####
Keff2_term_1=[[J*g,i,(i+1)%L] for i in range(L)] # PBC
Keff2_term_2=[[h*g,i] for i in range(L)]
# define static list
Keff_static=[["zy",Keff2_term_1],["yz",Keff2_term_1],["y",Keff2_term_2]]
Keff_02=hamiltonian(Keff_static,[],dtype=np.complex128,basis=basis)
```

```
Keff_02*=-np.pi**2/(8.0*Omega**2)
```

Next, we need to find $H_F^{(0+2)} = \exp[-iK_{\text{eff}}^{(2)}(0)]H_{\text{eff}}^{(0+2)}\exp[iK_{\text{eff}}^{(2)}(0)]$. To this end, we make use of the `hamiltonian` class method `rotate_by` which conveniently provides a function for this purpose. By specifying the optional argument `generator=True`, `rotate_by` recognises the operator B as a generator and defines a linear transformation to 'rotate' a `hamiltonian` object A via $\exp(aB)A\exp(a^*B^\dagger)$ for any complex-valued number a. Although we do not use it directly here, it is also useful for the user to become familiar with the documentation of the `exp_op` class which provides the matrix exponential, cf. App. C, which contains a variety of useful methods. For instance, $\exp(zB)A$ can be obtained using `exp_op(B,a=z).dot(A)`, while $A\exp(zB)$ is `A.dot(exp_op(B,a=z)`[7] for any complex number `z`.

```
##### rotate Heff to stroboscopic basis #####
# e^{-1j*Keff_02} Heff_02 e^{+1j*Keff_02}
HF_02 = Heff_02.rotate_by(Keff_02,generator=True,a=-1j)
```

Now that we have concluded the initialisation of the approximate Floquet Hamiltonian, it is time to discuss how to study the dynamics of the system. We start by defining a vector of times `t`, particularly suitable for the study of periodically driven systems. We initialise this time vector as an object of the `Floquet_t_vec` class. The arguments we need are the drive frequency `Omega`, the number of periods (here `100`), and the number of time points per period `len_T` (here set to `1`). Once initialised, `t` has many useful attributes, such as the time values `t.vals`, the drive period `t.T`, the stroboscopic times `t.strobo.vals`, or their indices `t.strobo.inds`. The `Floquet_t_vec` class has further useful properties, described in the documentation in App. C.

```
##### define time vector of stroboscopic times with 100 cycles #####
t=Floquet_t_vec(Omega,100,len_T=1) # t.vals=times, t.i=init. time, t.T=drive period
```

To calculate the exact stroboscopic Floquet Hamiltonian H_F, one can conveniently make use of the `Floquet` class. Currently, it supports three different ways of obtaining the Floquet Hamiltonian: (i) passing an arbitrary time-periodic `hamiltonian` object it will evolve each basis eigenstate for one period to obtain the evolution operator $U(T)$. This calculation can be parallelised using the Python module `joblib`, activated by setting the optional argument `n_jobs`. (ii) one can pass a list of static `hamiltonian` objects, accompanied by a list of time steps to apply each of these Hamiltonians at. In this case, the `Floquet` class will make use of the matrix exponential to find $U(T)$. Instead, here we choose, (iii), to use a single dynamic `hamiltonian` object $H(t)$, accompanied by a list of times $\{t_i\}$ to evaluate it at, and a list of time steps $\{\delta t_i\}$ to compute the time-ordered matrix exponential as $\prod_i \exp(-iH(t_i)\delta t_i)$. The `Floquet` class calculates the quasienergies `EF` folded in the interval $[-\Omega/2, \Omega/2]$ by default. If required, the user may further request the set of Floquet states by setting `VF=True`, the Floquet Hamiltonian, `HF=True`, and/or the Floquet phases – `thetaF=True`. For more information on `Floquet_t_vec`, the user is advised to consult the package documentation, see App. C.

```
##### calculate exact Floquet eigensystem #####
t_list=np.array([0.0,t.T/4.0,3.0*t.T/4.0])+np.finfo(float).eps # times to evaluate H
dt_list=np.array([t.T/4.0,t.T/2.0,t.T/4.0]) # time step durations to apply H for
Floq=Floquet({'H':H,'t_list':t_list,'dt_list':dt_list},VF=True) # call Floquet class
VF=Floq.VF # read off Floquet states
```

[7] One can also use the syntax `A.rdot(exp_op(a*B))` and `exp_op(z*B).rdot(A)`, respectively, for multiplication from the right.

```
EF=Floq.EF # read off quasienergies
```

As discussed in the main text, we choose for the initial state the ground state[8] of the approximate Hamiltonian $H_F^{(0+2)}$. Here, we demonstrate how to fully diagonalise a **hamiltonian** object using the function **eigh**. Note that to find only the ground state it is, in fact, much more efficient to use the sparse matrix Lanczos-based function **eigsh**, as in the example of Sec. 2.1.

```
##### calculate initial state (GS of HF_02) and its energy
EF_02, VF_02 = HF_02.eigh()
EF_02, psi_i = EF_02[0], VF_02[:,0]
```

Finally, we can calculate the time-dependence of the energy density $\mathcal{E}(t)$ and the entanglement entropy density $s_{\text{ent}}(t)$. This is done using the **measurements** function **obs_vs_time**. If one evolves with a constant Hamiltonian (which is effectively the case for stroboscopic time evolution), $\mathcal{QuSpi N}$ offers two different but equivalent options, that we now discuss. (i) As a first required argument of **obs_vs_time** one passes a tuple **(psi_i,E,V)** with the initial state, the spectrum, and the eigenbasis of the Hamiltonian to do the evolution with. The second argument is the time vector (here **t.vals**), and the third one – the operator one would like to measure (here the approximate energy density **HF_02/L**. If the observable is time-dependent, **obs_vs_time** will evaluate it at the appropriate times: $\langle\psi(t)|\mathcal{O}(t)|\psi(t)\rangle$. To obtain the entanglement entropy, **obs_vs_time** calls the **measurements** function **ent_entropy**, whose arguments are passed using the variable **Sent_args**. **ent_entropy** requires to pass the **basis**, and optionally – the subsystem **chain_subsys** which would otherwise be set to the first **L/2** sites of the chain. To learn more about how to obtain the reduced density matrix or other features of **ent_entropy**, consult the documentation, App. C.

```
##### time-dependent measurements
# calculate measurements
Sent_args = {"basis":basis,"chain_subsys":[j for j in range(L/2)]}
meas = obs_vs_time((psi_i,EF,VF),t.vals,[HF_02/L],Sent_args=Sent_args)
```

The other way to calculate a time-dependent observable (ii) is more generic and works for arbitrary time-dependent Hamiltonians. It makes use of Schrödinger evolution to find the time-dependent state using the **evolve** method of the **hamiltonian** class. While we introduced **evolve** in Sec. 2.1, here we explain an important feature: if the optional argument **iterate=True** is passed, then $\mathcal{QuSpi N}$ will not do the calculation of the state immediately; instead – it will create a generator object. By doing so one can avoid the causal loop over times to first find the state, and then looping once more over time to evaluate observables. The **evolve** method typically works for larger system sizes, than the ones that allow full ED. One can then simply pass the generator **psi_t** into **obs_vs_time** instead of the initial tuple.

```
# alternative way by solving Schroedinger's eqn
psi_t = H.evolve(psi_i,t.i,t.vals,iterate=True,rtol=1E-9,atol=1E-9)
meas = obs_vs_time(psi_t,t.vals,[HF_02/L],Sent_args=Sent_args)
```

The output of **obs_vs_time** is a dictionary. Extracting the energy density and entanglement entropy density values as a function of time, is as easy as:

```
# read off measurements
```

[8] The approximate Floquet Hamiltonian is unfolded[CITE FAPT review] and, thus, the ground state is well-defined.

```
Energy_t = meas["Expt_time"]
Entropy_t = meas["Sent_time"]["Sent"]
```

Last, we compute the infinite-time values of the energy density, the entropy of the infinite-time reduced density matrix, as well as the diagonal entropy. They are, in fact, closely related to the expectation values of the Diagonal ensemble of the initial state in the Floquet basis. The `measurements` tool contains the function `diag_ensemble` specifically designed for this purpose. The required arguments are the system size `L`, the initial state `psi_i`, as well as the Floquet spectrum `EF` and states `VF`. The optional arguments are packed in the auxiliary dictionary `DE_args`, and contain the observable `Obs`, the diagonal entropy `Sd_Renyi`, and the entanglement entropy of the reduced DM `Srdm_Renyi` with its arguments `Srdm_args`. The additional label `_Renyi` is used since in general one can also compute the Renyi entropy with parameter α, if desired. The function `diag_ensemble` will automatically return the densities of the requested quantities, unless the flag `densities=False` is specified. It has more features which allow one to calculate the temporal and quantum fluctuations of an observable at infinite times (i.e. in the Diagonal ensemble), and return the diagonal density matrix. Moreover, it can do additional averages of all diagonal ensemble quantities over a user-specified energy distribution, which may prove useful in calculating thermal expectations at infinite times, cf. App. C.

```
##### calculate diagonal ensemble measurements
DE_args = {"Obs":HF_02,"Sd_Renyi":True,"Srdm_Renyi":True,"Srdm_args":Sent_args}
DE = diag_ensemble(L,psi_i,EF,VF,**DE_args)
Ed = DE["Obs_pure"]
Sd = DE["Sd_pure"]
Srdm=DE["Srdm_pure"]
```

The complete code including the lines that produce Fig. 2 is available in Fig. 2.

2.3 Quantised Light-Atom Interactions in the Semi-classical Limit: Recovering the Periodically Driven Atom

Physics Setup—The last example we show deals with the quantisation of the (monochromatic) electromagnetic (EM) field. For the purpose of our little study, we take a two-level atom (i.e. a single-site spin chain) and couple it to a single photon mode (i.e. a quantum harmonic oscillator). The Hamiltonian reads

$$H = \Omega a^\dagger a + \frac{A}{2}\frac{1}{\sqrt{N_{\rm ph}}}\left(a^\dagger + a\right)\sigma^x + \Delta\sigma^z, \tag{12}$$

where the operator $a^\dagger$ creates a photon in the mode, and the atom is modelled by a two-level system described by the Pauli spin operators $\sigma^{x,y,z}$. The photon frequency is Ω, $N_{\rm ph}$ is the average number of photons in the mode, A – the coupling between the EM field $E = \sqrt{N_{\rm ph}^{-1}}\left(a^\dagger + a\right)$ and the dipole operator σ^x, and Δ measures the energy difference between the two atomic states.

An interesting question to ask is under what conditions the atom can be described[9] by the

[9] Strictly speaking the Hamiltonian $H_{\rm sc}(t)$ describes the spin dynamics in the rotating frame of the photon, defined by $a \to ae^{-i\Omega t}$; however, all three observables of interest: $a^\dagger a$, and $\sigma^{y,z}$ are invariant under this transformation.

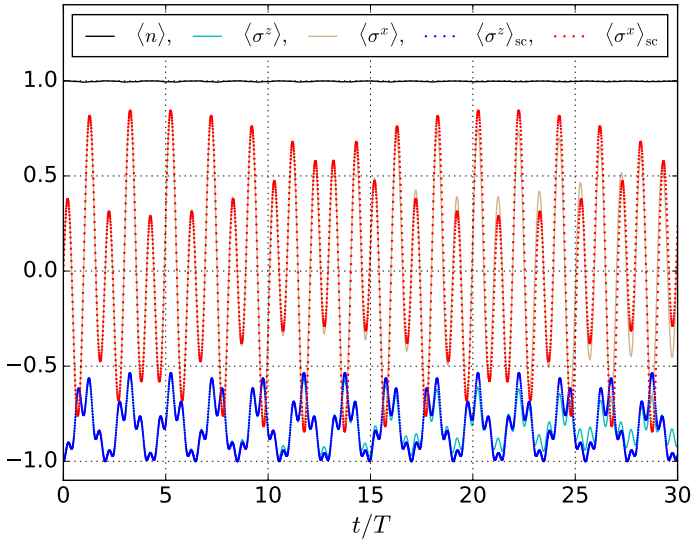


Figure 3: Emergent effective periodically driven dynamics in the semi-classical limit of the quantised light-atom interaction. The solid lines represent expectation values in the spin-photon basis, while dashed lines – the corresponding semi-classical quantities. The parameters are $A/\Delta = 1$, $\Omega/\Delta = 3.5$. The photon Hilbert space has a total number of $N_{\rm ph,tot} = 60$ states, and the mean number of photons in the initial coherent state is $N_{\rm ph} = 30$.

time-periodic semi-classical Hamiltonian:

$$H_{\rm sc}(t) = A \cos \Omega t \, \sigma^x + \Delta \sigma^z. \tag{13}$$

Curiously, despite its simple form, one cannot solve in a closed form for the dynamics generated by the semi-classical Hamiltonian $H_{\rm sc}(t)$.

To address the above question, we prepare the system such that the atom is in its ground state, while we put the photon mode in a coherent state with mean number of photons $N_{\rm ph}$, as required to by the semi-classical regime[CITE Haroche]:

$$|\psi_i\rangle = |{\rm coh}(N_{\rm ph})\rangle| \downarrow \rangle. \tag{14}$$

We then calculate the exact dynamics generated by the spin-photon Hamiltonian H, measure the Pauli spin matrix σ^z which represents the energy of the atom, σ^x – the dipole operator, and the photon number $n = a^\dagger a$:

$$\langle \mathcal{O} \rangle = \langle \psi_i | {\rm e}^{itH} \mathcal{O} \, {\rm e}^{-itH} | \psi_i \rangle, \qquad \mathcal{O} = n, \sigma^z, \sigma^y, \tag{15}$$

and compare these to the semi-classical expectation values

$$\langle \mathcal{O} \rangle_{\rm sc} = \langle \downarrow | \mathcal{T}_t {\rm e}^{i \int_0^t H_{\rm sc}(t') {\rm d}t'} \mathcal{O} \, \mathcal{T}_t {\rm e}^{-i \int_0^t H_{\rm sc}(t') {\rm d}t'} | \downarrow \rangle, \qquad \mathcal{O} = \sigma^z, \sigma^y. \tag{16}$$

Figure 3 a shows a comparison between the quantum and the semi-classical time evolution of all observables $\mathcal{O}$ as defined above.

Code Analysis—We used the following compact $\mathcal{Q}^{\rm u}\mathcal{S}\rho\text{¡}\mathcal{N}$ code to produce these results. First we load the required classes, methods and functions to do the calculation:

```
from qspin.basis import spin_basis_1d,photon_basis # Hilbert space bases
from qspin.operators import hamiltonian # Hamiltonian and observables
from qspin.tools.measurements import obs_vs_time # t_dep measurements
from qspin.tools.Floquet import Floquet,Floquet_t_vec # Floquet Hamiltonian
from qspin.basis.photon import coherent_state # HO coherent state
import numpy as np # generic math functions
```

Next, we define the model parameters as follows:

```
##### define model parameters #####
Nph_tot=60 # total number of photon states
Nph=Nph_tot/2 # mean number of photons in initial coherent state
Omega=3.5 # drive frequency
A=0.8 # spin-photon coupling strength (drive amplitude)
```

To set up the spin-photon Hamiltonian, we first build the site-coupling lists. The `ph_energy` list does not require the specification of a lattice site index, since the latter is not defined for the photon sector. The `at_energy` list, on the other hand, requires the input of the lattice site for the σ^z operator: since we consider a single two-level system or, equivalently – a single-site chain, this index is `0`. The spin-photon coupling lists `absorb` and `emit` also require the site index which refers to the corresponding Pauli matrices: in this model – `0` again due to dimensional constraints.

```
# define operator site-coupling lists
ph_energy=[[Omega]] # photon energy
at_energy=[[Delta,0]] # atom energy
absorb=[[A/(2.0*np.sqrt(Nph)),0]] # absorption term
emit=[[A/(2.0*np.sqrt(Nph)),0]] # emission term
```

To build the static operator list, we use the `|` symbol in the operator string to distinguish the spin and photon operators: spin operators always come to the left of the `|`-symbol, while photon operators – to the right. For convenience, the identity operator `I` can be omitted, such that `I|n` is the same as `|n`, and `z|I` is equivalent to `z|`, respectively. The dynamic list is empty since the spin-photon Hamiltonian is time-independent.

```
# define static and dynamics lists
static=[["|n",ph_energy],["x|-",absorb],["x|+",emit],["z|",at_energy]]
dynamic=[]
```

To build the spin-photon basis, we call the function `photon_basis` and use `spin_basis_1d` as the first argument. We need to specify the number of spin lattice sites, and the total number of harmonic oscillator (a.k.a photon) states. Building the Hamiltonian works as in Sec. 2.1 and 2.2.

```
# compute atom-photon basis
basis=photon_basis(spin_basis_1d,L=1,Nph=Nph_tot)
# compute atom-photon Hamiltonian H
H=hamiltonian(static,dynamic,dtype=np.float64,basis=basis)
```

We now set up the time-periodic semi-classical Hamiltonian which is defined on the spin Hilbert space only; thus we use a `spin_basis_1d` basis object. The existence of a non-empty dynamic list to define the time-dependence.

```
# define operators
dipole_op=[[A,0]]
# define periodic drive and its parameters
```

```
def drive(t,Omega):
    return np.cos(Omega*t)
drive_args=[Omega]
# define semi-classical static and dynamic lists
static_sc=[["z",at_energy]]
dynamic_sc=[["x",dipole_op,drive,drive_args]]
# compute semi-classical basis
basis_sc=spin_basis_1d(L=1)
# compute semi-classical Hamiltonian H_{sc}(t)
H_sc=hamiltonian(static_sc,dynamic_sc,dtype=np.float64,basis=basis_sc)
```

Next, we define the initial state as a product state, see Eq. (14). Notice that in the $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathcal{N}$ `spin_basis_1d` basis convention the state $|\downarrow\rangle = (1,0)^t$. This is because the spin basis states are coded using their bit representations and the state of all spins pointing down is assigned the integer `0`. To define the oscillator (a.k.a. photon) coherent state with mean photon number N_{ph}, we use the function `coherent_state`: its first argument is the eigenvalue of the annihilation operator a, while the second argument is the total number of oscillator states[10].

```
# define atom ground state
psi_at_i=np.array([1.0,0.0]) # spin-down eigenstate of \sigma^z
# define photon coherent state with mean photon number Nph
psi_ph_i=coherent_state(np.sqrt(Nph),Nph_tot+1)
# compute atom-photon initial state as a tensor product
psi_i=np.kron(psi_at_i,psi_ph_i)
```

The next step is to define a vector of stroboscopic times, using the class `Floquet_t_vec`. Unlike in Sec. 2.2, here we are also interested in the non-stroboscopic times in between the perfect periods lT. Thus, we omit the optional argument `len_T` making use of the default value set to `len_T=100`, meaning that there are now 100 time points within each period.

```
# define time vector over 30 driving cycles with 100 points per period
t=Floquet_t_vec(Omega,30) # t.i = initial time, t.T = driving period
```

We now time evolve the initial state both in the atom-photon, and the semi-classical cases using the `hamiltonian` class method `evolve`, as before. Once again, we define the solution `psi_t` as a generator expression using the optional argument `iterate=True`.

```
# evolve atom-photon state with Hamiltonian H
psi_t=H.evolve(psi_i,t.i,t.vals,iterate=True,rtol=1E-9,atol=1E-9)
# evolve atom GS with semi-classical Hamiltonian H_sc
psi_sc_t=H_sc.evolve(psi_at_i,t.i,t.vals,iterate=True,rtol=1E-9,atol=1E-9)
```

Last, we define the observables of interest, using the `hamiltonian` class with unit coupling constants. Since each observable represents a single operator, we refrain from defining operator lists and set up the observables in-line. Note that the main difference below (apart from the `|` notation) in defining the Pauli operators in the atom-photon and the semi-classical cases, is the basis argument. The Python dictionaries `obs_args` and `obs_args_sc` represent another way of passing optional keyword arguments to the hamiltonian function. Here we also disable the automatic symmetry and hermiticity checks.

[10] Since the oscillator ground state is denoted by $|0\rangle$, the state $|N_{\mathrm{ph}}\rangle$ is the $(N_{\mathrm{ph}}+1)^{\mathrm{st}}$ state of the oscillator basis.

```
# define observables parameters
obs_args={"basis":basis,"check_herm":False,"check_symm":False}
obs_args_sc={"basis":basis_sc,"check_herm":False,"check_symm":False}
# in atom-photon Hilbert space
n=hamiltonian([["|n", [[1.0  ]] ]],[],dtype=np.float64,**obs_args)
sz=hamiltonian([["z|",[[1.0,0]] ]],[],dtype=np.float64,**obs_args)
sy=hamiltonian([["y|",  [[1.0,0]] ]],[],dtype=np.complex128,**obs_args)
# in the semi-classical Hilbert space
sz_sc=hamiltonian([["z",[[1.0,0]] ]],[],dtype=np.float64,**obs_args_sc)
sy_sc=hamiltonian([["y",[[1.0,0]] ]],[],dtype=np.complex128,**obs_args_sc)
```

Finally, we calculate the time-dependent expectation values using the `measurements` tool function `obs_vs_time`. Its arguments are the time-dependent state `psi_t`, the vector of times `t.vals`, and a tuple of all observables of interest, and were discussed in Sec. 2.2. `obs_vs_time` returns a dictionary with all time-dependent expectations stored under the key `"Expt_time"`. They can be accessed by array slicing in the order in which the observables appear in the tuple argument, as shown in lines `75` and `78`, respectively.

```
# in atom-photon Hilbert space
Obs_t = obs_vs_time(psi_t,t.vals,(n,sz,sy))["Expt_time"]
O_n, O_sz, O_sy = Obs_t[:,0], Obs_t[:,1], Obs_t[:,2]
# in the semi-classical Hilbert space
Obs_sc_t = obs_vs_time(psi_sc_t,t.vals,(sz_sc,sy_sc))["Expt_time"]
O_sz_sc, O_sy_sc = Obs_sc_t[:,0], Obs_sc_t[:,1]
```

The complete code including the lines that produce Fig. 3 is available in Fig. 3.

3 Future Perspectives for $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{i}\mathcal{N}$

We have shown that the $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{i}\mathcal{N}$ functionality allows the user to do many different kinds of ED calculations of 1-dimensional systems with option of using a wide range of possible symmetries. In addition to the features we have dicussed in this article there are many other functions which we have implemented which are all listed in the Documentation (Appendix C). Some important ones we missed include, the tensor_basis class which constructs a new basis object implementing the tensor product of two individual basis objects. This is useful for studying interacting hard-core boson chains where the number of conserved for each chain. Another class which is useful is the HamiltonianOperator class. This class does the matrix vector product "on the fly" which significantly reduces the amount of memory needed to do this operation. This is useful for diagonalizing large spin chains with Lanczos as it only requires on the order of a hundred calls of the matrix vector product to solve for a few eigen values and eigen vectors.

We have set up the code to make it simple to extend to different types of systems. We are currently working towards adding the 1-dimension symmetries for spinless and spinful fermions as well as higher spins and bosons. Farther into the future we may implement a number of two dimensional lattices as well as their symmetries. We also welcome anyone who is interested in contributing to this project to reach out to the Authors with any questions they may have about the package organization. All modifications can be proposed through the pull request system on github.com.

Although $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{i}\mathcal{N}$ passed all tests we could think of so far, there may still be some bugs

lurking out there. Therefore, we would much appreciate it, if the users could report these bugs to the "Issues" forum on the $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{i}\mathcal{N}$ repository. With the report we request that the user please add a segment of code which reproduces the bug. As a rule of thumb, bug reports are most useful when the code segment is as short as possible but contains the necessary annotations and comments so it can be followed and, at the same time, the Hamiltonian used is the simplest one which displays the bug.

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...

Author contributions This is optional. If desired, contributions should be succinctly described in a single short paragraph, using author initials.

Funding information Authors are required to provide funding information, including relevant agencies and grant numbers with linked author's initials.

A Installation Guide in a Few Steps

$\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{i}\mathcal{N}$ is currently only being supported for Python 2.7 and so one must make sure to install this version of Python. The Authors recommend the use of Anaconda to install Python and manage your Python packages. It is free to download here, or for a lighter installation you can use miniconda which can be found here.

A.1 Mac OS X/Linux

To install Anaconda/miniconda all one has to do is execute the installation script with administrative privilege. To do this open up the terminal and go to the folder containing the downloaded installation file and execute the following command:

```
sudo bash > installation_file <
```

You will be prompted to enter your password. Follow the prompts of the installation. We recommend that you allow the installer to prepend the installation directory to your PATH variable which will make sure this installation of Python will be called when executing a Python script in the terminal. If this is not done then you will have to do this manually in your bash profile file:

```
export PATH="path_to/anaconda/bin:$PATH"
```

Installing via Anaconda.—Once you have Anaconda/miniconda installed, all you have to do to install $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{i}\mathcal{N}$ is to execute the following command into the terminal:

```
conda install -c weinbe58 qspin
```

If asked to install new packages just say 'yes'. To keep the code up-to-date, just run this command regularly.

Installing Manually.—Installing the package manually is not recommended unless the above method failed. Note that you must have NumPy, SciPy, and Joblib installed before

installing $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{i}\mathcal{N}$. Once all the prerequisite packages are installed, one can download the source code from github and then extract the code to whichever directory one desires. Open the terminal and go to the top level directory of the source code and execute:

```
Python setup.py install --record install\_file.txt
```

This will compile the source code and copy it to the installation directory of Python recording the installation location to `install_file.txt`. To update the code, you must first completely remove the current version installed and then install the new code. The `install_file.txt` can be used to remove the package by running:

```
cat install\_file.txt | xargs rm -rf.
```

A.2 Windows

To install Anaconda/miniconda on Windows, download the installer and execute it to install the program. Once Anaconda/miniconda is installed open the conda terminal and do one of the following to install the package:

Installing via Anaconda.—Once you have Anaconda/miniconda installed all you have to do to install $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{i}\mathcal{N}$ is to execute the following command into the terminal:

```
conda install -c weinbe58 qspin
```

If asked to install new packages just say 'yes'. To update the code just run this command regularly.

Installing Manually.—Installing the package manually is not recommended unless the above method failed. Note that you must have NumPy, SciPy, and Joblib installed before installing $\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{i}\mathcal{N}$. Once all the prerequisite packages are installed, one can download the source code from github and then extract the code to whichever directory one desires. Open the terminal and go to the top level directory of the source code and then execute:

```
Python setup.py install --record install\_file.txt
```

This will compile the source code and copy it to the installation directory of Python and record the installation location to `install_file.txt`. To update the code you must first completely remove the current version installed and then install the new code.

B Complete Example Codes

$\mathcal{Q}^{\mathrm{u}}\mathcal{S}\rho\mathrm{i}\mathcal{N}$ *Example Code* 1: Adiabatic Control of Parameters in MBL Phases

```
from qspin.operators import hamiltonian # Hamiltonians and operators
from qspin.basis import spin_basis_1d # Hilbert space spin basis
from qspin.tools.measurements import ent_entropy, diag_ensemble # entropies
from numpy.random import ranf,seed # pseudo random numbers
from joblib import delayed,Parallel # parallelisation
import numpy as np # generic math functions
from time import time # timing package
#
##### define simulation parameters #####
n_real=20 # number of disorder realisations
n_jobs=2 # number of spawned processes used for parallelisation
#
##### define model parameters #####
L=10 # system size
Jxy=1.0 # xy interaction
Jzz_0=1.0 # zz interaction at time t=0
h_MBL=3.9 # MBL disorder strength
h_ETH=0.1 # delocalised disorder strength
vs=np.logspace(-2.0,0.0,num=20,base=10) # log_2-spaced vector of ramp speeds
#
##### set up Heisenberg Hamiltonian with linearly varying zz-interaction #####
# define linear ramp function
v = 1.0 # declare ramp speed variable
def ramp(t):
    return (0.5 + v*t)
ramp_args=[]
# compute basis in the 0-total magnetisation sector (requires L even)
basis = spin_basis_1d(L,Nup=L/2,pauli=False)
# define operators with OBC using site-coupling lists
J_zz = [[Jzz_0,i,i+1] for i in range(L-1)] # OBC
J_xy = [[Jxy/2.0,i,i+1] for i in range(L-1)] # OBC
# static and dynamic lists
static = [["+-",J_xy],["-+",J_xy]]
dynamic =[["zz",J_zz,ramp,ramp_args]]
# compute the time-dependent Heisenberg Hamiltonian
H_XXZ = hamiltonian(static,dynamic,basis=basis,dtype=np.float64)
#
##### calculate diagonal and entanglement entropies #####
def realization(vs,H_XXZ,basis,real):
    """
    This function computes the entropies for a single disorder realisation.
    --- arguments ---
    vs: vector of ramp speeds
    H_XXZ: time-dep. Heisenberg Hamiltonian with driven zz-interactions
    basis: spin_basis_1d object containing the spin basis
    n_real: number of disorder realisations; used only for timing
    """
    ti = time() # start timer
```

```
    #
    global v # declare ramp speed v a global variable
    #
    seed() # the random number needs to be seeded for each parallel process
    #
    # draw random field uniformly from [-1.0,1.0] for each lattice site
    unscaled_fields=-1+2*ranf((basis.L,))
    # define z-field operator site-coupling list
    h_z=[[unscaled_fields[i],i] for i in range(basis.L)]
    # static list
    disorder_field = [["z",h_z]]
    # compute disordered z-field Hamiltonian
    no_checks={"check_herm":False,"check_pcon":False,"check_symm":False}
    Hz=hamiltonian(disorder_field,[],basis=basis,dtype=np.float64,**no_checks)
    # compute the MBL and ETH Hamiltonians for the same disorder realisation
    H_MBL=H_XXZ+h_MBL*Hz
    H_ETH=H_XXZ+h_ETH*Hz
    #
    ### ramp in MBL phase ###
    v=1.0 # reset ramp speed to unity
    # calculate the energy at infinite temperature for initial MBL Hamiltonian
    eigsh_args={"k":2,"which":"BE","maxiter":1E10,"return_eigenvectors":False}
    Emin,Emax=H_MBL.eigsh(time=0.0,**eigsh_args)
    E_inf_temp=(Emax+Emin)/2.0
    # calculate nearest eigenstate to energy at infinite temperature
    E,psi_0=H_MBL.eigsh(time=0.0,k=1,sigma=E_inf_temp,maxiter=1E10)
    psi_0=psi_0.reshape((-1,))
    # calculate the eigensystem of the final MBL hamiltonian
    E_final,V_final=H_MBL.eigh(time=(0.5/vs[-1]))
    # evolve states and calculate entropies in MBL phase
    run_MBL=[_do_ramp(psi_0,H_MBL,basis,v,E_final,V_final) for v in vs]
    run_MBL=np.vstack(run_MBL).T
    #
    ###  ramp in ETH phase ###
    v=1.0 # reset ramp speed to unity
    # calculate the energy at infinite temperature for initial ETH hamiltonian
    Emin,Emax=H_ETH.eigsh(time=0.0,**eigsh_args)
    E_inf_temp=(Emax+Emin)/2.0
    # calculate nearest eigenstate to energy at infinite temperature
    E,psi_0=H_ETH.eigsh(time=0.0,k=1,sigma=E_inf_temp,maxiter=1E10)
    psi_0=psi_0.reshape((-1,))
    # calculate the eigensystem of the final ETH hamiltonian
    E_final,V_final=H_ETH.eigh(time=(0.5/vs[-1]))
    # evolve states and calculate entropies in ETH phase
    run_ETH=[_do_ramp(psi_0,H_ETH,basis,v,E_final,V_final) for v in vs]
    run_ETH=np.vstack(run_ETH).T # stack vertically elements of list run_ETH
    # show time taken
    print "realization {0}/{1} took {2:.2f} sec".format(real+1,n_real,time()-ti)
    #
    return run_MBL,run_ETH
#
##### evolve state and evaluate entropies #####
def _do_ramp(psi_0,H,basis,v,E_final,V_final):
```

```
    """
    Auxiliary function to evolve the state and calculate the entropies after the
    ramp.
    --- arguments ---
    psi_0: initial state
    H: time-dependent Hamiltonian
    basis: spin_basis_1d object containing the spin basis (required for Sent)
    E_final, V_final: eigensystem of H(t_f) at the end of the ramp t_f=1/(2v)
    """
    # determine total ramp time
    t_f = 0.5/v
    # time-evolve state from time 0.0 to time t_f
    psi = H.evolve(psi_0,0.0,t_f)
    # calculate entanglement entropy
    subsys = range(basis.L/2) # define subsystem
    Sent = ent_entropy(psi,basis,chain_subsys=subsys)["Sent"]
    # calculate diagonal entropy in the basis of H(t_f)
    S_d = diag_ensemble(basis.L,psi,E_final,V_final,Sd_Renyi=True)["Sd_pure"]
    #
    return np.asarray([S_d,Sent])
#
##### produce data for n_real disorder realisations #####
"""
# alternative way without parallelisation
data = np.asarray([realization(vs,H_XXZ,basis,i) for i in xrange(n_real)])
"""
data = np.asarray(Parallel(n_jobs=n_jobs)(delayed(realization)(vs,H_XXZ,basis,i) for
     i in xrange(n_real)))
run_MBL,run_ETH = zip(*data) # extract MBL and data
# average over disorder
mean_MBL = np.mean(run_MBL,axis=0)
mean_ETH = np.mean(run_ETH,axis=0)
#
##### plot results #####
import matplotlib.pyplot as plt
### MBL plot ###
fig, pltarr1 = plt.subplots(2,sharex=True) # define subplot panel
# subplot 1: diag enetropy vs ramp speed
pltarr1[0].plot(vs,mean_MBL[0],label="MBL",marker=".",color="blue") # plot data
pltarr1[0].set_ylabel("$s_d(t_f)$",fontsize=22) # label y-axis
pltarr1[0].set_xlabel("$v/J_{zz}(0)$",fontsize=22) # label x-axis
pltarr1[0].set_xscale("log") # set log scale on x-axis
pltarr1[0].grid(True,which='both') # plot grid
pltarr1[0].tick_params(labelsize=16)
# subplot 2: entanglement entropy vs ramp speed
pltarr1[1].plot(vs,mean_MBL[1],marker=".",color="blue") # plot data
pltarr1[1].set_ylabel("$s_\mathrm{ent}(t_f)$",fontsize=22) # label y-axis
pltarr1[1].set_xlabel("$v/J_{zz}(0)$",fontsize=22) # label x-axis
pltarr1[1].set_xscale("log") # set log scale on x-axis
pltarr1[1].grid(True,which='both') # plot grid
pltarr1[1].tick_params(labelsize=16)
# save figure
fig.savefig('example1_MBL.pdf', bbox_inches='tight')
```

```
#
### ETH plot ###
fig, pltarr2 = plt.subplots(2,sharex=True) # define subplot panel
# subplot 1: diag enetropy vs ramp speed
pltarr2[0].plot(vs,mean_ETH[0],marker=".",color="green") # plot data
pltarr2[0].set_ylabel("$s_d(t_f)$",fontsize=22) # label y-axis
pltarr2[0].set_xlabel("$v/J_{zz}(0)$",fontsize=22) # label x-axis
pltarr2[0].set_xscale("log") # set log scale on x-axis
pltarr2[0].grid(True,which='both') # plot grid
pltarr2[0].tick_params(labelsize=16)
# subplot 2: entanglement entropy vs ramp speed
pltarr2[1].plot(vs,mean_ETH[1],marker=".",color="green") # plot data
pltarr2[1].set_ylabel("$s_\mathrm{ent}(t_f)$",fontsize=22) # label y-axis
pltarr2[1].set_xlabel("$v/J_{zz}(0)$",fontsize=22) # label x-axis
pltarr2[1].set_xscale("log") # set log scale on x-axis
pltarr2[1].grid(True,which='both') # plot grid
pltarr2[1].tick_params(labelsize=16)
# save figure
fig.savefig('example1_ETH.pdf', bbox_inches='tight')
#
plt.show() # show plots
```

$\mathcal{Q}^{u}\mathcal{S}\rho\text{¡}\mathcal{N}$ *Example Code* 2: Heating in Periodically Driven Spin Chains

```
from qspin.operators import hamiltonian # Hamiltonians and operators
from qspin.basis import spin_basis_1d # Hilbert space spin basis
from qspin.tools.measurements import obs_vs_time, diag_ensemble # t_dep measurements
from qspin.tools.Floquet import Floquet, Floquet_t_vec # Floquet Hamiltonian
import numpy as np # generic math functions
#
##### define model parameters #####
L=14 # system size
J=1.0 # spin interaction
g=0.809 # transverse field
h=0.9045 # parallel field
Omega=4.5 # drive frequency
#
##### set up alternating Hamiltonians #####
# define time-reversal symmetric periodic step drive
def drive(t,Omega):
    return np.sign(np.cos(Omega*t))
drive_args=[Omega]
# compute basis in the 0-total momentum and +1-parity sector
basis=spin_basis_1d(L=L,kblock=0,pblock=1)
# define PBC site-coupling lists for operators
x_field_pos=[[+g,i] for i in range(L)]
x_field_neg=[[-g,i] for i in range(L)]
z_field=[[h,i]      for i in range(L)]
J_nn=[[J,i,(i+1)%L] for i in range(L)] # PBC
# static and dynamic lists
static=[["zz",J_nn],["z",z_field],["x",x_field_pos]]
dynamic=[["zz",J_nn,drive,drive_args],
         ["z",z_field,drive,drive_args],["x",x_field_neg,drive,drive_args]]
# compute Hamiltonians
H=0.5*hamiltonian(static,dynamic,dtype=np.float64,basis=basis)
#
##### set up second-order van Vleck Floquet Hamiltonian #####
# zeroth-order term
Heff_0=0.5*hamiltonian(static,[],dtype=np.float64,basis=basis)
# second-order term: site-coupling lists
Heff2_term_1=[[+J**2*g,i,(i+1)%L,(i+2)%L] for i in range(L)] # PBC
Heff2_term_2=[[+J*g*h, i,(i+1)%L] for i in range(L)] # PBC
Heff2_term_3=[[-J*g**2,i,(i+1)%L] for i in range(L)] # PBC
Heff2_term_4=[[+J**2*g+0.5*h**2*g,i] for i in range(L)]
Heff2_term_5=[[0.5*h*g**2,        i] for i in range(L)]
# define static list
Heff_static=[["zxz",Heff2_term_1],
             ["xz",Heff2_term_2],["zx",Heff2_term_2],
             ["yy",Heff2_term_3],["zz",Heff2_term_2],
             ["x",Heff2_term_4],
             ["z",Heff2_term_5]                        ]
# compute van Vleck Hamiltonian
Heff_2=hamiltonian(Heff_static,[],dtype=np.float64,basis=basis)
Heff_2*=-np.pi**2/(12.0*Omega**2)
# zeroth + second order van Vleck Floquet Hamiltonian
```

```
Heff_02=Heff_0+Heff_2
#
##### set up second-order van Vleck Kick operator #####
Keff2_term_1=[[J*g,i,(i+1)%L] for i in range(L)] # PBC
Keff2_term_2=[[h*g,i] for i in range(L)]
# define static list
Keff_static=[["zy",Keff2_term_1],["yz",Keff2_term_1],["y",Keff2_term_2]]
Keff_02=hamiltonian(Keff_static,[],dtype=np.complex128,basis=basis)
Keff_02*=-np.pi**2/(8.0*Omega**2)
#
##### rotate Heff to stroboscopic basis #####
# e^{-1j*Keff_02} Heff_02 e^{+1j*Keff_02}
HF_02 = Heff_02.rotate_by(Keff_02,generator=True,a=-1j)
#
##### define time vector of stroboscopic times with 100 cycles #####
t=Floquet_t_vec(Omega,100,len_T=1) # t.vals=times, t.i=init. time, t.T=drive period
#
##### calculate exact Floquet eigensystem #####
t_list=np.array([0.0,t.T/4.0,3.0*t.T/4.0])+np.finfo(float).eps # times to evaluate H
dt_list=np.array([t.T/4.0,t.T/2.0,t.T/4.0]) # time step durations to apply H for
Floq=Floquet({'H':H,'t_list':t_list,'dt_list':dt_list},VF=True) # call Floquet class
VF=Floq.VF # read off Floquet states
EF=Floq.EF # read off quasienergies
#
##### calculate initial state (GS of HF_02) and its energy
EF_02, VF_02 = HF_02.eigh()
EF_02, psi_i = EF_02[0], VF_02[:,0]
#
##### time-dependent measurements
# calculate measurements
Sent_args = {"basis":basis,"chain_subsys":[j for j in range(L/2)]}
meas = obs_vs_time((psi_i,EF,VF),t.vals,[HF_02/L],Sent_args=Sent_args)
"""
# alternative way by solving Schroedinger's eqn
psi_t = H.evolve(psi_i,t.i,t.vals,iterate=True,rtol=1E-9,atol=1E-9)
meas = obs_vs_time(psi_t,t.vals,[HF_02/L],Sent_args=Sent_args)
"""
# read off measurements
Energy_t = meas["Expt_time"]
Entropy_t = meas["Sent_time"]["Sent"]
#
##### calculate diagonal ensemble measurements
DE_args = {"Obs":HF_02,"Sd_Renyi":True,"Srdm_Renyi":True,"Srdm_args":Sent_args}
DE = diag_ensemble(L,psi_i,EF,VF,**DE_args)
Ed = DE["Obs_pure"]
Sd = DE["Sd_pure"]
Srdm=DE["Srdm_pure"]
#
##### plot results #####
import matplotlib.pyplot as plt
import pylab
# define legend labels
str_E_t = "$\\mathcal{E}(lT)$"
```

```
str_Sent_t = "$s_\mathrm{ent}(lT)$"
str_Ed = "$\\overline{\mathcal{E}}$"
str_Srdm = "$\\overline{s}_\mathrm{rdm}$"
str_Sd = "$s_d^F$"
# plot infinite-time data
fig = plt.figure()
plt.plot(t.vals/t.T,Ed*np.ones(t.vals.shape),"b--",linewidth=1,label=str_Ed)
plt.plot(t.vals/t.T,Srdm*np.ones(t.vals.shape),"r--",linewidth=1,label=str_Srdm)
plt.plot(t.vals/t.T,Sd*np.ones(t.vals.shape),"g--",linewidth=1,label=str_Sd)
# plot time-dependent data
plt.plot(t.vals/t.T,Energy_t,"b-o",linewidth=1,label=str_E_t,markersize=3.0)
plt.plot(t.vals/t.T,Entropy_t,"r-s",linewidth=1,label=str_Sent_t,markersize=3.0)
# label axes
plt.xlabel("$\\#\ \\mathrm{periods}\\ l$",fontsize=18)
# set y axis limits
plt.ylim([-0.6,0.7])
# display legend
plt.legend(loc="lower right",ncol=2,fontsize=18)
# update axis font size
plt.tick_params(labelsize=16)
# turn on grid
plt.grid(True)
# save figure
fig.savefig('example2.pdf', bbox_inches='tight')
# show plot
plt.show()
```

$\mathcal{Q}^{u}\mathcal{S}\rho_{i}\mathcal{N}$ *Example Code* 3: Quantised Light-Atom Interactions in the Semi-classical Limit

```
from qspin.basis import spin_basis_1d,photon_basis # Hilbert space bases
from qspin.operators import hamiltonian # Hamiltonian and observables
from qspin.tools.measurements import obs_vs_time # t_dep measurements
from qspin.tools.Floquet import Floquet,Floquet_t_vec # Floquet Hamiltonian
from qspin.basis.photon import coherent_state # HO coherent state
import numpy as np # generic math functions
#
##### define model parameters #####
Nph_tot=60 # total number of photon states
Nph=Nph_tot/2 # mean number of photons in initial coherent state
Omega=3.5 # drive frequency
A=0.8 # spin-photon coupling strength (drive amplitude)
Delta=1.0 # difference between atom energy levels
#
##### set up photon-atom Hamiltonian #####
# define operator site-coupling lists
ph_energy=[[Omega]] # photon energy
at_energy=[[Delta,0]] # atom energy
absorb=[[A/(2.0*np.sqrt(Nph)),0]] # absorption term
emit=[[A/(2.0*np.sqrt(Nph)),0]] # emission term
# define static and dynamics lists
static=[["|n",ph_energy],["x|-",absorb],["x|+",emit],["z|",at_energy]]
dynamic=[]
# compute atom-photon basis
basis=photon_basis(spin_basis_1d,L=1,Nph=Nph_tot)
# compute atom-photon Hamiltonian H
H=hamiltonian(static,dynamic,dtype=np.float64,basis=basis)
#
##### set up semi-classical Hamiltonian #####
# define operators
dipole_op=[[A,0]]
# define periodic drive and its parameters
def drive(t,Omega):
    return np.cos(Omega*t)
drive_args=[Omega]
# define semi-classical static and dynamic lists
static_sc=[["z",at_energy]]
dynamic_sc=[["x",dipole_op,drive,drive_args]]
# compute semi-classical basis
basis_sc=spin_basis_1d(L=1)
# compute semi-classical Hamiltonian H_{sc}(t)
H_sc=hamiltonian(static_sc,dynamic_sc,dtype=np.float64,basis=basis_sc)
#
##### define initial state #####
# define atom ground state
psi_at_i=np.array([1.0,0.0]) # spin-down eigenstate of \sigma^z
# define photon coherent state with mean photon number Nph
psi_ph_i=coherent_state(np.sqrt(Nph),Nph_tot+1)
# compute atom-photon initial state as a tensor product
psi_i=np.kron(psi_at_i,psi_ph_i)
#
```

```
##### calculate time evolution #####
# define time vector over 30 driving cycles with 100 points per period
t=Floquet_t_vec(Omega,30) # t.i = initial time, t.T = driving period
# evolve atom-photon state with Hamiltonian H
psi_t=H.evolve(psi_i,t.i,t.vals,iterate=True,rtol=1E-9,atol=1E-9)
# evolve atom GS with semi-classical Hamiltonian H_sc
psi_sc_t=H_sc.evolve(psi_at_i,t.i,t.vals,iterate=True,rtol=1E-9,atol=1E-9)
#
##### define observables #####
# define observables parameters
obs_args={"basis":basis,"check_herm":False,"check_symm":False}
obs_args_sc={"basis":basis_sc,"check_herm":False,"check_symm":False}
# in atom-photon Hilbert space
n=hamiltonian([["|n", [[1.0  ]] ]],[],dtype=np.float64,**obs_args)
sz=hamiltonian([["z|",[[1.0,0]] ]],[],dtype=np.float64,**obs_args)
sy=hamiltonian([["y|",  [[1.0,0]] ]],[],dtype=np.complex128,**obs_args)
# in the semi-classical Hilbert space
sz_sc=hamiltonian([["z",[[1.0,0]] ]],[],dtype=np.float64,**obs_args_sc)
sy_sc=hamiltonian([["y",[[1.0,0]] ]],[],dtype=np.complex128,**obs_args_sc)
#
##### calculate expectation values #####
# in atom-photon Hilbert space
Obs_t = obs_vs_time(psi_t,t.vals,(n,sz,sy))["Expt_time"]
O_n, O_sz, O_sy = Obs_t[:,0], Obs_t[:,1], Obs_t[:,2]
# in the semi-classical Hilbert space
Obs_sc_t = obs_vs_time(psi_sc_t,t.vals,(sz_sc,sy_sc))["Expt_time"]
O_sz_sc, O_sy_sc = Obs_sc_t[:,0], Obs_sc_t[:,1]
##### plot results #####
import matplotlib.pyplot as plt
import pylab
# define legend labels
str_n = "$\\langle n\\rangle,$"
str_z = "$\\langle\\sigma^z\\rangle,$"
str_x = "$\\langle\\sigma^x\\rangle,$"
str_z_sc = "$\\langle\\sigma^z\\rangle_\\mathrm{sc},$"
str_x_sc = "$\\langle\\sigma^x\\rangle_\\mathrm{sc}$"
# plot spin-photon data
fig = plt.figure()
plt.plot(t.vals/t.T,O_n/Nph,"k",linewidth=1,label=str_n)
plt.plot(t.vals/t.T,O_sz,"c",linewidth=1,label=str_z)
plt.plot(t.vals/t.T,O_sy,"tan",linewidth=1,label=str_x)
# plot semi-classical data
plt.plot(t.vals/t.T,O_sz_sc,"b.",marker=".",markersize=1.8,label=str_z_sc)
plt.plot(t.vals/t.T,O_sy_sc,"r.",marker=".",markersize=2.0,label=str_x_sc)
# label axes
plt.xlabel("$t/T$",fontsize=18)
# set y axis limits
plt.ylim([-1.1,1.4])
# display legend horizontally
plt.legend(loc="upper right",ncol=5,columnspacing=0.6,numpoints=4)
# update axis font size
plt.tick_params(labelsize=16)
# turn on grid
```

```
plt.grid(True)
# save figure
fig.savefig('example3.pdf', bbox_inches='tight')
# show plot
plt.show()
```

C Package Documentation

The complete up-to-date documentation for the package is available online under:

https://github.com/weinbe58/qspin

References