QuSpin: a Python Package for Dynamics and Exact Diagonalisation of Quantum Many Body Systems.
Part II: bosons, fermions and higher spins

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Abstract

We present a major update to QuSpin, *SciPostPhys.2.1.003* – an open-source Python package for exact diagonalization and quantum dynamics of arbitrary boson, fermion and spin many-body systems, supporting the use of various symmetries in one dimension and (imaginary) time evolution following a user-specified driving protocol. We explain how to use the new features of QuSpin using seven detailed examples of various complexity: (i) the transverse-field Ising model and the Jordan-Wigner transformation, (ii) free particle systems: the SSH model, (iii) the many-body localised Fermi-Hubbard model, (iv) the Bose-Hubbard model in a ladder geometry, (v) nonlinear (imaginary) time evolution and the Gross-Pitaevskii equation, (vi) integrability breaking and thermalising dynamics in the spin-1 transverse-field Ising model, and (vii) Bose-Fermi mixtures. This easily accessible package can serve various purposes, including educational and cutting-edge experimental and theoretical research.

Contents

1 Which Problems can I Study with QuSpin?

- re-label numbering of examples to match order in text.

Understanding the physics of many-body quantum condensed matter systems often involves a great deal of numerical simulations, be it to gain intuition about the complicated problem of interest, or because the latter does not admit an analytical solution which can be expressed in a closed form. This motivates the development of open-source packages [CITE], the purpose of which is to facilitate the study of condensed matter systems, without the need to understand and implement complicated numerical methods which required years to understand and fully develop. Here, we report on a major upgrade to QuSpin [1] – a Python library for exact diagonalisation (ED) and simulation of the dynamics in arbitrary quantum many-body systems.

Although ED methods are vastly outperformed by more sophisticated numerical techniques in the study of equilibrium problems [CITE], as of present date ED remains essential for most dynamical non-equilibrium problems. The reason for this often times relies on the fact that the underlying physics of these problems cannot be explained without taking into consideration the contribution from high-energy states excited during the evolution. Some prominent examples of such problems include the study of many-body localisation (MBL) [CITE], the Eigenstate Thermalisation hypothesis [CITE], quantum quench dynamics [CITE], periodically-driven systems [CITE], adiabatic and counter-diabatic state preparation, applications of Machine Learning to non-equilibrium physics [CITE], optimal control [CITE], and many more **did I forget smth important?**.

It is, thus, arguably useful to have a toolbox available at our disposal which allows one to quickly simulate and study these and related nonequilibrium problems. As such, QuSpin offers easy access to performing numerical simulations, which can facilitate the development and inspiration of new ideas and the discovery of novel phenomena, eliminating the cost of spending time to develop a reliable code. Besides theorists, the new version of QuSpin will hopefully even prove valuable to experimentalists working on problems containing dynamical setups, as it can help students and researchers focus on perfecting the experiment, rather than worry about writing the supporting simulation code. Last but not least, with the computational processing power growing higher than ever before, the role played by simulations for theoretical research becomes increasingly more important too. It can, therefore, be expected that in the near future quantum simulations become an integral part of the standard physics university curriculum, and having easily accessible toolboxes, such as QuSpin, is one of the required prerequisites for this anticipated change.

2 How do I use the New Features of QuSpin?

New in QuSpin 2.0, we have added the following features and toolboxes:

- ...

Installing QuSpin is quick and efficient; just follow the steps outlined in App. A.

Before we carry on, we refer the interested reader to examples (i)-(iv) from the original QuSpin paper [1]. The examples below focus predominantly on the newly introduced features, and are thus to be considered complementary. We emphasize that, since they serve the purpose of explaining how to use QuSpin, for the sake of brevity we shall not discuss the interesting physics related to the interpretation of the results.

2.1 The Spectrum of the Transverse Field Ising Model and the Jordan-Wigner Transformation

This example shows how to

- construct fermionic hopping, p-wave pairing and on-site potential terms, and spin$-1/2$ interactions and transverse fields,
- implement periodic and anti-periodic boundary conditions,
- use particle conservation modulo 2, spin inversion, reflection, and translation symmetries,
- handle the default built-in particle conservation and symmetry checks,
- obtain the spectrum of a QuSpin Hamiltonian.

Physics Setup—The transverse field Ising (TFI) chain is paradigmatic in our understanding of quantum phase transitions, since it represents an exactly solvable model[CITE Sachdev]. The Hamiltonian is given my

$$H = \sum_{j=0}^{L-1} -J\sigma^z_{j+1}\sigma^z_j - h\sigma^x_j, \tag{1}$$

where the nearest-neighbour (nn) spin interaction is J, h denotes the transverse field, and σ^α_j are the Pauli spin-1/2 matrices. We use periodic boundary conditions and label the L lattice sites $0, \dots, L-1$ to conform with Python's convention. This model has gapped, fermionic elementary excitations, and exhibits a phase transition from an antiferromagnet to a paramagnet at $(h/J)_c = 1$ CHECK!. The Hamiltonian possesses the following symmetries: magnetisation conservation, parity (reflection w.r.t. the centre of the chain), spin inversion, and (many-body) momentum conservation.

In one dimension, the TFI Hamiltonian can be mapped to spinless p-wave superconducting fermions via the Jordan-Wigner (JW) transformation[CITE Sachdev, other paper]:

$$c_i = \prod_{j<i} \sigma^z_j \sigma^-_i, \qquad c^\dagger_i = \prod_{j<i} \sigma^z_j \sigma^+_i, \tag{2}$$

where the fermionic operators satisfy $\{c_i, c^\dagger_j\} = \delta_{ij}$. The Hamiltonian is readily shown to take the form

$$H = \sum_{j=0}^{L-1} J\left(-c^\dagger_j c_{j+1} + c_j c^\dagger_{j+1}\right) + J\left(-c^\dagger_j c^\dagger_{j+1} + c_j c_{j+1}\right) + 2h\left(n_j - \frac{1}{2}\right). \tag{3}$$

In the fermionic representation, the spin zz-interaction maps to nn hopping and a p-wave pairing term with coupling constant J, while the transverse field translates to an on-site potential shift of magnitude h. In view of the implementation of the model using QuSpin, we have ordered the terms such that the site index is growing to the right, which comes at the cost of a few negative signs due to the fermion statistics. We emphasize that this ordering is not dictated by QuSpin, but it is merely our choice to adopt it here for the sake of consistency. The fermion Hamiltonian posses the symmetries: particle conservation modulo 2, parity and (many-body) "momentum" conservation.

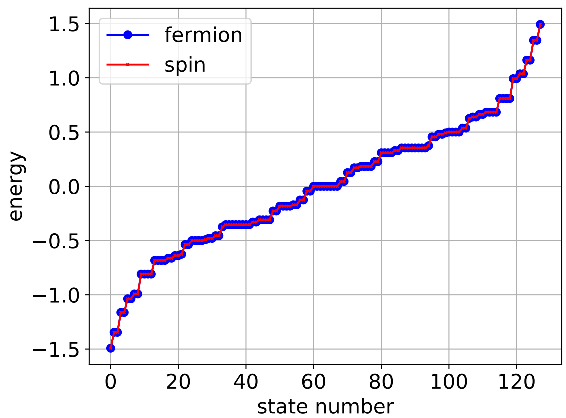
Here, we are interested in studying the spectrum of the TFI model in both the spin and fermion representations. However, if one naïvely carries out the JW transformation, and computes the spectra of Eqs. (1) and (3), one might be surprised that they do not match exactly. The reason lies in the form of the boundary condition required to make the JW mapping exact – a subtle issue often left aside in favour of discussing the interesting physics of the TFI model itself.

We recall that the starting is the periodic boundary condition imposed on the spin Hamiltonian in Eq. (1). Due to the symmetries of the spin Hamiltonian (1), we can define the JW transformation on every symmetry sector separately. To make the JW mapping exact, we supplement Eq. (2) with the following boundary conditions: (i) the negative spin-inversion symmetry sector maps to the fermion Hamiltonian (3) with *periodic* boundary conditions (PBC) and *odd* total number of fermions; (ii) the positive spin-inversion symmetry sector maps to the fermion Hamiltonian (3) with *anti-periodic* boundary conditions (APBC) and *even* total number of fermions. Anti-periodic boundary conditions differ from PBC by a negative sign attached to all coupling constants that cross a single, fixed lattice bond (the bond itself is arbitrary as all bonds are equal for PBC). APBC and PBC are special cases of the more general twisted boundary conditions where, instead of a negative sign, one attaches an arbitrary phase factor.

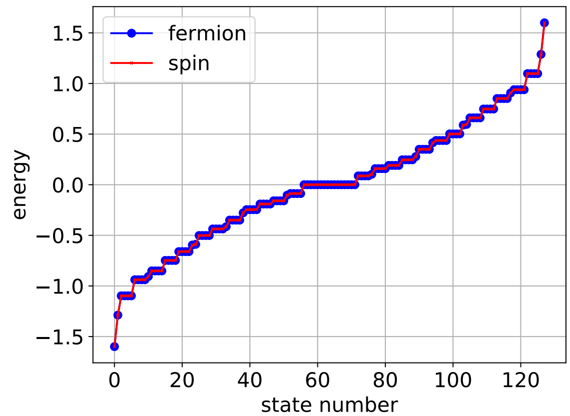
In the following, we show how to compute the spectra of the Hamiltonians in Eqs. (1) and (3) with the correct boundary conditions using QuSpin. Figure 1 shows that they match exactly in both the PBC and APBC cases discussed above.

Code Analysis—We begin by loading the QuSpin operator and basis constructors, as well as some standard Python libraries.

```
from quspin.operators import hamiltonian # Hamiltonians and operators
```



(a) negative spin inversion/PBC sector



(b) positive spin inversion/APBC sector

Figure 1: Comparison of the spectra of the spin and fermion representation of the transverse field Ising Hamiltonian in the spin (1) and fermion (3) representations. The degeneracy in the spectrum is due to the remaining parity and momentum conservations which could but are not taken into account (see text). The parameters are $J = 1.0$, $h = \sqrt{2}$, and $L = 8$.

```
from quspin.basis import spin_basis_1d, fermion_basis_1d # Hilbert space spin basis
import numpy as np # generic math functions
import matplotlib.pyplot as plt # figure/plot library
```

First, we define the models parameters.

```
##### define model parameters #####
L=8 # system size
J=1.0 # spin zz interaction
h=np.sqrt(2) # z magnetic field strength
```

We have to consider two cases when computing the spectrum, as discussed in the theory section above. In one case, the fermionic system has PBC and the particle number sector is odd, while the spins are constrained to the negative spin inversion symmetry sector, while in the second – the fermion model has APBC with even particle number sector, and the spin model is considered in the positive spin inversion sector. To this end, we introduce the variables `zblock` $\in \{\pm 1\}$ and `PBC` $\in \{\pm 1\}$, where `PBC` $= -1$ denotes APBC. Note than the only meaningful combinations are (`zblock`, `PBC`) $= (-1, 1), (1, -1)$, which we loop over:

```
# loop over spin inversion symmetry block variable and boundary conditions
for zblock,PBC in zip([-1,1],[1,-1]):
```

Within this loop, the code is divided in two independent parts: first, we compute the spectrum of the TFI system, and then – that of the equivalent fermionic model. Let us discuss the spins.

```
    ##### define spin model
```

In QuSpin, operators are stored as sparse lists. These lists contain two parts: (i) the lattice sites on which the operator acts together with the coupling strength, which we call a *site-coupling* list, and (ii) the types of the operators involved, i.e. the *operator-string*. For example, the operator $\mathcal{O} = g\sum_{j=0}^{L-1}\sigma_j^\mu$ can be uniquely represented by the site-coupling list `[[g,0],[g,1],...,[g,L-1]]`, and the information that it is the Pauli matrix μ. The components lists are nothing but the tuples of the field strength and the site index `[g,j]`. It is straightforward to generalise this to non-uniform fields `g`→`g[j]`. Similarly, any two-body operator $\mathcal{O} = J_{zz}\sum_{j=0}^{L-1}\sigma_j^\mu\sigma_{j+1}^\nu$ can be fully represented by the two sites it acts on, and its coupling strength: `[J,j,j+1]`. We then stack up these elementary lists together into the site-coupling list: `[[J,0,1],[J,1,2],...,[J,L-2,L-1],[J,L-1,0]]`.

```
    # site-coupling lists (PBC for both spin inversion sectors)
    h_field=[[-h,i] for i in range(L)]
    J_zz=[[-J,i,(i+1)%L] for i in range(L)] # PBC
```

Notice the way we defined the periodic boundary condition for the spin-spin interaction using the modulo operator `%`, which effectively puts a coupling between sites $L-1$ and 0. We mention in passing that the above procedure generalises so one can define any multi-body local or nonlocal operator using QuSpin.

In order to specify the types of the on-site single-particle operators, we use operator strings. For instance, the transverse field operator $\mathcal{O} = g\sum_{j=0}^{L-1}\sigma_j^x$ becomes `['x',h_field]`, while the two-body interaction is `['zz',J_zz]`. It is important to notice that the order of the letters in the operator string corresponds to the order the operators are listed in the site-coupling lists. Putting everything into one final list yields the `static` list for the spin model:

```
    # define spin static and dynamic lists
    static_spin =[["zz",J_zz],["x",h_field]] # static part of H
```

In QuSpin, the user can define both static and dynamic operators. Since this example does not contain any time evolution, we postpone the explanation of how to use dynamic lists to Sec. 2.5, and use an empty list instead.

```
    dynamic_spin=[] # time-dependent part of H
```

The last step before we can construct the Hamiltonian is to build the basis for it. This is done using the basis constructors. For spin systems, we use `spin_basis_1d` which allows to use the operator strings `'z','+','-','I'`, and for spin-1/2 additionally `'x','y'`. The first and required argument is the number of sites L. Optional arguments are used to parse symmetry sectors. For instance, if we want to construct an operator in the spin-inversion block with quantum number $+1$, we can conveniently do this using the flag `zblock=1`.

```
    # construct spin basis in pos/neg spin inversion sector depending on APBC/PBC
    basis_spin = spin_basis_1d(L=L,zblock=zblock)
```

Having specified the static and dynamic lists, as well as the basis, building up the Hamiltonian is a one-liner, using the `hamiltonian` constructor. The required arguments in order of appearance are the `static` and `dynamic` lists, respectively. Optional arguments include the `basis`, and the precision or data type `dtype`. If no basis is passed, the constructor uses `spin_basis_1d` by default. The default data type is `np.complex128`.

```
    # build spin Hamiltonians
    H_spin=hamiltonian(static_spin,dynamic_spin,basis=basis_spin,dtype=np.float64)
```

The Hamiltonian is stored as a Scipy sparse matrix for efficiency. It can be cast to a full array for a more convenient inspection using the attribute `H.toarray()`. To calculate its spectrum, we use the attribute `H.eigenvalsh()`, which returns all eigenvalues. Other attributes for diagonalisation were discussed in Example 0, c.f. Ref. [1].

```
    # calculate spin energy levels
    E_spin=H_spin.eigvalsh()
```

Let us now move to the second part of the loop which defines the fermionic p-wave superconductor. We start by defining the site-coupling list for the local potential

```
    ##### define fermion model
    # define site-coupling lists for external field
    h_pot=[[2.0*h,i] for i in range(L)]
```

Let us focus on the case of periodic boundary conditions `PBC=1` first.

```
    if PBC==1: # periodic BC: odd particle number subspace only
```

In the fermion model, we have two types of two-body terms: hopping terms $c_i^\dagger c_{i+1} - c_i c_{i+1}^\dagger$, and pairing terms $c_i^\dagger c_{i+1}^\dagger - c_i c_{i+1}$. While QuSpin allows any ordering of the operators, for the sake of consistency we set a convention: the site indices grow to the right. To take into account the opposite signs resulting from the fermion statistics, we have to code the site-coupling lists for all four terms separately. This is analogous to the spin-spin interaction above:

```
        # define site-coupling lists (including boudary couplings)
        J_pm=[[-J,i,(i+1)%L] for i in range(L)] # PBC
        J_mp=[[+J,i,(i+1)%L] for i in range(L)] # PBC
        J_pp=[[-J,i,(i+1)%L] for i in range(L)] # PBC
        J_mm=[[+J,i,(i+1)%L] for i in range(L)] # PBC
```

To construct a fermionic operator, we make use of the basis constructor `fermion_basis_1d`. Once again, we pass the number of sites `L`. As we explained in the analysis above, we need to consider all odd particle number sectors in the case of PBC. This is done by specifying the particle number sector `Nf`.

```
        # construct fermion basis in the odd particle number subsector
        basis_fermion = fermion_basis_1d(L=L,Nf=range(1,L+1,2))
```

In the case of APBC, we first construct all two-body site-coupling lists as if the boundaries were open, and supplement the APBC links with negative coupling strength in the end:

```
    elif PBC==-1: # anti-periodic BC: even particle number subspace only
        # define bulk site coupling lists
        J_pm=[[-J,i,i+1] for i in range(L-1)]
        J_mp=[[+J,i,i+1] for i in range(L-1)]
        J_pp=[[-J,i,i+1] for i in range(L-1)]
        J_mm=[[+J,i,i+1] for i in range(L-1)]
        # add boundary coupling between sites (L-1,0)
        J_pm.append([+J,L-1,0]) # APBC
        J_mp.append([-J,L-1,0]) # APBC
        J_pp.append([+J,L-1,0]) # APBC
        J_mm.append([-J,L-1,0]) # APBC
```

The construction of the basis is the same, except that this time we need all even particle number sectors:

```
        # construct fermion basis in the even particle number subsector
        basis_fermion = fermion_basis_1d(L=L,Nf=range(0,L+1,2))
```

As before, we need to specify the type of operators that go in the fermion Hamiltonian using operator string lists. The `fermion_basis_1d` class accepts the following strings `'+'`,`'-'`,`'n'`,`'I'`, and additionally the particle-hole symmetrised density operator `'z'` $= n - 1/2$. The static and dynamic lists read as

```
    # define fermionic static and dynamic lists
    static_fermion =[["+-",J_pm],["-+",J_mp],["++",J_pp],["--",J_mm],['z',h_pot]]
    dynamic_fermion=[]
```

Constructing and diagonalising the fermion Hamiltonian is the same as for the spin-1/2 system. Note that one can disable the automatic built-in checks for particle conservation `check_pcon=False` and all other symmetries `check_symm=False` if one wishes to suppress the checks.

```
    # build fermionic Hamiltonian
    H_fermion=hamiltonian(static_fermion,dynamic_fermion,basis=basis_fermion,
                            dtype=np.float64,check_pcon=False,check_symm=False)
    # calculate fermionic energy levels
    E_fermion=H_fermion.eigvalsh()
```

The complete code including the lines that produce Fig. 1 is available in Example Code 2.

2.2 Free Particle Systems: the Fermionic SSH Chain

This example shows how to

- construct free-particle Hamiltonians in real space,
- implement translation invariance with a two-site unit cell and construct the single-particle momentum-space block-diagonal Hamiltonian using the `block_diag_hamiltonian` function,
- compute non-equal time correlation functions,
- time evolve multiple quantum states simultaneously.

Physics Setup—The Su-Schrieffer-Heeger (SSH) model of a free-particle on a dimerised chain is widely used in one spatial dimension to introduce the concepts of edge states, topology, Berry phase, etc. The Hamiltonian is given by

$$H = \sum_{j=0}^{L-1} -(J + (-1)^j \delta J) \left(c_j c_{j+1}^\dagger - c_j^\dagger c_{j+1} \right) + \Delta (-1)^j n_j, \tag{4}$$

where $\{c_i, c_j^\dagger\} = \delta_{ij}$ obey fermionic commutation relations. The uniform part of the hopping matrix element is J, the bond dimerisation is defined by δJ, and Δ is the staggered potential. We work with periodic boundary conditions.

Below, we show how one can use QuSpin to study the physics of free fermions in the SSH chain. One way of doing this would be to work in the many-body (Fock space) basis, see Sec. 2.3. However, whenever the particles are non-interacting, the exponential scaling of the Hilbert space dimension with the number of lattice sites imposes an artificial limitation on the

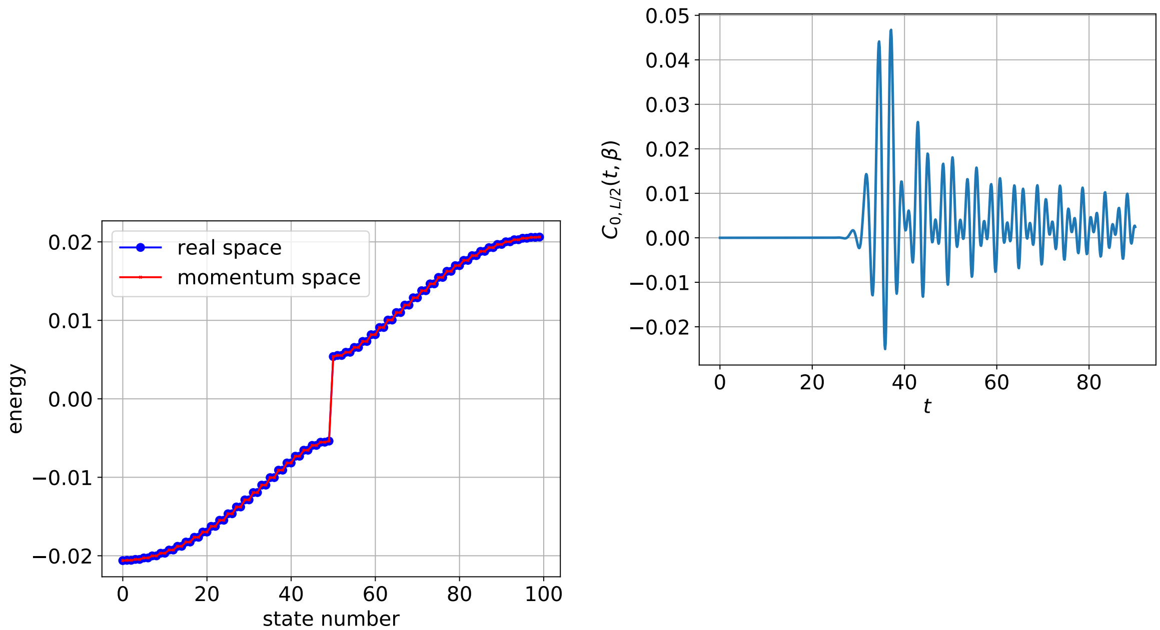


Figure 2: (a) the spectrum of the SSH Hamiltonian in real and momentum space. (b) The non-equal time correlator $C_{i=0,j=L/2}(t)$, cf. Eq. (6) as a function of time. The parameters are $\delta J/J = 0.1$, $\Delta/J = 0.5$, $J\beta = 100.0$ and $L = 100$.

system sizes one can do. Luckily, with no interactions present, the many-body wave functions factorise in a product of single-particle states. Hence, it is possible to study the behaviour of many free bosons and fermions by simulating the physics of a single particle, and populating the states according to bosonic or fermionic statistics, respectively.

Making use of translation invariance, a straightforward Fourier transformation to momentum space, $a_k = \sqrt{2/L}\sum_{j:\text{even}}^{L-1} \mathrm{e}^{-ikj} c_j$ and $b_k = \sqrt{2/L}\sum_{j:\text{odd}}^{L-1} \mathrm{e}^{-ikj} c_j$, casts the SSH Hamiltonian in the following form

$$H = \sum_{k\in\mathrm{BZ}'} (a_k^\dagger, b_k^\dagger) \begin{pmatrix} \Delta & -(J+\delta J)\mathrm{e}^{-ik} - (J-\delta J)\mathrm{e}^{+ik} \\ -(J+\delta J)\mathrm{e}^{+ik} - (J-\delta J)\mathrm{e}^{-ik} & -\Delta \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix}, \tag{5}$$

where the reduced Brillouin zone is defined as $\mathrm{BZ}' = [-\pi/2, \pi/2)$. We thus see that the Hamiltonian reduces further to a set of independent 2×2 matrices. The spectrum of the SSH model is gapped and, thus, has two bands, see Fig. 2a.

Since we are dealing with free fermions, the ground state is the Fermi sea, $|\mathrm{FS}\rangle$, defined by filling up the lowest band completely. We are interested in measuring the real-space non-equal time correlation function

$$C_{ij}(t) = \langle \mathrm{FS}|n_i(t)n_j(0)|\mathrm{FS}\rangle = \langle \mathrm{FS}(t)|n_i(0)\underbrace{U(t,0)n_j(0)|\mathrm{FS}\rangle}_{|\mathrm{nFS}(t)\rangle}. \tag{6}$$

To evaluate the correlator numerically, we shall use the right-hand side of this equation.

As we are studying free particles, it is enough to work with the single-particle states. For instance, the Fermi sea can be obtained as $|\mathrm{FS}\rangle = \prod_{k\leq k_F} c_k^\dagger|0\rangle$. Denoting the on-site density operator by n_i, one can cast the correlator in momentum space in the following form:

$$C_{ij}(t) = \sum_{k \leq k_F} \langle k | n_i(t) \hat{n}_j(0) | k \rangle. \tag{7}$$

If we want to consider finite-temperature β^{-1}, the above formula generalises to

$$C_{ij}(t, \beta) = \sum_{k \in \mathrm{BZ}'} n_{\mathrm{FD}}(k, \beta) \langle k | n_i(t) n_j(0) | k \rangle, \tag{8}$$

where $n_{\mathrm{FD}}(k, \beta) = 1/(\exp(\beta E_k) + 1)$ is the Fermi-Dirac distribution at temperature β^{-1}, with E_k the SSH dispersion. Figure 2b) shows the time evolution of $C_{ij}(t, \beta)$ for two sites, separated by the maximal distance on the ring: $L/2$.

Code Analysis.—Let us explain how one can do all this quickly and efficiently using QuSpin. As always, we start by loading the required packages and libraries.

```
from quspin.operators import hamiltonian,exp_op # Hamiltonians and operators
from quspin.basis import fermion_basis_1d # Hilbert space fermion basis
from quspin.tools.block_tools import block_diag_hamiltonian # block diagonalisation
import numpy as np # generic math functions
import matplotlib.pyplot as plt # plotting library
try: # import python 3 zip function in python 2 and pass if already using python 3
    import itertools.izip as zip
except ImportError:
    pass
```

After that, we define the model parameters

```
##### define model parameters #####
L=100 # system size
J=1.0 # uniform hopping contribution
deltaJ=0.1 # bond dimerisation
Delta=0.5 # staggered potential
beta=100.0 # set inverse temperature for Fermi-Dirac distribution
```

In the following, we construct the fermionic SSH Hamiltonian first in real space. We then show how one can also construct it in momentum space where, provided we use periodic boundary conditions, it appears bock-diagonal. Let us define the fermionic site-coupling lists. Once again, we emphasise that fermion systems require special care in defining the hopping terms: Eq. (4) is conveniently cast in the form where all site indices on the operators grow to the right, and all signs due to the fermion statistics are explicitly spelt out.

```
##### construct single-particle Hamiltonian #####
# define site-coupling lists
hop_pm=[[-J-deltaJ*(-1)**i,i,(i+1)%L] for i in range(L)] # PBC
hop_mp=[[+J+deltaJ*(-1)**i,i,(i+1)%L] for i in range(L)] # PBC
stagg_pot=[[Delta*(-1)**i,i] for i in range(L)]
```

Defining the `static` list assigns the specific SSH operator structure. Since our problem does not possess any explicit time dependence, we leave the `dynamic` list empty.

```
# define static and dynamic lists
static=[["+-",hop_pm],["-+",hop_mp],['n',stagg_pot]]
dynamic=[]
```

Setting up the fermion basis with the help of the constructor `fermion_basis_1d` proceeds as smoothly as in Sec. 2.1. Notice a cheap trick: by specifying a total of `Nf=1` fermion in the lattice, QuSpin actually allows to define single-particle models, as a special case of the more general many-body Hamiltonians. Compared to many body models, however, due to the exponentially reduced Hilbert space size, this allows us to scale up the system size `L`.

```
# define basis
basis=fermion_basis_1d(L,Nf=1)
```

We then build the real-valued SSH Hamiltonian in real space by passing the static and dynamic lists, as well as the basis and the data type. After that, we and diagonalise it, storing all eigenenergies and eigenstates.

```
# build real-space Hamiltonian
H=hamiltonian(static,dynamic,basis=basis,dtype=np.float64)
# diagonalise real-space Hamiltonian
E,V=H.eigh()
```

For translation invariant single-particle models, however, the user might prefer to use momentum space, where the Hamiltonian becomes block diagonal, as we showed above. This can be achieved using QuSpin's `block_tools`. The idea behind this tool is simple: the main purpose is to create the full Hamiltonian in block-diagonal form, where the blocks correspond to pre-defined quantum numbers. In our case, we would like to use momentum or `kblock`'s. Note that the unit cell in the SSH model contains two sites, which we encode using the variable `a=2`. Thus, we can create a list of dictionaries `blocks`, each element of which defines a single symmetry block. If we combine all blocks, we exhaust the full Hilbert space. All other basis arguments, such as the system size, we store in the variable `basis_args`. We invite the interested user to check the package documentation for additional optional arguments and functionality of `block_tools`, cf. App. C. We mention in passing that this procedure is independent of the symmetry, and can be done using all symmetries supported by QuSpin, not only translation.

```
##### compute Fourier transform and momentum-space Hamiltonian #####
# define basis blocks and arguments
blocks=[dict(Nf=1,kblock=i,a=2) for i in range(L//2)] # only L//2 distinct momenta
basis_args = (L,)
```

To create the block-diagonal Hamiltonian, we invoke the `block_diag_hamiltonian` method. It takes both requires and optional arguments, and returns the transformation which block-diagonalises the Hamiltonian (in our case the Fourier transform) and the block-diagonal Hamiltonian object. Required arguments, in order of appearance, are the `blocks`, the `static` and `dynamic` lists, the basis constructor, `basis_args`, and the data type. Since we expect the matrix elements of the momenum-space Hamiltonian to contain the Fourier factors $\exp(-ik)$, we know to choose a complex data type. `block_diag_hamiltonian` also accepts some optional arguments, such as the flags for disabling the automatic built-in symmetry checks. More about this function can be found in the documentation, cf. App. C.

```
# construct block-diagonal Hamiltonian
FT,Hblock = block_diag_hamiltonian(blocks,static,dynamic,fermion_basis_1d,
                              basis_args,np.complex128,get_proj_kwargs=dict(pcon=True))
```

We can then use all functions and methods of the `hamiltonian` class to manipulate the block-diagonal Hamiltonian, for instance the diagonalisation routines:

```python
# diagonalise momentum-space Hamiltonian
Eblock,Vblock=Hblock.eigh()
```

We now proceed to calculate the correlation function from Eq. (6). To this end, we shall split the correlator according to the RHS of Eq. (6). Thus, the strategy is to evolve both the Fermi sea $|\mathrm{FS}(t)\rangle$ and the auxiliary state $|\mathrm{nFS(t)}\rangle$ in time, and compute the expectation value of the time-independent operator $n_i(0)$ in between the two states as a function of time. Last, keep in mind that we do not need to construct the Fermi sea as a many-body state explicitly, so we rather work with single-particle states.

The first step is to collect all momentum eigenstates into the columns of the array `psi`. We then build the operators $n_{j=0}$ and $n_{j=L/2}$ in real space.

```python
##### prepare the density observables and initial states #####
# grab single-particle states and treat them as initial states
psi0=Vblock
# construct operator n_1 = $n_{j=0}$
n_1_static=[['n',[[1.0,0]]]]
n_1=hamiltonian(n_1_static,[],basis=basis,dtype=np.float64,
                check_herm=False,check_pcon=False)
# construct operator n_2 = $n_{j=L/2}$
n_2_static=[['n',[[1.0,L//2]]]]
n_2=hamiltonian(n_2_static,[],basis=basis,dtype=np.float64,
                check_herm=False,check_pcon=False)
```

Next, we transform these two operators to momentum space using the method `rotate_by()`. Setting the flag `generator=False` treats the Fourier transform `FT` as a unitary transformation, rather than a generator of a unitary transformation.

```python
# transform n_j operators to momentum space
n_1=n_1.rotate_by(FT,generator=False)
n_2=n_2.rotate_by(FT,generator=False)
```

Let us proceed with the time-evolution. We first define the time vector `t` and the state `n_psi0`.

```python
##### evaluate nonequal time correlator <FS|n_2(t) n_1(0)|FS> #####
# define time vector
t=np.linspace(0.0,90.0,901)
# calcualte state acted on by n_1
n_psi0=n_1.dot(psi0)
```

We can perform the time evolution in two ways: (i) we calculate the time-evolution operator `U` using the `exp_op` class, and apply it to the momentum states `psi0` and `n_psi0`. The `exp_op` class calculates the matrix exponential $\exp(aH)$ of an operator H multiplied by a complex number a. One can also conveniently compute a series of matrix exponentials $\exp(aHt)$ for every time t by specifying the stating point `start`, endpoint `stop` and the number of elements `num` which define the time array t via `t=np.linspace(start,stop,num)`. Last, by parsing the flag `iterate=True` we create a python generator – a pre-defined object evaluated only at the time it is called, i.e. not pre-computed, which can save both time and memory.

```python
# construct time-evolution operator using exp_op class (sometimes faster)
U = exp_op(Hblock,a=-1j,start=t.min(),stop=t.max(),num=len(t),iterate=True)
# evolve states
psi_t=U.dot(psi0)
n_psi_t = U.dot(n_psi0)
```

Another way of doing the time evolution, (ii), is to use the `evolve()` method of the `hamiltonian` class. The idea here is that every Hamiltonian defines a generator of time translations. This method solves the Schrödinger equation using SciPy's ODE integration routines, see App. C for more details. The required arguments, in order of appearance, are the initial state, the initial time, and the time vector. The `evolve()` method also supports the option to create the output as a generator using the flag `iterate=True`. Both ways (i) and (ii) time-evolve all momentum states `psi` at once.

```
# alternative method for time evolution using Hamiltonian class
#psi_t=Hblock.evolve(psi0,0.0,t,iterate=True)
#n_psi_t=Hblock.evolve(n_psi0,0.0,t,iterate=True)
```

To evaluate the correlator, we first preallocate memory by defining the empty array `correlators`, which will be filled with the correlator in every single-particle momentum mode $|k\rangle$. Using generators then allows us to loop only once over time to obtain the time-evolved states `psi_t` and `n_psi_t`. In doing so, we evaluate the expectation value $\langle \mathrm{FS}(t)|n_i(0)|\mathrm{nFS}(t)\rangle$ using the `matrix_ele()` method of the `hamiltonian` class. The flag `diagonal=True` makes sure only the diagonal matrix elements are calculated[1] and returned as a one-dimensional array.

```
# preallocate variable
correlators=np.zeros(t.shape+psi0.shape[1:])
# loop over the time-evolved states
for i, (psi,n_psi) in enumerate( zip(psi_t,n_psi_t) ):
    correlators[i,:]=n_2.matrix_ele(psi,n_psi,diagonal=True).real
```

Finally, we weigh all singe-state correlators by the Fermi-Dirac distribution to obtain the finite-temperature non-equal time correlation function $C_{0,L/2}(t,\beta)$.

```
# evaluate correlator at finite temperature
n_FD=1.0/(np.exp(beta*E)+1.0)
correlator = (n_FD*correlators).sum(axis=-1)
```

The complete code including the lines that produce Fig. 2 is available in Example Code 3.

2.3 Many-Body Localization in the Fermi-Hubbard Model

This example shows how to:

- construct Hamiltonians for spinful fermions using the `tensor_basis` class.
- how to use `ops_dict()` class to construct Hamiltonians with varying parameters.
- use new basis functionality to construct simple product states
- use `obs_vs_time` functionality to measure observables as a function of time

A class of exciting new problems in the field of non-equalibrium physics is that of Many-body localised (MBL) models. The MBL transition is a dynamical phase transition in the eigenstates of a many-body Hamiltonian. Driven primarily by quenched disorder, the transition is distinguished by the system having ergodic eigenstates in the weak disorder limit

[1] Recall that `psi_t` and `n_psi_t` contain many time-evolved states, and if one uses the default `diagonal=False`, all off-diagonal matrix elements will be computed as well, so the result will be a two-dimensional array

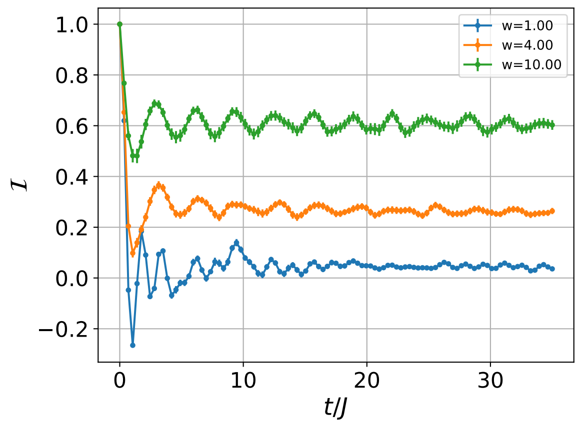


Figure 3: Sublattice imbalance I as a function of time, averaged over 100 disorder realizations for different disorder strengths. This data was taken on a chain of length $L = 8$.

and non-ergodic eigenstates in the strong disorder limit. The MBL phase is reminiscent of integrable systems as one can construct quasi-local integrals of motion, but these integrals of motion are much more robust in the sense that they are not sensitive to small perturbations as is the case in many classes of integrable systems[CITE MBL misc].

Motivated by recent experiments in cold atomic gasses [CITE Bloch MBL I think there are a few others too] we explore MBL in the context of fermions using QuSpin. The model we will consider is the Fermi-Hubbard model with quenched random disorder which has the following Hamiltonian:

$$H = -J \sum_{i=0,\sigma}^{L-2} \left(c^\dagger_{i\sigma} c_{i+1,\sigma} - c_{i\sigma} c^\dagger_{i+1,\sigma} \right) + U \sum_{i=0}^{L-1} n_{i\uparrow} n_{i\downarrow} + \sum_{i=0,\sigma}^{L-1} V_i n_{i\sigma} \tag{9}$$

where $c_{i\sigma}$ and $c^\dagger_{i\sigma}$ are the fermionic creation and annihilation operators on site i for spin σ, respectively. We will work in the sector of $1/4$ filling for both up and down spins. Preparing an initial configuration of fermions of alternating spin on every other site, we will then measure the sublattice imbalance [CITE exp]:

$$I = (N_A - N_B)/N_{\mathrm{tot}} \tag{10}$$

where A and B refer to the different sublattices of the chain and N is the particle number. Evolving the initial state under the Hamiltonian (9) we will calculate the time dependence of the imbalance which will give us information about the ergodicity of the Hamiltonian (or the lack thereof). If the Hamiltonian is ergodic then this quantity will decay to 0 in the limit $t \to \infty$ as one would expect due to thermalising dynamics, while if the Hamiltonian is MBL then some memory of its initial state will be retained, and therefore th imbalance will remain non-zero even at infinite times.

Because the Hilbert space dimension grows so quickly for this Hamiltonian with the lattice size, we will only consider the dynamics after a finite amount of time, and even with this it is a fairly long calculation to do, due to, (say which parts take longest time)

Code Analysis— Once again we start out by loading a set of libraries which we need to proceed with the simulation of MBL fermions.

```python
from quspin.operators import hamiltonian,exp_op,ops_dict # operators
from quspin.basis import tensor_basis,fermion_basis_1d # Hilbert spaces
from quspin.tools.measurements import obs_vs_time # calculating dynamics
import numpy as np # general math functions
from numpy.random import uniform,choice # tools for doing random sampling
from time import time # tool for calculating computation time
```

While we already encountered most of these libraries and functions, in this example we introduce the `ops_dict()` class which defines an operator, parametrized by multiple parameters, as opposed to the Hamiltonian which is only parametrized by time. Also, since this example requires us to do many different disorder realisations, we use **NumPy**'s random number library to do random sampling. We load `uniform` to generate the uniformly distributed random potential as well as `choice` which we use to estimate the uncertainties of the disorder averages using a bootstrap re-sampling procedure which we explain below below, or in App.?. In order to time how long each realization takes, we use the `time` function from python's `time` library.

After importing all the required libraries and functions we set up the parameters for the simulation including the number of realizations `n_real`, and the physical couplings `J`, U, the number of up and down fermions, etc.

```python
##### setting parameters for simulation
# simulation parameters
n_real = 100 # number of realizations
n_boot = 100 # number of bootstrap samples to calculate error
# physical parameters
L = 8 # system size
N = L//2 # number of particles
N_up = N//2 + N % 2 # number of fermions with spin up
N_down = N//2 # number of fermions with spin down
w_list = [1.0,4.0,10.0] # disorder strength
J = 1.0 # hopping strength
U = 5.0 # interaction strength
# range in time to evolve system
start,stop,num=0.0,35.0,101
t = np.linspace(start,stop,num=num,endpoint=True)
```

Next we set up the basis, introducing here the `tensor_basis` constructor class. In its full-fledged generality, `tensor_basis` takes n basis objects which it then uses to construct the matrix elements in the tensor product space:

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n. \tag{11}$$

Here we consider the case of two Hilbert spaces, $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, one for fermions with spin up and one for spin-down fermions[2]. One disadvantage of using the tensor basis is that it does not allow for the use of symmetries, beyond particle-conservation (magnetisation in the case of spin systems). we'll have to change this later when we have the ladder classes.

```python
###### create the basis
# build the two bases to tensor together to spinful fermions
basis_up = fermion_basis_1d(L,Nf=N_up) # up basis
basis_down = fermion_basis_1d(L,Nf=N_down) # down basis
basis = tensor_basis(basis_up,basis_down) # spinful fermions
```

[2] to construct a `tensor_basis` object in general: `t_basis = tensor_basis(basis_1,basis_2,...,basis_n)`

The next step in the procedure is to set up the site-coupling and operator lists:

```
##### create model
# define site-coupling lists
hop_right = [[-J,i,i+1] for i in range(L-1)] # hopping to the right OBC
hop_left = [[J,i,i+1] for i in range(L-1)] # hopping to the left OBC
int_list = [[U,i,i] for i in range(L)] # onsite interaction
# site-coupling list to create the sublattice imbalance observable
sublat_list = [[(-1.0)**i/N,i] for i in range(0,L)]
# create static lists
operator_list_0 = [
            ["+-|", hop_left], # up hop left
            ["-+|", hop_right], # up hop right
            ["|+-", hop_left], # down hop left
            ["|-+", hop_right], # down hop right
            ["n|n", int_list], # onsite interaction
            ]
imbalance_list = [["n|",sublat_list],["|n",sublat_list]]
```

Notice here that the `"|"` character is used to separate the operators which belong to the up (left side of tensor product) and down (right side of tensor product) Hilbert spaces in `basis`. If no string in present the operator is assumed to be the identity `'I'`. The site-coupling list, on the other hand, does not require separating the two sides of the tensor product, as it is assumed that the operator string lines up with the correct site index when the `'|'` character is removed.

In the last couple of lines defining model (see below), we create a python `dictionary` object in which we add static operator lists as `values`, indexed by a particular string known as the corresponding `key`. This dictionary, which we refer to as `operator_dict`, is then passed into the `ops_dict()` class which, for each `key` in `operator_dict`, constructs the operator listed in the site-coupling list for that `key`. When one wants to evaluate this operator for a particular set of parameters, one uses a second dictionary (see `params_dict` below give line number) with the same keys as `operator_dict`: the value corresponding to each key in the `params_dict` multiples the operator stored at that same key in `operator_dict`. This allows one to parametrize many-body operators in more complicated and general ways. In the present example, we define a key for the Fermi-Hubbard Hamiltonian, and then, as we need to change the disorder strength in between realisations, we also define keys for the local density operator for both up and down spins on each site. By doing this, we can then construct any disordered Hamiltonian by specify the disorder at each site, and changing its value from one realisation to another.

```
# create operator dictionary for ops_dict class
# add key for Hubbard hamiltonian
operator_dict=dict(H0=operator_list_0)
# add keys for local potential in each site
for i in range(L):
    # add to dictioanry keys h0,h1,h2,...,hL with local potential operator
    operator_dict["n"+str(i)] = [["n|",[[1.0,i]]],["|n",[[1.0,i]]]]
```

The `ops_dict()` class constructs operators in almost an identical manner as a `hamiltonian()` class with the exception that there is no dynamic list. Next, we construct our initial state with the fermions dispersed over the lattice on every other site. To get the index of the `basis` state which this initial state corresponds to, one can use the `index` function of the `tensor_basis` class. This function takes a string or integer representing the product state for each of the Hilbert spaces and then searches to find the full product state, returning the corresponding index. We can then create an empty array **psi_0** of dimension the total Hilbert space size, and insert unity at the index corresponding to the initial state. This allows us to easily define the many-body product state used in the rest of the simulation.

```
###### setting up operators
# set up hamiltonian dictionary and observable (imbalance I)
no_checks = dict(check_pcon=False,check_symm=False,check_herm=False)
H_dict = ops_dict(operator_dict,basis=basis,**no_checks)
I = hamiltonian(imbalance_list,[],basis=basis,**no_checks)
# strings which represent the initial state
s_up = "".join("1000" for i in range(N_up))
s_down = "".join("0010" for i in range(N_down))
# basis.index accepts strings and returns the index
# which corresponds to that state in the basis list
i_0 = basis.index(s_up,s_down) # find index of product state
psi_0 = np.zeros(basis.Ns) # allocate space for state
psi_0[i_0] = 1.0 # set MB state to be the given product state
print("H-space size: {:d}, initial state: |{:s}>(x)|{:s}>".format(basis.Ns,s_up,
    s_down))
```

Now that the operators are all set up, we can proceed with the simulation of the dynamics. First, we define a function which, given a disorder realization of the local potential, calculates the time evolution of $\mathcal{I}(t)$. We shall guide the reader through this function step by step. The syntax for this begins as follows:

```
# define function to do dynamics for different disorder realizations.
def real(H_dict,I,psi_0,w,t,i):
    # body of function goes below
    ti = time() # start timing function for duration of reach realisation
```

The first step is to construct the Hamiltonian from the **disorder** list which is as simple as

```
    # create a parameter list which specifies the onsite potential with disorder
    params_dict=dict(H0=1)
    for j in range(L):
        params_dict["n"+str(j)] = uniform(-w,w)
    # using the parameters dictionary construct a hamiltonian object with those
    # parameters defined in the list
    H = H_dict.tohamiltonian(params_dict)
```

using the **tohamiltonian()** method of **H_dict** class, which accepts as argument the dictionary **params_dict**, which shares the same keys as **operator_dict**, but whose values are determined by the **disorder** list which changes from one realisation to another.

Once the Hamiltonian has been constructed we want to time-evolve the initial state with it. To this end, we use the fact that, for time-independent Hamiltonians, the time-evolution operator coincides with the matrix exponential $\exp(-itH)$. In QuSpin, a convenient way to define matrix exponentials is offered by the **exp_op** class. Given an operator A , it calculates $\exp(atA)$ for any complex-valued number a. The time grid for t is specified using the optional arguments **start**, **stop** and **num**. If the latter are omitted, default is $t = 1$. The **exp_op** objects are either a list of arrays, the elements of which correspond to the operator $\exp(atA)$ at the times defined or, if **iterate=True** a generator for this list is returned. Here, we use **exp_op** to create a generator list containing the time-evolved states as follows

```
    # use exp_op to get the evolution operator
    U = exp_op(H,a=-1j,start=t.min(),stop=t.max(),num=len(t),iterate=True)
    psi_t = U.dot(psi_0) # get generator psi_t for time evolved state
```

To calculate the expectation value of the imbalance operator in time, we use the `obs_vs_time` function. Since the usage of this function was extensively discussed in Example2 and Example3 of Ref. [1], here we only mention that it accepts a (collection of) state(s) [or a generator] `psi_t`, a time vector `t`, and a dictionary `dict(I=I)`, whose values are the observables to calculate the expectation value of. The function returns a dictionary, the keys of which correspond to the keys every observable was defined under.

```
    # use obs_vs_time to evaluate the dynamics
    t = U.grid # extract time grid stored in U, and defined in exp_op
    obs_t = obs_vs_time(psi_t,t,dict(I=I))
```

The function ends by printing the time of executing and returning the value for I as a function of time for this realization

```
    # print reporting the computation time for realization
    print("realization {}/{} completed in {:.2f} s".format(i+1,n_real,time()-ti))
    # return observable values
    return obs_t["I"]
```

Now we are all set to run the disorder realizations for the different disorder strengths which in principle can be spilt up over multiple simulations, e.g. using `joblib` [c.f. Example2 from Ref. [1]] but for completeness we do all of the calculations in one script.

```
###### looping over diffent disorder strengths
for w in w_list:
    I_data = np.vstack([real(H_dict,I,psi_0,w,t,i) for i in range(n_real)])
```

Last, we calculate the average and its error bars using bootstrap re-sampling (See Appendix??)

```
    ##### averaging and error estimation
    I_avg = I_data.mean(axis=0) # get mean value of I for all time points
    # generate bootstrap samples
    bootstrap_gen = (I_data[choice(n_real,size=n_real)].mean(axis=0) for i in range(
    n_boot))
    # generate the fluctuations about the mean of I
    sq_fluc_gen = ((bootstrap-I_avg)**2 for bootstrap in bootstrap_gen)
    I_error = np.sqrt(sum(sq_fluc_gen)/n_boot)
```

The complete code including the lines that produce Fig. 3 is available in Example Code 4.

2.4 The Bose-Hubbard Model on Translationally Invariant Ladder

This example shows how to:

- construct interacting Hamiltonians for bosonic systems.
- construct a Hamiltonian on a ladder geometry.
- use the `block_ops` class to evolve a state over several symmetry sectors at once.
- measure the entanglement entropy of a state on the ladder.

Physics Setup— In this example we use QuSpin to simulate the dynamics of the Bose-Hubbard model (BHM) on a ladder geometry. The BHM is a minimal model for interacting lattice bosons which is most often experimentally realizable in cold atom experiments [CITE]. The Hamiltonian is given by

$$H_{\mathrm{BHM}} = -J\sum_{\langle ij\rangle}\left(a_i^\dagger a_j + \mathrm{h.c.}\right) + \frac{U}{2}\sum_i n_i(n_i-1) \tag{12}$$

where a_i and $a_i^\dagger$ are bosonic creation and annihilation operators on site i, respectively, and $\langle ij\rangle$ denotes nearest neighbors on the ladder. We consider a half-filled ladder of length L with $N = 2L$ sites and cylindrical boundary condition i.e. a periodic boundary condition along the ladder leg direction. We are interested in the limit $U/J \gg 1$ and, therefore, we restrict the local Hilbert space to allow at most two particles per site, effectively using a total of three states per site: empty, singly and doubly occupied.

The system is initialised in a random Fock state, and then evolved with the Hamiltonian (12). Since the BHM is non-integrable, we expect that the system eventually thermalizes so that the long-time occupation becomes roughly uniform over the entire system. Besides the local density, we also measure the entanglement entropy between the two legs of the ladder.

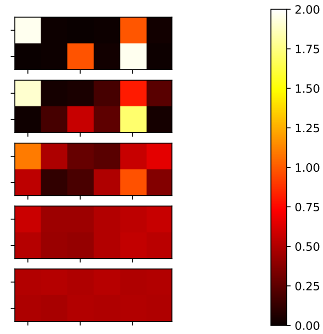
As we consider a translational invariant ladder, the Hilbert space factorizes into subspaces corresponding to the different many-body momentum blocks. This is similar to what was discussed in Sec. 2.2 for the SSH model, but slightly different as we consider translations of the *many-body* Fock states as opposed to the single particle states [2]. In certain cases, it happens that, even though the Hamiltonian features symmetries, the initial state does not obey them, as is the case in the present example, where the initial state is a random Fock state. Thus, in this section we project the wavefunction to the different symmetry sectors and evolve each of the projections separately under the Hamiltonian for that symmetry sector. After the evolution, each of these block wavefunctions is transformed back to the local Fock space basis, and summed up to recover the properly evolved initial state. We can then measure quantities such as the on-site density and the entanglement entropy. Figure 4 shows...

Code Analysis—Let us now show how one can simulate this system using QuSpin. Following the code structure of previous examples, we begin by loading the modules needed for the computation:

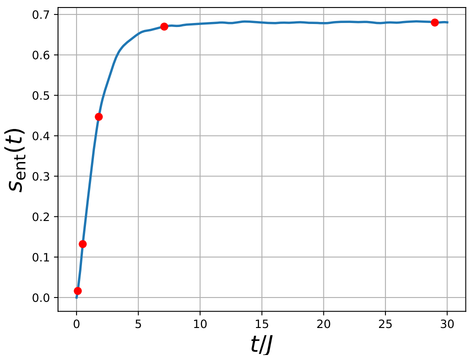
```python
from __future__ import print_function, division #import python 3 functions
from quspin.operators import hamiltonian # Hamiltonians and operators
from quspin.basis import boson_basis_1d # bosonic Hilbert space
from quspin.tools.block_tools import block_ops # dynamics in symmetry blocks
import numpy as np # general math functions
import matplotlib.pyplot as plt # plotting
import matplotlib.animation as animation # animating movie of dynamics
```

First, we set up the model parameters defining the length of the ladder `L`, the total number of sites in the chain `N=2*L`, as well as the filling factor for the bosons `nb`, and the maximum number of states per site (i.e. the local on-site Hilbert space dimension) `sps`. The hopping matrix elements $J_\perp$, $J_{\parallel,1}$, and $J_{\parallel,2}$ (see Fig. 1create figure showing ladder and couplings etc...) correspond to the python script variables `J_perp`, `J_par_1`, and `J_par_2`, respectively. The on-site interaction is denoted by `U`.

```python
##### define model parameters
# initial see for random number generator
```



(b) local density of bosons as a function of time. Later times appearing farther down the page.



(a) Entanglement entropy density between the two legs of the ladder as a function of time.

Figure 4: Quantities measured in the BHM: (a) the leg-to-leg entanglement entropy density and (b) the local density on each site as a function of time. The red dots on the entanglement plot shows the time points at which the snapshots of the local density are taken. The parameters are $U/J = 20$, and $L = 6$.

```
np.random.seed(0) # seed is 0 to produce plots from QuSpin2 paper
# setting up parameters of simulation
L = 6 # length of chain
N = 2*L # number of sites
nb = 0.5 # density of bosons
sps = 3 # number of states per site
J_par_1 = 1.0 # top side of ladder hopping
J_par_2 = 1.0 # bottom side of ladder hopping
J_perp =  0.5 # rung hopping
U = 20.0 # Hubbard interaction
```

Let us proceed to construct the Hamiltonian and the observables for the problem. For bosonic systems, we have `'+'`,`'-'` `'n'`, and `'I'` as available Fock space operators to use. In order to set up the local Hubbard interaction, we first split it up in two terms: $U/2\sum_i n_i(n_i-1) = -U/2\sum_i n_i + U/2\sum_i n_i^2$. Thus, we need two coupling lists:

```
##### set up Hamiltonian and observables
# define site-coupling lists
int_list_1 = [[-0.5*U,i] for i in range(N)] # interaction $-U/2 \sum_i n_i$
int_list_2 = [[0.5*U,i,i] for i in range(N)] # interaction: $U/2 \num_i n_i^2$
```

QuSpin *Example Code* 1: Translationally Invariant Ladder Geometry

```
#schematic of how the ladder lattice is set up coupling parameters:
# -: J_par_1
```

```
# ^: J_par_2
# |: J_perp
#
^ 1 ^ 3 ^ 5 ^ 7 ^ 9 ^
  |   |   |   |   |
- 0 - 2 - 4 - 6 - 8 -
#
# translations (i -> i+2):
#
 ^ 9 ^ 1 ^ 3 ^ 5 ^ 7 ^
   |   |   |   |   |
 - 8 - 0 - 2 - 4 - 6 -
#
# if J_par_1=J_par_2, one can use regular chain parity (i -> N - i):
#
 - 8 - 6 - 4 - 2 - 0 -
   |   |   |   |   |
 - 9 - 7 - 5 - 3 - 1 -
#
# combination of two ladder parity operators!
```

We also define the hopping site-coupling list. In general, QuSpin can set up the Hamiltonian on any graph (thus, including higher-dimensions). By labelling te lattice sites conveniently, we can define the ladder geometry, as shown in Fig. 1. For the ladder geometry we are interested in, there are three types of hopping on a ladder geometry: one along each of the two legs with tunnelling matrix elements `J_par_1` and `J_par_1`, respectively, and the transverse hopping along the rungs of the ladder with strength `J_perp`. The even sites correspond to the bottom leg while the odds sites are the top leg of the ladder. Therefore, the hopping on the bottom/top leg is defined by `[J_par_...,i,(i+2)%N]`, while the rung hopping (from the top leg to the bottom leg) is defined by `[J_perp,i,(i+1)%N]`.

```python
# setting up hopping lists
hop_list = [[-J_par_1,i,(i+2)%N] for i in range(0,N,2)] # PBC bottom leg
hop_list.extend([[-J_par_2,i,(i+2)%N] for i in range(1,N,2)]) # PBC top leg
hop_list.extend([[-J_perp,i,i+1] for i in range(0,N,2)]) # perp/rung hopping
hop_list_hc = [[J.conjugate(),i,j] for J,i,j in hop_list] # add h.c. terms
```

where we used the `list_1.extend(list_2)` method to concatenate two lists together[3].

Next, we define the static and dynamic lists, which are needed to construct the Hamiltonian.

```python
# set up static and dynamic lists
static = [
            ["+-",hop_list], # hopping
            ["-+",hop_list_hc], # hopping h.c.
            ["nn",int_list_2], # U n_i^2
            ["n",int_list_1] # -U n_i
        ]
dynamic = [] # no dynamic operators
```

[3]Note that the `extend` function is done inplace so if one tries to do `new_list=list_1.extend(list_2)`, `new_list` will be `None` and `list_1` will have all of the elements of `list_2` appended to it.

Instead of creating a **hamiltonian** class object in real space, we use the **block_ops** class to set up the Hamiltonian in a block-diagonal form in momentum space, similar to the SSH model, c.f.Sec. 2.2. In order to reduce the computational cost, the state is evolved in momentum space and projected to the Fock basis after the calculation. The purpose of **block_ops** is to provide a simple interface for solving the Schrödinger equation when an initial state does not obey the symmetries of the Hamiltonian it is evolved under. We have seen an example of this in Sec. 2.2 when trying to measure non-equal space-time correlation functions of local operators in a translational invariant system, while in this section we explicitly start out with a state which does not obey translation invariance. To construct the **block_ops** object we use the follow set of lines, explained below:

```
# create block_ops object
blocks=[dict(kblock=kblock) for kblock in range(L)] # blocks to project on to
baisis_args = (N,) # boson_basis_1d manditory arguments
basis_kwargs = dict(nb=nb,sps=sps,a=2) # boson_basis_1d optional args
get_proj_kwargs = dict(pcon=True) # set projection to full particle basis
H_block = block_ops(blocks,static,dynamic,boson_basis_1d,baisis_args,np.complex128,
                    basis_kwargs=basis_kwargs,get_proj_kwargs=get_proj_kwargs)
```

First, we create a list of dictionaries **blocks** which define the different symmetry sectors to project the initial state to before doing the time evolution[4]. this dict is not created until an evolution routine is called The optional arguments **basis_args** and **basis_kwargs** apply to every symmetry sector. Last, **get_proj_kwargs** contains the optional arguments to construct the projectors[5]. For more information about this class we refer the user to the Documentation, c.f. App. C.

Finally, we define the local density operators using the **boson_basis_1d** class.

```
# setting up basis for local fock basis
basis = boson_basis_1d(N,nb=nb,sps=sps)
# setting up observables
no_checks = dict(check_herm=False,check_symm=False,check_pcon=False)
n_list = [hamiltonian([["n",[[1.0,i]]]],[],basis=basis,dtype=np.float64,**no_checks)
     for i in range(N)]
```

Having set up the Hamiltonian, we now proceed to the time-evolution part of the problem. We begin by defining the initial random state in the Fock basis.

```
# set up initial state
i0 = np.random.randint(basis.Ns) # pick random state from basis set
psi = np.zeros(basis.Ns,dtype=np.float64)
psi[i0] = 1.0
# print info about setup
state_str = "".join(str(int((basis[i0]//basis.sps**i)%basis.sps)) for i in range(N))
print("total H-space size: {}, initial state: |{}>".format(basis.Ns,state_str))
```

Next we define the times at which we would like to solve the Schrödinger equation. Below, we use the **exp_op** class to compute the time-evolution operator as the exponential of the Hamiltonian, see Sec. 2.3. Therefore, we consider linearly spaced time points defined by the variables **start**,**stop**, and **num**.

[4] block_ops will not evolve in those symmetry sectors for which the projection is 0.

[5] In this case setting pcon=True means that the projector takes the state *from* the symmetry reduced basis *to* the fixed particle number basis.

```python
# setting up parameters for evolution
start,stop,num = 0,30,301 # 0.1 equally spaced points
times = np.linspace(start,stop,num)
```

To calculate the states as a function of time, we use the `expm` function of the `block_ops` class to first construct the unitary evolution operator as the matrix exponential of the time-independent Hamiltonian[6]. We define the `expm` function to have almost identical arguments as that of the `exp_op` class, but with some major exceptions. For one, because the Hamiltonian factorizes in a block-diagonal form, the evolution over each block can be done separately (e.g. just trivially loop through the blocks sequentially). In some cases, however, e.g. for single particle Hamiltonians [see Sec. 2.2], there are a lot of small blocks, and it actually makes sense to calculate the matrix exponential in block diagonal form which is achieved by setting the optional argument `block_diag=True`. Another optional argument, `n_jobs=int`, allows the user to spawn multiple python processes which do the calculations for the different blocks simultaneously for `n_jobs>1`. On most systems these processes will be distributed over multiple CPUs which can speed up the calculations if there are resources for this available. This also works in conjunction with the `block_diag` where each process creates its own block diagonal matrix for the calculation. Once all the calculations for each block are completed, the results are combined and conveniently projected back to the original local Fock basis.

```python
# calculating the evolved states
n_jobs = 1 # paralelisation: increase to see if calculation runs faster!
psi_t = H_block.expm(psi,a=-1j,start=start,stop=stop,num=num,block_diag=False,n_jobs
    =n_jobs)
```

We can now use the time dependent states calculated to compute the expectation value of the local density

```python
# calculating the local densities as a function of time
expt_n_t = np.vstack([n.expt_value(psi_t).real for n in n_list]).T
# reshape data for plotting
n_t = np.zeros((num,2,L))
n_t[:,0,:] = expt_n_t[:,0::2]
n_t[:,1,:] = expt_n_t[:,1::2]
```

We can also compute the entanglement entropy between the two legs of the adder. In the newer versions of QuSpin we have moved the entanglement entropy calculations to the basis classes themselves (keeping of course backwards compatible functions from older versions). The rational behind this is that this calculation is highly dependent on the type of system one is studying. Below, we show how to use the *basis* object to calculate the entanglement entropy. We note in passing that this function can also calculate the reduced density matrix and its eigenvalues for pure and mixed states. Once again we refer the reader to the Documentation to learn more about how to use this function, see App. C.

```python
# calculating entanglement entropy
sub_sys_A = range(0,N,2) # bottom side of ladder
gen = (basis.ent_entropy(psi,sub_sys_A=sub_sys_A)["Sent_A"]/L for psi in psi_t.T[:])
ent_t = np.fromiter(gen,dtype=np.float64,count=num)
```

The complete code including the lines that produce Fig. 4 is available in Example Code 5.

[6] For time dependent Hamiltonians, the `block_ops` class contains a method called `evolve`, see App. C.

2.5 The Gross-Pitaevskii Equation and Nonlinear Time Evolution

This example shows how to

- simulate time-dependent nonlinear equations of motion
- use imaginary time dynamics to find a lowest energy configuration

Physics Setup—The Gross-Pitaevskii wave equation (GPE) has been shown to govern the physics of weakly-interacting bosonic systems. It constitutes the starting point for studying Bose-Einstein condensates, but can also appear in non-linear optics, and represents the natural description of Hamiltonian mechanics in the wave picture. One of its interesting features is that it can exhibits chaotic classical dynamics, a physical manifestation of the presence of a cubic non-linear term.

Here, we study the time-dependent GPE on a one-dimensional lattice:

$$\begin{aligned} i\partial_t \psi_j(t) &= -J\left(\psi_{j-1}(t)+\psi_{j+1}(t)\right)+\frac{1}{2}\kappa_{\mathrm{trap}}(t)(j-j_0)^2\psi_j(t)+U|\psi_j(t)|^2\psi_j(t), \\ \kappa_{\mathrm{trap}}(t) &= (\kappa_f-\kappa_i)t/t_{\mathrm{ramp}}+\kappa_i \end{aligned} \tag{13}$$

where J is the hopping matrix element, $\kappa_{\mathrm{trap}}(t)$ – the harmonic trap strength which varies slowly in time over a scale t_{ramp}, and U – the mean-field interaction strength. The lattice sites are labelled by $j=0,\dots,L-1$, and j_0 is the centre of the 1d chain. We set the lattice constant to unity, and use open boundary conditions.

Whenever $U=0$, the system is non-interacting and the GPE reduces to the Heisenberg EOM for the bosonic field operator $\hat{\psi}_j(t)$. Thus, for the purposes of using QuSpin to simulate the GPE, it is instructive to cast Eq. (13) in the following generic form

$$i\partial_t\vec{\psi}(t)=H_{\mathrm{sp}}(t)\vec{\psi}(t)+U\vec{\psi}^*(t)\circ\vec{\psi}(t)\circ\vec{\psi}(t), \tag{14}$$

where $[\vec{\psi}(t)]_j=\psi_j(t)$, and $\circ$ represents the element-wise multiplication

$$\vec{\psi}(t)\circ\vec{\phi}(t)=\Big(\psi_0(t)\phi_0(t),\psi_1(t)\phi_1(t),\dots,\psi_{L-1}(t)\phi_{L-1}(t)\Big)^t.$$

The time-dependent single-particle Hamiltonian in real space is represented as an $L\times L$ matrix, $H_{\mathrm{sp}}(t)$, which comprises the hopping term, and the harmonic trap.

We want to initiate the time-evolution of the system at $t=0$ in its lowest energy state. To this end, we can define a 'ground state' for the GPE equation, in terms of the configuration which minimises the energy of the system:

$$\begin{aligned} \vec{\psi}_{\mathrm{GS}} &= \inf_{\vec{\psi}}\left(\vec{\psi}^t H_{\mathrm{sp}}(0)\vec{\psi}+\frac{U}{2}\sum_{j=0}^{L-1}|\psi_j|^4\right), \\ &= \inf_{\psi_j}\left(-J\sum_{j=0}^{L-2}(\psi^*_{j+1}\psi_j+\mathrm{c.c.})+\frac{1}{2}\kappa_{\mathrm{trap}}(0)\sum_{j=0}^{L-1}(j-j_0)^2|\psi_j|^2+\frac{U}{2}\sum_{j=0}^{L-1}|\psi_j|^4\right). \end{aligned} \tag{15}$$

One way to find the configuration $\vec{\psi}_{\mathrm{GS}}$, is to solve the GPE in imaginary time ($it\to\tau$), which induces exponential decay in all modes of the system, which singles out the lowest-energy state in the longer run. In doing so, we keep the norm of the solution fixed:

$$\begin{aligned}\partial_\tau\vec{\varphi}(\tau) &= -\Big[H_{\mathrm{sp}}(0)\vec{\varphi}(\tau) + U\vec{\varphi}^*(\tau)\circ\vec{\varphi}(\tau)\circ\vec{\varphi}(\tau)\Big], \qquad ||\vec{\varphi}(\tau)|| = \mathrm{const.},\\ \vec{\psi}_{\mathrm{GS}} &= \lim_{\tau\to\infty}\vec{\varphi}(\tau)\end{aligned} \tag{16}$$

Once we have the initial state $\vec{\psi}_{\mathrm{GS}}$, we evolve it according to the time-dependent GPE, Eq. (13), and track down the time evolution of the condensate density $\rho_j(t) = |\psi_j(t)|^2$. Fig. ??? shows the result.

Code Analysis—In the following, we demonstrate how one can code the above physics using QuSpin. As usual, we begin by loading the necessary packages:

```python
from quspin.operators import hamiltonian # Hamiltonians and operators
from quspin.basis import boson_basis_1d # Hilbert space boson basis
from quspin.tools.measurements import evolve # nonlinear evolution
import numpy as np # generic math functions
import matplotlib.pyplot as plt # plot library
```

Next, we define the model parameters. We distinguish between static parameters and dynamic parameters – those involved in the time-dependent trap widening.

```python
##### define model parameters #####
L=300 # system size
# calculate centre of chain
if L%2==0:
    j0 = L//2-0.5 # centre of chain
else:
    j0 = L//2 # centre of chain
sites=np.arange(L)-j0
# static parameters
J=1.0 # hopping
U=1.0 # Bose-Hubbard interaction strength
# dynamic parameters
kappa_trap_i=0.001 # initial chemical potential
kappa_trap_f=0.0001 # final chemical potential
t_ramp=40.0/J # set total ramp time
```

In order to do time evolution, we code up the trap widening protocol from Eq. (13) in the function **ramp**. Since we want to make use of QuSpin's time-dependent operator features, the first argument must be the time **t**, followed by all protocol parameters. These same parameters are then explicitly stored in the variable **ramp_args**.

```python
# ramp protocol
def ramp(t,kappa_trap_i,kappa_trap_f,t_ramp):
    return  (kappa_trap_f - kappa_trap_i)*t/t_ramp + kappa_trap_i
# ramp protocol parameters
ramp_args=[kappa_trap_i,kappa_trap_f,t_ramp]
```

With this, we are ready to construct the single-particle Hamiltonian $H_{\mathrm{sp}}(t)$. The first step is to define the site-coupling lists, and the static and dynamic lists. Note that the dynamic list, which defines the harmonic potential in the single-particle Hamiltonian, contains four elements: apart from the operator string and the corresponding site-coupling list, the third and fourth elements are the time-dependent function **ramp** and its argument list **ramp_args**, and this order is crucial.

```python
##### construct single-particle Hamiltonian #####
# define site-coupling lists
hopping=[[-J,i,(i+1)%L] for i in range(L-1)]
trap=[[0.5*(i-j0)**2,i] for i in range(L)]
# define static and dynamic lists
static=[["+-",hopping],["-+",hopping]]
dynamic=[['n',trap,ramp,ramp_args]]
```

To create the single-particle Hamiltonian, we choose to use the bosonic basis constructor `boson_basis_1d` specifying the number sector to `Nb=1` boson for the entire lattice, and a local Hilbert space of `sps=2` states per site (empty and filled).

```python
# define basis
basis = boson_basis_1d(L,Nb=1,sps=2)
```

Then we call the `hamiltonian` constructor to build the single-particle matrix. We can obtain the single-particle ground state without fully diagonalising this matrix, by using the sparse diagonalisation attribute `Hsp.eigsh()`. The `eigsh()` routine accepts the optional flags `k=1` and `'which'='SA'` which restrict the routine to find the first eigenstate starting from the bottom of the spectrum, i.e. the ground state.

```python
# build Hamiltonian
Hsp=hamiltonian(static,dynamic,basis=basis,dtype=np.float64)
E,V=Hsp.eigsh(time=0.0,k=1,which='SA')
```

Having set up the Hsmiltonian, the next step in the simulation is to compute the ground state of the GPE using imaginary time evolution from Eq. (16). To this end, we first define the function `GPE_imag_time` which evaluate the RHS. It is required that the first argument for this function is (imaginary) time `tau`, followed by the state `phi`. All other arguments, such as the single-particle Hamiltonian and the interaction strength are listed last. Note that we evaluate the time-dependent Hamiltonian at `time=0`, since we are interested in finding the GPE GS for the initial trap coniguration κ_i. Similar to before, we store these optional arguments in a list which we call `GPE_params`.

```python
##### imaginary-time evolution to compute GS of GPE #####
def GPE_imag_time(tau,phi,Hsp,U):
    """
    This function solves the real-valued GPE in imaginary time:
    $$ -\dot\phi(\tau) = Hsp(t=0)\phi(\tau) + U |\phi(\tau)|^2 \phi(\tau) $$
    """
    return -( Hsp.dot(phi,time=0) + U*np.abs(phi)**2*phi )
# define ODE parameters
GPE_params = (Hsp,U)
```

Any initial value problem requires us to pick an initial state. In the case of imaginary evolution, this state can often be arbitrary, but needs to possess the same symmetries as the true GPE ground state. Here, we choose the ground state of the single-particle Hamiltonian for an initial state, and normalise it to one particle per site. We also define the imaginary time vector `tau`. This array has to contain sufficiently long times so that we make sure we end up in the long imaginary time limit $\tau \to \infty$, as required by Eq. (16). Since imaginary time evolution is not unitary, QuSpin will be normalising the vector every τ-step. Thus, one also needs to make sure these steps are small enough to avoid convergence problems with the ODE solver.

```python
# define initial state to flow to GS from
```

```python
phi0=V[:,0]*np.sqrt(L) # initial state normalised to 1 particle per site
# define imaginary time vector
tau=np.linspace(0.0,35.0,71)
```

Performing imaginary time evolution is done using the `evolve()` method of the `measurements` tool. This function accepts an initial state `phi0`, initial time `tau[0]`, and a time vector `tau` and solves any user-defined ODE, here `GPE_imag_time`. The parameters of the ODE are passed using the keyword argument `f_params=GPE_params`. To ensure the normalisation of the state at each τ-step we use the flag `imag_time=True`. Real-valued output can be specified by `real=True`. Last, we request `evolve()` to create a generator object using the keyword argument `iterate=True`. Many of the keyword arguments of `evolve()` are the same as in the `H.evolve()` method of the `hamiltonian` class: for instance, one can choose a specific SciPy solver and its arguments, or the solver's absolute and relative tolerance. We refer the interested reader to the documentation, cf. App. C.

```python
# evolve state in imaginary time
psi_tau = evolve(phi0,tau[0],tau,GPE_imag_time,f_params=GPE_params,
                            imag_time=True,real=True,iterate=True)
```

Looping over the generator `phi_tau` we have access to the solution, which we display in a form of a movie:

```python
# display state evolution
for i,psi0 in enumerate(psi_tau):
    # compute energy
    E_GS=(Hsp.matrix_ele(psi0,psi0,time=0) + 0.5*U*np.sum(np.abs(psi0)**4) ).real
    # plot wave function
    plt.plot(sites, abs(phi0)**2, color='r',marker='s',alpha=0.2,
                                        label='$|\\phi_j(0)|^2$')
    plt.plot(sites, abs(psi0)**2, color='b',marker='o',
                                label='$|\\phi_j(\\tau)|^2$' )
    plt.xlabel('$\\mathrm{lattice\\ sites}$',fontsize=14)
    plt.title('$J\\tau=%0.2f,\\ E_\\mathrm{GS}(\\tau)=%0.4fJ$'%(tau[i],E_GS)
                                                                ,fontsize=14)
    plt.ylim([-0.01,max(abs(phi0)**2)+0.01])
    plt.legend(fontsize=14)
    plt.draw() # draw frame
    plt.pause(0.005) # pause frame
    plt.clf() # clear figure
plt.close()
```

Last, we use our GPE ground state, to time-evolve it in real time according to the trap widening protocol `ramp`, hard-coded into the single-particle Hamiltonian. We proceed analogously – first we define the real-time GPE and the time vector. In defining the GPE function, we split the ODE into a time-independent static part and a time-dependent dynamic part. The single-particle Hamiltonian for the former is accessed using the `hamiltonian` attribute `Hsp.static` which returns a SciPy sparse array. We can then manually add the non-linear cubic mean-field interaction term. In order to access the time-dependent part of the Hamiltonian, and evaluate it, we loop over the dynamic list `Hsp.dynamic`, which is a list consisting of the corresponding operator `Hd` together with the time-dependent function `f` which multiplies it, and its arguments `f_args`. In the very end, we multiply the final output vector by the Schrödinger $-i$, which ensures the unitarity of real-time evolution.

```
##### real-time evolution of GPE #####
def GPE(time,psi):
    """
    This function solves the complex-valued time-dependent GPE:
    $$ i\dot\psi(t) = Hsp(t)\psi(t) + U |\psi(t)|^2 \psi(t) $$
    """
    # solve static part of GPE
    psi_dot = Hsp.static.dot(psi) + U*np.abs(psi)**2*psi
    # solve dynamic part of GPE
    for Hd,f,f_args in Hsp.dynamic:
        psi_dot += f(time,*f_args)*Hd.dot(psi)
    return -1j*psi_dot
# define real time vector
t=np.linspace(0.0,t_ramp,101)
```

To perform the real-time evolution explicitly we once again use the **evolve()** function. This time, however, since the solution of the GPE is anticipated to be complex-valued, and because we do not do imaginary time, we do not need to pass the flags **real** and **imag_time**. Instead, we decided to show the flags for the relative and absolute tolerance of the solver.

```
# time-evolve state according to GPE
psi_t = evolve(psi0,t[0],t,GPE,iterate=True,atol=1E-12,rtol=1E-12)
```

Finally, we can enjoy the movie displaying real-time evolution

```
# display state evolution
for i,psi in enumerate(psi_t):
    # compute energy
    E=(Hsp.matrix_ele(psi,psi,time=t[i]) + 0.5*U*np.sum(np.abs(psi)**4) ).real
    # compute trap
    kappa_trap=ramp(t[i],kappa_trap_i,kappa_trap_f,t_ramp)*(sites)**2
    # plot wave function
    plt.plot(sites, abs(psi0)**2, color='r',marker='s',alpha=0.2
                                ,label='$|\\psi_{\\mathrm{GS},j}|^2$')
    plt.plot(sites, abs(psi)**2, color='b',marker='o',label='$|\\psi_j(t)|^2$')
    plt.plot(sites, kappa_trap,'--',color='g',label='$\\mathrm{trap}$')
    plt.ylim([-0.01,max(abs(psi0)**2)+0.01])
    plt.xlabel('$\\mathrm{lattice\\ sites}$',fontsize=14)
    plt.title('$Jt=%0.2f,\\ E(t)-E_\\mathrm{GS}=%0.4fJ$'%(t[i],E-E_GS),fontsize=14)
    plt.legend(loc='upper right',fontsize=14)
    plt.draw() # draw frame
    plt.pause(0.00005) # pause frame
    plt.clf() # clear figure
plt.close()
```

The complete code including the lines that produce Fig. ?? is available in Example Code 6.

2.6 Integrability Breaking and Thermalising Dynamics in the Spin-1 Transverse-Field Ising Model

This example shows how to:

- construct Hamiltonians for Higher spin operators.
- find ground state of a Hamiltonian

- use obs_vs_time function with costume user defined generator to calculate the expectation value of operators as a function of time.
- use the new functionality of the basis class to calculate the entanglement entropy for higher spin.

Physics Setup— In the previous section we introduced the TFI model and showed how one can solve the problem using the Jordan-Wigner transformation. This transformation allows one to get an exact analytic solution to the Hamiltonian (when the system obeys translational invariance). The fact that this solution exists in deeply connected to the notion of Integrability which has implications of how the system responds to a periodic modulation [CITE]. For non-integrable system when periodic driving, energy is no longer conserved and so generically one would expect that the system will heat up to infinite temperature, while in an integrable system, even though energy is not conserved, there are an extensive number of other static conserved quantities which may be conserved under the drive. If this is the case, then the system will not heat up at long times, but instead reach some steady state. By simply taking the transverse field ising model and promoting the spin-1/2 operators to spin-1, there is no longer a simple mapping to a quadratic Hamiltonian and therefore the model is no longer integrable. Here we will show this explicitly by driving the two different systems and checking it they heat or not. To do this we will define two Hamiltonians

$$H_{zz} = -\sum_{i=0}^{L-1} S^z_i S^z_{i+1}, \qquad H_x = -\sum_{i=0}^{L-1} S^x_i \tag{17}$$

and evolve the ferromagnetic ground state of H_{zz} with the following piecewise periodic Hamiltonian:

$$H(t) = H_{zz} - A\,\mathrm{sgn}\left(\cos(\Omega t)\right) H_x \tag{18}$$

where Ω is the driving frequency, T – the corresponding period, and A – the driving amplitude. As the Hamiltonian obeys translation,parity and spin-inversion symmetries we will use this to speed up the evolution by working in the symmetry sector which contains the ground state.

need equation to show application of unitaries In order to measure the difference in heating between spin-1 and spin-1/2 we measure the expectation value of H_{zz} as a function of time. This operator has a symmetric spectrum and so following ref.[CITE heading papers] we define Q:

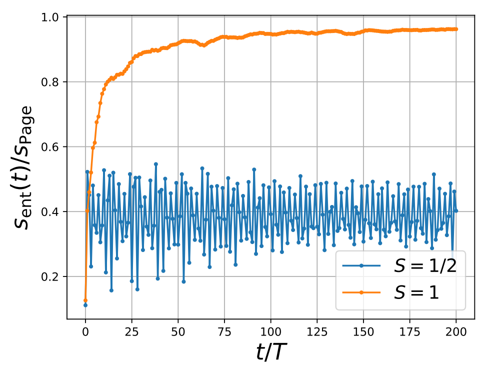
$$Q(t) = \left\langle \psi(t) \left| \frac{2\left(H_{zz} - E_{\mathrm{min}}\right)}{E_{\mathrm{max}} - E_{\mathrm{min}}} \right| \psi(t) \right\rangle = \left\langle \psi(t) \left| \frac{H_{zz} - E_{\mathrm{min}}}{-E_{\mathrm{min}}} \right| \psi(t) \right\rangle \tag{19}$$

where the last equality comes from the symmetry of the spectrum: $E_{\mathrm{max}} = -E_{\mathrm{min}}$. This quantity is defined such that an infinite temperature state has $Q = 1$. Another measure of heating we will use is the entanglement entropy density

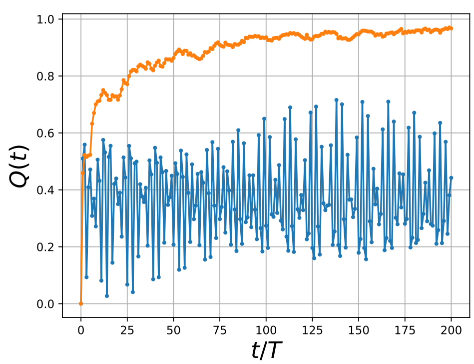
$$s_{\mathrm{ent}}(t) = -\frac{1}{|\mathrm{A}|}\mathrm{tr}_{\mathrm{A}}\left[\rho_{\mathrm{A}}(t)\log\rho_{\mathrm{A}}(t)\right], \qquad \rho_{\mathrm{A}}(t) = \mathrm{tr}_{\mathrm{A}^c}|\psi(t)\rangle\langle\psi(t)| \tag{20}$$

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

Code Analysis—Now we explain how to carry out the proposed study using QuSpin. We assume the reader has basic familiarity with QuSpin to set up simple time-dependent Hamiltonians. As is customary, we begin by loading the required Python libraries and packages:



(b) $s_{\rm ent}(t)/s_{\rm Page}$ for $t = nT$



(a) $Q(t)$ for $t = nT$

Figure 5: Comparing the dynamics of $Q(t)$ (a) and $s_{\rm ent}(t)$ (b) for $S = 1$ (orange) and $S = 1/2$ (blue) at stroboscopic times ($t = nT$). For $S = 1$ and $S = 1/2$ we take $L = 11$ and 18 respectively as to make sure the many-body Hilbert spaces have roughly the same number of state. $s_{\rm ent}$ is normalized by the Page entropy per site[CITE Page]. Note that for both systems $\Omega = 4$.

```python
from __future__ import print_function, division
from quspin.operators import ops_dict,hamiltonian,exp_op
from quspin.basis import spin_basis_1d # spin basis constructor
from quspin.tools.measurements import obs_vs_time # calculating dynamics
from quspin.tools.Floquet import Floquet_t_vec # period-spaced time vector
import numpy as np # general math functions
import matplotlib.pyplot as plt
```

Then, we define the model parameters. Note that we chose all physical couplings to be unity, so the only parameters are the drive frequency and the drive amplitude, which is set equal to the driving frequency [this is chosen arbitrarily]. Also, since the Hilbert space dimensions for the spin-1/2 and spin-1 systems scale differently with the length of the chain, we shall keep two variables, labelled by `L_12` and `L_1`, respectively. In general, all variables indexed by `_12` and `_1` in the code refer to spin-1/2 and spin-1 quantities, respectively.

```python
###### define model parameters
L_12 = 18 # length of chain for spin 1/2
L_1 = 11 # length of chain for spin 1
Omega = 2.0 # drive frequency
A = 2.0 # drive amplitude
```

Let us now define the spin bases. To this end, we make use of the `spin_basis_1d` constructor. Notice the optional argument `S`, which accepts a string (integer or half-integer) to specify the spin vector size. Requesting symmetry blocks works as usual, by using the corresponding optional arguments.

```python
###### setting up bases ######
basis_12 = spin_basis_1d(L_12,S="1/2",kblock=0,pblock=1,zblock=1) # spin 1/2 basis
basis_1 = spin_basis_1d(L_1,S="1"  ,kblock=0,pblock=1,zblock=1) # spin 1 basis
# print information about the basis
print("S = {S:3s}, L = {L:2d}, Size of H-space: {Ns:d}".format(S="1/2",L=L_12,Ns=basis_12.Ns))
print("S = {S:3s}, L = {L:2d}, Size of H-space: {Ns:d}".format(S="1"  ,L=L_1,Ns=basis_1.Ns))
```

To set up the site-coupling lists for the two operators in the Hamiltonian we proceed in the usual manner. Using them, we can call the `hamiltonian` constructor to define $-\sum_j S^z_j S^z_{j+1}$ and $-\sum_j S^x_j$. Here we keep the operators separate, in order to do the periodic step-drive evolution, which is why we do not need to define separate static and dynamic lists. We repeat this for both the spin-1/2 and the spin-1 systems.

```python
###### setting up operators in hamiltonian ######
# setting up site-coupling lists
Jzz_12 = [[-1.0,i,(i+1)%L_12] for i in range(L_12)]
hx_12  = [[-1.0,i] for i in range(L_12)]
Jzz_1 = [[-1.0,i,(i+1)%L_1] for i in range(L_1)]
hx_1  = [[-1.0,i] for i in range(L_1)]
# spin-1/2
Hzz_12 = hamiltonian([["zz",Jzz_12]],[],basis=basis_12,dtype=np.float64)
Hx_12  = hamiltonian([["+",hx_12],["-",hx_12]],[],basis=basis_12,dtype=np.float64)
# spin-1
Hzz_1 = hamiltonian([["zz",Jzz_1]],[],basis=basis_1,dtype=np.float64)
Hx_1  = hamiltonian([["+",hx_1],["-",hx_1]],[],basis=basis_1,dtype=np.float64)
```

In order to do time evolution, we need to define the initial state of our system. In this case, we start from the ground state of the Hamiltonian $-\sum_j S^z_j S^z_{j+1}$. We remind the reader that, since we work in a specific symmetry sector, this state may no longer be a product state. To this end, we employ the **eigsh()** method for sparse hermitian matrices of the **hamiltonian** class, where we explicitly specify that we are interested in getting a single (**k=1**) smallest algebraic (i.e. ground state) eigenenergy, and the corresponding eigenstate (a.k.a. the ground state), c.f. Example 1 in Ref. [1] for more details [PUT LINK TO GITHUB].

```
###### calculate initial states ######
# calculating bandwidth for non-driven hamiltonian
[E_12_min],psi_12 = Hzz_12.eigsh(k=1,which="SA") #
[E_1_min],psi_1 = Hzz_1.eigsh(k=1,which="SA")
# set up the initial states
psi0_12 = psi_12.ravel()
psi0_1 = psi_1.ravel()
```

Let us now move on to simulating the evolution due to the periodic step-drive. Before we begin, we note that QuSpin contains a build-in **Floquet** class which can be useful for studying this and other periodically-driven systems, see Example 3 in Ref. [1] [PUT LINK TO GITHUB]. Here, instead, we focus on manually evolving the state. First. we define the number of periods we would like to stroboscopically evolve our system for. Stroboscopic evolution is one where all quantities are evaluated at integer multiple of the driving period. To set up a time vector, which explicitly hits all those points, we use the **Floquet_t_vec** class, which accepts as arguments the frequency **Omega**, the number of periods **nT**, and the number of points per period **len_T**. The **Floquet_t_vec** class creates an object which has many useful attributes, including the stroboscopic times and their indices, the period, the starting point, etc. We invite the interested reader to check out the documentation [PUT LINK] for more information.

```
# stroboscopic time vector
nT = 200 # number of periods to evolve to
t=Floquet_t_vec(Omega,nT,len_T=1) # t.vals=t, t.i=initial time, t.T=drive period
```

Since the Hamiltonian is piece-wise constant, we can simulate the time evolution by exponentiating the separate terms. Note that, since we choose the driving phase (Floquet gauge) to yield a time-symmetric Hamiltonian, i.e. $H(-t) = H(t)$, this results in evolving the system with the Hamiltonians $H_{zz} + AH_x$, $H_{zz} - AH_x$, $H_{zz} + AH_x$ for the durations $T/4, T/2, T/4$, respectively (think of the phase of the drive as that of a rectilinear cosine drive). To compute the matrix exponential of a static operator, we make use of the **exp_op** class, where $\exp(zB)$ =**exp_op(B,a=z)** for some complex number z and some operator B.

```
# creating generators of time evolution using exp_op class
U1_12 = exp_op(Hzz_12+A*Hx_12,a=-1j*t.T/4)
U2_12 = exp_op(Hzz_12-A*Hx_12,a=-1j*t.T/2)
U1_1 = exp_op(Hzz_1+A*Hx_1,a=-1j*t.T/4)
U2_1 = exp_op(Hzz_1-A*Hx_1,a=-1j*t.T/2)
```

In order to evolve the state itself, we demonstrate how to construct a user-defined generator function **evolve_gen()**, which takes the initial state, the number of periods, and a sequence of unitaries within a period to apply them on the state. The generator character of the function means that it will not execute the loops when called for the first time, but rather store information about them, and return the values one by one when prompted to do so later on. This is useful since otherwise we would have to loop over all times to evolve the state first, and then again to compute the observables, As we can we below, the generator function allows us to get away with a single loop.

```python
# user-defined generator for stroboscopic dynamics
def evolve_gen(psi0,nT,*U_list):
    yield psi0
    for i in range(nT): # loop over number of periods
        for U in U_list: # loop over unitaries
            psi0 = U.dot(psi0)
        yield psi0
# get generator objects for time-evolved states
psi_12_t = evolve_gen(psi0_12,nT,U2_12,U1_12,U2_12)
psi_1_t = evolve_gen(psi0_1,nT,U2_1,U1_1,U2_1)
```

Finally, we are ready to compute the time-dependent quantities of interest. In order to calculate the expectation $\langle\psi(t)|H_{zz}|\psi(t)\rangle$ QuSpin has a routine called `obs_vs_time()`. It accepts the time-dependent state `psi_12_t` (or its generator), the time vector `t.vals` to evaluate the observable at, and a dictionary, which contains all observables of interest (here `Hzz_12`). The output of `obs_vs_time()` is a dictionary which contains the results: every observable was passed in by a string (here `"E"`), under which its expectation value will appear, evaluated at the requested times. Further, if one specifies the optional argument `return_state=True`, the time-evolved state is also returned under the string `"psi_t"`.

```python
###### compute expectation values of observables ######
# measure Hzz as a function of time
Obs_12_t = obs_vs_time(psi_12_t,t.vals,dict(E=Hzz_12),return_state=True)
Obs_1_t = obs_vs_time(psi_1_t,t.vals,dict(E=Hzz_1),return_state=True)
```

In fact, `obs_vs_time()` can also compute the entanglement entropy at every point of time (see documentation [PUT LINK]). Instead, we decided to show how one can do this using the new functionality of the `basis` class. Each basis constructor comes with a function method `ent_entropy()` which evaluates the entanglement entropy of a given state, and may return the reduced density matrix upon request. To compute the entanglement, the user needs to pass the state (here `Obs_12_t["psi_t"]`), and a subsystem to define the partition for computing the entanglement. The method `ent_entropy()` can handle vectorised calculations, and will compute the entanglement of the state for each point of time. The output is stored in a dictionary, and the entanglement entropy can be accessed with the key `"Sent_A"`. Finally, to obtain the entanglement entropy density, we also normalise the results by the size of the subsystem of interest.

```python
# calculating the entanglement entropy density
Sent_t_12 = basis_12.ent_entropy(Obs_12_t["psi_t"],sub_sys_A=range(L_12//2))["Sent_A"]/(L_12//2)
Sent_t_1 = basis_1.ent_entropy(Obs_1_t["psi_t"],sub_sys_A=range(L_1//2))["Sent_A"]/(L_1//2)
```

In order get an intuition about the amount of entanglement cause in the system by the drive, we use as a reference entanglement the corresponding Page values, which are a measure of...

```python
# calculate Page entropy density values
s_p_12 = np.log(2)-2.0**(-L_12//2-L_12)/(2*(L_12//2))
s_p_1 = np.log(3)-3.0**(-L_1//2-L_1)/(2*(L_1//2))
```

The complete code including the lines that produce Fig. 5 is available in Example Code 7.

2.7 Out-of-Equilibrium Bose-Fermi Mixtures

The last example in our tutorial shows how to:

- construct Hamiltonians for Bose-Fermi mixtures using the `tensor_basis` class
- periodically drive one subsystem (here the fermions)
- use new basis functionality to construct simple product states in the tensor basis
- use `obs_vs_time` functionality to compute the evolution of the entanglement entropy of the bosons with the fermions.

Physics Setup—The interest in the Bose-Fermi Hubbard model is motivated from different areas of condensed matter and atomic physics. Studying the dressing of (interacting) fermionic atoms submerged in a superfluid Bose gas, the development of the sympathetic cooling technique to cool down spin-polarised fermions which do not interact in the s-wave channel, etc., are only a few of the experimental platforms for the rich physics it hides. On the theoretical side, the BFH model is seen as a playground for the understanding of exotic phases of matter, such as the coexistence of superfluid and checkerboard order, supersolid states, and the emergence of dressed compound particles. It is also a natural candidate for the search of supersymmetry in condensed matter.

In this section, we study the generation of interspecies entanglement, in a spinless Bose-Fermi mixture, caused by an external time-dependent drive. The Hamiltonian for the system reads

$$\begin{aligned} H(t) &= H_\mathrm{b} + H_\mathrm{f}(t) + H_\mathrm{bf}, \\ H_\mathrm{b} &= -J_\mathrm{b}\sum_j\left(b^\dagger_{j+1}b_j + \mathrm{h.c.}\right) - \frac{U_\mathrm{bb}}{2}\sum_j n^\mathrm{b}_j + \frac{U_\mathrm{bb}}{2}\sum_j n^\mathrm{b}_j n^\mathrm{b}_j, \\ H_\mathrm{f}(t) &= -J_\mathrm{f}\sum_j\left(c^\dagger_{j+1}c_j - c_{j+1}c^\dagger_j\right) + A\cos\Omega t\sum_j(-1)^j n^\mathrm{f}_j + U_\mathrm{ff}\sum_j n^\mathrm{f}_j n^\mathrm{f}_{j+1}, \\ H_\mathrm{bf} &= U_\mathrm{bf}\sum_j n^\mathrm{b}_j n^\mathrm{f}_j, \end{aligned} \tag{21}$$

where the operator $b^\dagger_j$ ($c^\dagger_j$) creates a boson (fermion) on site j, and the corresponding density is $n^\mathrm{b}_j = b^\dagger_j b_j$ ($n^\mathrm{f}_j = c^\dagger_j c_j$). The hopping matrix elements are denoted by J_b and J_f, respectively. The bosons are subject to an on-site interaction of strength U_bb, while the spin-polarised fermion-fermion interaction U_ff is effective on neighbouring sites. The bosonic and fermionic sectors are coupled through an on-site interspecies density-density interaction U_bf. We assume unit filling for the bosons and half-filling for the fermions.

The BF mixture is initially prepared in the product state $|b\rangle|f\rangle = ...$ A low-frequency periodic drive of amplitude A and frequency Ω couples to the staggered potential in the fermions sector, and pumps energy into the system. We study the growth of the entanglement $S_\mathrm{ent}(t)$ between the two species, see Fig.???

$$S_\mathrm{ent}(t) = -\mathrm{tr}_\mathrm{b}\left(\rho_\mathrm{b}(t)\log\rho_\mathrm{b}(t)\right), \quad \rho_\mathrm{b}(t) = \mathrm{tr}_\mathrm{f}|\psi(t)\rangle\langle\psi(t)|, \tag{22}$$

where tr_b (tr_f) is the trace over the boson (fermion) sector, respectively.
Code Analysis—...

3 New Horizons for QuSpin

- 2D lattices
- single-particle Hamiltonian class
- Liouville dynamics

We would much appreciate it if the users could report bugs using the issues forum in the QuSpin online repository.

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A Installation Guide in a Few Steps

QuSpin is currently only being supported for Python 2.7 and Python 3.5 and so one must make sure to install this version of Python. We recommend the use of the free package manager Anaconda which installs Python and manages its packages. For a lighter installation, one can use miniconda.

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 QuSpin is to execute the following command into the terminal:

```
$ conda install -c weinbe58 quspin
```

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 the Python packages NumPy, SciPy, and Joblib installed before installing QuSpin. 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 QuSpin is to execute the following command into the terminal:

```
> conda install -c weinbe58 quspin
```

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 QuSpin. 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 Basic Use of Command Line to Run Python

In this appendix we will review how to use the command line for Windows and OS X/Linux to navigate your computer's folders/directories and run the Python scripts.

B.1 Mac OS X/Linux

Some basic commands:

- change directory:

```
$ cd < path_to_directory >
```

- list files in current directory:

```
$ ls
```

  list files in another directory:

```
$ ls < path_to_directory >
```

- make new directory:

```
$ mkdir <path>/< directory_name >
```

- copy file:

```
$ cp < path >/< file_name > < new_path >/< new_file_name >
```

- move file or change file name:

```
$ mv < path >/< file_name > < new_path >/< new_file_name >
```

- remove file:

```
$ rm < path_to_file >/< file_name >
```

Unix also has an auto complete feature if one hits the TAB key. It will complete a word or stop when it matches more than one file/folder name. The current directory is denoted by "." and the directory above is "..". Now, to execute a Python script all one has to do is open your terminal and navigate to the directory which contains the python script. To execute the script just use the following command:

```
$ python script.py
```

It's that simple!

B.2 Windows

Some basic commands:

- change directory:

```
> cd < path_to_directory >
```

- list files in current directory:

```
> dir
```

  list files in another directory:

```
> dir < path_to_directory >
```

- make new directory:

```
> mkdir <path>\< directory_name >
```

- copy file:

```
> copy < path >\< file_name > < new_path >\< new_file_name >
```

- move file or change file name:

```
> move < path >\< file_name > < new_path >\< new_file_name >
```

- remove file:

```
> erase < path >\< file_name >
```

Windows also has a auto complete feature using the TAB key but instead of stopping when there multiple files/folders with the same name, it will complete it with the first file alphabetically. The current directory is denoted by "." and the directory above is "..".

B.3 Execute Python Script (any operating system)

To execute a Python script all one has to do is open up a terminal and navigate to the directory which contains the Python script. Python can be recognised by the extension `.py`. To execute the script just use the following command:

```
python script.py
```

It's that simple!

C Package Documentation

In QuSpin quantum many-body operators are represented as matrices. The computation of these matrices are 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++ shared library. These libraries are then easily interfaced with Python, but can run orders of magnitude faster than pure Python code [3]. The matrices are stored in a sparse matrix format using the sparse matrix library of SciPy [4]. This allows QuSpin to easily interface with mature Python packages, such as NumPy, SciPy, any many others. 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 [5, 6, 7, 4]. Moreover, we have included specific functionality in QuSpin 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. The complete up-to-date documentation for the package is available online under:

https://github.com/weinbe58/QuSpin/#quspin

D Complete Example Codes

In this appendix, we give the complete python scripts for the dix examples discussed in Sec. 2. In case the reader has trouble with the TAB spaces when copying from the code environments below, the scripts can be downloaded from github at:

https://github.com/weinbe58/QuSpin/tree/master/examples

QuSpin *Example Code* 2: The Spectrum of the Transverse Field Ising Model and the Jordan-Wigner Transformation

```
from quspin.operators import hamiltonian # Hamiltonians and operators
from quspin.basis import spin_basis_1d, fermion_basis_1d # Hilbert space spin basis
import numpy as np # generic math functions
import matplotlib.pyplot as plt # figure/plot library
#
##### define model parameters #####
L=8 # system size
J=1.0 # spin zz interaction
h=np.sqrt(2) # z magnetic field strength
#
# loop over spin inversion symmetry block variable and boundary conditions
for zblock,PBC in zip([-1,1],[1,-1]):
    #
    ##### define spin model
    # site-coupling lists (PBC for both spin inversion sectors)
    h_field=[[-h,i] for i in range(L)]
    J_zz=[[-J,i,(i+1)%L] for i in range(L)] # PBC
    # define spin static and dynamic lists
    static_spin =[["zz",J_zz],["x",h_field]] # static part of H
    dynamic_spin=[] # time-dependent part of H
    # construct spin basis in pos/neg spin inversion sector depending on APBC/PBC
    basis_spin = spin_basis_1d(L=L,zblock=zblock)
    # build spin Hamiltonians
    H_spin=hamiltonian(static_spin,dynamic_spin,basis=basis_spin,dtype=np.float64)
    # calculate spin energy levels
    E_spin=H_spin.eigvalsh()
    #
    ##### define fermion model
    # define site-coupling lists for external field
    h_pot=[[2.0*h,i] for i in range(L)]
    if PBC==1: # periodic BC: odd particle number subspace only
        # define site-coupling lists (including boudary couplings)
        J_pm=[[-J,i,(i+1)%L] for i in range(L)] # PBC
        J_mp=[[+J,i,(i+1)%L] for i in range(L)] # PBC
        J_pp=[[-J,i,(i+1)%L] for i in range(L)] # PBC
        J_mm=[[+J,i,(i+1)%L] for i in range(L)] # PBC
        # construct fermion basis in the odd particle number subsector
        basis_fermion = fermion_basis_1d(L=L,Nf=range(1,L+1,2))
    elif PBC==-1: # anti-periodic BC: even particle number subspace only
        # define bulk site coupling lists
        J_pm=[[-J,i,i+1] for i in range(L-1)]
        J_mp=[[+J,i,i+1] for i in range(L-1)]
```

```
    J_pp=[[-J,i,i+1] for i in range(L-1)]
    J_mm=[[+J,i,i+1] for i in range(L-1)]
    # add boundary coupling between sites (L-1,0)
    J_pm.append([+J,L-1,0]) # APBC
    J_mp.append([-J,L-1,0]) # APBC
    J_pp.append([+J,L-1,0]) # APBC
    J_mm.append([-J,L-1,0]) # APBC
    # construct fermion basis in the even particle number subsector
    basis_fermion = fermion_basis_1d(L=L,Nf=range(0,L+1,2))
# define fermionic static and dynamic lists
static_fermion =[["+-",J_pm],["-+",J_mp],["++",J_pp],["--",J_mm],['z',h_pot]]
dynamic_fermion=[]
# build fermionic Hamiltonian
H_fermion=hamiltonian(static_fermion,dynamic_fermion,basis=basis_fermion,
                        dtype=np.float64,check_pcon=False,check_symm=False)
# calculate fermionic energy levels
E_fermion=H_fermion.eigvalsh()
#
##### plot spectra
plt.plot(np.arange(H_fermion.Ns),E_fermion/L,marker='o'
                                ,color='b',label='fermion')
plt.plot(np.arange(H_spin.Ns),E_spin/L,marker='x'
                                ,color='r',markersize=2,label='spin')
plt.xlabel('state number',fontsize=16)
plt.ylabel('energy',fontsize=16)
plt.xticks(fontsize=16)
plt.yticks(fontsize=16)
plt.legend(fontsize=16)
plt.grid()
plt.tight_layout()
plt.show()
```

QuSpin *Example Code* 3: Free Particle Systems: the Fermionic SSH Chain

```python
from quspin.operators import hamiltonian,exp_op # Hamiltonians and operators
from quspin.basis import fermion_basis_1d # Hilbert space fermion basis
from quspin.tools.block_tools import block_diag_hamiltonian # block diagonalisation
import numpy as np # generic math functions
import matplotlib.pyplot as plt # plotting library
try: # import python 3 zip function in python 2 and pass if already using python 3
    import itertools.izip as zip
except ImportError:
    pass
##### define model parameters #####
L=100 # system size
J=1.0 # uniform hopping contribution
deltaJ=0.1 # bond dimerisation
Delta=0.5 # staggered potential
beta=100.0 # set inverse temperature for Fermi-Dirac distribution
##### construct single-particle Hamiltonian #####
# define site-coupling lists
hop_pm=[[-J-deltaJ*(-1)**i,i,(i+1)%L] for i in range(L)] # PBC
hop_mp=[[+J+deltaJ*(-1)**i,i,(i+1)%L] for i in range(L)] # PBC
stagg_pot=[[Delta*(-1)**i,i] for i in range(L)]
# define static and dynamic lists
static=[["+-",hop_pm],["-+",hop_mp],['n',stagg_pot]]
dynamic=[]
# define basis
basis=fermion_basis_1d(L,Nf=1)
# build real-space Hamiltonian
H=hamiltonian(static,dynamic,basis=basis,dtype=np.float64)
# diagonalise real-space Hamiltonian
E,V=H.eigh()
##### compute Fourier transform and momentum-space Hamiltonian #####
# define basis blocks and arguments
blocks=[dict(Nf=1,kblock=i,a=2) for i in range(L//2)] # only L//2 distinct momenta
basis_args = (L,)
# construct block-diagonal Hamiltonian
FT,Hblock = block_diag_hamiltonian(blocks,static,dynamic,fermion_basis_1d,
                        basis_args,np.complex128,get_proj_kwargs=dict(pcon=True))
# diagonalise momentum-space Hamiltonian
Eblock,Vblock=Hblock.eigh()
##### prepare the density observables and initial states #####
# grab single-particle states and treat them as initial states
psi0=Vblock
# construct operator n_1 = $n_{j=0}$
n_1_static=[['n',[[1.0,0]]]]
n_1=hamiltonian(n_1_static,[],basis=basis,dtype=np.float64,
                check_herm=False,check_pcon=False)
# construct operator n_2 = $n_{j=L/2}$
n_2_static=[['n',[[1.0,L//2]]]]
n_2=hamiltonian(n_2_static,[],basis=basis,dtype=np.float64,
                check_herm=False,check_pcon=False)
# transform n_j operators to momentum space
n_1=n_1.rotate_by(FT,generator=False)
```

```
n_2=n_2.rotate_by(FT,generator=False)
##### evaluate nonequal time correlator <FS|n_2(t) n_1(0)|FS> #####
# define time vector
t=np.linspace(0.0,90.0,901)
# calcualte state acted on by n_1
n_psi0=n_1.dot(psi0)
# construct time-evolution operator using exp_op class (sometimes faster)
U = exp_op(Hblock,a=-1j,start=t.min(),stop=t.max(),num=len(t),iterate=True)
# evolve states
psi_t=U.dot(psi0)
n_psi_t = U.dot(n_psi0)
# alternative method for time evolution using Hamiltonian class
#psi_t=Hblock.evolve(psi0,0.0,t,iterate=True)
#n_psi_t=Hblock.evolve(n_psi0,0.0,t,iterate=True)
# preallocate variable
correlators=np.zeros(t.shape+psi0.shape[1:])
# loop over the time-evolved states
for i, (psi,n_psi) in enumerate( zip(psi_t,n_psi_t) ):
    correlators[i,:]=n_2.matrix_ele(psi,n_psi,diagonal=True).real
# evaluate correlator at finite temperature
n_FD=1.0/(np.exp(beta*E)+1.0)
correlator = (n_FD*correlators).sum(axis=-1)
##### plot spectra
plt.plot(np.arange(H.Ns),E/L,
                    marker='o',color='b',label='real space')
plt.plot(np.arange(Hblock.Ns),Eblock/L,
                    marker='x',color='r',markersize=2,label='momentum space')
plt.xlabel('state number',fontsize=16)
plt.ylabel('energy',fontsize=16)
plt.xticks(fontsize=16)
plt.yticks(fontsize=16)
plt.legend(fontsize=16)
plt.grid()
plt.tight_layout()
plt.show()
##### plot correlator
plt.plot(t,correlator,linewidth=2)
plt.xlabel('$t$',fontsize=16)
plt.ylabel('$C_{0,L/2}(t,\\beta)$',fontsize=16)
plt.xticks(fontsize=16)
plt.yticks(fontsize=16)
plt.grid()
plt.tight_layout()
plt.show()
```

QuSpin *Example Code* 4: Many-Body Localisation in the Fermi-Hubbard Model

```
from __future__ import print_function, division
from quspin.operators import hamiltonian,exp_op,ops_dict # operators
from quspin.basis import tensor_basis,fermion_basis_1d # Hilbert spaces
from quspin.tools.measurements import obs_vs_time # calculating dynamics
import numpy as np # general math functions
from numpy.random import uniform,choice # tools for doing random sampling
from time import time # tool for calculating computation time
import matplotlib.pyplot as plt # plotting
#
##### setting parameters for simulation
# simulation parameters
n_real = 100 # number of realizations
n_boot = 100 # number of bootstrap samples to calculate error
# physical parameters
L = 8 # system size
N = L//2 # number of particles
N_up = N//2 + N % 2 # number of fermions with spin up
N_down = N//2 # number of fermions with spin down
w_list = [1.0,4.0,10.0] # disorder strength
J = 1.0 # hopping strength
U = 5.0 # interaction strength
# range in time to evolve system
start,stop,num=0.0,35.0,101
t = np.linspace(start,stop,num=num,endpoint=True)
#
###### create the basis
# build the two bases to tensor together to spinful fermions
basis_up = fermion_basis_1d(L,Nf=N_up) # up basis
basis_down = fermion_basis_1d(L,Nf=N_down) # down basis
basis = tensor_basis(basis_up,basis_down) # spinful fermions
#
##### create model
# define site-coupling lists
hop_right = [[-J,i,i+1] for i in range(L-1)] # hopping to the right OBC
hop_left = [[J,i,i+1] for i in range(L-1)] # hopping to the left OBC
int_list = [[U,i,i] for i in range(L)] # onsite interaction
# site-coupling list to create the sublattice imbalance observable
sublat_list = [[(-1.0)**i/N,i] for i in range(0,L)]
# create static lists
operator_list_0 = [
            ["+-|", hop_left], # up hop left
            ["-+|", hop_right], # up hop right
            ["|+-", hop_left], # down hop left
            ["|-+", hop_right], # down hop right
            ["n|n", int_list], # onsite interaction
            ]
imbalance_list = [["n|",sublat_list],["|n",sublat_list]]
# create operator dictionary for ops_dict class
# add key for Hubbard hamiltonian
operator_dict=dict(H0=operator_list_0)
# add keys for local potential in each site
```

```python
for i in range(L):
    # add to dictioanry keys h0,h1,h2,...,hL with local potential operator
    operator_dict["n"+str(i)] = [["n|",[[1.0,i]]],["|n",[[1.0,i]]]]
#
###### setting up operators
# set up hamiltonian dictionary and observable (imbalance I)
no_checks = dict(check_pcon=False,check_symm=False,check_herm=False)
H_dict = ops_dict(operator_dict,basis=basis,**no_checks)
I = hamiltonian(imbalance_list,[],basis=basis,**no_checks)
# strings which represent the initial state
s_up = "".join("1000" for i in range(N_up))
s_down = "".join("0010" for i in range(N_down))
# basis.index accepts strings and returns the index
# which corresponds to that state in the basis list
i_0 = basis.index(s_up,s_down) # find index of product state
psi_0 = np.zeros(basis.Ns) # allocate space for state
psi_0[i_0] = 1.0 # set MB state to be the given product state
print("H-space size: {:d}, initial state: |{:s}>(x)|{:s}>".format(basis.Ns,s_up,s_down))
#
# define function to do dynamics for different disorder realizations.
def real(H_dict,I,psi_0,w,t,i):
    # body of function goes below
    ti = time() # start timing function for duration of reach realisation
    # create a parameter list which specifies the onsite potential with disorder
    params_dict=dict(H0=1)
    for j in range(L):
        params_dict["n"+str(j)] = uniform(-w,w)
    # using the parameters dictionary construct a hamiltonian object with those
    # parameters defined in the list
    H = H_dict.tohamiltonian(params_dict)
    # use exp_op to get the evolution operator
    U = exp_op(H,a=-1j,start=t.min(),stop=t.max(),num=len(t),iterate=True)
    psi_t = U.dot(psi_0) # get generator psi_t for time evolved state
    # use obs_vs_time to evaluate the dynamics
    t = U.grid # extract time grid stored in U, and defined in exp_op
    obs_t = obs_vs_time(psi_t,t,dict(I=I))
    # print reporting the computation time for realization
    print("realization {}/{} completed in {:.2f} s".format(i+1,n_real,time()-ti))
    # return observable values
    return obs_t["I"]
#
###### looping over diffrent disorder strengths
for w in w_list:
    I_data = np.vstack([real(H_dict,I,psi_0,w,t,i) for i in range(n_real)])
    ##### averaging and error estimation
    I_avg = I_data.mean(axis=0) # get mean value of I for all time points
    # generate bootstrap samples
    bootstrap_gen = (I_data[choice(n_real,size=n_real)].mean(axis=0) for i in range(n_boot))
    # generate the fluctuations about the mean of I
    sq_fluc_gen = ((bootstrap-I_avg)**2 for bootstrap in bootstrap_gen)
    I_error = np.sqrt(sum(sq_fluc_gen)/n_boot)
```

```
    ##### plotting results
    plt.errorbar(t,I_avg,I_error,marker=".",label="w={:.2f}".format(w))
# configuring plots
plt.xlabel("$t/J$",fontsize=18)
plt.ylabel("$\mathcal{I}$",fontsize=18)
plt.grid(True)
plt.tick_params(labelsize=16)
plt.legend(loc=0)
plt.tight_layout()
plt.savefig('fermion_MBL.pdf', bbox_inches='tight')
plt.show()
```

QuSpin *Example Code* 5: The Bose-Hubbard Model on Translationally Invariant Ladder

```
from __future__ import print_function, division #import python 3 functions
from quspin.operators import hamiltonian # Hamiltonians and operators
from quspin.basis import boson_basis_1d # bosonic Hilbert space
from quspin.tools.block_tools import block_ops # dynamics in symmetry blocks
import numpy as np # general math functions
import matplotlib.pyplot as plt # plotting
import matplotlib.animation as animation # animating movie of dynamics
#
##### define model parameters
# initial see for random number generator
np.random.seed(0) # seed is 0 to produce plots from QuSpin2 paper
# setting up parameters of simulation
L = 6 # length of chain
N = 2*L # number of sites
nb = 0.5 # density of bosons
sps = 3 # number of states per site
J_par_1 = 1.0 # top side of ladder hopping
J_par_2 = 1.0 # bottom side of ladder hopping
J_perp =  0.5 # rung hopping
U = 20.0 # Hubbard interaction
#
##### set up Hamiltonian and observables
# define site-coupling lists
int_list_1 = [[-0.5*U,i] for i in range(N)] # interaction $-U/2 \sum_i n_i$
int_list_2 = [[0.5*U,i,i] for i in range(N)] # interaction: $U/2 \num_i n_i^2$
# setting up hopping lists
hop_list = [[-J_par_1,i,(i+2)%N] for i in range(0,N,2)] # PBC bottom leg
hop_list.extend([[-J_par_2,i,(i+2)%N] for i in range(1,N,2)]) # PBC top leg
hop_list.extend([[-J_perp,i,i+1] for i in range(0,N,2)]) # perp/rung hopping
hop_list_hc = [[J.conjugate(),i,j] for J,i,j in hop_list] # add h.c. terms
# set up static and dynamic lists
static = [
            ["+-",hop_list], # hopping
            ["-+",hop_list_hc], # hopping h.c.
            ["nn",int_list_2], # U n_i^2
            ["n",int_list_1] # -U n_i
        ]
dynamic = [] # no dynamic operators
# create block_ops object
blocks=[dict(kblock=kblock) for kblock in range(L)] # blocks to project on to
baisis_args = (N,) # boson_basis_1d manditory arguments
basis_kwargs = dict(nb=nb,sps=sps,a=2) # boson_basis_1d optional args
get_proj_kwargs = dict(pcon=True) # set projection to full particle basis
H_block = block_ops(blocks,static,dynamic,boson_basis_1d,baisis_args,np.complex128,
                    basis_kwargs=basis_kwargs,get_proj_kwargs=get_proj_kwargs)
# setting up basis for local fock basis
basis = boson_basis_1d(N,nb=nb,sps=sps)
# setting up observables
no_checks = dict(check_herm=False,check_symm=False,check_pcon=False)
n_list = [hamiltonian([["n",[[1.0,i]]]],[],basis=basis,dtype=np.float64,**no_checks)
     for i in range(N)]
```

```python
##### do time evolution
# set up initial state
i0 = np.random.randint(basis.Ns) # pick random state from basis set
psi = np.zeros(basis.Ns,dtype=np.float64)
psi[i0] = 1.0
# print info about setup
state_str = "".join(str(int((basis[i0]//basis.sps**i)%basis.sps)) for i in range(N))
print("total H-space size: {}, initial state: |{}>".format(basis.Ns,state_str))
# setting up parameters for evolution
start,stop,num = 0,30,301 # 0.1 equally spaced points
times = np.linspace(start,stop,num)
# calculating the evolved states
n_jobs = 1 # paralelisation: increase to see if calculation runs faster!
psi_t = H_block.expm(psi,a=-1j,start=start,stop=stop,num=num,block_diag=False,n_jobs=n_jobs)
# calculating the local densities as a function of time
expt_n_t = np.vstack([n.expt_value(psi_t).real for n in n_list]).T
# reshape data for plotting
n_t = np.zeros((num,2,L))
n_t[:,0,:] = expt_n_t[:,0::2]
n_t[:,1,:] = expt_n_t[:,1::2]
# calculating entanglement entropy
sub_sys_A = range(0,N,2) # bottom side of ladder
gen = (basis.ent_entropy(psi,sub_sys_A=sub_sys_A)["Sent_A"]/L for psi in psi_t.T[:])
ent_t = np.fromiter(gen,dtype=np.float64,count=num)
# plotting static figures
"""
fig, ax = plt.subplots(nrows=5,ncols=1)
im=[]
im_ind = []
for i,t in enumerate(np.logspace(-1,np.log10(stop-1),5,base=10)):
    j = times.searchsorted(t)
    im_ind.append(j)
    im.append(ax[i].imshow(n_t[j],cmap="hot",vmax=n_t.max(),vmin=0))
    ax[i].tick_params(labelbottom=False,labelleft=False)
cax = fig.add_axes([0.85, 0.1, 0.03, 0.8])
fig.colorbar(im[2],cax)
plt.savefig("boson_density.pdf")
plt.figure()
plt.plot(times,ent_t,lw=2)
plt.plot(times[im_ind],ent_t[im_ind],marker="o",linestyle="",color="red")
plt.xlabel("$t/J$",fontsize=20)
plt.ylabel("$s_\mathrm{ent}(t)$",fontsize=20)
plt.grid()
plt.savefig("boson_entropy.pdf")
plt.show()
"""
# setting up two plots to animate side by side
fig, (ax1,ax2) = plt.subplots(1,2)
fig.set_size_inches(10, 5)
ax1.set_xlabel(r"$t/J$",fontsize=18)
ax1.set_ylabel(r"$s_\mathrm{ent}$",fontsize=18)
ax1.grid()
```

```
line1, = ax1.plot(times, ent_t, lw=2)
line1.set_data([],[])
im = ax2.matshow(n_t[0],cmap="hot")
fig.colorbar(im)
def run(i): # function to update frame
    # set new data for plots
    line1.set_data(times[:i],ent_t[:i])
    im.set_data(n_t[i])
    return im, line1
ani = animation.FuncAnimation(fig, run, range(num),interval=50)
plt.show()
#
"""
#schematic of how the ladder lattice is set up coupling parameters:
# -: J_par_1
# ^: J_par_2
# |: J_perp
#
^ 1 ^ 3 ^ 5 ^ 7 ^ 9 ^
  |   |   |   |   |
- 0 - 2 - 4 - 6 - 8 -
#
# translations (i -> i+2):
#
 ^ 9 ^ 1 ^ 3 ^ 5 ^ 7 ^
   |   |   |   |   |
 - 8 - 0 - 2 - 4 - 6 -
#
# if J_par_1=J_par_2, one can use regular chain parity (i -> N - i):
#
 - 8 - 6 - 4 - 2 - 0 -
   |   |   |   |   |
 - 9 - 7 - 5 - 3 - 1 -
#
# combination of two ladder parity operators!
"""
```

QuSpin *Example Code* 6: The Gross-Pitaevskii Equation and Nonlinear Time Evolution

```python
from quspin.operators import hamiltonian # Hamiltonians and operators
from quspin.basis import boson_basis_1d # Hilbert space boson basis
from quspin.tools.measurements import evolve # nonlinear evolution
import numpy as np # generic math functions
import matplotlib.pyplot as plt # plot library
#
##### define model parameters #####
L=300 # system size
# calculate centre of chain
if L%2==0:
    j0 = L//2-0.5 # centre of chain
else:
    j0 = L//2 # centre of chain
sites=np.arange(L)-j0
# static parameters
J=1.0 # hopping
U=1.0 # Bose-Hubbard interaction strength
# dynamic parameters
kappa_trap_i=0.001 # initial chemical potential
kappa_trap_f=0.0001 # final chemical potential
t_ramp=40.0/J # set total ramp time
# ramp protocol
def ramp(t,kappa_trap_i,kappa_trap_f,t_ramp):
    return  (kappa_trap_f - kappa_trap_i)*t/t_ramp + kappa_trap_i
# ramp protocol parameters
ramp_args=[kappa_trap_i,kappa_trap_f,t_ramp]
#
##### construct single-particle Hamiltonian #####
# define site-coupling lists
hopping=[[-J,i,(i+1)%L] for i in range(L-1)]
trap=[[0.5*(i-j0)**2,i] for i in range(L)]
# define static and dynamic lists
static=[["+-",hopping],["-+",hopping]]
dynamic=[['n',trap,ramp,ramp_args]]
# define basis
basis = boson_basis_1d(L,Nb=1,sps=2)
# build Hamiltonian
Hsp=hamiltonian(static,dynamic,basis=basis,dtype=np.float64)
E,V=Hsp.eigsh(time=0.0,k=1,which='SA')
#
##### imaginary-time evolution to compute GS of GPE #####
def GPE_imag_time(tau,phi,Hsp,U):
    """
    This function solves the real-valued GPE in imaginary time:
    $$ -\dot\phi(\tau) = Hsp(t=0)\phi(\tau) + U |\phi(\tau)|^2 \phi(\tau) $$
    """
    return -( Hsp.dot(phi,time=0) + U*np.abs(phi)**2*phi )
# define ODE parameters
GPE_params = (Hsp,U)
# define initial state to flow to GS from
phi0=V[:,0]*np.sqrt(L) # initial state normalised to 1 particle per site
```

```
# define imaginary time vector
tau=np.linspace(0.0,35.0,71)
# evolve state in imaginary time
psi_tau = evolve(phi0,tau[0],tau,GPE_imag_time,f_params=GPE_params,
                            imag_time=True,real=True,iterate=True)
#
# display state evolution
for i,psi0 in enumerate(psi_tau):
    # compute energy
    E_GS=(Hsp.matrix_ele(psi0,psi0,time=0) + 0.5*U*np.sum(np.abs(psi0)**4) ).real
    # plot wave function
    plt.plot(sites, abs(phi0)**2, color='r',marker='s',alpha=0.2,
                                        label='$|\\phi_j(0)|^2$')
    plt.plot(sites, abs(psi0)**2, color='b',marker='o',
                                label='$|\\phi_j(\\tau)|^2$' )
    plt.xlabel('$\\mathrm{lattice\\ sites}$',fontsize=14)
    plt.title('$J\\tau=%0.2f,\\ E_\\mathrm{GS}(\\tau)=%0.4fJ$'%(tau[i],E_GS)
                                                            ,fontsize=14)
    plt.ylim([-0.01,max(abs(phi0)**2)+0.01])
    plt.legend(fontsize=14)
    plt.draw() # draw frame
    plt.pause(0.005) # pause frame
    plt.clf() # clear figure
plt.close()
#
##### real-time evolution of GPE #####
def GPE(time,psi):
    """
    This function solves the complex-valued time-dependent GPE:
    $$ i\dot\psi(t) = Hsp(t)\psi(t) + U |\psi(t)|^2 \psi(t) $$
    """
    # solve static part of GPE
    psi_dot = Hsp.static.dot(psi) + U*np.abs(psi)**2*psi
    # solve dynamic part of GPE
    for Hd,f,f_args in Hsp.dynamic:
        psi_dot += f(time,*f_args)*Hd.dot(psi)
    return -1j*psi_dot
# define real time vector
t=np.linspace(0.0,t_ramp,101)
# time-evolve state according to GPE
psi_t = evolve(psi0,t[0],t,GPE,iterate=True,atol=1E-12,rtol=1E-12)
#
# display state evolution
for i,psi in enumerate(psi_t):
    # compute energy
    E=(Hsp.matrix_ele(psi,psi,time=t[i]) + 0.5*U*np.sum(np.abs(psi)**4) ).real
    # compute trap
    kappa_trap=ramp(t[i],kappa_trap_i,kappa_trap_f,t_ramp)*(sites)**2
    # plot wave function
    plt.plot(sites, abs(psi0)**2, color='r',marker='s',alpha=0.2
                                ,label='$|\\psi_{\\mathrm{GS},j}|^2$')
    plt.plot(sites, abs(psi)**2, color='b',marker='o',label='$|\\psi_j(t)|^2$')
    plt.plot(sites, kappa_trap,'--',color='g',label='$\\mathrm{trap}$')
```

```
    plt.ylim([-0.01,max(abs(psi0)**2)+0.01])
    plt.xlabel('$\\mathrm{lattice\\ sites}$',fontsize=14)
    plt.title('$Jt=%0.2f,\\ E(t)-E_\\mathrm{GS}=%0.4fJ$'%(t[i],E-E_GS),fontsize=14)
    plt.legend(loc='upper right',fontsize=14)
    plt.draw() # draw frame
    plt.pause(0.00005) # pause frame
    plt.clf() # clear figure
plt.close()
```

QuSpin *Example Code* 7: Integrability Breaking and Thermalising Dynamics in the Spin-1 Transverse-Field Ising Model

```
from __future__ import print_function, division
from quspin.operators import ops_dict,hamiltonian,exp_op
from quspin.basis import spin_basis_1d # spin basis constructor
from quspin.tools.measurements import obs_vs_time # calculating dynamics
from quspin.tools.Floquet import Floquet_t_vec # period-spaced time vector
import numpy as np # general math functions
import matplotlib.pyplot as plt
#
###### define model parameters
L_12 = 18 # length of chain for spin 1/2
L_1 = 11 # length of chain for spin 1
Omega = 2.0 # drive frequency
A = 2.0 # drive amplitude
#
###### setting up bases ######
basis_12 = spin_basis_1d(L_12,S="1/2",kblock=0,pblock=1,zblock=1) # spin 1/2 basis
basis_1 = spin_basis_1d(L_1,S="1"  ,kblock=0,pblock=1,zblock=1) # spin 1 basis
# print information about the basis
print("S = {S:3s}, L = {L:2d}, Size of H-space: {Ns:d}".format(S="1/2",L=L_12,Ns=basis_12.Ns))
print("S = {S:3s}, L = {L:2d}, Size of H-space: {Ns:d}".format(S="1"  ,L=L_1,Ns=basis_1.Ns))
#
###### setting up operators in hamiltonian ######
# setting up site-coupling lists
Jzz_12 = [[-1.0,i,(i+1)%L_12] for i in range(L_12)]
hx_12  = [[-1.0,i] for i in range(L_12)]
Jzz_1 = [[-1.0,i,(i+1)%L_1] for i in range(L_1)]
hx_1  = [[-1.0,i] for i in range(L_1)]
# spin-1/2
Hzz_12 = hamiltonian([["zz",Jzz_12]],[],basis=basis_12,dtype=np.float64)
Hx_12  = hamiltonian([["+",hx_12],["-",hx_12]],[],basis=basis_12,dtype=np.float64)
# spin-1
Hzz_1 = hamiltonian([["zz",Jzz_1]],[],basis=basis_1,dtype=np.float64)
Hx_1  = hamiltonian([["+",hx_1],["-",hx_1]],[],basis=basis_1,dtype=np.float64)
#
###### calculate initial states ######
# calculating bandwidth for non-driven hamiltonian
[E_12_min],psi_12 = Hzz_12.eigsh(k=1,which="SA") #
[E_1_min],psi_1 = Hzz_1.eigsh(k=1,which="SA")
# set up the initial states
psi0_12 = psi_12.ravel()
psi0_1 = psi_1.ravel()
#
###### time evolution ######
# stroboscopic time vector
nT = 200 # number of periods to evolve to
t=Floquet_t_vec(Omega,nT,len_T=1) # t.vals=t, t.i=initial time, t.T=drive period
# creating generators of time evolution using exp_op class
U1_12 = exp_op(Hzz_12+A*Hx_12,a=-1j*t.T/4)
```

```python
U2_12 = exp_op(Hzz_12-A*Hx_12,a=-1j*t.T/2)
U1_1 = exp_op(Hzz_1+A*Hx_1,a=-1j*t.T/4)
U2_1 = exp_op(Hzz_1-A*Hx_1,a=-1j*t.T/2)
# user-defined generator for stroboscopic dynamics
def evolve_gen(psi0,nT,*U_list):
    yield psi0
    for i in range(nT): # loop over number of periods
        for U in U_list: # loop over unitaries
            psi0 = U.dot(psi0)
        yield psi0
# get generator objects for time-evolved states
psi_12_t = evolve_gen(psi0_12,nT,U2_12,U1_12,U2_12)
psi_1_t = evolve_gen(psi0_1,nT,U2_1,U1_1,U2_1)
#
###### compute expectation values of observables ######
# measure Hzz as a function of time
Obs_12_t = obs_vs_time(psi_12_t,t.vals,dict(E=Hzz_12),return_state=True)
Obs_1_t = obs_vs_time(psi_1_t,t.vals,dict(E=Hzz_1),return_state=True)
# calculating the entanglement entropy density
Sent_t_12 = basis_12.ent_entropy(Obs_12_t["psi_t"],sub_sys_A=range(L_12//2))["Sent_A"]/(L_12//2)
Sent_t_1 = basis_1.ent_entropy(Obs_1_t["psi_t"],sub_sys_A=range(L_1//2))["Sent_A"]/(L_1//2)
# calculate Page entropy density values
s_p_12 = np.log(2)-2.0**(-L_12//2-L_12)/(2*(L_12//2))
s_p_1 = np.log(3)-3.0**(-L_1//2-L_1)/(2*(L_1//2))
#
###### plotting results ######
plt.plot(t.strobo.inds,(Obs_12_t["E"]-E_12_min)/(-E_12_min),marker='.',markersize=5,label="$S=1/2$")
plt.plot(t.strobo.inds,(Obs_1_t["E"]-E_1_min)/(-E_1_min),marker='.',markersize=5,label="$S=1$")
plt.grid()
plt.ylabel("$Q(t)$",fontsize=20)
plt.xlabel("$t/T$",fontsize=20)
plt.savefig("TFIM_Q.pdf")
plt.figure()
plt.plot(t.strobo.inds,Sent_t_12/s_p_12,marker='.',markersize=5,label="$S=1/2$")
plt.plot(t.strobo.inds,Sent_t_1/s_p_1,marker='.',markersize=5,label="$S=1$")
plt.grid()
plt.ylabel("$s_{\mathrm{ent}}(t)/s_\mathrm{Page}$",fontsize=20)
plt.xlabel("$t/T$",fontsize=20)
plt.legend(loc=0,fontsize=16)
plt.savefig("TFIM_S.pdf")
plt.show()
```


References

[1] P. Weinberg and M. Bukov, *QuSpin: a Python Package for Dynamics and Exact Diagonalisation of Quantum Many Body Systems part I: spin chains*, SciPost Phys. **2**, 003 (2017),

doi:10.21468/SciPostPhys.2.1.003.

[2] A. W. Sandvik, *Computational studies of quantum spin systems*, AIP Conference Proceedings **1297**(1), 135 (2010), doi:http://dx.doi.org/10.1063/1.3518900.

[3] S. Behnel, R. Bradshaw, C. Citro, L. Dalcin, D. S. Seljebotn and K. Smith, *Cython: The best of both worlds*, Computing in Science & Engineering **13**(2), 31 (2011), doi:http://dx.doi.org/10.1109/MCSE.2010.118.

[4] E. Jones, T. Oliphant, P. Peterson *et al.*, *SciPy: Open source scientific tools for Python* (2001–).

[5] S. v. d. Walt, S. C. Colbert and G. Varoquaux, *The numpy array: A structure for efficient numerical computation*, Computing in Science & Engineering **13**(2), 22 (2011), doi:http://dx.doi.org/10.1109/MCSE.2011.37.

[6] T. E. Oliphant, *Python for scientific computing*, Computing in Science & Engineering **9**(3), 10 (2007), doi:http://dx.doi.org/10.1109/MCSE.2007.58.

[7] K. J. Millman and M. Aivazis, *Python for scientists and engineers*, Computing in Science & Engineering **13**(2), 9 (2011), doi:http://dx.doi.org/10.1109/MCSE.2011.36.