ALF Tutorial

The *ALF* (*A*lgorithms for *L*attice *F*ermions) project release ?.? tutorial

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The ALF package provides a general code for auxiliary-field Quantum Monte Carlo simulations and default analysis. In this tutorial we show how users from beginners to specialists can profit from ALF. This document is divided in two parts:

Part I. The first, introductory part of the tutorial is based on ALF's python interface – `pyALF` – which greatly simplifies using the code, making it ideal for: *obtaining benchmark* results for established models; *getting started* with QMC and ALF; or just *quickly running* a simulation.

Part II. The second part is independent of the first and aimed at more advanced users who want to simulate their own systems. It guides the user on how to modify the package's Fortran source code and presents the resources implemented to facilitate this task.

This document is intended to be self-contained, but the interested reader should check ALF's documentation, which contains a thorough, systematic description of the package's latest (development) version.

Notice that the latest stable release of ALF is ALF 2.0 – the correspondent tutorial can be found at https://git.physik.uni-wuerzburg.de/ALF/ALF_Tutorial/-/tree/master/Tutorial-ALF-2.0 .

Part I. Just run it

What follows is a collection of self-explanatory Jupyter notebooks written in Python, each centered on a detailed example followed by a few simple exercises. The notebooks printed below can be found, together with the necessary files and an increasing number of additional notebooks exploring ALF's capabilities, in the pyALF repository.

Requirements

You can download pyALF from its repository linked above or, from the command line:

```
git clone https://git.physik.uni-wuerzburg.de/ALF/pyALF.git
```

To run the notebooks you need the following installed in your machine:

- Python and packages SciPy, NumPy and matplotlib
- Jupyter
- the libraries Lapack and Blas
- a Fortran compiler, such as `gfortran` or `ifort`,

where the last two are required by the main package ALF. Also, add pyALF's path to your environment variable `PYTHONPATH`. In Linux, this can be achieved, e.g., by adding the following line to `.bashrc`:

```
export PYTHONPATH="/local/path/to/pyALF:$PYTHONPATH"
```

Python and its packages can be easily installed on a variety of platforms using the Anaconda distribution – check its installation instructions for your system. Then, from Anaconda, you can issue the command

```
conda install -c anaconda  ipython jupyterlab scipy numpy matplotlib
```

Anaconda is recommended due to its convenience, but the system's package management (e.g., apt-get) or Python's own package management, pip3, can be used instead if preferred – see, for instance, SciPy installation instructions.

A Fortran compiler and the libraries needed for ALF can be installed in a Debian-based Linux via

```
sudo apt-get install  gfortran liblapack-dev make
```

In MacOS, gfortran can be found at `https://gcc.gnu.org/wiki/GFortranBinaries#MacOS`, where detailed instructions are available. You will need to have Xcode as well as the Apple developer tools installed.

For Windows and other Linuxes and Unixes, please check the Tutorials' repository README.

Starting

Jupyter notebooks are run through a Jupyter server[1] started, e.g., from the command line:

```
jupyter notebook
```

(or, depending on the installation, `jupyter-notebook`) which opens the "notebook dashboard" in your default browser, where you can navigate through your file structure to the pyALF directory. There you will find the interface's core module, `py_alf.py`, some auxiliary files, and notebooks such as the ones included below. Have fun.

Notebooks

1. A minimal ALF run

In this bare-bones example we use the pyALF interface to run the canonical Hubbard model on a default configuration: a 6×6 square grid, with interaction strength $U = 4$ and inverse temperature $\beta = 5$.

Bellow we go through the steps for performing the simulation and outputting observables.

---

1. Import `Simulation` class from the `py_alf` python module, which provides the interface with ALF:

[1]:
```
import os
from py_alf import Simulation                # Interface with ALF
```

2. Create an instance of `Simulation`, setting parameters as desired:

[2]:
```
sim = Simulation(
    "Hubbard",                                # Hamiltonian
    {                                         # Model and simulation parameters for each Simulation instance
    "Model": "Hubbard",                       # Base model
    "Lattice_type": "Square"},                # Lattice type
    alf_dir=os.getenv('ALF_DIR', './ALF'),    # Directory with ALF source code. Gets it from
                                              # environment variable ALF_DIR, if present
)
```

[1] Note that pyALF can also be used to start a simulation from the command line, without starting a Jupyter server or using a notebook. For instance: `python3.7 Run.py -R -alfdir /home/debian/ALF-1.2/ -config "Intel" -executable_R Hubbard -mpi True` starts a parallel run of the Hubbard model, using ALF compiled with `ifort`. Notice that `Run.py` requires a configuration file `Sims`, which defines the simulation parameters. An entry of `Sims` might read as: `"Model": "Hubbard", "Lattice_type": "Square", "L1": 4, "L2": 4, "NBin": 5, "ham_T": 0.0, "Nsweep" : 2000, "Beta": 1.0, "ham_chem": -1.0`

3. Compile ALF, downloading it first from the ALF repository if not found locally. This may take a few minutes:

```
[3]: sim.compile()                                   # Compilation needs to be performed only once
```

```
Compiling ALF... Done.
```

4. Perform the simulation as specified in `sim`:

```
[4]: sim.run()                                       # Perform the actual simulation in ALF
```

```
Prepare directory "/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square"
for Monte Carlo run.
Create new directory.
Run /home/stafusa/ALF/ALF/Prog/Hubbard.out
```

5. Perform some simple analyses:

```
[5]: sim.analysis()                                  # Perform default analysis; list observables
```

```
Analysing Ener_scal
Analysing Part_scal
Analysing Pot_scal
Analysing Kin_scal
Analysing Den_eq
Analysing SpinZ_eq
Analysing Green_eq
Analysing SpinXY_eq
Analysing SpinT_eq
Analysing SpinXY_tau
Analysing SpinZ_tau
Analysing Den_tau
Analysing Green_tau
Analysing SpinT_tau
```

6. Store computed observables list:

```
[6]: obs = sim.get_obs()                             # Dictionary for the observables
```

```
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square/Kin_scalJ 1
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square/Part_scalJ 1
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square/Ener_scalJ 1
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square/Pot_scalJ 1
```

which are available for further analyses. For instance, the internal energy of the system (and its error) is accessed by:

```
[7]: obs['Ener_scalJ']['obs']
```

```
[7]: array([[-29.893866,   0.109235]])
```

---

7. Running again: The simulation can be resumed to increase the precision of the results.

```
[8]: sim.run()
     sim.analysis()
     obs2 = sim.get_obs()
     print(obs2['Ener_scalJ']['obs'])
     print("\nRunning again reduced the error from ", obs['Ener_scalJ']['obs'][0][1]," to ",␣
      ↪obs2['Ener_scalJ']['obs'][0][1], ".")
```

```
Prepare directory "/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square"
for Monte Carlo run.
Resuming previous run.
Run /home/stafusa/ALF/ALF/Prog/Hubbard.out
Analysing Ener_scal
Analysing Part_scal
Analysing Pot_scal
Analysing Kin_scal
Analysing Den_eq
Analysing SpinZ_eq
Analysing Green_eq
Analysing SpinXY_eq
Analysing SpinT_eq
Analysing SpinXY_tau
Analysing SpinZ_tau
Analysing Den_tau
Analysing Green_tau
Analysing SpinT_tau
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square/Kin_scalJ 1
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square/Part_scalJ 1
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square/Ener_scalJ 1
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square/Pot_scalJ 1
[[-29.839345   0.049995]]

Running again reduced the error from  0.109235  to  0.049995 .
```

Note: To run a fresh simulation - instead of performing a refinement over previous run(s) - the Monte Carlo run directory should be deleted before rerunning.

1.1. Exercises

1. Rerun once again and check the new improvement in precision.
2. Look at a few other observables (`sim.analysis()` outputs the names of those available).
3. Change the lattice size by adding, e.g., `"L1": 4,` and `"L2": 1,` to the simulation parameters definitions of `sim` (step 2).

2. Trotter systematic error - Hubbard on the square lattice

In this example we use the pyALF interface to run ALF with the Mz choice of Hubbard-Stratonovich transformation (i.e., coupled to the z-component of the spin) on a 6×6 site square lattice, at $U/t = 4$ half-band filling, and inverse temperature $\beta t = 5$.

We carry out a systematic $\Delta\tau t$ extrapolation keeping $\Delta\tau t L_{\text{Trotter}} = 2$ constant. Recall that the formulation of the auxiliary field QMC approach is based on the symmetric Trotter decomposition

$$e^{-\Delta\tau\left(\hat{A}+\hat{B}\right)} = e^{-\Delta\tau\hat{A}/2}e^{-\Delta\tau\hat{B}}e^{-\Delta\tau\hat{A}/2} + \mathcal{O}\left(\Delta\tau^3\right)$$

The overall error produced by this approximation is of the order $\Delta\tau^2$.

Bellow we go through the steps for performing this extrapolation: setting the simulation parameters, running it and analysing the data. A reference plot for this analyses is found in ALF documentation, Sec. 2.3.2 (Symmetric Trotter decomposition).

---

1. Import `Simulation` class from the `py_alf` python module, which provides the interface with ALF, as well as mathematics and plotting packages:

[1]:
```python
import os
from py_alf import Simulation            # Interface with ALF
#
import numpy as np                       # Numerical library
from scipy.optimize import curve_fit     # Numerical library
import matplotlib.pyplot as plt          # Plotting library
```

2. Create instances of `Simulation`, specifying the necessary parameters, in particular the different $\Delta\tau$ values:

[8]:
```python
sims = []                                # Vector of Simulation instances
print('dtau values used:')
for dtau in [0.05, 0.1, 0.2]:           # Values of dtau
    print(dtau)
    sim = Simulation(
        'Hubbard',                       # Hamiltonian
        {                                # Model and simulation parameters for each Simulation instance
        'Model': 'Hubbard',             #    Base model
        'Lattice_type': 'Square',       #    Lattice type
        'L1': 6,                        #    Lattice length in the first unit vector direction
        'L2': 6,                        #    Lattice length in the second unit vector direction
        'Checkerboard': False,          #    Whether checkerboard decomposition is used or not
        'Symm': True,                   #    Whether symmetrization takes place
        'ham_T': 1.0,                   #    Hopping parameter
        'ham_U': 4.0,                   #    Hubbard interaction
        'ham_Tperp': 0.0,               #    For bilayer systems
        'beta': 5.0,                    #    Inverse temperature
        'Ltau': 0,                      #    '1' for time-displaced Green functions; '0' otherwise
        'NSweep': 200,                  #    Number of sweeps per bin
        'NBin': 10,                     #    Number of bins
        'Dtau': dtau,                   #    Only dtau varies between simulations, Ltrot=beta/Dtau
        'Mz': True,                     #    If true, sets the M_z-Hubbard model: Nf=2, N_sum=1,
        },                              #             HS field couples to z-component of magnetization
        alf_dir=os.getenv('ALF_DIR', './ALF'), # Directory with ALF source code. Gets it from
                                               # environment variable ALF_DIR, if present
    )
    sims.append(sim)
```

```
dtau values used:
0.05
0.1
0.2
```

3. Compile ALF, downloading it first if not found locally. This may take a few minutes:

```
[3]: sims[0].compile()                       # Compilation needs to be performed only once
```

```
Compiling ALF... Done.
```

4. Perform the simulations, as specified in each element of `sim`:

```
[9]: for i, sim in enumerate(sims):
         sim.run()                           # Perform the actual simulation in ALF
```

```
Prepare directory "/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square_L1=
6_L2=6_Checkerboard=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=5.0_Dtau=0.05_Mz=
True" for Monte Carlo run.
Create new directory.
Run /home/stafusa/ALF/ALF/Prog/Hubbard.out
Prepare directory "/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square_L1=
6_L2=6_Checkerboard=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=5.0_Dtau=0.1_Mz=T
rue" for Monte Carlo run.
Create new directory.
Run /home/stafusa/ALF/ALF/Prog/Hubbard.out
Prepare directory "/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square_L1=
6_L2=6_Checkerboard=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=5.0_Dtau=0.2_Mz=T
rue" for Monte Carlo run.
Create new directory.
Run /home/stafusa/ALF/ALF/Prog/Hubbard.out
```

5. Calculate the internal energies:

```
[10]: ener = np.empty((len(sims), 2))           # Matrix for storing energy values
      dtaus = np.empty((len(sims),))            # Matrix for Dtau values, for plotting
      for i, sim in enumerate(sims):
          print(sim.sim_dir)                    # Directory containing the simulation output
          sim.analysis()                        # Perform default analysis
          dtaus[i] = sim.sim_dict['Dtau']                       # Store Dtau value
          ener[i] = sim.get_obs(['Ener_scalJ'])['Ener_scalJ']['obs']   # Store internal energy
```

```
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square_L1=6_L2=6_Checkerboard
=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=5.0_Dtau=0.05_Mz=True
Analysing Ener_scal
Analysing Part_scal
Analysing Pot_scal
Analysing Kin_scal
Analysing Den_eq
Analysing SpinZ_eq
Analysing Green_eq
Analysing SpinXY_eq
Analysing SpinT_eq
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square_L1=6_L2=6_Checkerboard
=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=5.0_Dtau=0.05_Mz=True/Ener_scalJ 1
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square_L1=6_L2=6_Checkerboard
=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=5.0_Dtau=0.1_Mz=True
Analysing Ener_scal
Analysing Part_scal
Analysing Pot_scal
Analysing Kin_scal
Analysing Den_eq
Analysing SpinZ_eq
Analysing Green_eq
Analysing SpinXY_eq
Analysing SpinT_eq
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square_L1=6_L2=6_Checkerboard
=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=5.0_Dtau=0.1_Mz=True/Ener_scalJ 1
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square_L1=6_L2=6_Checkerboard
=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=5.0_Dtau=0.2_Mz=True
Analysing Ener_scal
Analysing Part_scal
Analysing Pot_scal
Analysing Kin_scal
Analysing Den_eq
Analysing SpinZ_eq
Analysing Green_eq
Analysing SpinXY_eq
Analysing SpinT_eq
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_Square_L1=6_L2=6_Checkerboard
=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=5.0_Dtau=0.2_Mz=True/Ener_scalJ 1
```

[11]:
```
print('For Dtau values', dtaus, 'the measured energies are:\n', ener)
```

```
For Dtau values [0.05 0.1  0.2 ] the measured energies are:
 [[-29.743579   0.058593]
 [-29.76641    0.047186]
 [-29.84635    0.057173]]
```

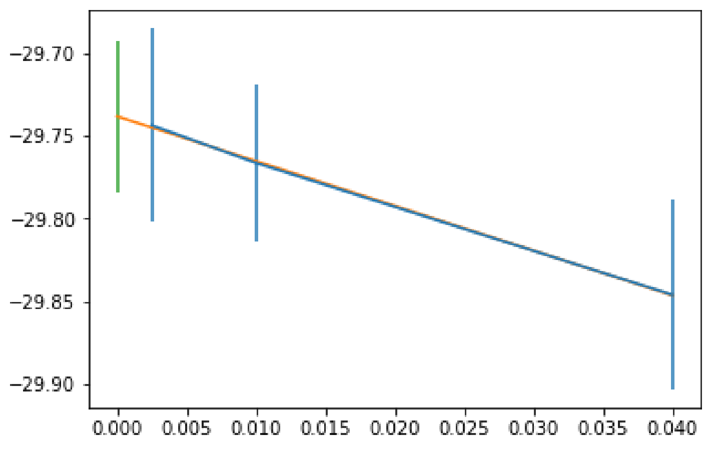
[12]:
```
plt.errorbar(dtaus**2, ener[:, 0], ener[:, 1])

def func(x, y0, a):
    return y0 + a*x**2
popt1, pcov = curve_fit(func, dtaus, ener[:, 0], sigma=ener[:, 1], absolute_sigma=True)
perr1 = np.sqrt(np.diag(pcov))
print(popt1, perr1)
xs = np.linspace(0., dtaus.max())
plt.plot(xs**2, func(xs, *popt1))

plt.errorbar(0, popt1[0], perr1[0])
```

```
[-29.73817034  -2.71266175] [0.04573724 2.02039198]
```

[12]:
```
<ErrorbarContainer object of 3 artists>
```



2.1. Exercises

1. Try out the four different combinations for `Checkerboard` and `Symm` settings in order to observe their effect on the output and run time. Reference: Sec. 2.3.2 - Symmetric Trotter decomposition - of the ALF documentation, especially Fig. 2.

3. Testing against ED - Hubbard on a ring

In this example we use the pyALF interface to run ALF with the Mz choice of Hubbard Stratonovitch transformation on a four site ring, at $U/t = 4$ and inverse temperature $\beta t = 2$. For this set of parameters, the exact internal energy reads:

$$\left\langle -t \sum_{\langle i,j\rangle,\sigma} \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + U\sum_{i=1}^{N} \hat{n}_{i,\uparrow}\hat{n}_{j,\downarrow} \right\rangle = -1.47261997t$$

To reproduce this result we will have to carry out a systematic $\Delta\tau t$ extrapolation keeping $\Delta\tau t L_{\text{Trotter}} = 2$ constant.
Recall that the formulation of the auxiliary field QMC approach is based on the Trotter decomposition

$$e^{-\Delta\tau\left(\hat{A}+\hat{B}\right)} = e^{-\Delta\tau\hat{A}/2}e^{-\Delta\tau\hat{B}}e^{-\Delta\tau\hat{A}/2} + \mathcal{O}\left(\Delta\tau^3\right)$$

The overall error produced by this approximation is of the order $\Delta\tau^2$.

Bellow we go through the steps for performing this extrapolation: setting the simulation parameters, running it and analyzing the data.

---

1. Import `Simulation` class from the `py_alf` python module, which provides the interface with ALF, as well as mathematics and plotting packages:

[1]:
```
import os
from py_alf import Simulation             # Interface with ALF
#
import numpy as np                        # Numerical library
from scipy.optimize import curve_fit      # Numerical library
import matplotlib.pyplot as plt           # Plotting library
```

2. Create instances of `Simulation`, specifying the necessary parameters, in particular the different $\Delta\tau$ values:

[19]:
```
sims = []                                 # Vector of Simulation instances
print('dtau values used:')
for dtau in [0.05, 0.1, 0.2]:            # Values of dtau
    print(dtau)
    sim = Simulation(
        'Hubbard',                        # Hamiltonian
        {                                 # Model and simulation parameters for each Simulation instance
        'Model': 'Hubbard',               #    Base model
        'Lattice_type': 'N_leg_ladder',   #    Lattice type
        'L1': 4,                          #    Lattice length in the first unit vector direction
        'L2': 1,                          #    Lattice length in the second unit vector direction
        'Checkerboard': False,            #    Whether checkerboard decomposition is used or not
        'Symm': True,                     #    Whether symmetrization takes place
        'ham_T': 1.0,                     #    Hopping parameter
        'ham_U': 4.0,                     #    Hubbard interaction
        'ham_Tperp': 0.0,                 #    For bilayer systems
        'beta': 2.0,                      #    Inverse temperature
        'Ltau': 0,                        #    '1' for time-displaced Green functions; '0' otherwise
        'NSweep': 1000,                   #    Number of sweeps per bin
        'NBin': 100,                    #    Number of bins
        'Dtau': dtau,                   #    Only dtau varies between simulations, Ltrot=beta/Dtau
        'Mz': True,                     #    If true, sets the M_z-Hubbard model: Nf=2, N_sum=1,
        },                              #             HS field couples to z-component of magnetization
        alf_dir=os.getenv('ALF_DIR', './ALF'), # Directory with ALF source code. Gets it from
                                         # environment variable ALF_DIR, if present
    )
    sims.append(sim)
```

```
dtau values used:
0.05
0.1
0.2
```

3. Compile ALF, downloading it first if not found locally. This may take a few minutes:

```
[3]: sims[0].compile()                        # Compilation needs to be performed only once
```

```
Compiling ALF... Done.
```

4. Perform the simulations, as specified in each element of `sim`:

```
[20]: for i, sim in enumerate(sims):
          sim.run()                           # Perform the actual simulation in ALF
```

```
Prepare directory "/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_N_leg_ladd
er_L1=4_L2=1_Checkerboard=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=2.0_Dtau=0.
05_Mz=True" for Monte Carlo run.
Create new directory.
Run /home/stafusa/ALF/ALF/Prog/Hubbard.out
Prepare directory "/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_N_leg_ladd
er_L1=4_L2=1_Checkerboard=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=2.0_Dtau=0.
1_Mz=True" for Monte Carlo run.
Create new directory.
Run /home/stafusa/ALF/ALF/Prog/Hubbard.out
Prepare directory "/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_N_leg_ladd
er_L1=4_L2=1_Checkerboard=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=2.0_Dtau=0.
2_Mz=True" for Monte Carlo run.
Create new directory.
Run /home/stafusa/ALF/ALF/Prog/Hubbard.out
```

5. Calculate the internal energies:

```
[21]: ener = np.empty((len(sims), 2))           # Matrix for storing energy values
      dtaus = np.empty((len(sims),))            # Matrix for Dtau values, for plotting
      for i, sim in enumerate(sims):
          print(sim.sim_dir)                    # Directory containing the simulation output
          sim.analysis()                        # Perform default analysis
          dtaus[i] = sim.sim_dict['Dtau']                     # Store Dtau value
          ener[i] = sim.get_obs(['Ener_scalJ'])['Ener_scalJ']['obs']   # Store internal energy
```

```
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_N_leg_ladder_L1=4_L2=1_Checke
rboard=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=2.0_Dtau=0.05_Mz=True
Analysing Ener_scal
Analysing Part_scal
Analysing Pot_scal
Analysing Kin_scal
Analysing Den_eq
Analysing SpinZ_eq
Analysing Green_eq
Analysing SpinXY_eq
Analysing SpinT_eq
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_N_leg_ladder_L1=4_L2=1_Checke
rboard=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=2.0_Dtau=0.05_Mz=True/Ener_sca
lJ 1
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_N_leg_ladder_L1=4_L2=1_Checke
rboard=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=2.0_Dtau=0.1_Mz=True
Analysing Ener_scal
Analysing Part_scal
Analysing Pot_scal
Analysing Kin_scal
Analysing Den_eq
Analysing SpinZ_eq
Analysing Green_eq
Analysing SpinXY_eq
Analysing SpinT_eq
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_N_leg_ladder_L1=4_L2=1_Checke
rboard=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=2.0_Dtau=0.1_Mz=True/Ener_scal
J 1
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_N_leg_ladder_L1=4_L2=1_Checke
rboard=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=2.0_Dtau=0.2_Mz=True
Analysing Ener_scal
Analysing Part_scal
Analysing Pot_scal
Analysing Kin_scal
Analysing Den_eq
Analysing SpinZ_eq
Analysing Green_eq
Analysing SpinXY_eq
Analysing SpinT_eq
/home/stafusa/ALF/pyALF/Notebooks/ALF_data/Hubbard_N_leg_ladder_L1=4_L2=1_Checke
rboard=False_Symm=True_T=1.0_U=4.0_Tperp=0.0_beta=2.0_Dtau=0.2_Mz=True/Ener_scal
J 1
```

[22]:
```
print('For Dtau values', dtaus, 'the measured energies are:\n', ener)
```

```
For Dtau values [0.05 0.1  0.2 ] the measured energies are:
 [[-1.474445  0.002606]
 [-1.477042  0.002152]
 [-1.490565  0.001943]]
```

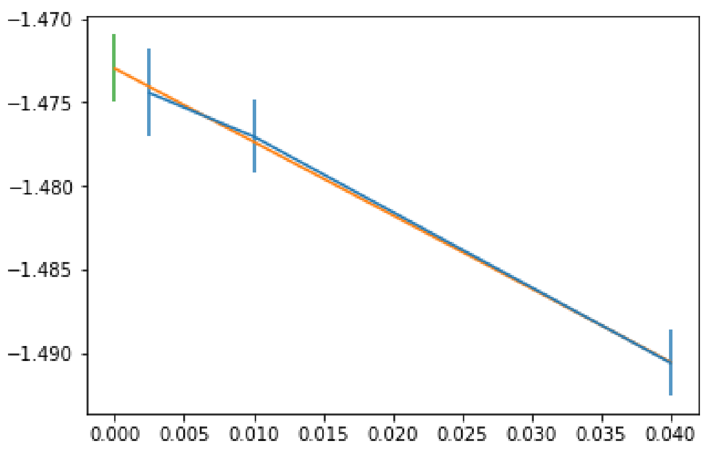
[23]:
```
plt.errorbar(dtaus**2, ener[:, 0], ener[:, 1])

def func(x, y0, a):
    return y0 + a*x**2
popt1, pcov = curve_fit(func, dtaus, ener[:, 0], sigma=ener[:, 1], absolute_sigma=True)
perr1 = np.sqrt(np.diag(pcov))
print(popt1, perr1)
xs = np.linspace(0., dtaus.max())
plt.plot(xs**2, func(xs, *popt1))

plt.errorbar(0, popt1[0], perr1[0])
```

```
[-1.47297574 -0.43843489] [0.00203182 0.07621841]
```

[23]:
```
<ErrorbarContainer object of 3 artists>
```



3.1. Exercises

1. Redo the extrapolation for different values of βt (e.g., for $\beta t = 1$, the internal energy is -0.62186692t, and for $\beta t = 4$, it is -1.90837196t).
2. Experiment with different settings for `Checkerboard` and `Symm`.

4. Projective algorithm

In this example we use the pyALF interface to run ALF's projective algorithm with the Mz choice of Hubbard Stratonovich transformation on a 4-site ring.

The projective approach is the method of choice if one is interested in ground-state properties. The starting point is a pair of trial wave functions, $|\Psi_{T,L/R}\rangle$, that are not orthogonal to the ground state $|\Psi_0\rangle$:

$$\langle\Psi_{T,L/R}|\Psi_0\rangle \neq 0.$$

The ground-state expectation value of any observable $\hat{O}$ can then be computed by propagation along the imaginary time axis:

$$\frac{\langle\Psi_0|\hat{O}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} = \lim_{\theta\to\infty} \frac{\langle\Psi_{T,L}|e^{-\theta\hat{H}}e^{-(\beta-\tau)\hat{H}}\hat{O}e^{-\tau\hat{H}}e^{-\theta\hat{H}}|\Psi_{T,R}\rangle}{\langle\Psi_{T,L}|e^{-(2\theta+\beta)\hat{H}}|\Psi_{T,R}\rangle},$$

where β defines the imaginary time range where observables (time displaced and equal time) are measured and τ varies from 0 to β in the calculation of time-displace observables. For further details, see Sec. 3 of ALF documentation.

---

1. Import `Simulation` class from the `py_alf` python module, which provides the interface with ALF, as well as numerical and plotting packages:

[1]:
```
from py_alf import Simulation              # Interface with ALF
#
import numpy as np                         # Numerical library
from scipy.optimize import curve_fit       # Numerical library
import matplotlib.pyplot as plt            # Plotting library
```

2. Create instances of `Simulation`, specifying the necessary parameters, in particular the `Projector` to `True`:

[2]:
```
sims = []                                  # Vector of Simulation instances
print('Theta values used:')
for theta in [5, 10, 20]:                  # Values of Theta
    print(theta)
    sim = Simulation(
        'Hubbard',                         # Hamiltonian
        {                                  # Model and simulation parameters for each Simulation instance
        'Model': 'Hubbard',                #    Base model
        'Lattice_type': 'N_leg_ladder',    #    Lattice type
        'L1': 4,                           #    Lattice length in the first unit vector direction
        'L2': 1,                           #    Lattice length in the second unit vector direction
        'Checkerboard': False,             #    Whether checkerboard decomposition is used or not
        'Symm': True,                      #    Whether symmetrization takes place
        'Projector': True,                 #    Whether to use the projective algorithm
        'Theta': theta,                    #    Projector parameter
        'ham_T': 1.0,                      #    Hopping parameter
        'ham_U': 4.0,                      #    Hubbard interaction
        'ham_Tperp': 0.0,                  #    For bilayer systems
        'beta': 1.0,                       #    Inverse temperature
        'Ltau': 0,                         #    '1' for time-displaced Green functions; '0' otherwise
        'NSweep': 400,                     #    Number of sweeps
        'NBin': 10,                        #    Number of bins
        'Dtau': 0.05,                      #    Only dtau varies between simulations, Ltrot=beta/Dtau
        'Mz': True,                        #    If true, sets the M_z-Hubbard model: Nf=2, N_sum=1,
        },                                 #             HS field couples to z-component of magnetization
        alf_dir='~/Programs/ALF',          # Local ALF copy, if present
    )
    sims.append(sim)
```

```
Theta values used:
5
10
20
```

3. Compile ALF, downloading it first if not found locally. This may take a few minutes:

[3]:
```
sims[0].compile()                        # Compilation needs to be performed only once
```

```
Compiling ALF... Done.
```

4. Perform the simulations, as specified in each element of `sim`:

[4]:
```
for i, sim in enumerate(sims):
    sim.run()                            # Perform the actual simulation in ALF
```

```
Prepare directory "/home/stafusa/ALF/pyALF/Hubbard_N_leg_ladder_L1=4_L2=1_Checke
rboard=False_Symm=True_Projector=True_Theta=5_T=1.0_U=4.0_Tperp=0.0_beta=1.0_Dta
u=0.05_Mz=True" for Monte Carlo run.
Create new directory.
Run /home/stafusa/Programs/ALF/Prog/Hubbard.out
Prepare directory "/home/stafusa/ALF/pyALF/Hubbard_N_leg_ladder_L1=4_L2=1_Checke
rboard=False_Symm=True_Projector=True_Theta=10_T=1.0_U=4.0_Tperp=0.0_beta=1.0_Dt
au=0.05_Mz=True" for Monte Carlo run.
Create new directory.
Run /home/stafusa/Programs/ALF/Prog/Hubbard.out
Prepare directory "/home/stafusa/ALF/pyALF/Hubbard_N_leg_ladder_L1=4_L2=1_Checke
rboard=False_Symm=True_Projector=True_Theta=20_T=1.0_U=4.0_Tperp=0.0_beta=1.0_Dt
au=0.05_Mz=True" for Monte Carlo run.
Create new directory.
Run /home/stafusa/Programs/ALF/Prog/Hubbard.out
```

5. Calculate the internal energies:

[6]:
```
%%capture
ener = np.empty((len(sims), 2))          # Matrix for storing energy values
thetas = np.empty((len(sims),))          # Matrix for Thetas values, for plotting
for i, sim in enumerate(sims):
    print(sim.sim_dir)                   # Directory containing the simulation output
    sim.analysis()                       # Perform default analysis
    thetas[i] = sim.sim_dict['Theta']                       # Store Theta value
    ener[i] = sim.get_obs(['Ener_scalJ'])['Ener_scalJ']['obs']  # Store internal energy
```

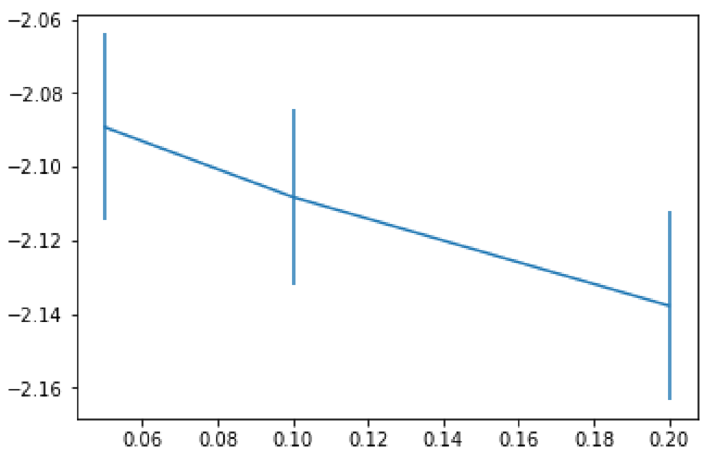
Where the *cell magic* `%%capture` suppresses the output of `sim.analysis()`, which lists the data directories and observables.

[7]:
```
print('For Theta values', thetas, 'the measured energies are:\n', ener)
```

```
For Theta values [ 5. 10. 20.] the measured energies are:
 [[-2.137697  0.025552]
 [-2.108235  0.023964]
 [-2.089294  0.025426]]
```

[8]:
```
plt.errorbar(1/thetas, ener[:, 0], ener[:, 1])
```

[8]:
```
<ErrorbarContainer object of 3 artists>
```



4.1. Exercises

1. A ladder system consists of chains assembled one next to the other, for instance, setting `L1=14`, `L2=3` defines a 3-leg ladder. It is a well-known result [Dagotto and Rice, *Science* 271 (1996), **5249**, pp. 618] that spin correlations in ladder systems decay as power laws (apart from logarithmic corrections) for odd-leg ladders, and exponentially for even-leg ladders. The paper presents numerical results for the Heisenberg model. How do these correlations behave for the Hubbard model at half-filling?

Part II. Getting your hands dirty - writing new code

A lot already comes implemented in ALF, but unavoidably, as one proceeds in their own investigations, a new model has to be implemented or a new observable defined – and for that, one must grapple with the package's Fortran source code. This second part of the tutorial consists in a set of guided exercises that exemplify how to make basic additions to the code, taking as starting point the template-like, relatively self-contained module `Hamiltonian_Hubbard_Plain_Vanilla_mod.F90`, which is also a good display of ALF's internal workings.

These worked-out exercises, together with ALF's modularity, boosted by its Predefined Structures, should make getting your hands dirty less daunting than it may sound.

Downloading and using the code and tutorial

One can use the ALF package downloaded automatically by the Python script in the first part of this tutorial, or manually, by typing

```
git clone https://git.physik.uni-wuerzburg.de/ALF/ALF.git
```

in a shell. Similarly, to download the tutorial, including solutions, enter:

```
git clone https://git.physik.uni-wuerzburg.de/ALF/ALF_Tutorial.git
```

The necessary environment variables and the directives for compiling the code are set by the script `configure.sh`: `source configure.sh GNU`, followed by the command `make`. Details and further options are described in the package's documentation found in its repository.

A workflow you can adopt for solving the exercises – or indeed using ALF in general – is the following:

1. Compile the modified Hamiltonian module, for instance:
   `make Hubbard_Plain_Vanilla`
2. Create a data directory with the content of `Start`:
   `cp -r ./Start ./Run && cd ./Run/`
3. Run its executable, e.g., serially:
   `$ALF_DIR/Prog/Hubbard_Plain_Vanilla.out`
4. Perform default analyses[2]:
   `$ALF_DIR/Analysis/ana.out *`

The structure of the data files and details on the analysis output can be found in ALF's documentation.

Exercise 1 – Dimensional crossover

Here we will modify the code so as to allow for different hopping matrix elements along the x and y directions of a square lattice.

1a) Modifying the hopping

To do so we start from the module `Hamiltonian_Hubbard_Plain_Vanilla_mod.F90`, which we here shorten to "`Vanilla`", found in `$ALF_DIR/Prog/Hamiltonians/`, proceeding as follows:

- Add `Ham_Ty` to the `VAR_Hubbard_Plain_Vanilla` name space in the parameter file `parameters`.
- Declare a new variable, `Ham_Ty`, in the module's specification (just search for the declaration of `Ham_T` in `Vanilla`).

[2]The `analysis.sh` bash script from earlier versions of ALF, run without arguments, is still available in the `Start` directory.

- Add `Ham_Ty` to the `VAR_Hubbard_Plain_Vanilla` name space (`namelist`) declaration at the `Ham_Set` subroutine of `Vanilla`.
- Modify the hopping matrix in the subroutine `Ham_Hop` in `Vanilla`:

```
 Do I = 1,Latt%N
   Ix = Latt%nnlist(I,1,0)
   Op_T(1,nf)%O(I,  Ix) = cmplx(-Ham_T,    0.d0, kind(0.D0))
   Op_T(1,nf)%O(Ix, I ) = cmplx(-Ham_T,    0.d0, kind(0.D0))
   If ( L2 > 1 ) then
      Iy = Latt%nnlist(I,0,1)
!!!!!!! Modifications for Exercise 1a
      !Op_T(1,nf)%O(I,  Iy) = cmplx(-Ham_T,    0.d0, kind(0.D0))
      !Op_T(1,nf)%O(Iy, I ) = cmplx(-Ham_T,    0.d0, kind(0.D0))
      Op_T(1,nf)%O(I,  Iy) = cmplx(-Ham_Ty,    0.d0, kind(0.D0))
      Op_T(1,nf)%O(Iy, I ) = cmplx(-Ham_Ty,    0.d0, kind(0.D0))
!!!!!!!
   endif
   Op_T(1,nf)%O(I,  I ) = cmplx(-Ham_chem, 0.d0, kind(0.D0))
   Op_T(1,nf)%P(i) = i
Enddo
```

Note: If you'd like to run the simulation using MPI, you should also add the broadcasting call for `Ham_Ty` to `Ham_Set`. It is a good idea as well to get the new simulation parameter written into the file `info`, also a change in `Ham_Set`.

In the directory `Solutions/Exercise_1` we have duplicated ALF's code and commented the changes that have to be carried out to the file `Hamiltonian_Hubbard_Plain_Vanilla_mod.F90`, found in the `Prog/Hamiltonians` directory. The solution directory also includes the modified and original modules, as well as reference data and the necessary `Start` directory (remember to copy its contents to every new `Run` directory, and to have a different `Run` directory for each simulation).

As an application of this code, we can once again consider a ladder system (e.g, a 2-leg ladder with `L1=14` and `L2=2`), for different values of `Ham_Ty`. The results you should obtain for the total spin correlation function (file `SpinT_eqJR`) are summarized in Fig. 1.

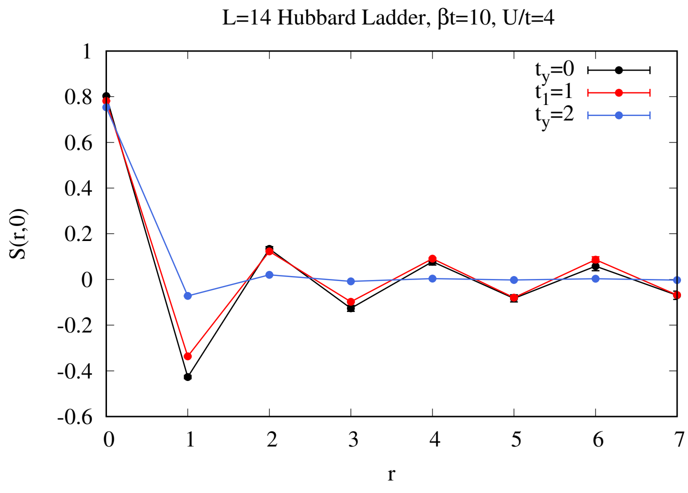


Figure 1: Spin correlation functions along one leg for the Hubbard ladder. As t_y grows the spin gap becomes large enough so as to detect the exponential decal of the spin correlation function on this small lattice size. The underlying physics of odd-even ladder systems is introduced in the article: Elbio Dagotto and T. M. Rice, Surprises on the way from one- to two-dimensional quantum magnets: The ladder materials, Science 271 (1996), no. 5249, 618–623.

1b) The SU(2) Hubbard-Stratonovich transformation

The SU(2) Hubbard-Stratonovich decomposition couples to the density and conserves spin rotational symmetry. Introduce into the module `Hamiltonian_Hubbard_mod.F90` and into the name space `VAR_Hubbard` the same changes done to the `Vanilla` module, described in the previous item, and enter `Mz=.F.` in the `parameters` file (in order to choose the $SU(N)$ Hubbard interaction) and compare results to those of the M_z decomposition above – especially with regard to numerical convergence.

Exercise 2 – Defining a new model: The one-dimensional t-V model

In this section, we will show what modifications have to be carried out for computing the physics of the one dimensional t-V model of spinless fermions.

$$\hat{H} = -t\sum_i \left(\hat{c}_i^\dagger \hat{c}_{i+a} + \hat{c}_{i+a}^\dagger \hat{c}_i\right) - \frac{V}{2}\sum_i \left(\hat{c}_i^\dagger \hat{c}_{i+a} + \hat{c}_{i+a}^\dagger \hat{c}_i\right)^2 . \tag{1}$$

The above form is readily included in the ALF since the interaction is written in terms of a perfect square. Expanding the square yields (up to a constant) the desired model:

$$\hat{H} = -t\sum_i \left(\hat{c}_i^\dagger \hat{c}_{i+a} + \hat{c}_{i+a}^\dagger \hat{c}_i\right) + V\sum_i \left(\hat{n}_i - 1/2\right)\left(\hat{n}_{i+a} - 1/2\right). \tag{2}$$

Note that the t-V model is already implemented in ALF in the module `Hamiltonian_tV_mod.F90` found in `Prog/Hamiltonians/`. While it can be used for checking your own results[3], you are not supposed to reproduce that implementation – which is more general and makes use of predefined structures – but instead to write a simpler one, based on the module `Hamiltonian_Hubbard_Plain_Vanilla_mod.F90` as detailed below.

2a) Define new model

In the directory `$ALF_DIR/Solutions/Exercise_2` we have duplicated the ALF and commented the changes that have to be carried out to the file `Hamiltonian_Hubbard_Plain_Vanilla_mod.F90`, which we here shorten to "`Vanilla`", found in `$ALF_DIR/Prog/Hamiltonians/`. The following are the essential steps to be carried out:

- Add the `VAR_t_V` name space in the file `parameters` and set the necessary variables – or simply rename the `VAR_Hubbard_Plain_Vanilla` name space to `VAR_t_V` and, within it, `Ham_U` to `Ham_Vint`. (Ignore the name space `VAR_tV`, which is used by the general implementation mentioned above.)
- Declare a new variable, `Ham_Vint`, in `Vanilla`'s specification.
- Add the `VAR_t_V` name space (`namelist`) declaration at the `Ham_Set` subroutine of `Vanilla`, containing the same variables the name space contains in `parameters`, and read it in.
- Still in the `Ham_set` subroutine of `Vanilla`: set `NF=1`, since we are working with spinless fermions; change the MPI broadcast call for `Ham_U` to broadcast `Ham_Vint` instead; and change similarly the output to the info file.
- In the `Ham_V` subroutine you have to add the new interaction. For a given bond at a given time slice, we need to decouple the interaction:

  $$e^{\Delta\tau\frac{V}{2}\left(\hat{c}_i^\dagger\hat{c}_{i+a}+\hat{c}_{i+a}^\dagger\hat{c}_i\right)^2} = \sum_{l=\pm1,\pm2}\gamma_l e^{\sqrt{\Delta\tau\frac{V}{2}}\eta_l\left(\hat{c}_i^\dagger\hat{c}_{i+a}+\hat{c}_{i+a}^\dagger\hat{c}_i\right)} = \sum_{l=\pm1,\pm2}\gamma_l e^{g\eta_l\left(\hat{c}_i^\dagger,\hat{c}_{i+a}^\dagger\right)O\left(\hat{c}_i,\hat{c}_{i+a}\right)^T} . \tag{3}$$

  Here is how this translates in the code (the new integer variable, `i2`, should be declared):

[3]A short simulation of the t-V model can be conveniently run using its Jupyter notebook available in pyALF.

```
Allocate(Op_V(Ndim,N_FL))
do nf = 1,N_FL
   do i  =  1, Ndim
      call Op_make(Op_V(i,nf),2)
   enddo
enddo
Do i = 1, Ndim  ! Runs over bonds = # of lattice sites in one-dimension.
   i2                 = Latt%nnlist(i,1,0)
   Op_V(i,nf)%P(1)    = i
   Op_V(i,nf)%P(2)    = i2
   Op_V(i,nf)%O(1,2) = cmplx(1.d0 ,0.d0, kind(0.d0))
   Op_V(i,nf)%O(2,1) = cmplx(1.d0 ,0.d0, kind(0.d0))
   Op_V(i,nf)%g       = sqrt(cmplx(Dtau*Ham_Vint/2.d0, 0.d0, kind(0.d0)))
   Op_V(i,nf)%alpha  = cmplx(0d0  ,0.d0, kind(0.d0))
   Op_V(i,nf)%type    = 2
   Call Op_set( Op_V(i,nf) )
enddo
```

- Finally, you have to update the `Obser` and `ObserT` routines for the calculation of equal- and time-displaced correlations. For the `t_V` model you can essentially use the same observables as for the `Hubbard_SU(2)` model in 1D – a step which requires a number of changes with respect to the `Vanilla` base, such as:

```
!!!!! Modifications for Exercise 2
!Zpot = Zpot*ham_U                         ! Vanilla
Zpot = Zpot*Ham_Vint                       ! t-V
!!!!!
```

  and

```
!Zrho = Zrho + Grc(i,i,1) +  Grc(i,i,2)  ! Vanilla
Zrho = Zrho + Grc(i,i,1)                  ! t-V
```

  with the observables being coded in the routine `Obser` as

```
Z = cmplx(dble(N_SUN), 0.d0, kind(0.D0))
Do I1 = 1,Ndim
   I = I1
   no_I = 1
   Do J1 = 1,Ndim
      J = J1
      no_J = 1
      imj = latt%imj(I,J)
      Obs_eq(1)%Obs_Latt(imj,1,no_I,no_J) =  Obs_eq(1)%Obs_Latt(imj,1,no_I,no_J) + &
      &                Z * GRC(I1,J1,1) * ZP*ZS  ! Green
      Obs_eq(2)%Obs_Latt(imj,1,no_I,no_J) =  Obs_eq(2)%Obs_Latt(imj,1,no_I,no_J) + &
      &                Z * GRC(I1,J1,1) * GR(I1,J1,1) * ZP*ZS  ! SpinZ
      Obs_eq(3)%Obs_Latt(imj,1,no_I,no_J) =  Obs_eq(3)%Obs_Latt(imj,1,no_I,no_J) + &
      &                ( GRC(I1,I1,1) * GRC(J1,J1,1) * Z + &
      &                  GRC(I1,J1,1) * GR(I1,J1,1 )       ) * Z * ZP*ZS  ! Den
   enddo
   Obs_eq(3)%Obs_Latt0(no_I) =  Obs_eq(3)%Obs_Latt0(no_I) + Z * GRC(I1,I1,1) * ZP * ZS
enddo
```

  among other changes - with similar ones in the `ObserT` routine.

  All necessary changes are implemented and clearly indicated in the solution provided in `Solutions/Exercise_2/Hamiltonian_Hubbard_Plain_Vanilla_mod-Exercise_2.F90`.

In the directory `Solutions/Exercise_2` we have duplicated ALF's code and commented the changes that have to be carried out to the file `Hamiltonian_Hubbard_Plain_Vanilla_mod.F90` in the `Prog/Hamiltonians` directory. The solution directory also includes reference data and the necessary

`Start` directory (remember to copy its contents to every new `Run` directory, and to have a different `Run` directory for each simulation).

You can now run the code for various values of V/t. A Jordan-Wigner transformation will map the `t_V` model onto the XXZ chain:

$$\hat{H} = J_{xx} \sum_i \hat{S}^x_i \hat{S}^x_{i+a} + \hat{S}^y_i \hat{S}^y_{i+a} + J_{zz} \sum_i \hat{S}^z_i \hat{S}^z_{i+a} \quad , \tag{4}$$

with $J_{zz} = V$ and $J_{xx} = 2t$. Hence, when $V/t = 2$ we reproduce the Heisenberg model. For $V/t > 2$ the model is in the Ising regime with long-range charge density wave order and is an insulator. In the regime $-2 < V/t < 2$ the model is metallic and corresponds to a Luttinger liquid. Finally, at $V/t < -2$ phase separation between hole rich and electron rich phases occur. Fig. 2 shows typical results for the density-density correlation function (file `Den_eqJR`).

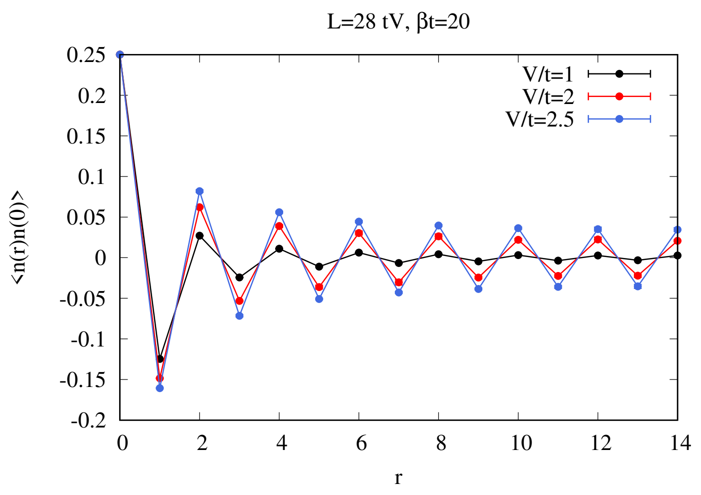


Figure 2: Density-Density correlation functions of the t-V model. In the Luttinger liquid phase, $-2 < V/t < 2$, it is known that the density-density correlations decay as $\langle n(r)n(0)\rangle \propto \cos(\pi r) r^{-(1+K_\rho)}$ with $(1+K_\rho)^{-1} = \frac{1}{2} + \frac{1}{\pi}\arcsin\left(\frac{V}{2|t|}\right)$ (A. Luther and I. Peschel, Calculation of critical exponents in two dimensions from quantum field theory in one dimension, Phys. Rev. B 12 (1975), 3908.) The interested reader can try to reproduce this result.

Exercise 3 – Adding a new observable

This exercise illustrates the modifications that are required to implement a new observable, the correlation function of the bond-hopping in the 1-dimensional Hubbard chain. This observable is interesting in many different setups. For example, the model studied here exhibits an emergent $SO(4)$ symmetry that relates the anti-ferromagnetic order parameter and the bond dimerization (I. Affleck, PRL 55, 1355 (1985); I. Affleck and F. D. M. Haldane, PRB 36, 5291 (1987)). Another example where this quantity is useful to investigate is the 1-dimensional Su-Schrieffer-Heger model describing an electron-phonon system.

3a) Applying Wick's theorem

Here the task is to define a new equal-time observable, the kinetic energy correlation, given by

$$\left\langle \hat{O}_{i,\delta} \hat{O}_{j,\delta'} \right\rangle - \left\langle \hat{O}_{i,\delta} \right\rangle \left\langle \hat{O}_{j,\delta'} \right\rangle = S_O\left(i-j, \delta, \delta'\right) \tag{5}$$

where i, j refer to the unit cells and δ encodes the bond label. Since we are working in 1D, there is only one bond per unit cell and $\delta = ax$ such that

$$\hat{O}_{i,x} = \sum_\sigma \left(\hat{c}^\dagger_{i,\sigma} \hat{c}_{i+ax,\sigma} + H.c. \right) . \tag{6}$$

Note that the first term of Eq. 5 is of the generic form $\sum_{\sigma,\sigma'} \left\langle \hat{c}^{\dagger}_{i_1,\sigma}\hat{c}_{i_2,\sigma}\hat{c}^{\dagger}_{j_1,\sigma'}\hat{c}_{j_2,\sigma'} \right\rangle$. This expectation value can be readily decomposed into single-particle Green functions by using Wick's theorem. It can be applied for a fixed field configuration Φ since the Hamiltonian $\hat{H}(\Phi)$ is then bi-linear in the fermion operators.

$$\sum_{\sigma,\sigma'} \left\langle \hat{c}^{\dagger}_{i_1,\sigma}\hat{c}_{i_2,\sigma}\hat{c}^{\dagger}_{j_1,\sigma'}\hat{c}_{j_2,\sigma'} \right\rangle_{\Phi} = \sum_{\sigma,\sigma'} \left(\left\langle \hat{c}^{\dagger}_{i_1,\sigma}\hat{c}_{i_2,\sigma} \right\rangle_{\Phi} \left\langle \hat{c}^{\dagger}_{j_1,\sigma'}\hat{c}_{j_2,\sigma'} \right\rangle_{\Phi} + \left\langle \hat{c}^{\dagger}_{i_1,\sigma}\hat{c}_{j_2,\sigma'} \right\rangle_{\Phi} \left\langle \hat{c}_{i_2,\sigma}\hat{c}^{\dagger}_{j_1,\sigma'} \right\rangle_{\Phi} \right) \quad (7)$$

The second term of vanishes for $\sigma \neq \sigma'$ due to flavor symmetry (Mz-decoupling used here in the vanilla version) or due to the $SU(2)$ symmetry (density decoupling available in the generic implementation of Hubbard model). The single-particle Green functions are provided in the `Obser` routine, where all equal-time observables are measured, as

$$GRC(i,j,\sigma) = \left\langle \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} \right\rangle_{\Phi} \quad (8)$$

$$GR(i,j,\sigma) = \left\langle \hat{c}_{i,\sigma}\hat{c}^{\dagger}_{j,\sigma} \right\rangle_{\Phi} . \quad (9)$$

3b) Necessary code modifications

In the directory `$ALF_DIR/Solutions/Exercise_3` we have duplicated the ALF and commented the changes that have to be carried out to the file `Hamiltonian_Hubbard_Plain_Vanilla_mod.F90` found in `$ALF_DIR/Prog/Hamiltonians/`, which we here shorten to "`Vanilla`". The following are the essential steps to be carried out:

- Introduce the new observable and allocate the memory required to store the measurements. This is done in the subroutine `Alloc_obs(Ltau)` by increasing the length of the array `Obs_eq` appropriately and adding a new case to specify the filename in which the results are stored on disc. (You might want to revisit this section later on to add the time-displaced version of the correlation function by changing `Obs_tau` in the same fashion.)
- The actual measurements are taken in the subroutine `Obser(GR,Phase,Ntau)`. While `GR` is passed to the subroutine, the first lines of code already implement the construct `GRC` $= 1 -$ `GR`^{T}. (This section does not have to be modified, but it is useful to keep this in mind for future reference when you implement a new model from scratch.)
- The measurement of an equal-time correlation function consists of two separate parts: the connected one given by the first term in Eq. 5, and the background, given by the second term.
- Implement the measurement of the connected part, stored as `Obs_eq`(6) in this example, using the Wick decomposition sketched above.
- Keep in mind that the background $\sum_i \left\langle \hat{O}_{i,\delta} \right\rangle \neq 0$ is non-vanishing and has to be measured separately (you can compare with the density correlation function), and is stored in `Obs_eq`(6)%`Obs_Latt0`(1).
- The analysis tool will then automatically combine both contributions and evaluate Eq. 5 using the jackknife method to estimate the mean and error or the correlation function.

The 1-D Hubbard exhibits an emergent $SO(4)$ symmetry:

$$\langle \bar{S}(r)S(0) \rangle \sim \frac{(-1)^r}{r} \ln^d(r) \quad (10)$$

$$\left\langle \hat{O}_{r,x}\hat{O}_{0,x} \right\rangle - \left\langle \hat{O}_{r,x} \right\rangle \left\langle \hat{O}_{0,x} \right\rangle \sim \frac{(-1)^r}{r} \ln^{\beta}(r) \quad (11)$$

where $d = 1/2$ and $\beta = -3/2$ (T. Sato, M. Hohenadler, et.al, ArXiv:2005.08996 (2020)) and this exercise provides all the tools required to study it. Beware of the large system sizes, and therefore long run times, that are required to extract the logarithmic scaling corrections. More details are discussed in the appendix of above reference (ArXiv:2005.08996).

Finally, it is straightforward to implement the time-displaced version of this correlation function, following essentially the same steps as described above. The observable is now stored in `Obs_tau`, the measurements are taken in `ObserT`, and you can find the implementation in the solution to this exercise as well.