Deckblatt

Contents

1 What changed regarding our first submission

1.1 Variables

We changed/deleted all our old variables depending on other parameters to be now only defined by dimensionless values, without changing their value in regards to our first submission. In our case of modularity where we work with the same variables in multiple python files it is also practical to add an extra python file for storing our constant variables (and some basic functions used in multiple other files). We can then import these global variables by "from variables import *".
This change worked with all the prior functions and tests except for testing the integrators in dependence of M or rather τ. We had to add an additional input for τ into the integrators (and therefore the tests) so that the dependence could be evaluated without having to define the integrators in the same file as the tests.

1.2 Modularity

As mentioned above, we improved our file management by implementing a modularity of files, dividing our prior one python file into now seven (and more for the second sub-project). The content of these modules did not change if not stated otherwise (variables, tests, convergence). The new file system is listed below:
- "variables.py": defining variables and few general functions
- "hamiltonian.py": defining potential and hamiltonian
- "test_hamiltonian.py": defining the tests for the hamiltonian and also running them for multiple N and dimensions
- "integrators.py": defining both the integrators

- "test_integrators.py": defining the tests for the integrators and also running them for multiple N and dimensions
- "test_integr_converg.py": testing the dependence of the integrators on M or rather τ
- "animation.py": defining functions for animation and animating

1.3 Tests

The tests we included in the sub-project 1 were in general not modified for this revision. We now ran these tests of the hamiltonian and integrators for multiple dimensions and N for proper testing. Here we take focus on $N = 5$, 10, 15 and 20; because the relevance of boundary conditions and resulting errors decrease for large N. The exact output for running the testing files is shown in the following figures for each of the N for 4 dimensions (hamiltonian) and 3 dimensions (integrators, due to long run-time). The tests are including "randomly" generated arrays, therefore we do these tests 10 times each and the maximum error (depending on the criteria) of each test is saved. Also notice that the output shows N as a float, it is an integer nonetheless.

```
Testing linearity of the hamiltonian 10 times. Maximum error:
    N                    1D                    2D                    3D                    4D
 5.0    3.03543989777123e-14   2.382173337059642e-13  6.844854043943255e-13   1.368970808788651e-12
10.0   2.842170943040401e-14  2.3437142008433856e-13  5.084229945850415e-13   1.850687635408088e-12
15.0  2.8916994303251375e-14   2.428351918216984e-13  6.844854043943255e-13  1.8225386545374702e-12
20.0   2.842170943040401e-14    2.31335954426011e-13   6.87429441225494e-13  1.4210854715202004e-12

Testing hermiticity of the hamiltonian 10 times. Maximum error:
    N                    1D                    2D                    3D                    4D
 5.0   3.351623381340333e-14  9.094947017729282e-13   7.332580706405269e-12  1.1647215137477994e-10
10.0   3.552713678800501e-14  3.691322511952926e-12    5.83850263709029e-11  1.8626593600314625e-09
15.0  1.1381166927749112e-13  3.749942721349417e-12  2.3283064365386963e-10   7.450935859821782e-09
20.0  1.1374233532693354e-13  7.290154618149881e-12   4.656834912388614e-10  2.9802429857090324e-08

Testing positivity of the hamiltonian 10 times. Number of times hamiltonian was negative:
    N 1D 2D 3D 4D
 5.0  0  0  0  0
10.0  0  0  0  0
15.0  0  0  0  0
20.0  0  0  0  0

Testing eigenvectors of the kinetic hamiltonian 10 times. Maximum error:
    N                    1D                    2D                    3D                    4D
 5.0  1.2434497875801753e-14  1.0800775465867404e-13  2.1796412355254754e-13  3.7765864436546257e-13
10.0   6.878105916320056e-14  2.8297091250436605e-13   5.684341886080801e-13   7.687336868637697e-13
15.0  1.8898569046946333e-13    4.96058580543691e-13   8.877964208322321e-13  1.2994969994968336e-12
20.0  1.6664651003666564e-13   3.784599012301946e-13  1.2144721902219863e-12   1.781252837098464e-12
```

Figure 1: Output of our test functions for the hamiltonian for multiple N and D; 10 iterations.

One can see that the errors for testing the linearity and eigenvectors are in the range of 10^{-14} to 10^{-12}, where for higher dimensions the error increases. It also seems that for higher N the errors also increase. But in some cases this could also be due to the "random" generation. We observe the same dependence for the hermiticity with errors up to 10^{-8} in 4D. The positivity of the hamiltonian was correct all the iterations.

Now our integrator tests. The unitarity of the strang-splitting integrator and linearity of both of the integrators are 10^{-15} which check with the expectation for these results. The unitarity errors of the second order integrator are as expected far larger even in 1D with 10^{-3} and rising for higher dimensions. This behaves similar to the energy conservation tests shows. The important detail is that no expected significant lowering of errors for higher N is seen, which is most likely due $N = 20$ still relatively small and the usage of randomly generated arrays, which also change the error maxima not insignificantly.

```
Testing unitarity of the Second-Order integrator 10 times. Maximum error:
    N                    1D                    2D                  3D
  5.0  0.00023134679866898544  0.29432925155303447  1406139.1332302373
 10.0   0.0001898018578345706  0.18635597133244697   382882.6616002843
 15.0  0.00012810589455369836  0.11910954315621969   193573.5679069894
 20.0  0.00013144001773945924  0.08550130886767437   163070.4338785969

Testing unitarity of the Strang-Splitting integrator 10 times. Maximum error:
    N                    1D                    2D                    3D
  5.0  7.771561172376096e-15   5.551115123125783e-15  3.9968028886505635e-15
 10.0  7.105427357601002e-15    5.10702591327572e-15  4.6629367034256575e-15
 15.0  5.218048215738236e-15  6.5503158452884236e-15   6.217248937900877e-15
 20.0  5.995204332975845e-15   6.217248937900877e-15   7.771561172376096e-15

Testing linearity of the Second-Order integrator 10 times. Maximum error:
    N                    1D                    2D                    3D
  5.0  4.449557262054371e-16  6.684427777288335e-16  1.1443916996305594e-15
 10.0  6.662783593823664e-16  9.063162369069397e-16   9.930136612989092e-16
 15.0  4.652682298944613e-16  6.280369834735101e-16  1.1102230246251565e-15
 20.0  4.494775313252277e-16  8.005932084973442e-16   9.930136612989092e-16

Testing linearity of the Strang-Splitting integrator 10 times. Maximum error:
    N                    1D                    2D                    3D
  5.0   8.899114524108741e-16  1.0532500405730103e-15  1.1102230246251565e-15
 10.0   6.719831536961551e-16   9.036560719766055e-16  1.1801832636420706e-15
 15.0  1.1226435567921847e-15  1.3426356273935429e-15  1.4895204919483639e-15
 20.0  1.0235750533041806e-15    1.11722656473849e-15   1.831026719408895e-15

Testing energy conservation of the Second-Order integrator 10 times. Maximum error:
    N                    1D                   2D                  3D
  5.0   0.0004240480834809546  0.6908244913065005  29.336258341952885
 10.0   0.0005974192230198128  0.7890433465539104  57.252187233938685
 15.0   0.0005299375140594975  1.0711009260218702   79.51799403587609
 20.0  0.00046080404873549696  1.1005977792368071  110.79809416852561

Testing energy conservation of the Strang-Splitting integrator 10 times. Maximum error:
    N                  1D                  2D                 3D
  5.0   0.742796708299295   3.113208245196745  8.071081532671315
 10.0  0.6411267020514231    4.11278953987653  10.83453933683154
 15.0  0.3458058145831373  2.8962394323939407  8.535507208949525
 20.0  0.2030570297923049  2.4407420552872168  6.300917385631578
```

Figure 2: Output of our test functions for the integrators for multiple N and D; 10 iterations.

Below, all the tests were run for one iteration for $N = 5$ and $D = 9$ as an additional testing.
With all these results we can safely conclude that our tests run (correctly) in more dimensions than $D = 1$, even for small N.

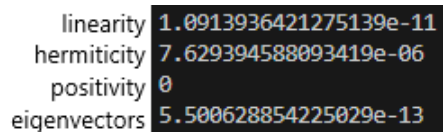

Figure 3: Output of our test functions for the hamiltonian for $N = 5$ and $D = 9$; 1 iteration.

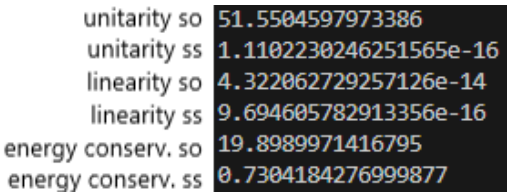

Figure 4: Output of our test functions for the integrators for $N = 5$ and $D = 9$; 1 iteration.

1.4 Convergence with rel() function xxxxxxxchange title

- Flo H

2 How the code works for the second sub-project

3 Workflow

4 Implementing conjugate-gradient and power method

5 Testing

!!! describe this time with detail and test all possible configurations!!!

6 Convergence of eigenvalues/eigenvectors

7 Appendix