Semiclassical Monte Carlo

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Contents

1 Files

- `HamiltonianMod.jl`: module to open the hamiltonian file format
- `scmc.jl`: the implementation itself
- `tests.jl`: unit tests
- `solve-rk8.jl`: used to plot the (non)conservation of energy and M with time

2 TODO How it works

1. ☒ Generate a random state vector
2. ☒ Monte Carlo steps for convergence
3. ☒ Compute known values, like energy or magnetization
4. ☒ Determine the step for decorrelation
5. ☒ Write RK8 (Dormand-Prince)
6. ☒ Compute (dynamical) structural factor
7. ☒ Put everything together

3 Data format

- state vector : `(3, Ns, Nx, Ny)`

4 Steps for MC simulations

1. Figure out the thermalization step using energy and magnetization
2. Figure out the stride looking at correlation
3. Run it ?

See the file `checkparams.jl` for these two steps.

5 Reproducing figure 4 from the SCMC paper

5.1 Target figures

5.2 TODO Fix the wrong $S\vec{q}(t)$ problem

5.2.1 TODO Simple try with a single sample

5.2.2 Possible explanations

- Code is wrong (still possible)
- Some scaling issue:
  - For the temperature => wrong phase

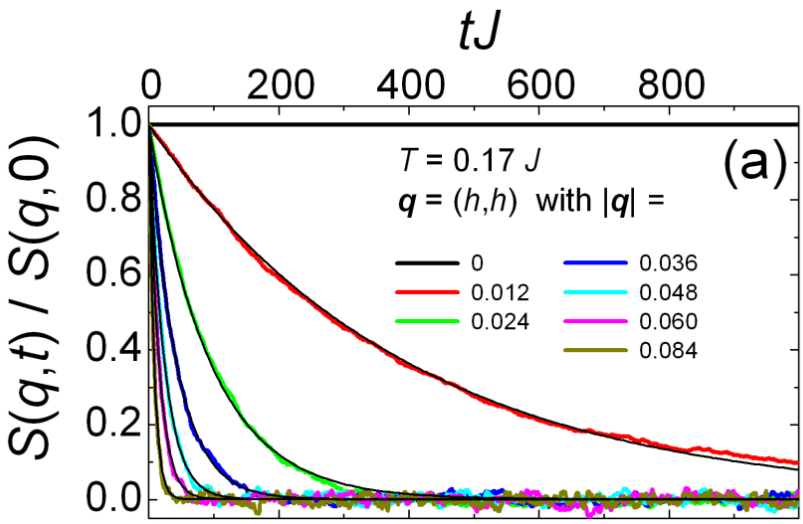


Figure 1: Figure 4 from the paper

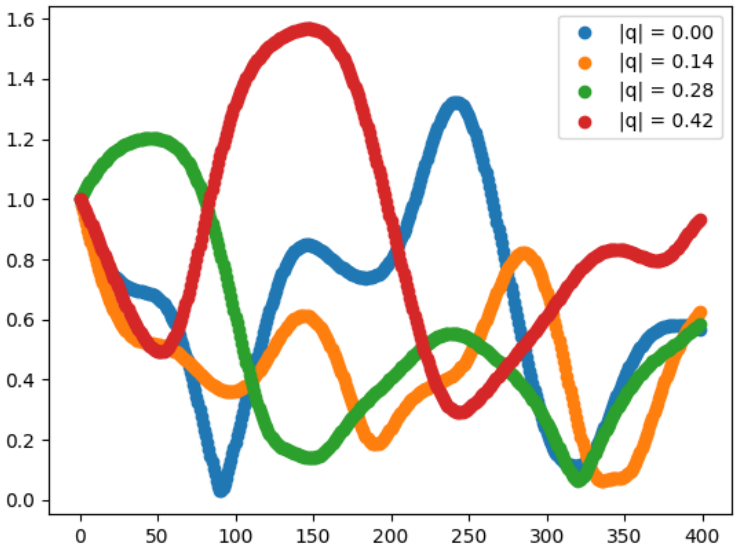


Figure 2: Only the first sample

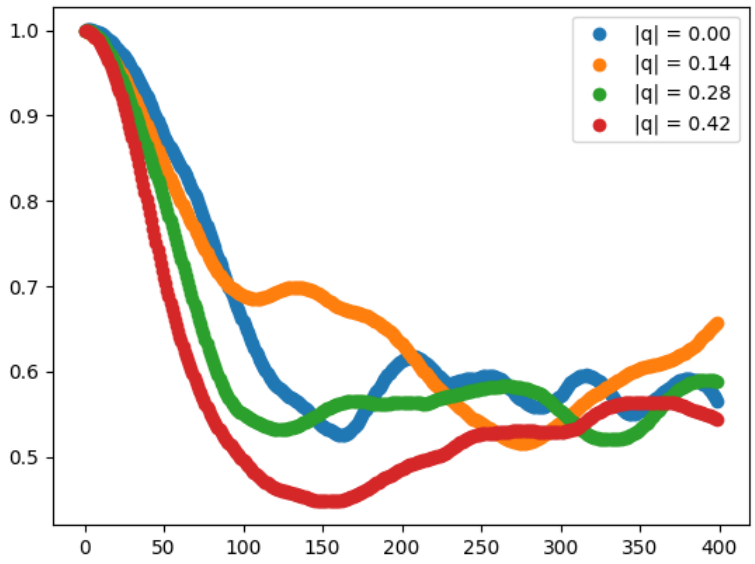


Figure 3: 74 samples

  - For the momentum space => perhaps with other kpoints it's fine

- Convergence issue ? Unlikely

5.2.3 WAIT Check energy and magnetization conservation

They are not conserved ! This was not occuring before, with the two spins system. Possibilities:

- bug in the code for for multiple unit cells
- the system was not special before (no thermalization), so even if the energy and magnetization moved a bit, it was likely to stay close

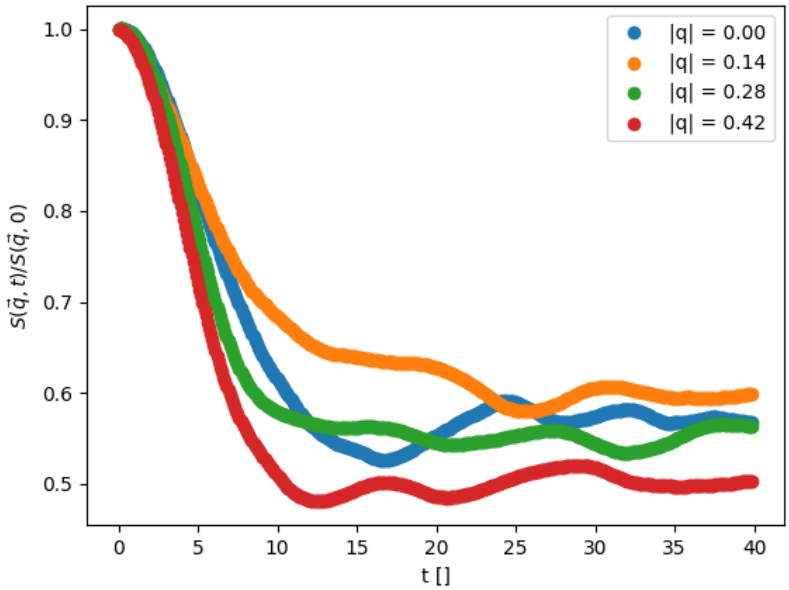
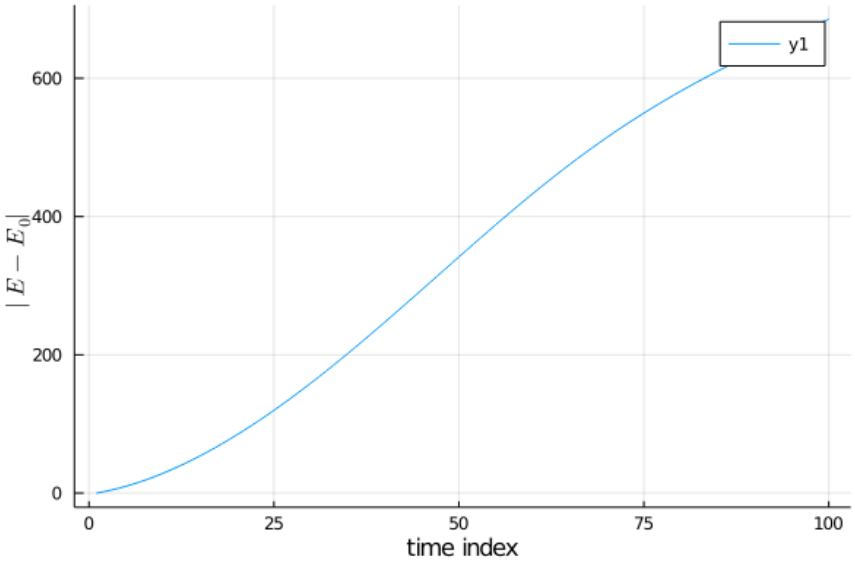


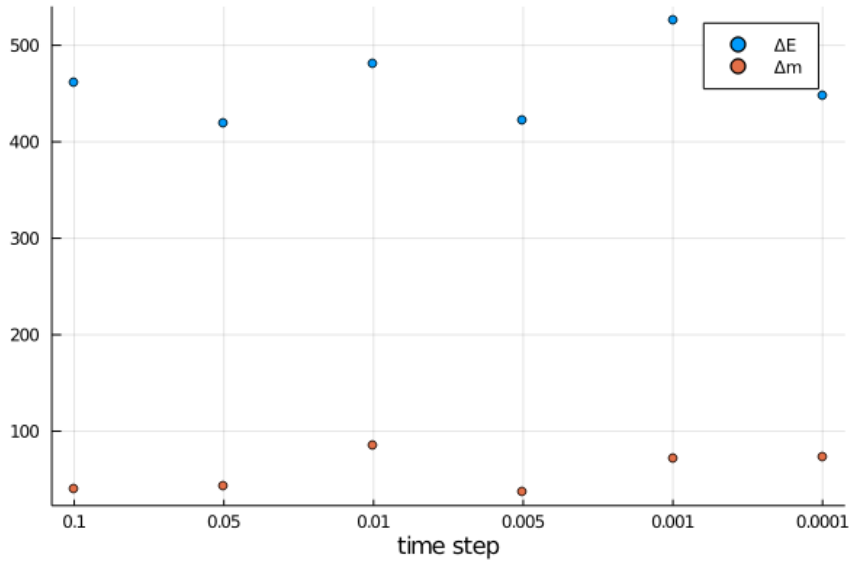
Figure 4: 403 samples

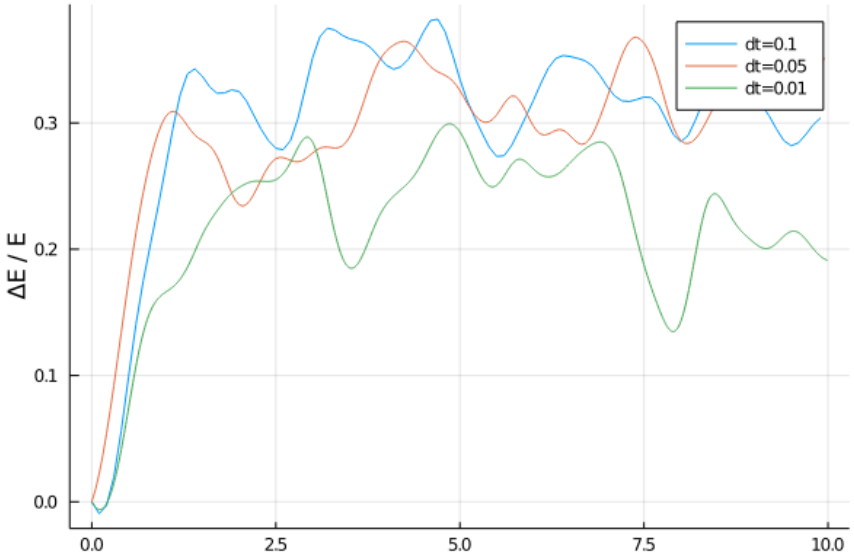


5.2.4 TODO Plotting the energy / magnetization non conservation as a function of the time step

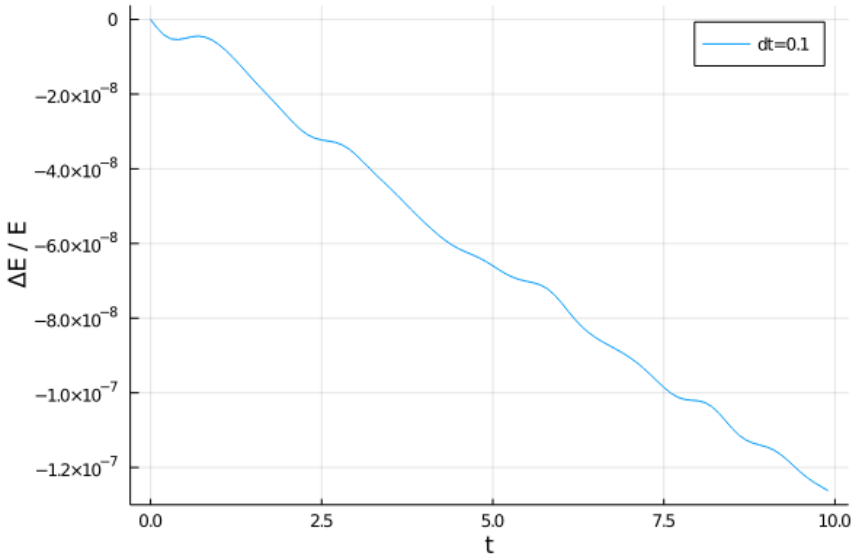
```
T = 0.17
L = 20
nt = round(Int, t / dt)
thermal = 20

dts = [0.1, 0.05, 0.01, 0.005, 0.001, 0.0001]
```





It is finally working ! I was making shallow copies of the couplings in the hamiltonian . . .



5.2.5 TODO Improve sampling with the time evolution