2018 Work Log

January

Week 1

Returned from vacation in s.e. asia on Monday. I started working with easy maintenance tasks on my code.

- Created a git `development` to keep the `master` branch stable at all times.
- Polished up the `cmake` build script so that libraries are either found or fetched and installed properly in a platform independent way. Took some trial and error.
- Added support for Travis-CI, so that a `git push` now triggers a build in `g++-7.2` and `clang++-5.0`, and reports pass/fail on the github page.
- Added support for reading parameters from a text file instead of hardcoding them into a namespace .
- Rewrite routines for finding files in the filesystem, making better use of `<std::experimental::filesystem>` features for finding input and output files.

Week 2

Continued on maintenance work. Almost finished

- Fixed some profiling issues. Timings were not clear enough.
- Fixed console output and implemented optional verbosity level, and optional timestamps.
- Started restructoring the algorithms using smart pointers everywhere, and using a Base class from which algorithms are derived (itebd, idmrg, fdmrg, xdmrg, etc). This modularization will speed up development time later, I believe.

Week 3

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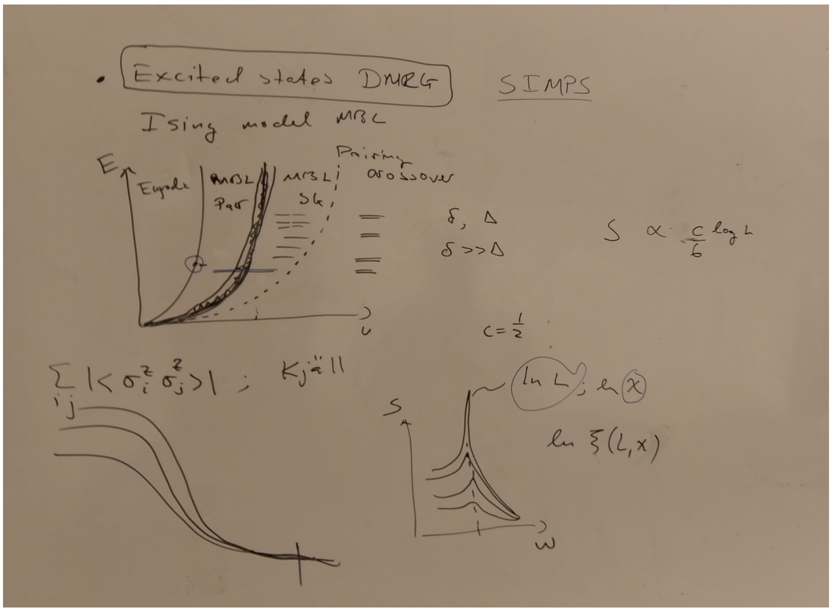
Week 4

This week I started a new project: excited-state DMRG. I am supposed to implement SIMPS or xDMRG and then study the MBL transition shown in the picture.



Other than that I continued the modularization, refactoring code. I'm trying to finish this as quickly as possible.

February

Week 1

- Finished modularization.
- Made another attempt to get Arpackc++ working to get eigenvalues of complex matrices. It worked!
- Added the excited states module and started working on that.

Week 2

- Changed the whole codebase to use complex numbers throughout. Having this double - complex switch is just messy, when complex numbers is "lingua franca" for MPS.
- The xDMRG procedure is quite simple! Simply find all eigenvectors to the local effective hamiltonian, i.e. $L - H - L$, where H is an MPO, and chose the eigenvector with greatest overlap to the current state. Starting with a randomly oriented spin chain this converges usually to a highly excited state. Unfortunaely it doesn't let us target a specific energy, but perhaps if we use SIMPS in the beginning to target a specific part of the spectrum,

we can then use xDMRG later to pinpoint a particular eigenstate in that region.

Week 3

- To gauge how close the algorithm is to an eigenstate, I returned to the issue of computing the variance $\langle \Delta H \rangle = \langle H^2 \rangle - \langle H \rangle^2$. The method by C.West using characteristic functions seems very promising... if I could just get it to work.

Week 4

- Continued working on variances.
- During the group meeting on Friday, a very fundamental error was pointed out to me. Essentially I hadn't been applying the unitary gates correctly; I applied them all, and then swapped. I am supposed to swap between every gate, and only then is a singla "tebd" step complete. It is amazing that I've gotten correct results all this time despite this flaw.

March

- The variance method by C.West works, almost. There is a discrepancy compared to the "double MPO - double environment" method I use for DMRG. Now I need to compute the variance using the regular method with the normal 2-site Hamiltonians. Turns out this is quite difficult, because the infinite number of crossterms need to be summed over. There are two places where this is described:
  - Zauner-Stauber, V., Vanderstraeten, L., Fishman, M. T., Verstraete, F., & Haegeman, J. (2017). Variational optimization algorithms for uniform matrix product states
  - Vanderstraeten, L. (n.d.). Tangent space methods for matrix product states