Quantum Dynamics of a System of Interacting Fermions

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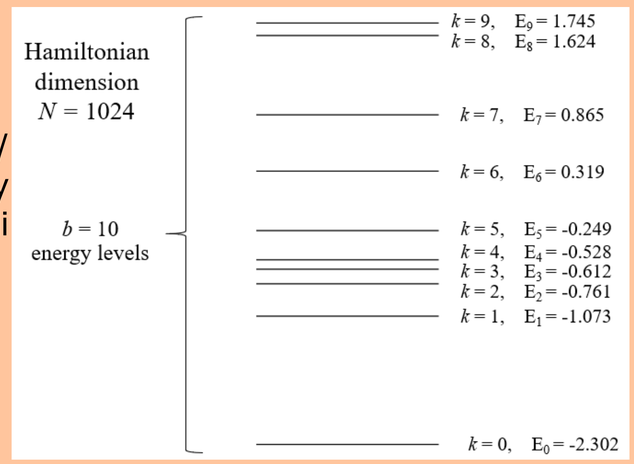
Abstract

This was a coding based project to numerically initialise and evolve a system of interacting fermions, with a number of occupiable single-body states and associated energies. The Hamiltonian matrix of many-body states and a random interaction matrix were formed and added together. Components for time evolution were evaluated. The system was then evolved from a chosen initial state and the results were analysed.

Overview of System

- Hamiltonian dimension $N = 2^b = 1024$
- Number of energy levels $b = 10$, each labelled by number k
- 0 or up to 1 fermion/ electron can occupy each level (Pauli exclusion principle)
- Energy level values taken from Gaussian distribution
- Fixed number of fermions $m = 5$



(A) *System of fermions*

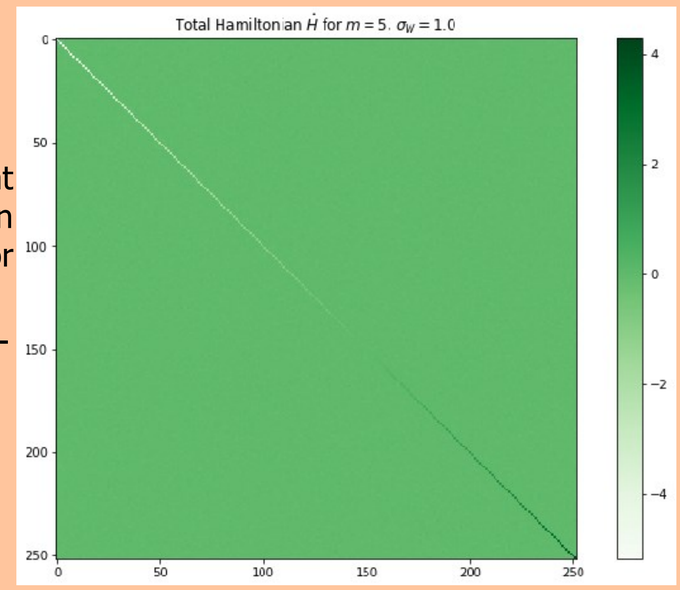
Forming the Total Hamiltonian

The bare Hamiltonian H_0 was formed, a diagonal matrix containing all many-body energy states.

This was sorted/permuted into states that share the same fermion number and in ascending energy, and the matrix for fermion number $m = 5$ was extracted.

A random interaction matrix W was formed using values taken from a Gaussian distribution, and interaction strength set to $\sigma_W = 1$.

The total Hamiltonian was formed: $\hat{H} = H_0 + W$



(B) *The total Hamiltonian for system with 5 fermions (sorted in ascending energies)*

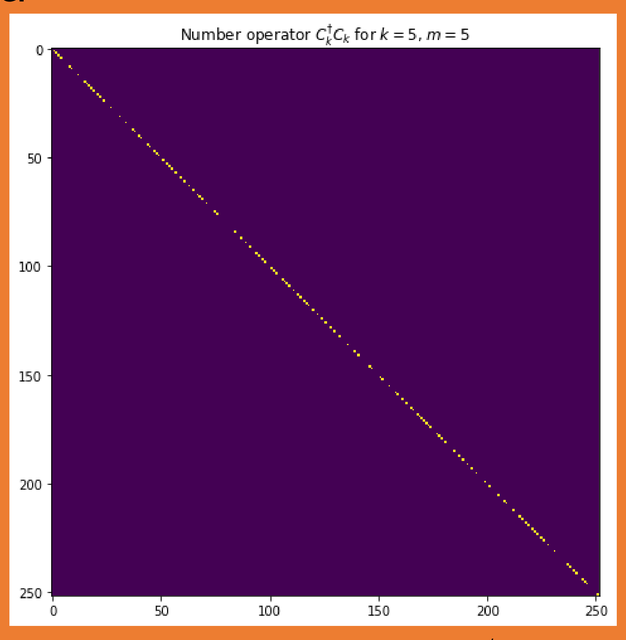
Obtaining components for time evolution

The main objective is to simulate the expectation value of occupation number at the kth level (over time): $\langle n_k \rangle = \mathrm{Tr}\left(C_k^\dagger \, C_k \; |\psi(t)\rangle \langle \psi(t)| \right)$

The components required for this and time evolution are:

Number Operator

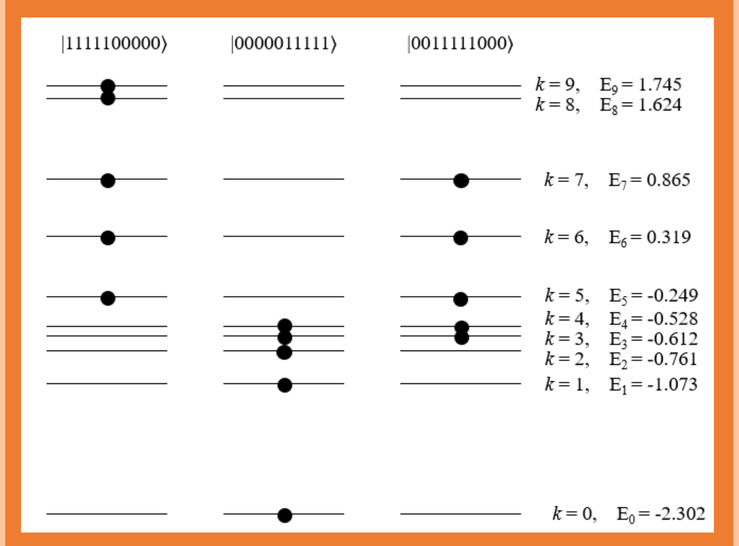
A diagonal matrix containing value 0/1 where the level k is unoccupied/occupied in a many-body state.



(C) *The number operator $C_5^\dagger C_5$*

Initial State

Any many-body state in the Total Hamiltonian could be set to be the initial state at time t=0. (D) displays three of these (filling top, bottom, and middle five levels).



(D) *Three example states of indexes 251, 0, 126*

Evolution Operator & Time Step

The eigenvalues and eigenvectors of $\hat{H}$ were used to compute the evolution operator:

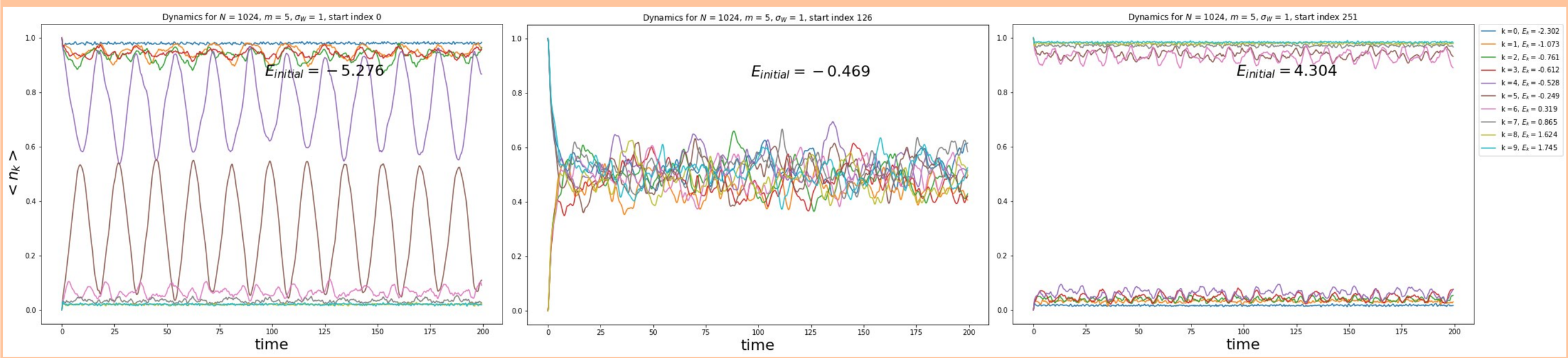
$$U_t = e^{-i\hat{H}t}$$

The time step Δt used was found using Fermi's Golden rule. DOS is a quantity referring to the density of states.

$$\Gamma = 2\pi \, \sigma_W^2 \, \mathrm{DOS} \qquad \Delta t = \frac{1}{10\,\Gamma}$$

Resulting Dynamics

The three initial states as in **(D)** were used to observe the dynamics. The results are in **(E).** State 0: dynamics seem frozen, except for levels $k = 4$ and 5, which seem to oscillate. State 126: all levels seem to be occupied throughout time. State 251: the dynamics seem frozen, as the top five levels remain occupied, and the bottom five unoccupied over time. It can be concluded from this result that the dynamics have a dependence on the initial state.



(E) *Dynamics observed from initial states of indexes 0, 126, 251*

Conclusion

A code was produced to numerically produce a system of fermions with random interactions occupying k single-particle states. Matrices for the Total Hamiltonian were formed, from which the components of time evolution were computed. With this, the dynamics over time of chosen initial states were simulated.