Simulating the Quantum Dynamics of Many-Body Systems using Graphical Processor Units

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1. Abstract

The aim of this project was to numerically simulate the dynamics of a many-body, isolated, quantum system of interacting identical fermions. The total Hamiltonian H was set up using a bare Hamiltonian H_0 and an interaction matrix W. The components for the evolution operator were defined to be able to evolve the system. This project mainly focused on the average occupation number $< n_k >$ and it was analysed as a function of time t, energy ϵ_k and interaction strength σ_W. Finally, the discrepancy between the simulation data and the Fermi-Dirac distribution was presented.

2. The Fermi – Dirac Distribution

- The Fermi-Dirac distribution is the standard prediction for a system of fermions.
- It describes the distribution of particles over multiple energy states in a thermalized state.
- It is defined by,

$$f(E) = \frac{1}{e^{\beta(E-\mu)} + 1}$$

where $\beta = \frac{1}{k_B T}$, μ is the chemical potential and E is the energy. These values were estimated in the project to be able to compare the function to the simulated data.

- The graph has a distinct step-function.

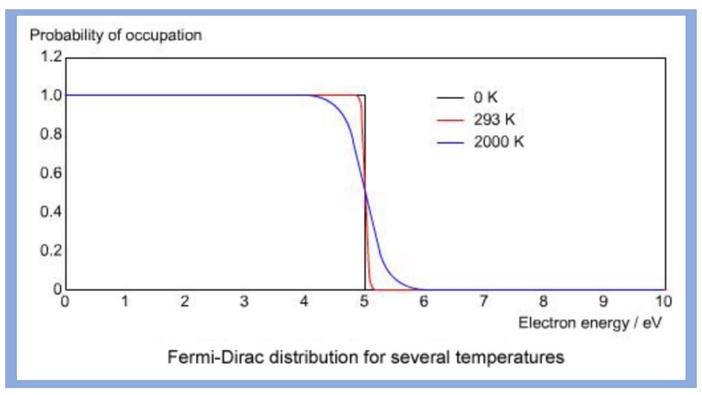

Figure 1: The Fermi-Dirac Distribution [1]

3. Many-Body Quantum Systems

- A system of m interacting fermions was set up in a many-body state.
- The number of energy levels b = 10 where labelled k.
- Each energy level had an occupation number, 0 or 1, to show an unfilled or filled energy level.
- The energies ϵ_k were taken from a Gaussian distribution.
- The states were represented using binary notation:
  - Length of binary notation = number of energy levels b.
  - Number of 1s (Hamming Weight) = Number of m electrons

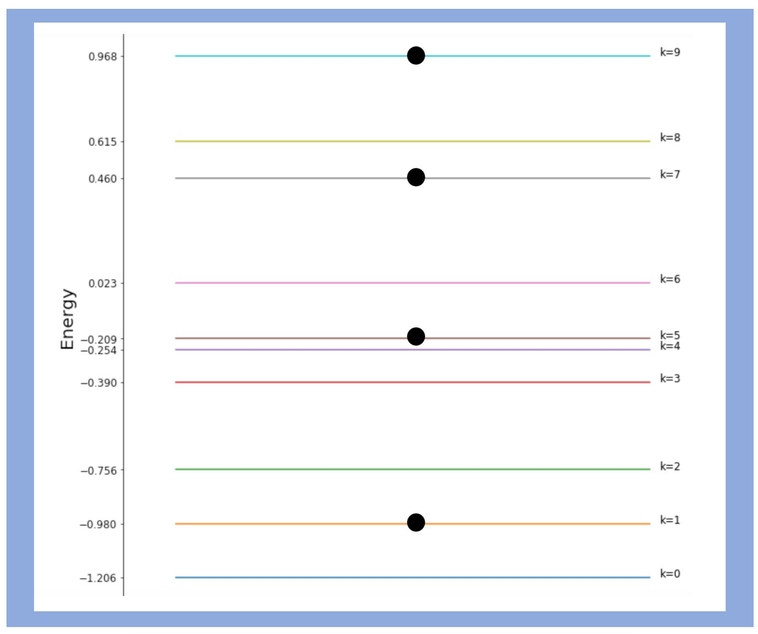

Figure 2: Example of a many-body state with binary representation |1010100010> and $m = 4$ electrons.

4. The Total Hamiltonian H

- The Total Hamiltonian was set up using the equation,

$$H = H_0 + W.$$

- The bare Hamiltonian H_0 is a N x N diagonal matrix of the single particle energies where $N = 2^b$ and is defined by,

$$H_0 = \sum_k \epsilon_k n_k,$$

where ϵ_k are the energies of each k energy level and n_k is the occupation number taking values 0 or 1.

- H_0 was sorted and permuted into sub-blocks of matching number of electrons m and with ascending energies.
- The sub-block with $m = 5$ was extracted for H.
- The interaction matrix W is a random diagonal matrix with entries given by the Gaussian distribution.

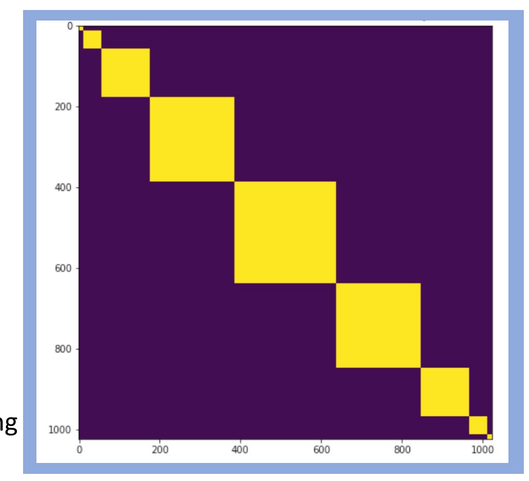

Figure 3: Sub-block representation of the sorted bare Hamiltonian.

5. Results

The project focused on varying the occupation number against time, interaction strength and finally energy which could then be compared to the Fermi-Dirac equation.

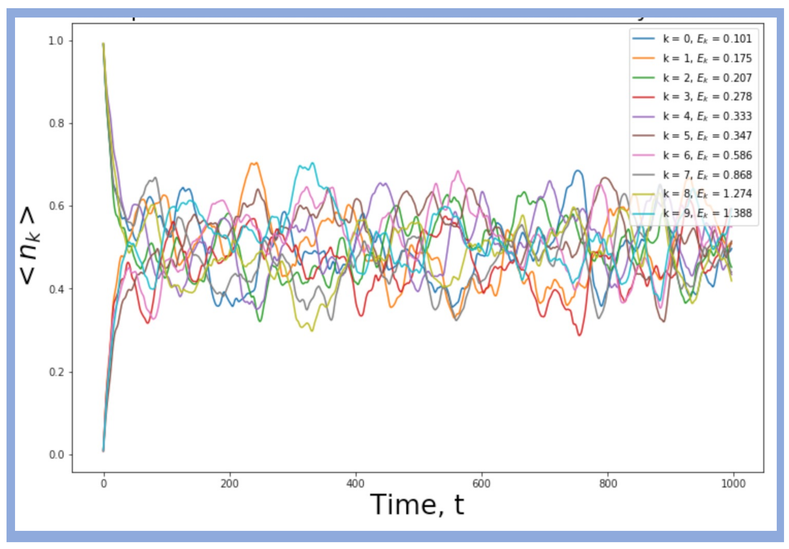

Figure 4: Occupation number as a function of time.

Discussion

For all k orbitals, the occupation number evolves to a stationary state with an average occupation number of 0.5 when the interaction strength $\sigma_W > 0.01$.

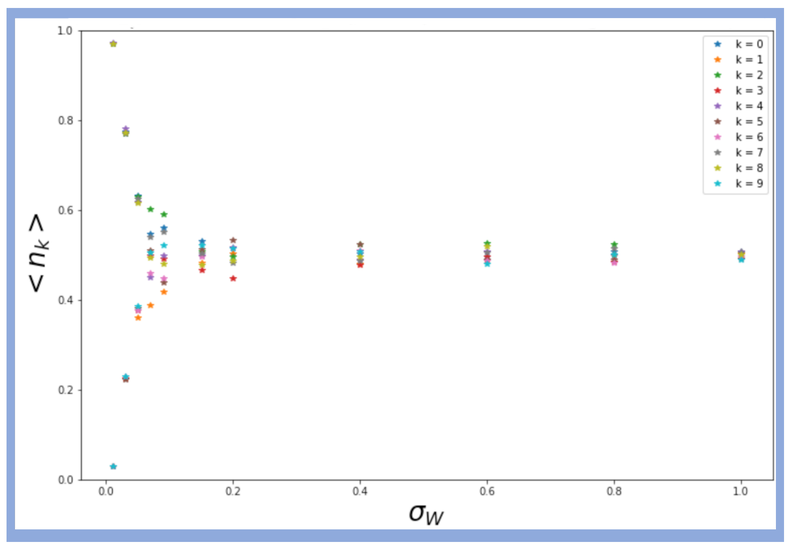

Figure 5: Occupation number as a function of interaction strength.

As the interaction strength σ_W increases, the occupation number $< n_k >$ settles towards 0.5.

At $\sigma_W > 0.01$, the system is frozen in its initial state.

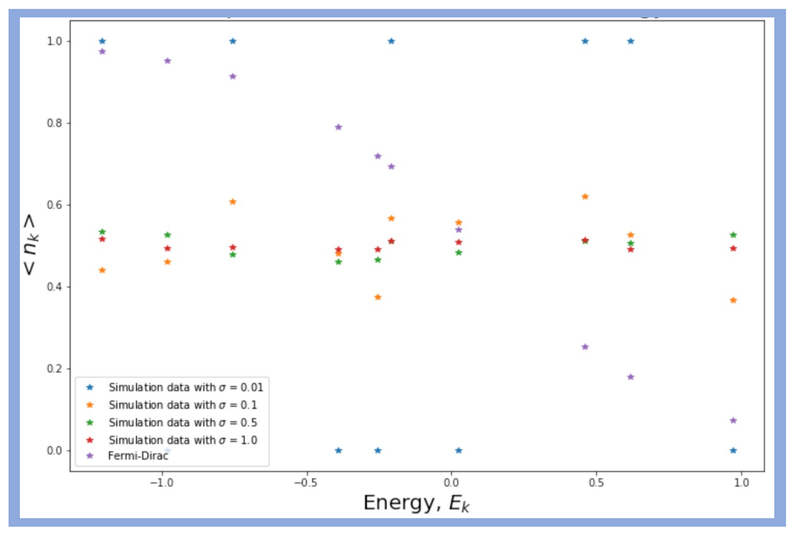

Figure 6: The estimated Fermi-Dirac distribution compared to the simulation data.

The estimated Fermi-Dirac distribution shows the distinct step-function.

The occupation number of the simulation data remains at 0.5 for $\sigma_W > 0.01$.

The simulation data does not follow the same distribution as the Fermi-Dirac distribution.

6. Conclusion

- The project numerically simulated a many-body quantum system of interacting fermions and observed how the average occupation number of each energy level evolves with time, energy and interaction strength.
- The occupation number as a function of time, Fig. 4, gradually reached an equilibrium state with a value of 0.5 for all k orbitals.
- The occupation number as a function of energy, Fig. 6, also followed the same trend and remained at a value of 0.5 with small fluctuations for all k orbitals.
- This does not follow the Fermi-Dirac distribution and therefore, one can assume the evolved system did not reach a thermal equilibrium.
- An example a system that reaches a stabilized state which is not thermal is called a Many-Body Localized (MBL) system.
- An increase in the interaction strength also caused the occupation number to go from a value that was frozen in its initial state to settling at 0.5 for all k orbitals.

References

[1] DoITPoMS, TLP Library Introduction to Semiconductors - The Fermi–Dirac Distribution, (accessed 02/03/2021)