Theory

Second Quantization

Second quantization, also referred to as the occupation number representation, is a formalism used to describe and analyze quantum many-body systems. In quantum field theory, it is known as canonical quantization, where fields (typically wave functions of matter) are treated as field operators, akin to how physical quantities (position, momentum, etc.) are treated as operators in first quantization. The foundational ideas of this method were introduced in 1927 by Paul Dirac and later developed by Pascual Jordan and Vladimir Fock.

In this approach, quantum many-body states are represented in the Fock state basis, constructed by populating each single-particle state with a certain number of identical particles. The second quantization formalism introduces creation ($c_i^\dagger$) and annihilation (c_i) operators to construct and handle the Fock states. These operators follow specific commutation or anti-commutation relations, which depend on whether the particles are bosons or fermions. For fermions, which obey the Pauli exclusion principle, the operators satisfy anti-commutation relations:

$$\{c_i, c_j\} = 0, \quad \{c_i^\dagger, c_j^\dagger\} = 0, \quad \{c_i, c_j^\dagger\} = \delta_{ij}$$

In this formalism, the Hamiltonian of a quantum many-body system can be expressed in terms of these creation and annihilation operators. For the specific problem of calculating the energy and correlation function for 3 electrons in an 8-site system, the Hamiltonian is given by:

$$H = -t \sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) + V \sum_i n_i n_{i+1}$$

where t represents the hopping term, V represents the interaction term between neighboring sites, and $n_i = c_i^\dagger c_i$ is the number operator at site i.

The goal is to solve this Hamiltonian using the second quantization formalism to obtain the ground state energy and the correlation functions. The process involves the following steps:

1. Construct the Fock Space: Define the basis states for the system, which, in this case, involves all possible configurations of 3 electrons in 8 sites.

2. Build the Hamiltonian Matrix: Express the Hamiltonian in matrix form using the creation and annihilation operators. Each element of the matrix corresponds to the transition amplitude between different basis states.

3. Diagonalize the Hamiltonian: Use numerical methods to diagonalize the Hamiltonian matrix and find the eigenvalues and eigenvectors. The lowest eigenvalue corresponds to the ground state energy of the system.

4. Calculate Correlation Functions: Once the ground state is obtained, calculate the correlation functions, such as the two-point correlation function $\langle c_i^\dagger c_j \rangle$, using the ground state wavefunction.

Density Matrix Renormalization Group (DMRG)

The Density Matrix Renormalization Group (DMRG) algorithm, pioneered by Steven White in 1992, is a variational optimization algorithm used by physicists to find the ground states of Hamiltonians for quantum many-body systems in low dimensions. Beyond being a numerical method, DMRG has bridged ideas from theoretical condensed matter physics and quantum information, enabling advances in fields such as quantum chemistry and the study of dissipative systems. It also led to the development and widespread use of tensor networks as mathematical representations of quantum many-body states, with applications extending beyond quantum systems. Today, DMRG is one of the most powerful and widely used methods for simulating strongly correlated quantum many-body systems.

Algorithm

The DMRG algorithm can be outlined as follows:

- Build all the operator matrices for a single-site Hamiltonian and the operators involved in the interactions between the site and the rest of the system.
- Start growing the blocks by adding single sites, as outlined in the exact diagonalization section. Assume the Hilbert space for the single site has dimension d.
- When the size of the blocks becomes larger than $d \times m$, start applying the density matrix truncation:

1. Using a suitable library routine (Lanczos, Davidson), diagonalize the full Hamiltonian (super-Hamiltonian) of the two combined blocks (superblock) to obtain the ground state $|\Psi\rangle = \sum_{ij} |i\rangle|j\rangle$.
2. Calculate the reduced density matrix of the left and right blocks. For symmetric systems, only one is needed.
3. For each block, diagonalize the density matrix to obtain the full spectrum and eigenvectors.
4. Truncate the basis by keeping only the m eigenvectors with the largest eigenvalues.
5. Rotate the Hamiltonian and the operators involved in the interactions between blocks to the new basis.
6. Add a new site to the left and right blocks to build new blocks of dimension $d \times m$, and reiterate the diagonalization and truncation steps. Stop when the desired system size is reached or the error in the energy is below a predefined tolerance.

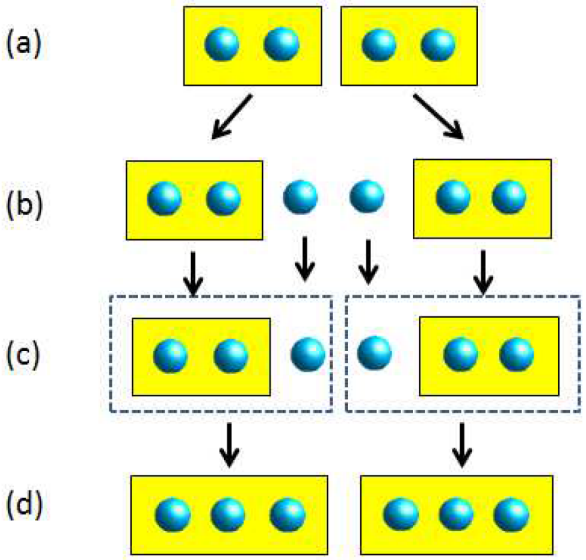

Figure 1: DMRG algorithm

Problem 1

In this problem, we solve the quantum many-body system of 8 sites with 3 electrons using second quantization and creation and annihilation operators, comparing the result to what we obtained in Homework 2. The Hamiltonian of our system is:

$$H = -t \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + V \sum_i n_i n_{i+1}$$

Where $c_i^\dagger$ is creation operator and is given by :

$$c_i^\dagger = \sigma_z^{\otimes i-1} \otimes \sigma_- \otimes I^{\otimes n-i}$$

After we built the Hamiltonian we impose fermionic statistics by finding the diagonal elements of N_{tot} equal to number of electrons and transform the Hamiltonian into those basis.

Result

The results using second quantization and the first quantization from Homework 2 for the ground state energy and correlation function are as follows:

(I have also added my first quantization code so you can verify that the results are the same).

Method	Value
Second Quantization (New)	-4.4939
First Quantization (Old)	-4.4939

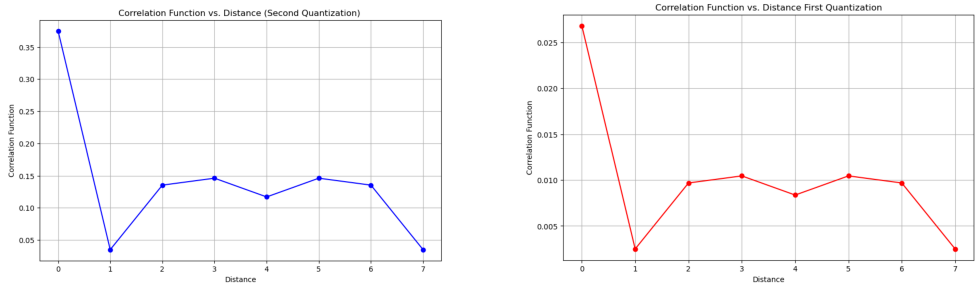

Figure 2: Comparison of results using second quantization (left) and first quantization (right).

Problem 2

In this problem, we solve the 1D Ising model for 60 spins using the Numerical Renormalization Group (NRG) method to find the ground state energy and average and correlation functions of $\langle S_x \rangle$, $\langle S_y \rangle$, $\langle S_x S_x \rangle$, $\langle S_z S_z \rangle$.

Result

The results for the ground state energy using the NRG method are:

Method	Value
NRG	-13.0889

The results for the correlation functions are given below:

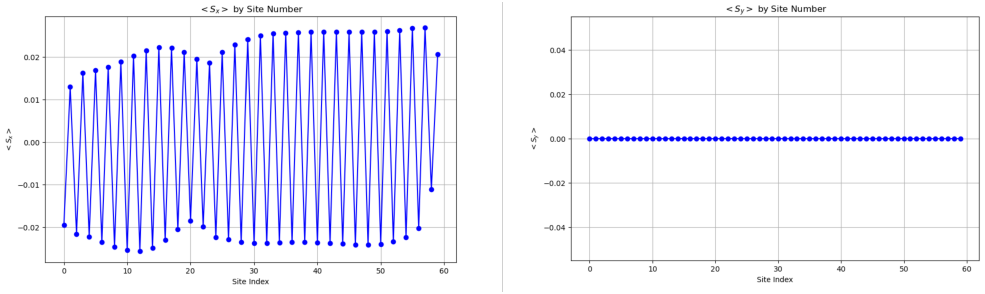

Figure 3: Correlation functions $\langle S_x \rangle$ and $\langle S_y \rangle$.

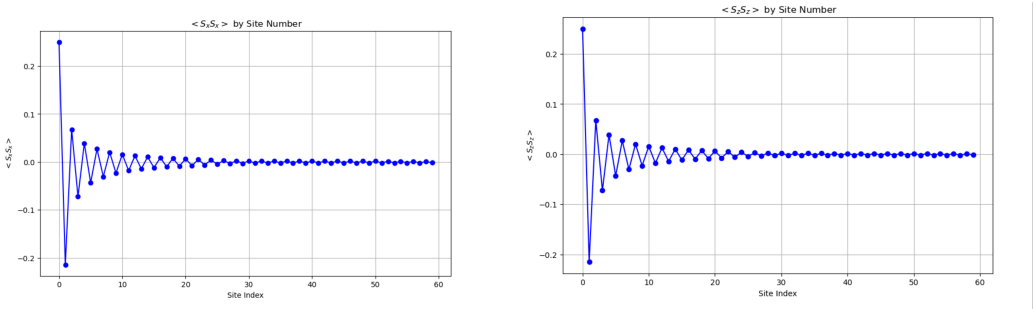

Figure 4: Correlation functions $\langle S_x S_x \rangle$ and $\langle S_z S_z \rangle$.

Problem 3

In this problem, we repeat Problem 2 using the DMRG method.

Result

The results for the ground state energy using the DMRG method are:

Parameter	Value
DMRG	-13.20119

The results for the correlation functions are given below:

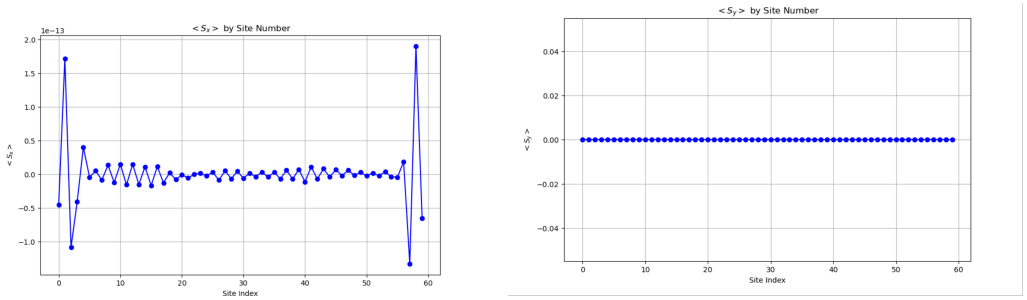

Figure 5: Correlation functions $\langle S_x \rangle$ and $\langle S_y \rangle$ (DMRG).

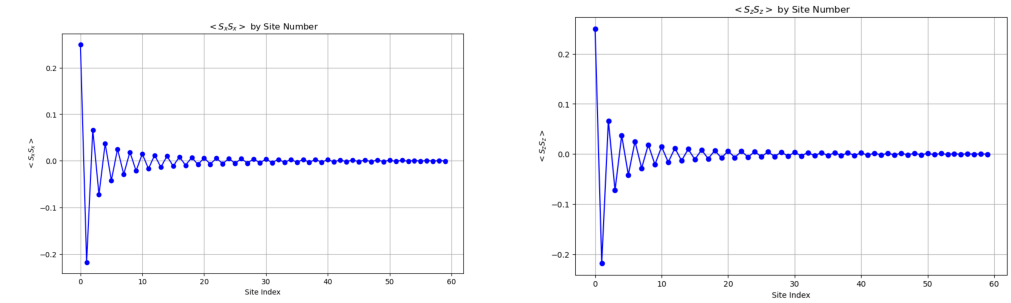

Figure 6: Correlation functions $\langle S_x S_x \rangle$ and $\langle S_z S_z \rangle$ (DMRG).

We observe that the results are consistent with those obtained using the NRG method.

References

1. The Density Matrix Renormalization Group and its time-dependent variants Adrian E. Feiguin Department of Physics and Astronomy, University of Wyoming, Wyoming, USA 82071

2. Wikipedia contributors. "Second quantization." Wikipedia, The Free Encyclopedia. Wikipedia, The Free Encyclopedia, last modified April 27, 2024. `https://en.wikipedia.org/wiki/Second_quantization`