Computational Physics
Set 2

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Introduction

In this report, we are dealing with solving Schrödinger equation for Np fermions, so we have to include fermionic statistics. The task is to translate the "Matlab" code to "Python" code, and represent the results and plot here.

Note that in all of the code, I set $\frac{\hbar^2}{m(dx)^2} = 1$.

Part 1 : Excitation energies of Np=2 fermions problem

In this part, we have two fermions and there is interaction between them, so the hamiltonian is:

$$H = -(T + T^{\dagger}) + \sum_{i=1}^{Np=2} V_1 n_i^{(1)} n_{i+1}^{(2)} \tag{1}$$

I set $V_1 = 5$ to solve it numerically. The excitation energies can be observed by Figure 1.

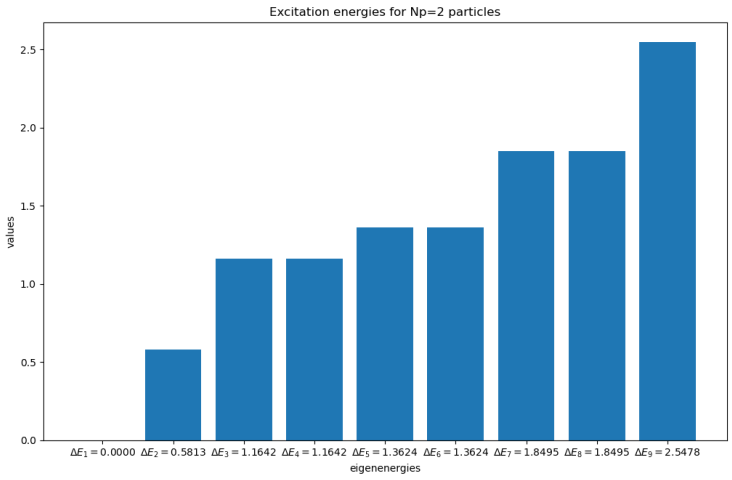

Figure 1: Excitation energies for Np=2 fermions

These are the values of excitation energies obtained by Running the code:
[0.0000, 0.5813, 1.1642, 1.1642, 1.3624, 1.3624, 1.8495, 1.8495, 2.5478]

Part 2 : Excitation energies of Np=3 fermions problem

In the case of Np=3 fermions, the hamiltonian of interacting fermions is:

$$H = -(T + T^{\dagger}) + \sum_{i=1}^{Np=3} V_1 n_i^{(1)} n_{i+1}^{(2)} \tag{2}$$

Setting $V_1 = 5$, we can see excitation energies from the bar chart in Figure 2.

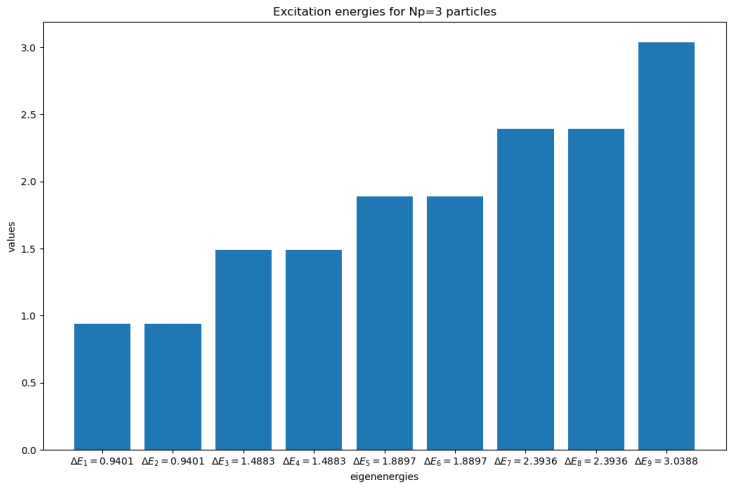

Figure 2: Excitation energies for Np=3 fermions

These are the values of excitation energies for Np=3 interacting fermions by running the code:
[0.9401, 0.9401, 1.4883, 1.4883, 1.8897, 1.8897, 2.3936, 2.3936, 3.0388]

Note the degeneracies occur in both Np=2 and Np=3 fermionic systems.

Part 3: Average number of particles for Np=3 fermions

In this part, we are dealing with Np=3 body problem for interacting fermions and we have to calculate average number of particles with respect to length. Average number of particles in j-th site is obtained by the formula:

$$\langle N_i \rangle = \langle \psi | N_j^{tot} | \psi \rangle \tag{3}$$

Note that I use ground state ψ_{gs} to evaluate all of the expectation values. Setting $V_1 = 5, V_2 = 0, V_3 = -5$, this can be observed in Figure 3.

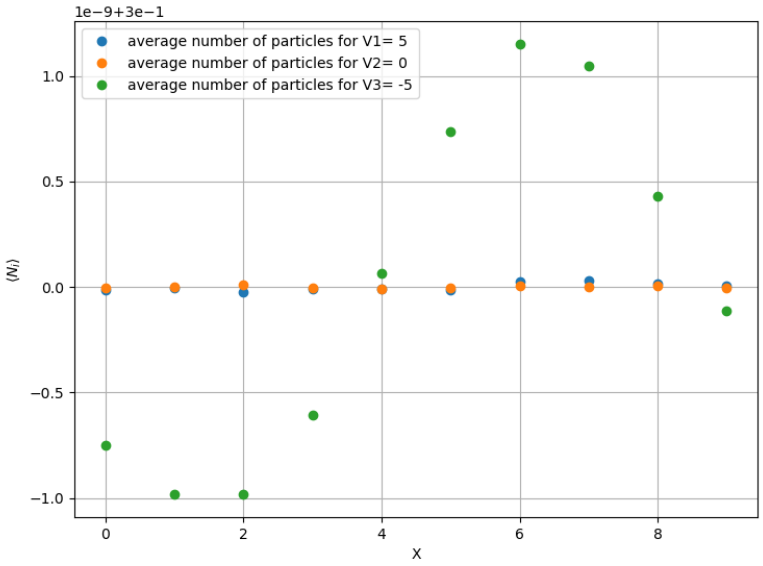

Figure 3: Average number of particles in the case of Np=3 fermions

You have to note that in all 3 cases, the average number in each point is approximately 0.3, and is a constant function of length, not sinusoidal for V_3 !

This can be easily seen by examining average number of particles in each site by the code (to 4 digits):

For $V_1 = 5$:

[0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000]

For $V_2 = 0$:
[0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000]
For $V_3 = -5$:
[0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000, 0.3000]

You can see that all of the values are constant(not only to the fourth digit, to more digits if you run the code). The non-constant shape is a consequence of the scale and resolution of y-axis (average number of particles).

Part 4: Correlation function of density-density for particles between i-th and j-th sites

Now we want to examine correlation function of density-density for Np=3 fermions between i-th and j-th sites. The correlation function between site i and j is given by this formula:

$$Corr(N_i, N_j) = \langle\psi|N_i^{tot}N_j^{tot}|\psi\rangle - \langle\psi|N_i^{tot}|\psi\rangle\langle\psi|N_j^{tot}|\psi\rangle \tag{4}$$

In general, we have to examine each i with each j, but in this case, as a consequence of translation symmetry, the correlation function is only a function of **difference of i and j**, or in other words, it's only function of **length**.

I again use the ground state ψ_{gs} to evaluate all of the expectation values. Setting $V_1 = 5, V_2 = 0, V_3 = -5$, the correlation function can be observed in Figure 4.

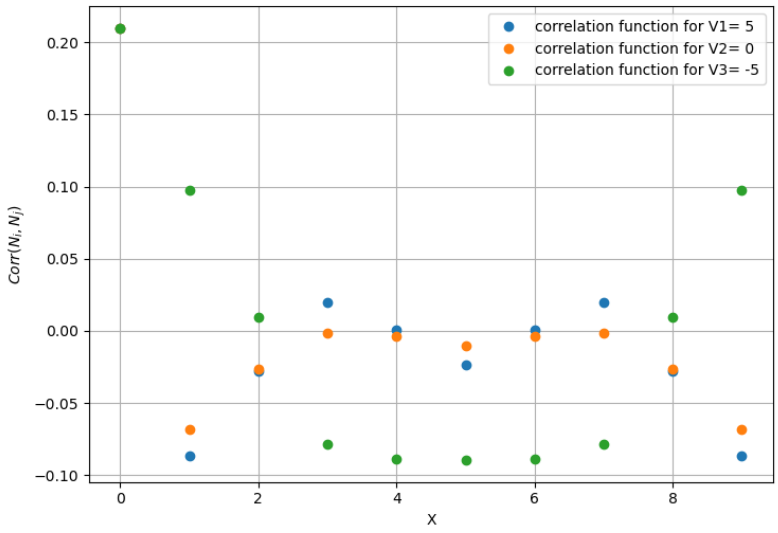

Figure 4: Correlation function of Np=3 fermionic system as a function of length

These are the values of correlation function obtained by running the code (to 4 digits):

For $V_1 = 5$:
[0.2100, -0.0863, -0.0278, 0.0199, 0.0009, -0.0234, 0.0009, 0.0199, -0.0278, -0.0863]

For $V_2 = 0$:
[0.2100, -0.0685, -0.0262, -0.0015, -0.0038, -0.0100, -0.0038, -0.0015, -0.02625, -0.0685

For $V_3 = -5$:
[0.2100, 0.0974, 0.0096, -0.0782, -0.0889, -0.0898, -0.0889, -0.0782, 0.0096, 0.0974]