Mean Field Approximation of Hubbard Model and its Application on Graphene nanoflakes.

A project submitted in partial fulfilment
of the Requirements for the Computational Physics course (P-452)

by

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1 Introduction

The solids that we deal with daily are multi-particle structures. Studying these kinds of quantum-mechanical multi-particle systems is a very difficult task. However, we begin with very simple structures and understand them with the help of various models. In the process of formulating and solving a model, we use approximations if the solution is too difficult to compute.

Hubbard model is one such model used to describe a solid with lattice sites that are arranged periodically (crystals). The Hubbard model Hamiltonian contains a hopping term that connects the wavefunction at two different sites and an onsite potential term. Despite its simplicity, Hubbard model is a very powerfool tool to study correlated fermion systems. In this report, we apply the mean field approximation to Hubbard model for solving the spin densities at the lattice sites of a Graphene nanoflake. The spin densities are then used to find the net spin density at the lattice sites.

2 The Hubbard model

To apply the Hubbard model, we first consider a regular array of fixed lattice sites. The atoms at the lattice sites are assigned only a single energy level, as opposed to the multiple energy levels an atom typically has. this is a good picture for a solid with just one energy band at the energy surface. The sites are then restricted by Pauli's exclusion principle to have a maximum of two electrons, both having opposite spins. The electrons can move around the lattice and interact with each other via Coulomb interaction. Two electrons occupying the same lattice will have the highest magnitude of coulomb interaction. Hubbard's model considers only this interaction in its Hamiltonian. The interaction term is non-zero if the site is doubly occupied and zero otherwise. There is no interaction between the fermions as different sites.

The kinetic energy is written in terms of creation and destruction operators. This term destroys an electron at a site and creates an electron at an adjacent site. The energy scale t, which governs the 'hopping', is determined by the overlap of the wavefunctions at the two sites. The hopping is only considered between nearest neighbors, as beyond that, the wavefunction is considered to die out.

Considering all this, we write the Hubbard Hamiltonian as,

$$\hat{H} = -t\Sigma_{\langle i,j,\rangle,\sigma}(c^{\dagger}_{j,\sigma}c_{i,\sigma} + c^{\dagger}_{i,\sigma}c_{j,\sigma}) + U\Sigma_j n_{j,\uparrow}n_{j,\downarrow} \tag{2.1}$$

The Hubbard Hamiltonian has a particle Hole-symmetry. In a Bipartite lattice (a lattice system where the lattice can be divided into two sublattices such that a site in one sublattice has neighbors that are members of the second sublattice.) there is high probability of an anti-ferromagnetic ordering existing in the system, where sites of one sublattice contain only one spin and a spin has only opposite spins as its neighbors.

Mean Field Approximation

The mean field theory provides effective and simple approximations for complex systems composed of a large number of interacting particles or components. Generally speaking, the theory is based on a principle of averaging the interaction effects exerted on each single particle by the others. We use the Mean field approximation to convert the quartic terms in the Hubbard Hamiltonian ($Uc^{\dagger}_{\downarrow}c_{\downarrow}c^{\dagger}_{\uparrow}c_{\uparrow}$) involving four fermionic operators into a quadratic term. The approach begins by expressing the number operators as an average value plus a deviation from the average:

$$n_{i\uparrow} = \langle n_{i\uparrow}\rangle + (n_{i\uparrow} - \langle n_{i\uparrow}\rangle)n_{i\downarrow} = \langle n_{i\downarrow}\rangle + (n_{i\downarrow} - \langle n_{i\downarrow}\rangle \tag{2.2}$$

Substituting these expressions into the Hubbard interaction term, and dropping the 'small' term (it's not really small!!) which is the product of the two deviations from the average yields,

$$\begin{aligned} n_{i\uparrow}n_{i\downarrow} &= [\langle n_{i\uparrow}\rangle + (n_{i\uparrow} - \langle n_{i\uparrow}\rangle)][\langle n_i\rangle + (n_i - \langle n_{i\downarrow}\rangle)] \\ &\approx \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle + \langle n_{i\downarrow}\rangle(n_{i\uparrow} - \langle n_{i\uparrow}\rangle) + \langle n_{i\uparrow}\rangle(n_{i\downarrow} - \langle n_{i\downarrow}\rangle) \\ &= n_{i\uparrow}\langle n_{i\downarrow}\rangle + n_{i\downarrow}\langle n_{i\uparrow}\rangle - \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle \end{aligned} \tag{2.3}$$

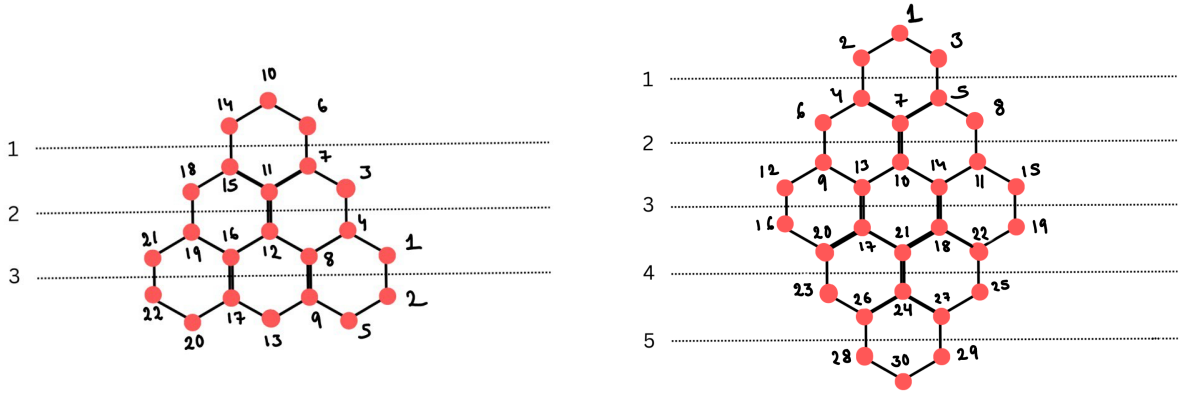
The up-spin fermions interact with the average density of the down-spin fermions, and similarly, the down-spin fermions interact with the average density of the up-spin fermions. These two terms overcount the original single interaction term, so the product of the average densities is subtracted. Within this mean-field replacement, the Hubbard Hamiltonian is now quadratic and takes the form,

$$\hat{H} = -t\Sigma_{\langle i,j,\rangle,\sigma}(c^{\dagger}_{j,\sigma}c_{i,\sigma} + c^{\dagger}_{i,\sigma}c_{j,\sigma}) + U(\Sigma_j(n_{j,\uparrow}\langle n_{j,\downarrow}\rangle + n_{j,\downarrow}\langle n_{j,\uparrow}\rangle + \langle n_{j,\uparrow}\rangle\langle n_{j,\downarrow}\rangle \tag{2.4}$$

This approximated Hamiltonian has all its terms quadratic, which means the matrix Hamiltonian can be written on a one-electron basis. The one-electron basis is obtained by applying the creation operators for different sites to the vacuum state. In this report, we only work with half-filled states, i.e., all the lattice sites have 1 electron.

3 Numerical solution of the mean field Hubbard model.

In this report, we construct two kinds of graphene nanoflakes - a triangular nanoflake and a diamond nanoflake. The steps involved in solving the spin densities at the lattice sites are as follows,



(a) Triangular system

(b) Diamond system

Figure 1: The two nanoflakes of Graphene.

3.1 Constructing the structure.

The two graphene structures are shown in figure 1. In the code, the size of the lattice is parametrized by the number of rows of the center. For instance, in the diamond lattice shown in the figure, the number of rows of centre is 5. The number of lattice sites is then calculated as,

$$\begin{aligned} n_r &= 2n - 1 \\ N_{lat} &= 2((n+1)^2 - 1) \end{aligned} \tag{3.1}$$

Here, the number of rows is denoted by n_r and the N_{lat} denotes the number of lattice sites. Similarly, the number of lattice sites for a triangular lattice is given by,

$$N_{lat} = (n_r + 1)(n_r + 3) - 2 \tag{3.2}$$

Then each lattice is numbered as shown in figures .

3.2 Constructing the Hamiltonian

The Hamiltonian is a 2Nx2N square matrix, where N is the number of lattice sites. It consists of four blocks of dimension N $\times$ N: the two blocks on the diagonal are pure spin-up and spin-down blocks and the two off-diagonal blocks mix spin-up and spin-down. According to the MF Hamiltonian, they are equal to zero (see Fig. 2 for an illustration of the block matrix). The tight binding term implies that the Hamiltonian matrix has terms of amplitude t for elements corresponding to neighboring sites. The second term of the Hamiltonian concerns diagonal elements in the single-electron basis. The diagonal elements in the spin- up (-down) block involve mean densities of down (up) spins.

The elements can be fed manually by inspecting which lattice index sites are nearest neighbors. However, in this paper, the construction of the matrix is automated, given the scheme of numbering shown in the figures is followed.

3.3 Iterative solutions for spin densities

The Hamiltonian of involves mean values of density operators, and it is therefore necessary to solve it self-consistently. Initial conditions for the mean densities are guessed and a Hamiltonian based on these mean values is built. In the next step, the initial Hamiltonian is diagonalized, resulting in eigenenergies and eigen-vectors. New mean values are computed by populating the eigen-vectors of N lowest energies, where N is the number of electrons in the system and a new Hamiltonian is generated, diagonalized, leading to new mean values. This loop is repeated until the difference between the input and output mean values is smaller than a given threshold, at which point the process is converged. The pseudo code for this iterative process is given in the appendices.

3.4 Computing the net spins at each site

The net spin at each site is calculated using the relation,

$$\sigma_{net} = (\langle n_{i,\uparrow} \rangle - \langle n_{i,\downarrow} \rangle)/2 \tag{3.3}$$

4 Results and Analysis

The structure was solved for two initial density values. The results for both cases are attached at the end of the report.

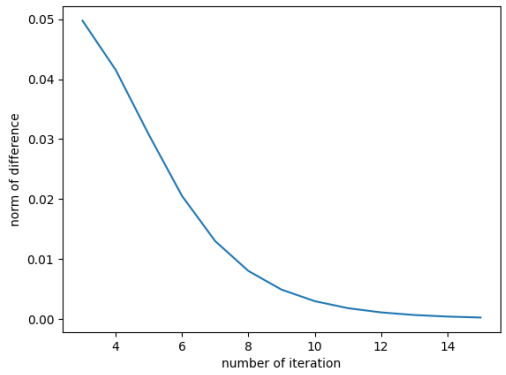
4.1 Triangular type lattice

The number of sites in one sublattice is more than the number of sites of the other sublattice. Hence, according to Lieb's condition, the total spin should be 1. Our simulation agrees with this condition as the net magnetization of this system turns out to be almost 1.

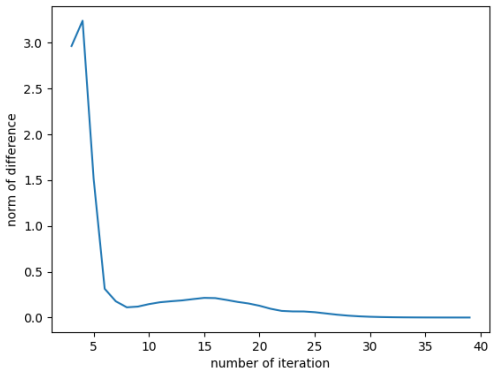
4.2 Diamond type lattice

Irrespective of the initial conditions, the net spin density at each site is close to zero. Hence, these types show no magnetic ordering, giving the net magnetization to be zero. The number of sites in each sublattice is 15. Hence, according to Lieb's condition for the Bipartite lattice, the total spin of the system should be zero.

The convergence is measured by plotting the norm of the difference between the electron densities at each site for two consecutive iterations. The plots are shown below.

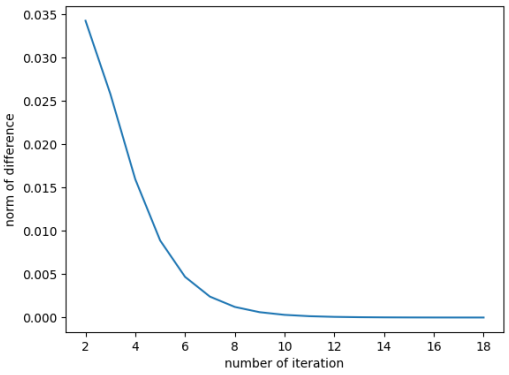


(a) Initial conditions - I

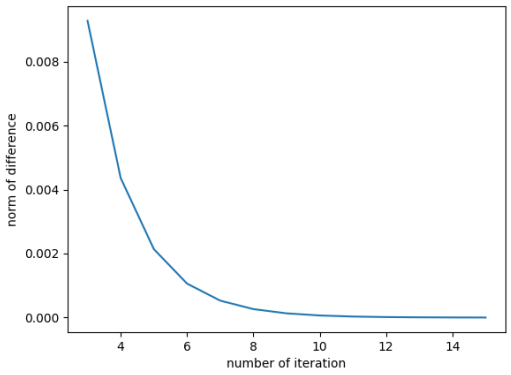


(b) Initial conditions - II

Figure 2: Plot showing the convergence rate for triangular type lattice



(a) Initial conditions - I



(b) Initial conditions - II

Figure 3: Plot showing the convergence rate for diamond type lattice

5 Conclusion

The Mean field Hubbard theory thus gives a very accurate picture of the magnetization of the system. The results agree with the Lieb condition for Bipartite lattices. However, we have only studied the spin of the system. In order to test its validity for graphene-based systems, the outcomes of this method can be compared with other computational approaches, like exact diagonalization and Quantum Monte Carlo simulations. This theory can be extended to other systems such as Bowtie nanoflakes and Graphene nanoribbons to study their magnetic ordering and spin.

6 References

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