Hubbard Model Assignment

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1 Introduction

The Hubbard model offers one of the most simple ways to get insight into how the interactions between electrons can give rise to insulating,magnetic,and even novel superconducting effects in a solid.It was written down in the early 1960'sand initially applied to understanding the behavior of the transition metal monoxides(FeO, NiO,CoO),compounds which are antiferromagnetic insulators,yet had been predicted to be metallic by methods which treats strong interactions less carefully.

Over the intervening years,the Hubbard model has been applied to the understanding of many systems,from'heavy fermion systems in the 1980's,to high temperature superconductors in the 1990's.Indeed,it is an amazing feature of the model that,despite its simplicity, its exhibits behavior relevant to many of the most subtle and beautiful properties of solid state systems.The Hubbard model has been studied by the full range of analytic techniques developed by condensed matter theorists,from simple mean field approaches to theoretical methods employing Feynman diagrams,expansions in the degeneracy of the number of 'flavors' (spin,orbital angular momentum),etc.

In the following description we develop a scheme for counting and defining basis states using binary numbers and ultimately finding the ground state eigenvalues and eigenstates by diagonalizing the hamiltonian

2 Hubbard Model Formulation

We start with defining a system of non-interacting fermions on a lattice with L sites. In second quantisation then the hopping/cross interaction terms may be written within the Hamiltonian as:

$$H_t = \Sigma_{ij} t_{ij} c_i^\dagger c_j \tag{1}$$

where

$$c_i^\dagger, c_j = \delta_{ij} \tag{2}$$

and the hopping term may be defined as

$$t_{ij} = \langle \phi_i | -\frac{\hbar^2 \Delta^2}{2m} + v | \phi_j \rangle = \int dx \phi_i(x) (-\frac{\hbar^2 \Delta^2}{2m} + v(x)) \phi_j(x)$$

(3)

Our problem may be furthur reduced if we only consider nearest neighbour interactions and substitute t_{ij} by -t so that the Hamiltonian becomes:

$$H_t = -t \Sigma_{<ij>} (c_i^\dagger c_j + c_j^\dagger c_i) \tag{4}$$

We have already considered the Kinetic Energy/ Hopping Term above as H_t. However if we have the situation where two electrons of opposite spin are paired up on the same orbital we need to add another interaction term:

$$H_U = U \Sigma_j (n_{j\uparrow} n_{j\downarrow} \tag{5}$$

Hence the total Hubbard Hamiltonian becomes:

$$H = H_t + H_U = -t \Sigma_{<ij>\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \Sigma_j n_{j\uparrow} n_{j\downarrow} \tag{6}$$

Now we need to find a way to represent our basis states. Our operations become easier if we represent each spin configuration as a binary number as follows. For example for N = 2, In the binary representation we use a 2*N bit representation for a N spin configuration. The first N bits from the left are for the $\downarrow$ and the remaining N bins for the $\uparrow$. If a spin is present we put 1 there and if not we set that position 0.

	beginner	expert	computer			
J	algebraic	picture	binary	$I_\downarrow$	$I_\uparrow$	I
1	$c^\dagger_{1\uparrow}c^\dagger_{0\uparrow}\|\rangle$	$\uparrow$ $\uparrow$	$\|00\rangle_\downarrow\|11\rangle_\uparrow$	0	3	3
2	$c^\dagger_{0\downarrow}c^\dagger_{0\uparrow}\|\rangle$	$\bigcirc$ $\uparrow\downarrow$	$\|01\rangle_\downarrow\|01\rangle_\uparrow$	1	1	5
3	$c^\dagger_{0\downarrow}c^\dagger_{1\uparrow}\|\rangle$	$\uparrow$ $\downarrow$	$\|01\rangle_\downarrow\|10\rangle_\uparrow$	1	2	6
4	$c^\dagger_{1\downarrow}c^\dagger_{0\uparrow}\|\rangle$	$\downarrow$ $\uparrow$	$\|10\rangle_\downarrow\|01\rangle_\uparrow$	2	1	9
5	$c^\dagger_{1\downarrow}c^\dagger_{1\uparrow}\|\rangle$	$\uparrow\downarrow$ $\bigcirc$	$\|10\rangle_\downarrow\|10\rangle_\uparrow$	2	2	10
6	$c^\dagger_{0\downarrow}c^\dagger_{1\downarrow}\|\rangle$	$\downarrow$ $\downarrow$	$\|11\rangle_\downarrow\|00\rangle_\uparrow$	3	0	12

Figure 1: Various Representations of Basis States

3 Counting Basis States

Now that we have our basis states we need to find a general method for counting them. We came up with the following methods.

3.1 Method 1

If we select J $\uparrow$ spins we need to count the number of ways of placing them at N sites. We need then to multiply this with the number of ways to arrange N - J $\downarrow$ spins at N sites. Thus we get

$$states = \Sigma_{j=0}^{N} C_j^N C_{N-j}^N \tag{7}$$

3.2 Method 2

Instead of counting in this manner we can have an alternate method for counting and simultaneously generating the Basis states in Binary representation. In a single loop we can generate 2^{2N} corresponding to 2N bits. Now we only choose those bits where the number of 1s does not exceed N. We saved the resulting binary numbers in a 2d array. By splitting each binary number from the middle we can retrieve the up and down kets.

N	Basis State Count
2	6
4	70
6	924
8	12870
10	184756

4 Defining operators and constructing the Hamiltonian

4.1 Counting and forming H_t operators

For each value of N since we are only taking nearest neighbour interactions we have N-1 interaction terms. Considering conjugate and up down spins, we have a total number of 4*(N-1) operator terms for the H_t Hamiltonian. For example if we look at the 4 terms for N = 2:

Country List				
Operator	Bit0	Bit1	Bit2	Bit3
$C^\dagger_{0\uparrow}C_{1\uparrow}$	0	0	-1	1
$C^\dagger_{1\uparrow}C_{0\uparrow}$	0	0	1	-1
$C^\dagger_{0\downarrow}C_{1\downarrow}$	-1	1	0	0
$C^\dagger_{1\downarrow}C_{0\downarrow}$	1	-1	0	0

We used +1 to represent the creation and -1 for the annihilation operator. "Operation" in binary here is defined as the addition of binary representations of operator and ϕ_2. For example:

$$C^\dagger_{0\uparrow}C_{1\uparrow}\left|\uparrow\uparrow \mathbf{O}\right\rangle = [0,0,-1,1] + [1,0,1,0] = [1,0,0,1] = \left|\downarrow \quad \uparrow\right\rangle \tag{8}$$

The only thing left to do is to

4.2 Counting and forming H_U operators

It is much more easier to create the H_U matrix. First of all it is only non zero for diagonal elements. Among the diagonal elements it is non zero for paired up spin kets only. An easy way to implement this is to sum up the Binary representations of up and down kets and select only those kets where 2 appears after addition.

5 Matrices computed for N = 2

Choosing t = 1 and U = 0.5. We obtained the following matrix for N = 2. The ground state energy was obtained as -1.7655.

0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.50	-1.00	-1.00	0.00	0.00
0.00	-1.00	0.00	0.00	-1.00	0.00
0.00	-1.00	0.00	0.00	-1.00	0.00
0.00	0.00	-1.00	-1.00	0.50	0.00
0.00	0.00	0.00	0.00	0.00	0.00

The following plot shows the probabilities of the different basis states for N = 2:

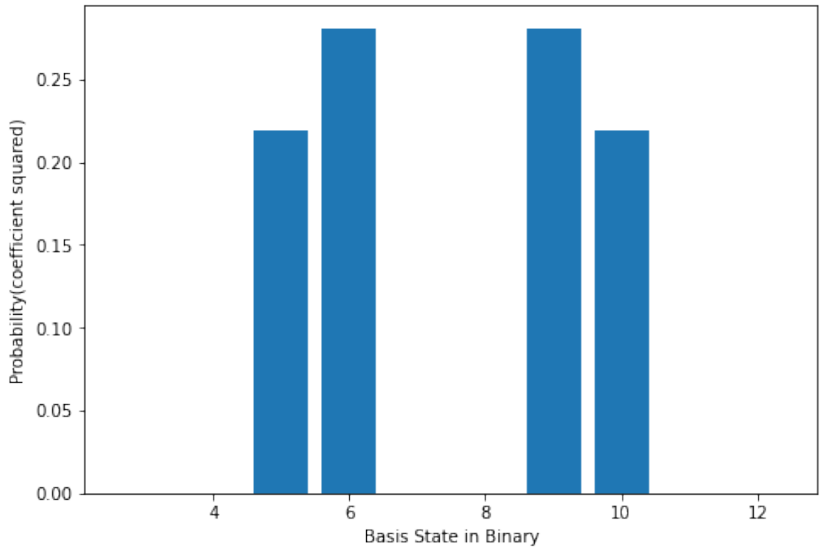

Figure 2: Basis State probabilities(N = 2)(U = 0.5)

Thus we obtain $|\downarrow \quad \uparrow\rangle$ *or* $|\uparrow \quad \downarrow\rangle$ with the maximum probability.

6 Matrices computed for other values of N and U

6.1 N = 2 cases

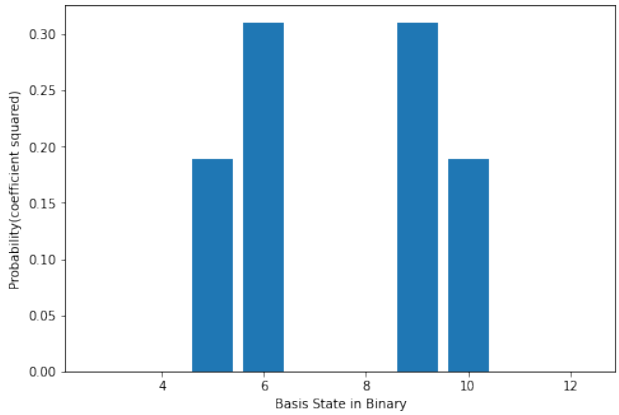

Figure 3: Basis State probabilities(N = 2)(U = 1)

$|\downarrow \quad \uparrow\rangle$ *or* $|\uparrow \quad \downarrow\rangle$ has the maximum probability.

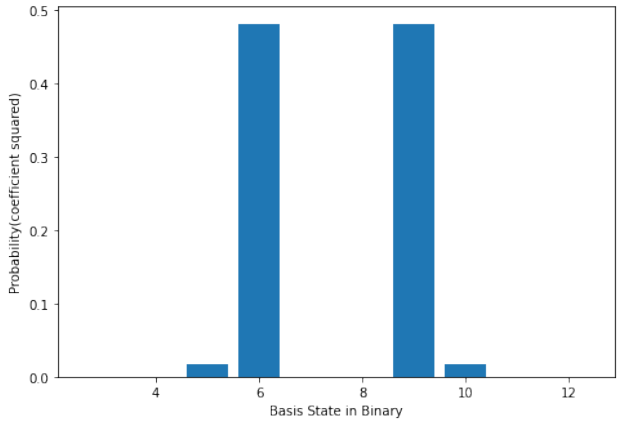

Figure 4: Basis State probabilities(N = 2)(U = 10)

$|\downarrow \quad \uparrow\rangle$ *or* $|\uparrow \quad \downarrow\rangle$ has the maximum probability.

6.2 N = 4 cases

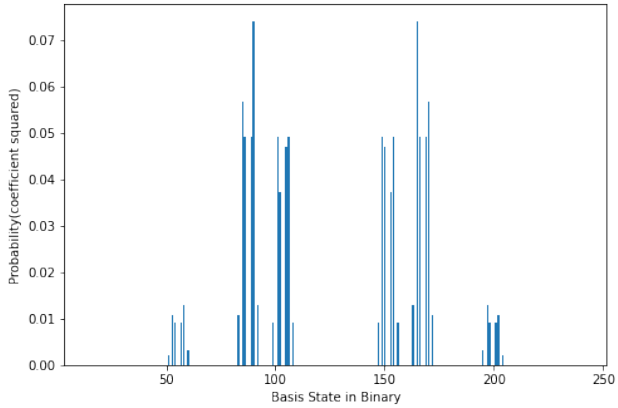

Figure 5: Basis State probabilities(N = 2)(U = 0.5)

$|\downarrow\ \uparrow\ \downarrow\ \uparrow\rangle$ or $|\uparrow\ \downarrow\ \uparrow\ \downarrow\rangle$ has the maximum probability.

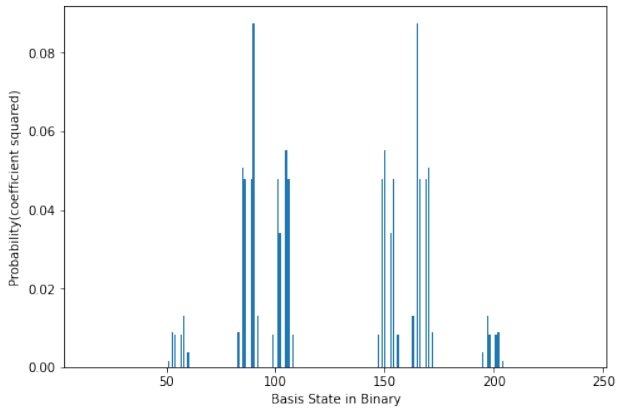

Figure 6: Basis State probabilities(N = 2)(U = 1)

$|\downarrow\ \uparrow\ \downarrow\ \uparrow\rangle$ or $|\uparrow\ \downarrow\ \uparrow\ \downarrow\rangle$ has the maximum probability.

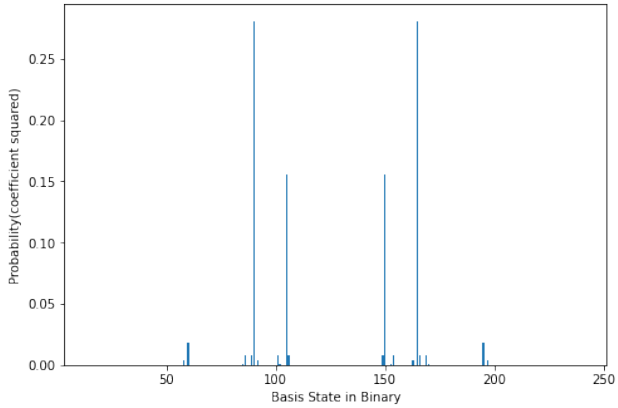

Figure 7: Basis State probabilities(N = 2)(U = 10)

$|\downarrow \uparrow \downarrow \uparrow\rangle$ or $|\uparrow \downarrow \uparrow \downarrow\rangle$ has the maximum probability.

6.3 N = 6 cases

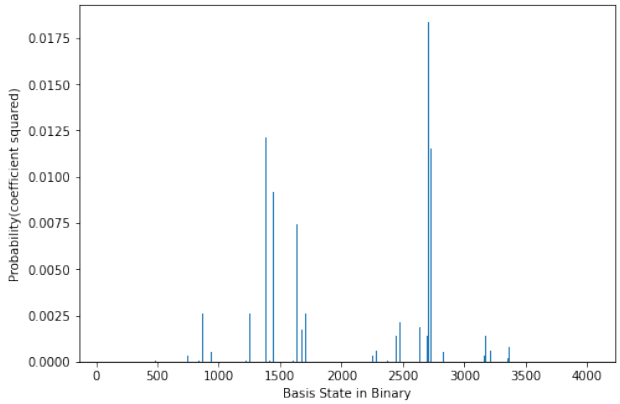

Figure 8: Basis State probabilities(N = 6)(U = 0.5)

$|\uparrow \downarrow \uparrow \downarrow \uparrow \downarrow\rangle$ or $|\downarrow \uparrow \downarrow \uparrow \downarrow \uparrow\rangle$ has the maximum probability.

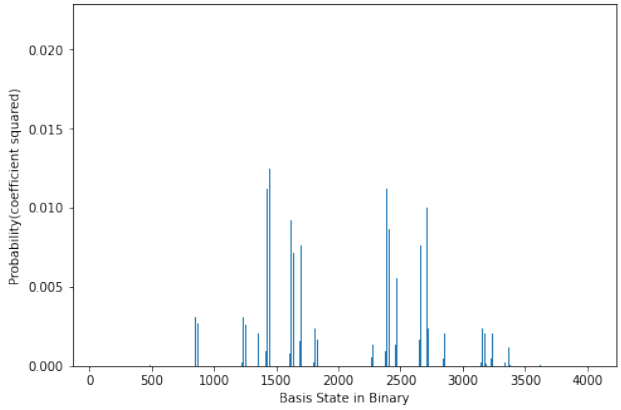

Figure 9: Basis State probabilities(N = 6)(U = 1)

$|\uparrow \downarrow \uparrow \downarrow \uparrow \downarrow\rangle$ or $|\downarrow \uparrow \downarrow \uparrow \downarrow \uparrow\rangle$ has the maximum probability.

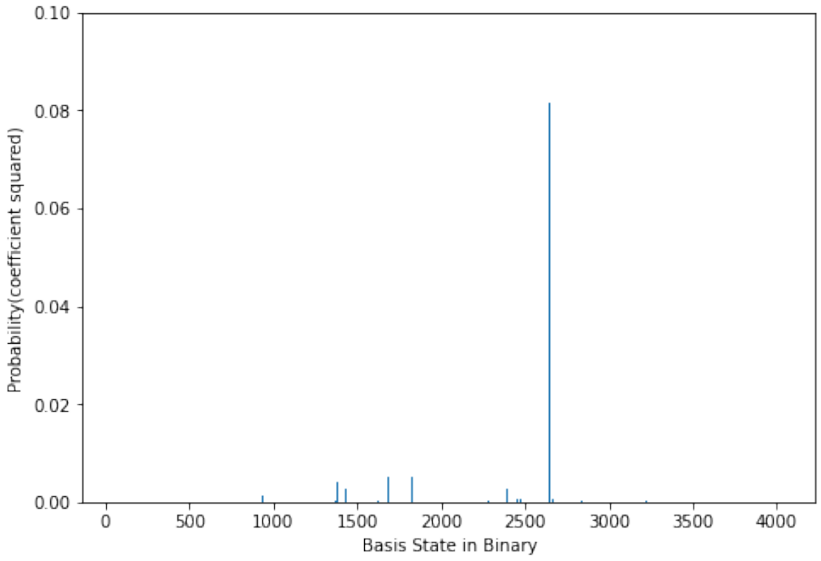

Figure 10: Basis State probabilities(N = 6)(U = 10)

$|\uparrow \downarrow \uparrow \downarrow \uparrow \downarrow\rangle$ or $|\downarrow \uparrow \downarrow \uparrow \downarrow \uparrow\rangle$ has the maximum probability.

7 Conclusion

We faced difficulties with constructing Hamiltonian Matrices for N = 8 and higher. We were thinking in the direction of sparse matrix implementations or ways to optimise the code where the Hamiltonian is constructed. The lanczos iteration gives the ground state energy at similar time complexity to the inbuilt scipy function.

8 References

1) arxiv.org/abs/0807.4878
2) Lanczos iteration code forked from github https://github.com/awietek
3) Youtube lectures on Lanczos iteration by Prof Slim Belhaiza