Exact Diagonalization of the Hubbard Model using Lanczos iteration

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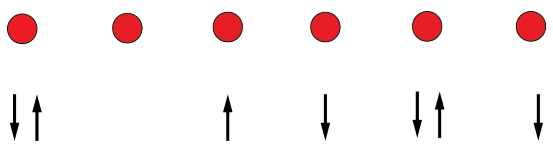
One Dimensional Hubbard model

$$H = H_{hop} + H_{int} = -t \sum_{<i,j>\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad (1)$$

- Introduced by John Hubbard in 1963.
- Endless source of interesting phenomena till date.
- Mott insulators, High Temperature superconductivity, Antiferromagnetism
- Basically, it introduces strong correlations between electrons through the interaction term, H_{int}
- Generally, hard to solve using numerics.



Dimensions

For a given system having say N sites, what are the total number of basis states possible? Answer is: quite a lot!

Sites	Dimensions
4	17364
6	3659878
8	810374138
10	185410906900
12	43308802153726

- For just 12 sites we reach hundreds of trillions of states!
- Number of elements in the Hamiltonian matrix will be square of that!
- Can we do anything to reduce this huge number?

Properties of the Hamiltonian

Total number of electrons

The Hamiltonian in (1) commutes with the total number of electrons, $\hat{N} = \sum_{i,\sigma} c^{\dagger}_{i\sigma} c_{i\sigma}$, i.e $[H, \hat{N}] = 0$, which means that any eigenfunction of the Hamiltonian has a fixed number of particles. So, we can **choose** to work with any number of electrons we please!

Spin sectors

The Hamiltonian, incredibly, also commutes with the up-spin and consequently down-spin number operators too, $[H, N_{\uparrow}] = 0$, where, $\hat{N}_{\uparrow} = \sum_i c^{\dagger}_{i\uparrow} c_{i\uparrow}$.

Half-filled system

The **half-filled** case is where the number of electrons in the system is the same as the number of sites, irrespective of spin.It has been of particular interest since it represents a natural situation where each atom(site) provides one electron to the system.
In this project we obtain the ground state wavefunctions of the Hubbard half-filled model using the Lanczos iteration algorithm.Subsequently, we check to see if these states display anti-ferromagnetism.
The dimensions are greatly reduced if we work with this number of electrons:

Sites	Dimensions	Reduced dimensions
4	17364	70
6	3659878	924
8	810374138	12870
10	185410906900	184756
12	43308802153726	2704156

Ordering the basis states

An example for $N = 2$. There are 3 spin sectors and 6 bases in total. Within a sector, the labels I are sectored. The elements in the Hamiltonian can be constructed by taking products $\langle\alpha| H |\beta\rangle$, between states $|\alpha\rangle$ and $|\beta\rangle$.However, since matrices are sparse, other techniques are employed.

S_z	**State**	$I_\downarrow$	$I_\uparrow$	$I = 2^N I_\downarrow + I_\uparrow$
2	$\|00\rangle_\downarrow \|11\rangle_\uparrow$	0	3	3
0	$\|01\rangle_\downarrow \|01\rangle_\uparrow$	1	1	5
0	$\|01\rangle_\downarrow \|10\rangle_\uparrow$	1	2	7
0	$\|10\rangle_\downarrow \|01\rangle_\uparrow$	2	1	9
0	$\|10\rangle_\downarrow \|10\rangle_\uparrow$	2	2	10
-2	$\|11\rangle_\downarrow \|00\rangle_\uparrow$	3	0	12

Table: Basis states for $N = 2$

The Lanczos Algorithm

- Since the dimensions of H is so large, normal methods like QR diagonalization do not apply.
- Lanczos iteration maps H, a $n \times n$ matrix to a smaller matrix $\mathrm{T}(m \times m)$, using an orthogonal transformation O where the columns of O are a set of m vectors generated recursively through the formula:

$$u_{k+1} = Hv_k - \alpha_k v_k - \beta_k v_{k-1}$$

where $\alpha_k = v_k^T H v_k$ and $\beta_k = v_{k-1}^T H v_k$.

$$T_{mm} = \begin{pmatrix} \alpha_1 & \beta_2 & & & & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & & \beta_m & \alpha_m \end{pmatrix}$$

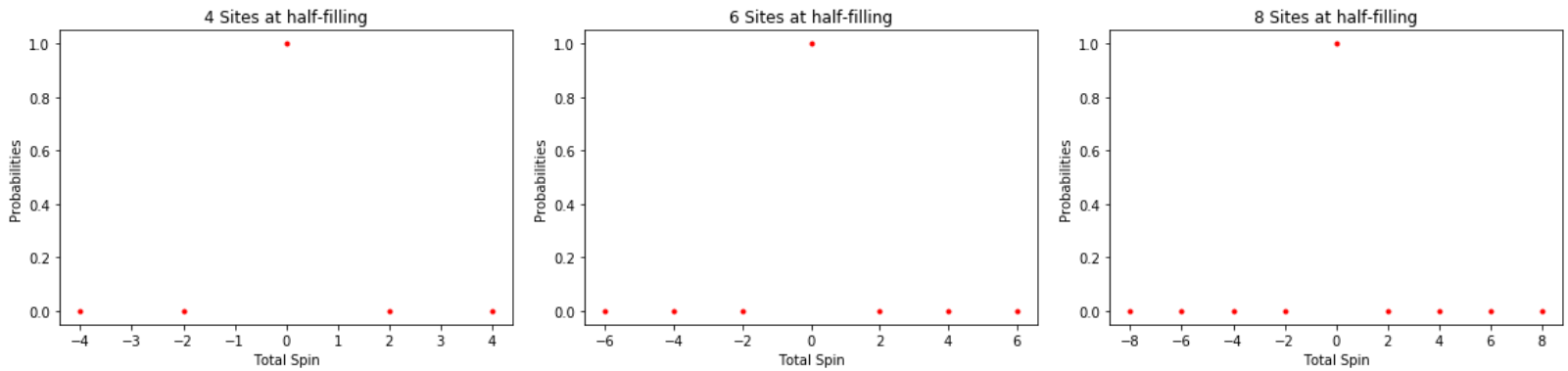
The Lanczos Algorithm

- $T = O^T H O$, is a tridiagonal matrix that can be diagonalized by usual methods.
- The largest eigenvalues of T approximate those of H.The eigenvectors are obtained through the transformation $x_k \approx O x_k^{'}$.
- Finding eigenvalues of large matrices is not a problem, as the algorithm needs to store only three **large** vectors per iteration.
- However, to get the eigenvectors, we need to store all m vectors which can take a toll on memory.
- Ground states have largest energy magnitude in half-filled Hubbard.

$$T_{mm} = \begin{pmatrix} \alpha_1 & \beta_2 & & & & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & & \beta_m & \alpha_m \end{pmatrix}$$

Ground states across spin sectors

We sum the probabilities in each spin sector and present the results for different cases. We see the for all the cases of $N = 4, 6$ and 8, the wavefunction is strictly limited to the spin-0 sector, as was expected:

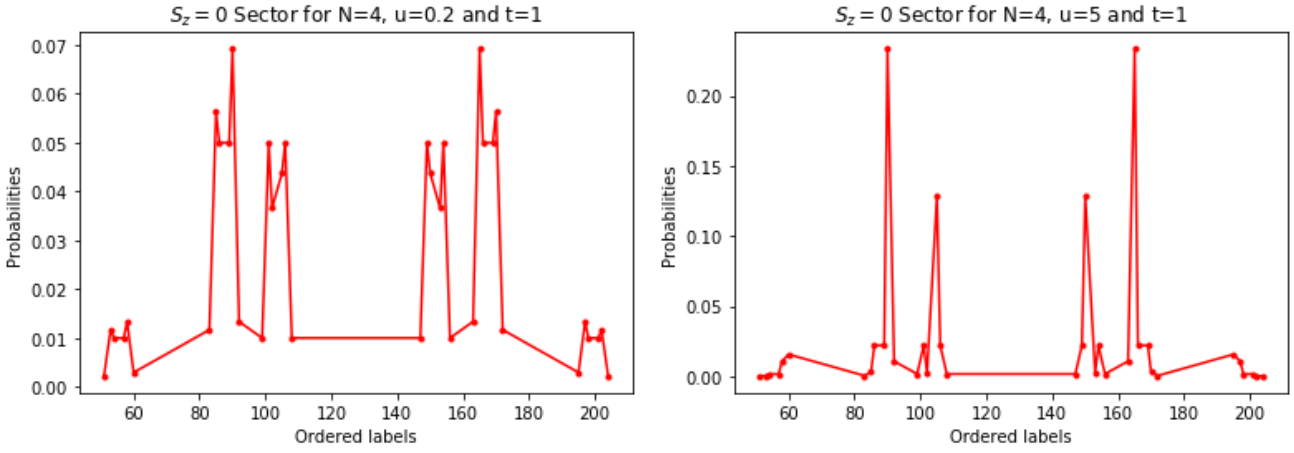


A closer look- Antiferromagnetism

We are interested in determining whether these ground states are anti-ferromagnetic.The fact that the wavefunction lies entirely in the $S_z = 0$ sector gives us hope, as anti-ferromagnetism in an even site chain would require an equal number of spin-up and spin-down electrons.
First of all we determine the labels of the required states.
$N = 4$ anti-ferro states are: $|\uparrow\downarrow\uparrow\downarrow\rangle \equiv |0101\rangle_{\downarrow} |1010\rangle_{\uparrow} \equiv I = 90$ and $|\downarrow\uparrow\downarrow\uparrow\rangle \equiv |1010\rangle_{\downarrow} |0101\rangle_{\uparrow} \equiv I = 165$
Similarly, the labels for $N = 6$ are 1386 and 2709, whereas $N = 8$, the labels are: 21930 and 43605.

A closer look- Antiferromagnetism, $N = 4$

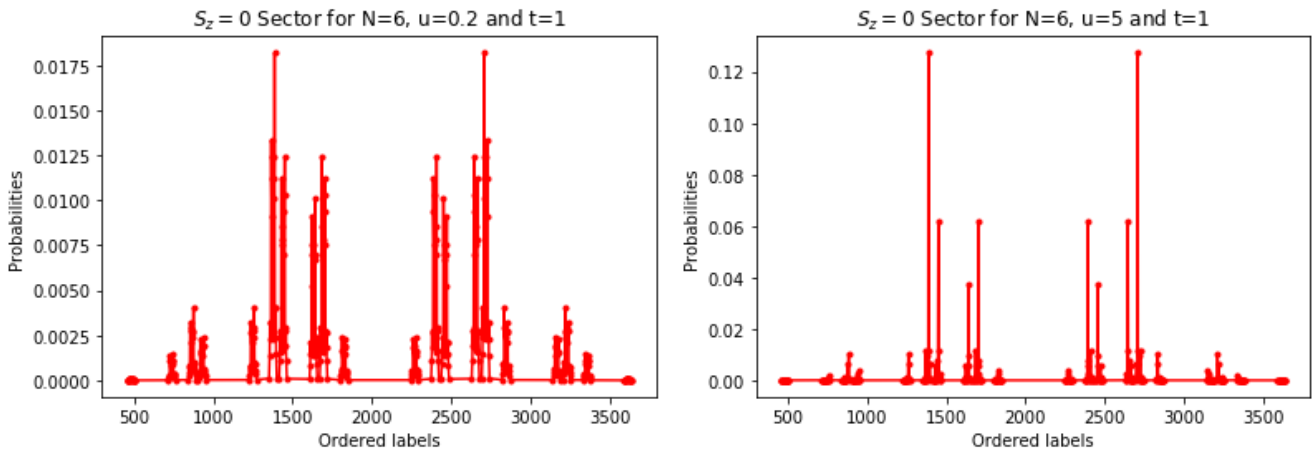
We present the distribution acquired for the $N = 4$ case, the eigenvalues are -4.276 and -1.657.(from left to right)



The peaks in both the graphs exactly correspond to the labels calculated earlier. A trend however, is noted, as the on-site repulsion, U increases there is more probability of two electrons not occupying a single site and hence there is more contribution from the anti-ferromagnetic states.

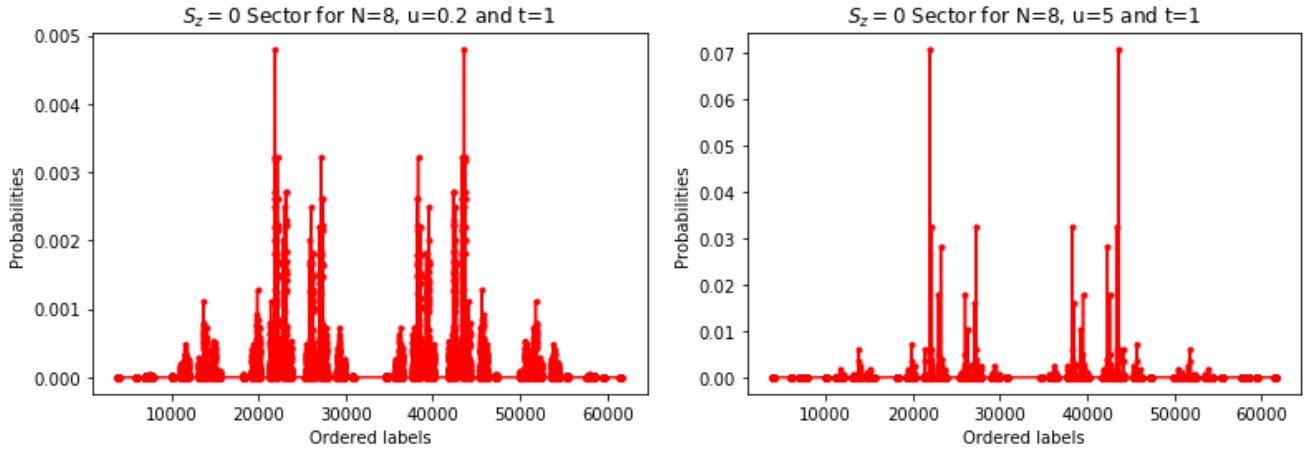
A closer look- Antiferromagnetism, $N = 6$

The case for 6 sites is similar,with eigenvalues of -6.694 and -2.624.The peaks correspond to labels of 1386 and 2709:



A closer look-Antiferromagnetism, $N = 8$

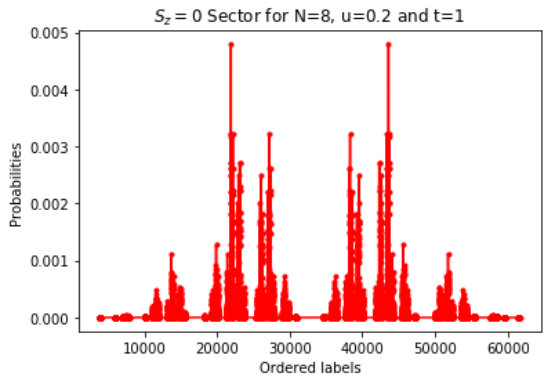
The case for 8 sites is similar with eigenvalues of -9.125 and -3.5934:



Peaks are exactly at the labels of 21930 and 43605.Hence, we can conclude that the Hubbard model indeed exhibits anti-ferromagnetism for these lattices.
In all these cases, an increase in on-site repulsion leads to sharper peaks and more anti-ferromagnetism.

An **even** closer look- Antiferromagnetism

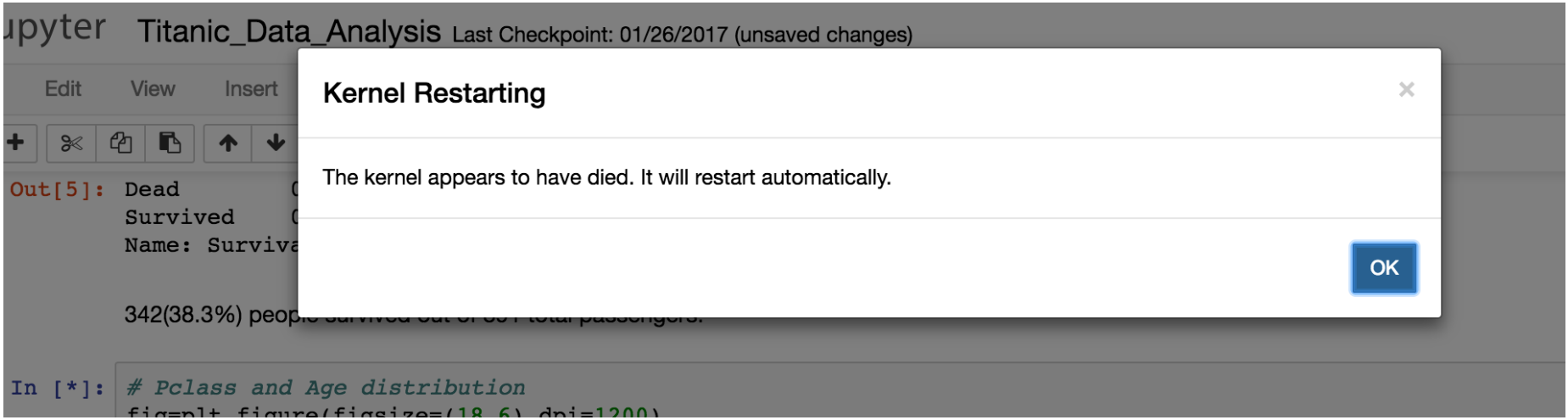
What are the two secondary cluster of peaks that are present in every graph?
For $N = 4$, it turns out that these "second" peaks refer to the states of $|\downarrow\downarrow\uparrow\uparrow\rangle \equiv 165$ and $|\downarrow\downarrow\uparrow\uparrow\rangle \equiv 165$
So, unlike the original anti-ferro states, which have one unit of $\uparrow$ and one of $\downarrow$ repeating alternatively, these states have instead $\uparrow\uparrow$ and $\downarrow\downarrow$ alternating!!
In fact, for all the other sizes too, it can be checked that these "secondary peaks" indeed correspond to such type of states.
What about three units repeating, $\uparrow\uparrow\uparrow$ and $\downarrow\downarrow\downarrow$? Do these correspond to the third largest peaks which are situated near the ends of the graphs?



The curious case of $N = 10$

- For just 10 sites at half-filling, there are 184756 basis states $\implies$ 10 million matrix elements! Lanczos iteration cannot be carried out for more than 50 steps.Bad results are produced where wavefunction isn't limited to just one sector.
- Can anything be done?
- An inspired guess would be to look for the ground state in the $S_z = 0$ sector. We can assume that just like its predecessors, the ground state would lie in this sector, which also makes sense from symmetry arguments(unless the GS suddenly decides to become degenerate).
- Working only in $S_z = 0$, the dimension is further reduced from 184756 to 63504.Quite a fall.
- If we use this for say 100 iterations, python gives some interesting results...

Oops!



Python literally died.

In conclusion

- Exact diagonalization is a **bad** idea for large systems.Analytical methods can prove to be far more powerful in extracting useful information.
- We successfully investigated and confirmed the existence of anti-ferromagnetism for ground states in sites of size 4, 6 and 8 using the Lanczos iteration method to exactly diagonalize the Hamiltonian. We also obtained the energy eigenvalues.
- The ground states are found to have some sort of fondness for **ordered** states.
- The cases for $N = 10$ and 12 were found to be beyond the reach of the humble 2 GB DDR3 RAM.