Exact Diagonalization Code

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1 Basis elements

For the 4-site Hubbard model at half filling with $S_z = 0$, there are in total 36 basis elements. I used a string of binaries to represent occupied and unoccupied momenta. Four entries represent four momenta, small to large, from right to left, shown below:

$$(a, b, c, d)$$
$$(3\pi/2, \pi, \pi/2, 0)$$

For example, $(0, 0, 1, 1)$ means momenta 0 and $\pi/2$ are occupied; $(1, 0, 1, 0)$ means momenta $\pi/2$ and $3\pi/2$ are occupied. I then gave each and every four-binary string a index:

$$0011 \to 1$$
$$0101 \to 2$$
$$0110 \to 3$$
$$1001 \to 4$$
$$1010 \to 5$$
$$1100 \to 6$$

Since we have in total four electrons, this is just half of the picture. The other half is constructed by adding another four-binary string to these six. The index of the final string is defined using $6\cdot(i-1)+j$, where i is the index for the first string, j is the index for the second string. For example, to construct the basis element that represents $0\uparrow 2\uparrow 0\downarrow 1\downarrow$, we use $(0, 1, 0, 1)$ and $(0, 0, 1, 1)$, since

$$(0, 1, 0, 1) \to 0\uparrow 2\uparrow$$
$$(0, 0, 1, 1) \to 0\downarrow 1\downarrow$$

The whole string then becomes

$$(0, 1, 0, 1, 0, 0, 1, 1) \to 0\uparrow 2\uparrow 0\downarrow 1\downarrow$$

Notice I put the string for up spins first. The index for the first string is 2, and the second one is 1, so the total index for $(0, 1, 0, 1, 0, 0, 1, 1)$ is then $6 \cdot (2 - 1) + 1 = \mathbf{7}$. Below I attach a figure showing all basis elements directly from the code.

2 Hamiltonian

The Hamiltonian I used is:

$$H = \sum_{k\sigma} \epsilon(k) n_{k\sigma} - \frac{U}{4} \sum_{k_1,k_2,k_3} c^\dagger_{k_1+k_2-k_3\uparrow} c^\dagger_{k_3\downarrow} c_{k_2\uparrow} c_{k_1\downarrow}, \tag{1}$$

where $\epsilon(k) = -2tcos(k)$. Note the minus sign here. It's because I swap the $c_{k_2\uparrow}$ and $c^\dagger_{k_3\downarrow}$ operators.

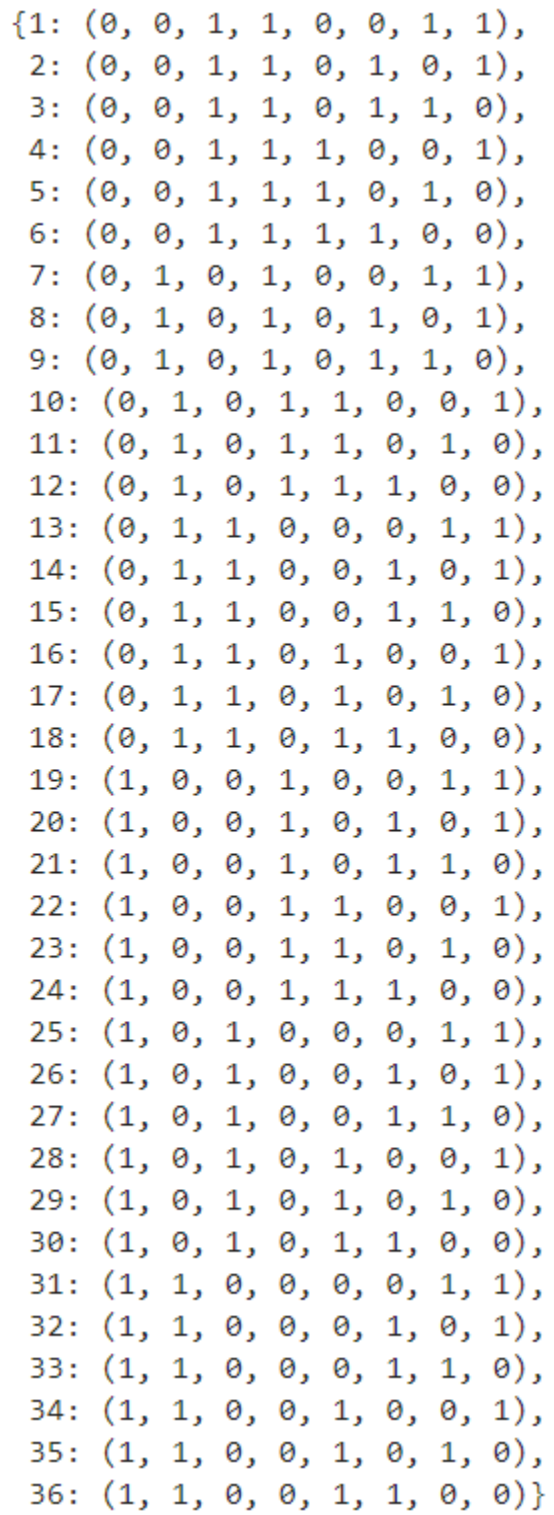

Figure 1: All 36 basis elements and their indices. The first four binaries are up spins, the second four are down spins.

3 Matrix construction

The U matrix is created by applying $c^{\dagger}_{k_1+k_2-k_3\uparrow}c^{\dagger}_{k_3\downarrow}c_{k_2\uparrow}c_{k_1\downarrow}$ operator to each basis element for different k_1, k_2, and k_3, and then project the resulted row vector onto column vectors. Indices k_1, k_2, and k_3 cover every possible excitation, for example, for the basis element $(0,1,1,0,1,1,0,0)$, k_1 can be 2 or 3, k_2 can be 5 or 6, and k_3 can be 0 or 1. Note here the indices are inverted, meaning 0 to 7 runs from the far right to the left-most index. Finally $k_1+k_2-k_3$ takes whichever index available. For example, if we picked $k_1=2$, $k_2=5$, $k_3=0$, and then the other index has to be $2+5-0=7$, to conserve momentum, the resulted state is $(1,1,0,0,1,0,0,1)$, the first annihilation operator commutes through 3 operators; the second commutes through 1 operator; the third commutes through 2 operators, and the last commutes through 0 operators. So the total sign is $+1$. $(1,1,0,0,1,0,0,1)$ has a total index of 34, so one of the possible excitation from $(0,1,1,0,1,1,0,0)$ is $|34\rangle$.

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row(18)
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[[1, '34'], [1, '4'], [-1, '29'], [1, '8'], [-1, '33'], [-1, '3']]
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Figure 2: $(0,1,1,0,1,1,0,0)$ has a total index of 18, therefore the function $row(18)$ outputs all possible excitations of this basis element, and their corresponding signs.

The corresponding matrix element is then constructed by projecting the row element onto columns, for example,

$$\langle 29|\, U\, |2\rangle = -1,$$
$$\langle 8|\, U\, |2\rangle = 1.$$

I then run the *row* function for all 36 basis elements, and then use such projection method to construct all $36x36$ matrix elements. That's the method I used in my exact diagonalization code.

The T matrix is simple. One just use a function that runs through a string of a basis element, recording all nonzero entries and their positions k. Using the equation $\epsilon(k) = -2cos(k)$ for all k values, and sum them all up. Here k takes values of $3\pi/3$, π, $\pi/2$, and 0, going from left to right.