

BUILDING SPARSE XX HAMILTONIAN

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The XX Hamiltonian is given by

$$H = J \sum_{j=1}^{N-1} \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y \right) - h \sum_{j=1}^N \sigma_j^z = H_{xy} + H_z, \quad (1)$$

where

$$\sigma_j^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_j^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_j^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2)$$

Notice that they come in pairs in the xy-Hamiltonian, such that

$$\sigma_j^x \sigma_{j+1}^x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \sigma_j^y \sigma_{j+1}^y = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}. \quad (3)$$

Therefore, the components of H are always real. Now, we can try to find a pattern. Let's assume $J = h = 1$ and start with the 2-site Hamiltonian.

$$H^{(2)} = \sigma^x \otimes \sigma^x + \sigma^y \otimes \sigma^y - \sigma^z \otimes \sigma^0 - \sigma^0 \otimes \sigma^z = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix}. \quad (4)$$

H_z is always going to have a single σ^z matrix with $N - 1$ identity matrices at the remaining sites. Then, we can write it as

$$H_z = - \sum_{i=0}^{N-1} \sigma^0 \otimes \cdots \otimes \sigma_i^z \otimes \cdots \otimes \sigma^0. \quad (5)$$

The following pattern is observed:

- If σ^z is at the N -th site position, then $1, -1$ alternate in the diagonal, namely

$$\sigma^0 \otimes \cdots \otimes \sigma^z = \text{diag}(1, -1, 1, -1, \dots, 1, -1)$$

- If σ^z is at the $(N-1)$ -th site position, then $1, 1, -1, -1$ alternate in the diagonal, namely

$$\sigma^0 \otimes \cdots \otimes \sigma^z \otimes \sigma^0 = \text{diag}(1, 1, -1, -1, \dots, 1, 1, -1, -1)$$

- If σ^z is at the first site position, then $\underbrace{1, \dots, 1}_{2^{N-1} \text{ times}}, \underbrace{-1, \dots, -1}_{2^{N-1} \text{ times}}$ alternate in the diagonal, namely

$$\sigma^z \otimes \cdots \otimes \sigma^0 = \text{diag}(1, 1, -1, -1, \dots, 1, 1, -1, -1)$$

Therefore, the j -th diagonal component of the i -th term of $-H_z$ is given by

$$F_{ij} = (-1)^{\lfloor \frac{j}{2^i} \rfloor}. \quad (6)$$

In this terms, the j -th diagonal component of $-H_z$ is

$$G_j = \sum_{i=0}^{N-1} F_{ij} = \sum_{i=0}^{N-1} (-1)^{\lfloor \frac{j}{2^i} \rfloor} \quad (7)$$

and finally,

$$H_z = -h \text{diag} (G_0, G_1, \dots, G_{2^N-1}) = -h \text{diag} \left(N, \sum_{i=0}^{N-1} (-1)^{\lfloor \frac{1}{2^i} \rfloor}, \dots, \sum_{i=0}^{N-1} (-1)^{\lfloor \frac{2^N-2}{2^i} \rfloor}, -N \right). \quad (8)$$

Now, we can work on the planar Hamiltonian H_{xy}

$$H_{xy}^{(2)} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (9)$$

$$H_{xy}^{(3)} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \end{pmatrix}, \quad (10)$$

$$H_{xy}^{(4)} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \end{pmatrix}. \quad (11)$$

We can build $H^{(n)}$ recursively by making $I \otimes H^{(n-1)}$ and then filling $(\pm 2^{n-2})$ -th diagonal (the main diagonal is taken as the 0-th diagonal) with 2s from its (2^{n-2}) -th to its $(2^{n-1} - 1)$ -th component.

As our approach is recursive, we start from the non-zero elements of $H_{xy}^{(2)}$ and build the non-zero elements of the next matrices. These matrices are symmetric, so we can work only with the lower triangular part.

From $H_{xy}^{(2)}$, ($N = 2$) the non-zero entries are

$$L_2 = \{(2, 1)\}. \quad (12)$$

For the next matrix, ($N = 3$),

$$L_3 = \{(2, 1), (\textcolor{red}{2} + 2^{N-1}, \textcolor{red}{1} + 2^{N-1}), (2^{N-1}, 2^{N-2}), (2^{N-1} + 1, 2^{N-2} + 1)\},$$

$$L_3 = \{(2, 1), (\textcolor{red}{6}, \textcolor{red}{5}), (\textcolor{blue}{4}, \textcolor{blue}{2}), (\textcolor{blue}{5}, \textcolor{blue}{3})\}. \quad (13)$$

For the next matrix, ($N = 4$),

$$L_4 = \{(2, 1), (6, 5), (4, 2), (5, 3), (\textcolor{red}{10}, \textcolor{red}{9}), (\textcolor{red}{14}, \textcolor{red}{13}), (\textcolor{red}{12}, \textcolor{red}{10}), (\textcolor{red}{13}, \textcolor{red}{11}), (\textcolor{blue}{8}, \textcolor{blue}{4}), (\textcolor{blue}{9}, \textcolor{blue}{5}), (\textcolor{blue}{10}, \textcolor{blue}{6}), (\textcolor{blue}{11}, \textcolor{blue}{7})\}. \quad (14)$$

The **red color** indicates copying the matrix in the bottom right part of the identity whereas **blue** accounts for filling the -2^{n-1} diagonal.

In general, the non-zero elements of $H_{xy}^{(N)}$, which have a value of $2J$, are located at

$$L_N = \{L_{N-1}, \{\textcolor{red}{L}_{N-1} \oplus (2^{N-1}, 2^{N-1})\}, \{(2^{N-1} + j, 2^{N-2} + j)\}_{j=0,1,\dots,2^{N-2}}\}. \quad (15)$$

Finally, the planar Hamiltonian can be built as

$$[H_{xy}]_{ij} = 2J\delta_{(i,j),L_N} \quad (16)$$