BUILDING SPARSE XX HAMILTONIAN

Alejandro Gómez Cadavid

1. Pure case

The XX Hamiltonian is given by

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

where

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

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

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

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.

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

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

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

The following pattern is observed:
- If σ^z is at the N-th site position, then $1, -1$ alternate in the diagonal, namely
$$\sigma^0 \otimes \cdots \otimes \sigma^z = \mathrm{diag}(1, -1, 1, -1, \cdots, 1, -1)$$
- If σ^z is at the (N-1)-th site position, then $1, 1, -1, -1$ alternate in the diagonal, namely
$$\sigma^0 \otimes \cdots \otimes \sigma^z \otimes \sigma^0 = \mathrm{diag}(1, 1, -1, -1, \cdots, 1, 1, -1, -1)$$
- If σ^z is at the first site position, then $\underbrace{1, \cdots, 1}_{2^{N-1} \text{ times}}, \underbrace{-1, \cdots, -1}_{2^{N-1} \text{ times}}$ alternate in the diagonal, namely
$$\sigma^z \otimes \cdots \otimes \sigma^0 = \mathrm{diag}(1, 1, -1, -1, \cdots, 1, 1, -1, -1)$$

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

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

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

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

and finally,

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

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

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

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

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

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

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

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

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

$$L_3 = \big\{(2,1), (6,5), (4,2), (5,3)\big\}. \tag{13}$$

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

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

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

$$\boxed{L_N = \big\{L_{N-1}, \big\{L_{N-1} \oplus (2^{N-1}, 2^{N-1})\big\}, \big\{(2^{N-1}+j, 2^{N-2}+j)\big\}_{j=0,1,\cdots,2^{N-2}}\big\}.} \tag{15}$$

Finally, the planar Hamiltonian can be built as

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

2. Impure case

The Hamiltonian is given by

$$H = J\sum_{j=1}^{N-1}\Big(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y\Big) - \sum_{j=1}^{N}\Big[h + \delta h(\delta_{j,p} + \delta_{j,q})\Big]\sigma_j^z = H_{xy} + H_z, \tag{17}$$

where q, p are the impurities positions

$$(p,q) = \left(\frac{N-d-1}{2}, \frac{N+d}{2}\right) \qquad \text{if} \quad N \quad \text{is even,} \tag{18}$$

$$(p,q) = \left(\frac{N-d-2}{2}, \frac{N+d}{2}\right) \qquad \text{if} \quad N \quad \text{is odd.} \tag{19}$$

The transverse Hamiltonian must be corrected to include impurities,

$$G_j = \sum_{i=0}^{N-1}\Big[h + \delta h(\delta_{j,p} + \delta_{j,q})\Big](-1)^{\lfloor\frac{j}{2^i}\rfloor} \tag{20}$$

and

$$H_z = -\,\mathrm{diag}\left(G_0, G_1, \cdots, G_{2^N-1}\right).$$
(21)