XY model chain

Jose Alejandro Montana Cortes

April 2020

At the very start we started defining what canonical typicality was and in that sense we started to find a problem that could be have the following properties

- It is necessary to know the precise state of the universe, so we have to be able to solve analytically our universe¹
- We also need to compute reduced states not only for single states but for products of two different states.

Having this in mind we present here an introduction to the XY model in 1D. The XY Hamiltonian models is a set of N spin 1/2 particles located on the sites of d- dimensional lattice. In the rest of the document when we refer to the XY model we will always be referring to the 1D XY model.

A chain of N spins where each spin is able to interact with its nearest neighbours and having the freedom in its spin to interact on the plane XY with an external magnetic field is described by the Hamiltonian

$$H_{XY} = -\frac{1}{2} \sum_{l=0}^{N-1} \left(\frac{1+\gamma}{2} \sigma_l^x \sigma_{l+1}^x + \frac{1-\gamma}{2} \sigma_l^y \sigma_{l+1}^y + \lambda \sigma_l^z \right)$$
(1)

where γ is so-called the anisotropy parameter and represents the difference between the strength of the xx interaction and the yy interaction², λ is the intensity of the external magnetic field and σ_l^i is the pauli matrix (i=x,y,z) acting over the l site of the chain.

The XY model is a model that has been widely studied for a variety of values of λ and γ and in some limits it has a correspondence to other models of interest in condensed matter³.

¹It is expensive specially we we talk about the Hilbert space which grows exponentially.

²Of course here we talk about the interaction in the spin space.

³Some examples of this are the boson Hubbard model in the limit of hard bosons, $\gamma=1$ correspond to the Ising model. The kitaev chain is equivalent to the XY model under a proper identification of the parameters $\mu,\,t$ and Δ with γ and λ

1 The spectrum

To find the spectrum of the Hamiltonian (1) we need to perform some transformations.

1.1 Jordan-Wigner Transformation

we first considert the non local transformation given by

$$\hat{b}_l = \left(\prod_{m < l} \sigma_m^z\right) \sigma_l^-, \quad \sigma_l^- = \frac{\sigma_l^x - i\sigma_l^y}{2}, \tag{2}$$

where these b_l represent spinless fermionic operators because they follow canonical anticommutation relation (CAR)

$$\left\{\hat{b}_i^{\dagger}, \hat{b}_j^{\dagger}\right\} = \left\{\hat{b}_i, \hat{b}_j\right\} = 0, \quad \left\{\hat{b}_i^{\dagger}, \hat{b}_j\right\} = \delta_{i,j}, \tag{3}$$

So inverting the transformation we get

$$\sigma_l^z = 1 - 2\hat{b}_l^{\dagger} \hat{b}_l
\sigma_l^x = \left(\prod_{m < l} \left(1 - 2\hat{b}_m^{\dagger} \hat{b}_m\right)\right) \left(\hat{b}_l^{\dagger} + \hat{b}_l\right)
\sigma_l^y = i \left(\prod_{m < l} \left(1 - 2\hat{b}_m^{\dagger} \hat{b}_m\right)\right) \left(\hat{b}_l^{\dagger} - \hat{b}_l\right),$$
(4)

so the terms of interaction in the Hamiltonian will look as

$$\hat{\sigma}_{l}^{x}\hat{\sigma}_{l+1}^{x} = \left(\hat{b}_{l}^{\dagger} - \hat{b}_{l}\right)\left(\hat{b}_{l+1}^{\dagger} + \hat{b}_{l+1}\right)
\hat{\sigma}_{l}^{y}\hat{\sigma}_{l+1}^{y} = -\left(\hat{b}_{l}^{\dagger} + \hat{b}_{l}\right)\left(\hat{b}_{l+1}^{\dagger} - \hat{b}_{l+1}\right)$$
(5)

so the Hamiltonian look like,

$$H_{XY} = -\frac{1}{2} \sum_{l} \left[\left(\hat{b}_{l+1}^{\dagger} \hat{b}_{l} + \hat{b}_{l}^{\dagger} \hat{b}_{l+1} \right) + \gamma \left(\hat{b}_{l}^{\dagger} \hat{b}_{l+1}^{\dagger} - \hat{b}_{l} \hat{b}_{l+1} \right) \right] - \frac{\lambda}{2} \sum_{l} \left(1 - 2 \hat{b}_{l}^{\dagger} \hat{b}_{l} \right), \tag{6}$$

after the transformation. The term of $-\lambda N/2$ is ignored since it cause only an gauge of the spectrum in the energy.

1.2 Fourier Transformation

It is possible to exploit an other symmetry in the system, to do so it is possible to consider periodic boundary conditions (PBC), which is done by identifying the spin in the site N with the spin in the site 1. After imposing this we have that the Fourier transform of the operator \hat{b}_l will look as

$$\hat{d}_k = \frac{1}{\sqrt{N}} \sum_{l=1}^{N} \hat{b}_l e^{-i\phi_k l},\tag{7}$$

with $\theta_k = \frac{2\pi}{N}k$.

Since the Fourier transformation is unitary, the operators \hat{d}_k will preserve the CAR.

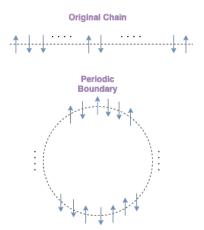


Figure 1: Illustration of what a boundary condition means in the case of our spin chain

The Hamiltonian can be then written in terms of the operators \hat{d}_k as

$$H_{XY} = \sum_{k=-(N-1)/2}^{(N-1)/2} (-\lambda + \cos \phi_k) \, \hat{d}_k^{\dagger} \hat{d}_k + \frac{i\gamma}{2} \sum_{k=-(N-1)/2}^{(N-1)/2} \sin \phi_k \left(\hat{d}_k \hat{d}_{-k} + h.c \right), \tag{8}$$

where we have ignored an additional term which is proportional to 1/N which will vanish for in the thermodynamic limit $N \to \infty$, which is our case of interest.

1.3 Bogoliubov - Valantin Transformation

As mentioned before fermionic quadratic Hamiltonians as the last one can easily be diagonalised via a Bogoliubov-Valantin transformation over the operators \hat{d}_k

$$\tilde{d}_k = u_k \hat{d}_k^{\dagger} + i v_k \hat{d}_{-k} \tag{9}$$

Since we want this transformation to preserve CAR, it is needed that $u_k^2 + v_k^2 = 1$, which implies that we can use the parametrization $u_k = \cos(\psi_k/2)$ and $v_k = \sin(\psi_k/2)$, with

$$\cos \frac{\psi_k}{2} = \frac{-\lambda + \cos \phi_k}{\sqrt{(\lambda - \cos \phi_k)^2 + (\gamma \sin \phi_k)^2}}$$
(10)

So finally our Hamiltonian will look as

$$H_{XY} = \sum_{-(N-1)/2}^{(N-1)/2} \tilde{\Lambda}_k \tilde{d}_k^{\dagger} \tilde{d}_k \tag{11}$$

with

$$\tilde{\Lambda}_k := \sqrt{\left(\lambda - \cos \phi_k\right)^2 + \left(\gamma \sin \phi_k\right)^2} \tag{12}$$

where the latter expression allow us to identify the critical regions of the model.

2 Fermionic Covariance Matrix for the XY model

Since we have to work with products of states which are completely characterised by its second moments, it turns out, for convenience, to work with the fermionic covariance matrix of the model XY. So to do this we need to be able to express the Hamiltonian (1) in terms of Majoranana fermions. This can be done by using an analogous of the Jordan Wigner transformation use to diagonalised the XY Hamiltonian but now we apply it to the 2N Majorana fermions

$$\hat{\gamma}_l = \left(\prod_{m < l} \hat{\sigma}_m^z\right) \hat{\sigma}_l^x, \quad \hat{\gamma}_{l+N} = \left(\prod_{m < l} \hat{\sigma}_m^z\right) \hat{\sigma}_l^y, \tag{13}$$

where again $l = 1, 2 \dots N - 1$

$$\begin{cases} \frac{-(N-1)}{2} & 0 & i & \frac{N-1}{2} \\ & \ddots & & \ddots \\ \frac{-(N-1)}{2} & 0 & i & \frac{N-1}{2} \\ \end{cases}$$
 Majorana
$$\begin{cases} \frac{N-1}{2} & & & \frac{N-1}{2} \\ \frac{N-1}{2} & & & \frac{3N-1}{2} \end{cases}$$

Figure 2: Illustration of how the spins in the chain are mapped to the Majorana fermions.

and similarly as before we have that

$$\hat{\gamma}_l \hat{\gamma}_{l+N} = \left(\prod_{m < l} \hat{\sigma}_m^z\right) \left(\prod_{m < l} \hat{\sigma}_m^z\right) \hat{\sigma}_l^x \hat{\sigma}_l^y = i \hat{\sigma}_l^z \tag{14}$$

$$\hat{\gamma}_{l+N}\hat{\gamma}_{l+1} = \left(\prod_{m< l} \hat{\sigma}_m^z\right) \hat{\sigma}_l^y \left(\prod_{m< l+1} \hat{\sigma}_m^z\right) \hat{\sigma}_{l+1}^x = \hat{\sigma}_l^y \hat{\sigma}_l^z \hat{\sigma}_{l+1}^x = i\hat{\sigma}_l^x \hat{\sigma}_{l+1}^x \qquad (15)$$

$$\hat{\gamma}_l \hat{\gamma}_{l+N+1} = \left(\prod_{m < l} \hat{\sigma}_m^z\right) \hat{\sigma}_l^x \left(\prod_{m < l+1} \hat{\sigma}_m^z\right) \hat{\sigma}_{l+1}^y = \hat{\sigma}_l^x \hat{\sigma}_l^z \hat{\sigma}_{l+1}^y = -i\hat{\sigma}_l^y \hat{\sigma}_{l+1}^y \qquad (16)$$

Which coincide, up to constant factors the three terms in the Hamiltonian (1). This will lead us to a Hamiltonian of the form

$$H_{XY} = \frac{i}{4} \sum_{\alpha,\beta=0}^{2N} \Omega_{\alpha\beta} \left[\hat{\gamma}_{\alpha}, \hat{\gamma}_{\beta} \right]$$
 (17)

where Ω is the antisymmetric matrix of the form

$$\Omega = \left[\begin{array}{c|c} 0 & \tilde{\Omega} \\ \hline -\tilde{\Omega}^T & 0 \end{array} \right],\tag{18}$$

with

$$\tilde{\Omega} = \begin{pmatrix}
\lambda & \frac{1-\gamma}{2} & 0 & 0 & \dots & 0 & \frac{1+\gamma}{2} \\
\frac{1+\gamma}{2} & \lambda & \frac{1-\gamma}{2} & 0 & \dots & 0 & 0 \\
0 & \frac{1+\gamma}{2} & \lambda & \frac{1-\gamma}{2} & \dots & 0 & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots \\
\frac{1-\gamma}{2} & 0 & 0 & 0 & \dots & \frac{1+\gamma}{2} & \lambda.
\end{pmatrix}$$
(19)

In general (18) can be diagonalised via an orthogonal transformation O^4

$$\Omega = O \left[\begin{array}{c|c} 0 & \omega \\ \hline \omega & 0 \end{array} \right] O^T, \tag{20}$$

where $O \in O(2N)$ and written in terms of two smaller orthogonal matrices

$$O = \begin{bmatrix} O_1 & 0 \\ \hline 0 & O_2 \end{bmatrix}, \tag{21}$$

and ω is a diagonal matrix of size $N \times N$ which holds excitation numbers -1/2 + n. By doing the product of matrices in (20) we can easily see that

$$\tilde{\Omega} = O_1 \omega O_2^T, \tag{22}$$

which is nothing but the singular value decomposition of the matrix $\tilde{\Omega}$. The latter result tell us that a fast way to construct the matrix O, which diagonalise Ω , is to focus on $\tilde{\Omega}$.

A fact that we can exploit is that as is shown in equation (19) $\tilde{\Omega}$ is a circulant real matrix, meaning that it can be easily diagonalised by means of a Fourier transform. So we can write

$$\tilde{\Omega}_{mn} = \frac{1}{N} \sum_{\theta_k \in (-\pi, \pi)} \omega(\theta_k) e^{\phi(\theta_k)} e^{i(m-n)\theta_k}$$
(23)

where $\omega(\theta_k) = \omega(\theta_k)^* = \omega(-\theta_k)$, $\phi(\theta_k) = -\phi(\theta_k)$ and are given by

$$\omega^{2}(\theta_{k}) := (\lambda - \cos \theta_{k})^{2} + \gamma^{2} \sin^{2} \theta_{k}$$
(24)

⁴This special relation provide us a way to transform from spacial modes to excitation in the chain, so that we can either excite the chain and see what the spatial modes are or the other way.

and

$$\phi(\theta_k) := \arctan\left(\frac{\lambda - \cos \theta_k}{-\gamma \sin \theta_k}\right). \tag{25}$$

So expanding the equation (23) we get

$$\widetilde{\Omega}_{mn} = \frac{1}{N} \left[\omega(0) + (-1)^{m-n} \omega(\pi) + 2 \sum_{0 < \theta_k < \pi} \omega(\theta_k) \cos(\theta_k(m-n) + \phi(\theta_k)) \right]
= \frac{\omega(0)}{N} + (-1)^{m-n} \frac{\omega(\pi)}{N} + \sum_{0 < \theta_k \le \pi} \omega(\theta_k) \left(u_m^c(\theta_k) v_n^c(\theta_k) + u_m^s(\theta_k) v_n^s(\theta_k) \right),$$
(26)

where

$$u_{m}^{c}\left(\theta_{k}\right) = \sqrt{\frac{2}{N}}\cos\left(m\theta_{k} + \phi\left(\theta_{k}\right)\right), \quad u_{m}^{s}\left(\theta_{k}\right) = \sqrt{\frac{2}{N}}\sin\left(m\theta_{k} + \phi\left(\theta_{k}\right)\right) \quad (27)$$

$$v_n^c(\theta_k) = \sqrt{\frac{2}{N}}\cos(n\theta_k), \quad u_n^s(\theta_k) = \sqrt{\frac{2}{N}}\sin(n\theta_k)$$
 (28)

Now defining $u^s(0) = v^s(\pi) = 0$ y $u^c(0) = v^c(\pi) = \frac{1}{\sqrt{N}}$, we have that $\tilde{\Omega}_{m,n}$ can be written as

$$\tilde{\Omega}_{mn} = \sum \omega \left(\theta_k\right) \left(u_m^c \left(\theta_k\right) v_n^c \left(\theta_k\right) + u_m^s \left(\theta_k\right) v_n^s \left(\theta_k\right)\right),\tag{29}$$

therefore the upper part of the Hamiltonian reads

$$H = \sum_{m,n=0}^{N-1} \frac{i}{4} \sum_{\theta_k=0}^{\pi} \omega(\theta_k) (u_m^c(\theta_k) v_n^c(\theta_k) + u_m^s(\theta_k) v_n^s(\theta_k)) [\hat{\gamma}_n, \hat{\gamma}_{m+N}]$$
(30)

$$H = \sum_{\theta_k=0}^{\pi} \omega\left(\theta_k\right) \left(\underbrace{\left[\hat{\gamma}_k^c, \hat{\gamma}_{k+N}^c\right]}_{1-2\sigma_k^z} + \underbrace{\left[\hat{\gamma}_k^s, \hat{\gamma}_{k+N}^s\right]}_{1-2\sigma_k^z}\right),\tag{31}$$

where

$$\hat{\gamma}_{k}^{c,s} := \sum_{n} u_{n}^{c,s} (\theta_{k}) \, \hat{\gamma}_{n}, \quad \hat{\gamma}_{k+N}^{c,s} := \sum_{n} v_{n}^{c,s} (\theta_{k}) \, \hat{\gamma}_{n+N}. \tag{32}$$

Now we look back on the fact that the fermionic covariance matrix defined by $\Gamma_{\alpha\beta} = \frac{1}{2i} \operatorname{tr} \left(\rho \left[\gamma_{\alpha}, \gamma_{\beta} \right] \right) = \frac{1}{2i} \langle \left[\gamma_{\alpha}, \gamma_{\beta} \right] \rangle$, so it is known that the transformation that brings Ω into its Williamson form, does the same on the fermionic covariance matrix. Therefore for a state $|\vec{n}\rangle$ an eigenstate of the base (c, s, θ_k) , where $m^{c,s}(\theta_k) - 1/2$, with $n^{c,s}(\theta_k)$ the occupation number of cosine, sin in the k-mode. We get

$$\tilde{\Gamma}_{mn} = \sum_{\theta_k}^{\pi} \left[m^c \left(\theta_k \right) u_m^c \left(\theta_k \right) v_n^c \left(\theta_k \right) + m^s \left(\theta_k \right) u_m^s \left(\theta_k \right) v_n^s \left(\theta_k \right) \right] \\
= \sum_{\theta_k}^{\pi} \left(\frac{m^c \left(\theta_k \right) + m^s \left(\theta_k \right)}{2} \right) \left(u_m^c \left(\theta_k \right) v_n^c \left(\theta_k \right) + u_m^s \left(\theta_k \right) v_n^s \left(\theta_k \right) \right) \\
+ \sum_{\theta_k}^{\pi} \left(\frac{m^c \left(\theta_k \right) - m^s \left(\theta_k \right)}{2} \right) \left(u_m^c \left(\theta_k \right) v_n^c \left(\theta_k \right) - u_m^s \left(\theta_k \right) v_n^s \left(\theta_k \right) \right),$$
(33)

by defining $m^{\pm}(\theta_k) = \frac{m^c(\theta_k) \pm m^s(\theta_k)}{2}$ and inverting the transformations above done we finally get that

$$\tilde{\Gamma}_{mn} = \sum_{\theta_k}^{\frac{\tilde{\Gamma}_{mn}^+}{\tilde{\Gamma}_{mn}^+}} + \sum_{\theta_k}^{\frac{\tilde{\Gamma}_{mn}^+}{\tilde{\Gamma}_{mn}^-}} + \sum_{\tilde{\Gamma}_{mn}^-}^{\frac{\tilde{\Gamma}_{mn}^+}{\tilde{\Gamma}_{mn}^-}} . \tag{34}$$

we notice that $\tilde{\Gamma}_{mn}^+$ is circulant, whereas $\tilde{\Gamma}_{mn}^-$ is not, nevertheless, notice that $\tilde{\Gamma}_{mn}^+ = \tilde{\Gamma}_{mn'}$, with n' a change on the index $n \to -n'$, this can be see as a rotation over the circle

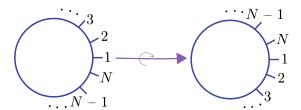


Figure 3: Meaning of the relabel done in the circulant matrix, which can be seen as a reflection over the circle

Explicitly we can write that if $\tilde{\Gamma}_{mn}^+$ has the shape

$$\begin{pmatrix}
a_0 & a_{-1} & \cdots & a_2 & a_1 \\
a_1 & a_0 & \cdots & a_3 & a_2 \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
a_{-1} & a_{-2} & a_{-3} & \cdots & a_0
\end{pmatrix},$$
(35)

Then $\tilde{\Gamma}_{mn}^-$ will be given by

$$\begin{pmatrix}
a_0 & a_1 & \cdots & a_{-2} & a_{-1} \\
a_1 & a_2 & \cdots & a_{-1} & a_0 \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
a_{-1} & a_0 & a_1 & \cdots & a_{-2}
\end{pmatrix}.$$
(36)

So we can notice 3 things, First, the FCM always can be written as a circulant matrix plus an anticirculant matrix. Second, in the Ground state, the FCM is circulant only, since the fermion occupation numbers $n^c(\theta_k) = n^s(\theta_k) = 0, \forall k$. Third, for a generic state, we have that in average the FCM matrix is always circulant, because $\langle n^c(\theta_k) \rangle = \langle n^s(\theta_k) \rangle$.

3 From the FCM to the Hamiltonian of the subsample

As mentioned before, the connection between the Hamiltonian and the fermionic covariance matrix can easily seen throughout the eigenvalues via

$$\lambda_k = \frac{1}{2} - n \tag{37}$$

where λ_k are the eigenvalues of the FCM and n is the ocupation number given by the Fermi distribution

$$n = \frac{1}{e^{\beta \varepsilon(\theta_k)} + 1}. (38)$$

So rearranging the terms we get

$$\beta \varepsilon(\theta_k) = \ln\left(\frac{1-n}{n}\right) \tag{39}$$