One-dimensional quantum spin chains

Gabriel T. Landi
University of São Paulo
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1 Introduction

1.1 XY, XX and TFIM

In these notes we are going to study a class of exactly soluble models which are at the heat of much of today's research in condensed matter physics and statistical mechanics. We consider a one-dimensional chain with L sites, each described by Pauli operators σ^i_α, with $\alpha \in \{x, y, z, +, -\}$ and $i = 1, \ldots, L$. The general Hamiltonian goes by the name of **XY model** and has the form

$$H = -\sum_{i=1}^{L} \left[J_x \sigma^i_x \sigma^{i+1}_x + J_y \sigma^i_y \sigma^{i+1}_y + g\sigma^i_z \right], \qquad \text{(XY model)}. \tag{1.1}$$

The first two terms describe a nearest-neighbor interaction in the xy plane, whereas the last describes a magnetic field pointing in the z direction. The model is called XY because the interaction is anisotropic. We usually define

$$J_x = J\left(\frac{1+\gamma}{2}\right), \qquad J_y = J\left(\frac{1-\gamma}{2}\right), \tag{1.2}$$

where $\gamma \in [0, 1]$ is called the **anisotropy parameter** and J is a constant. If $\gamma = 0$ the couplings in the x and y directions become equal and we refer to it, instead, as the **XX model**:

$$H = -\sum_{i=1}^{L} \left[J(\sigma^i_x \sigma^{i+1}_x + \sigma^i_y \sigma^{i+1}_y) + g\sigma^i_z \right], \qquad \text{(XX model)}. \tag{1.3}$$

In the opposite limit, if $\gamma = 1$ the y part of the interaction vanishes and we are left with

$$H = -\sum_{i=1}^{L} \left[J\sigma^i_x \sigma^{i+1}_x + g\sigma^i_z \right], \qquad \text{(TFIM)}. \tag{1.4}$$

This is called the **transverse field Ising model (TFIM)**. Sometimes this model is written in a slightly different way, as

$$H = -\sum_{i=1}^{L} \left[J\sigma^i_z \sigma^{i+1}_z + g\sigma^i_x \right], \tag{1.5}$$

That is, with $x \leftrightarrow z$. The term $J\sigma^i_z \sigma^{i+1}_z$ is the classical Ising model and $g\sigma^i_x$ is the transverse field. Eqs. (1.4) and (1.5) are physically equivalent: they simply correspond to a rotation of the Pauli operators around the y axis, by $\pi/2$.

1.2 Expressing the Hamiltonian in terms of $\sigma^i_\pm$

It is convenient to introduce the spin lowering and raising operators $\sigma^i_\pm$ from

$$\sigma^i_x = \sigma^i_+ + \sigma^i_-, \qquad \sigma^i_y = \frac{\sigma^i_+ - \sigma^i_-}{i}. \tag{1.6}$$

The inverse relations are

$$\sigma^i_\pm = \frac{\sigma^i_x \pm \sigma^i_y}{2}. \tag{1.7}$$

In terms of these operators we get

$$\sigma_x^i\sigma_x^{i+1} = \sigma_+^i\sigma_-^{i+1} + \sigma_-^i\sigma_+^{i+1} + \sigma_+^i\sigma_+^{i+1} + \sigma_-^i\sigma_-^{i+1} \tag{1.8}$$

$$\sigma_y^i\sigma_y^{i+1} = \sigma_+^i\sigma_-^{i+1} + \sigma_-^i\sigma_+^{i+1} - \sigma_+^i\sigma_+^{i+1} - \sigma_-^i\sigma_-^{i+1}. \tag{1.9}$$

All the changes are the minus signs in the last two terms. Plugging this in Eq. (1.1) and using also the parametrization (1.2), we then find

$$J_x\sigma_x^i\sigma_x^{i+1} + J_y\sigma_y^i\sigma_y^{i+1} = J\Big\{\sigma_+^i\sigma_-^{i+1} + \sigma_-^i\sigma_+^{i+1} + \gamma(\sigma_+^i\sigma_+^{i+1} + \sigma_-^i\sigma_-^{i+1})\Big\}. \tag{1.10}$$

We can also get rid of σ_z^i by writing

$$\sigma_z^i = 2\sigma_+^i\sigma_-^i - 1. \tag{1.11}$$

The easiest way to verify this is to just write down the 2×2 Pauli matrices

$$\sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \qquad \sigma_+ = \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}, \qquad \sigma_- = \begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}, \qquad \sigma_+\sigma_- = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}. \tag{1.12}$$

Combining these results, we can reexpress the Hamiltonian (1.1) as

$$H = -\sum_{i=1}^{L}\Big\{J(\sigma_+^i\sigma_-^{i+1} + \sigma_-^i\sigma_+^{i+1}) + J\gamma(\sigma_+^i\sigma_+^{i+1} + \sigma_-^i\sigma_-^{i+1}) + 2g\sigma_+^i\sigma_-^i\Big\}, \tag{1.13}$$

where I already neglect a constant $-gL$ that appears from the last term. If we forget about the term proportional to γ, this Hamiltonian looks quite a lot like the **tight-binding Hamiltonian** in second quantization. A term like $\sigma_+^i\sigma_-^{i+1}$ flips spin i up and spin $i+1$ down; it is pretty much the same idea as the hopping term $c_i^\dagger c_{i+1}$ in tight-binding (the term proportional to γ in (1.13) is a bit weird, I admit).

There is, however, one fundamental difference with respect to tight-binding: namely, the **algebra**. *Spin operators are neither bosonic nor fermionic.* They feel a bit fermionic because they can only describe two levels and $(\sigma_+^i)^2 = 0$. But they are not. Bosonic operators satisfy $[a_i, a_j^\dagger] = \delta_{ij}$ and fermionic operators satisfy $\{c_i, c_j^\dagger\} = \delta_{ij}$. The Pauli operators, on the other hand, satisfy something weird: if $i \neq j$ they commute:

$$[\sigma_-^i, \sigma_+^j] = 0, \qquad i \neq j \tag{1.14}$$

But when $i = j$, they anti-commute:

$$\{\sigma_-^i, \sigma_-^j\} = 1. \tag{1.15}$$

The Pauli operators are therefore neither fermionic nor bosonic.

The reason why the algebra matters is because these Hamiltonians are always diagonalized by introducing new operators which are *linear combinations* of the original

operators. In the language of second quantization, this could be for instance something like

$$d_\alpha = \sum_i U_{i\alpha} c_i,$$

for some unitary U. What is special about bosonic and fermionic operators is that linear combinations preserve the algebra (as long as U is unitary, of course). With Pauli operators this is not the case. For instance, suppose we were to try to naively define new Pauli operators in a similar way:

$$\tilde{\sigma}^\alpha_- = \sum_i U_{i\alpha} \sigma^i_-,$$

If we then try to see what happens, for instance, with Eq. (1.15), we find

$$\{\tilde{\sigma}^\alpha_-, \tilde{\sigma}^\alpha_+\} = \sum_{ij} U_{i\alpha} U_{j\alpha} \{\sigma^i_-, \sigma^j_+\}.$$

We know how to deal with this anti-commutator when $i = j$. But we have no idea what to do when $i \neq j$. Thus, we cannot proceed any further with this expression, which means that the algebra of the $\tilde{\sigma}^\alpha_\pm$ will be a mess.

2 Jordan-Wigner transformation

A day may come when the hopes of Men fail. But it is not this day. Quite incredibly, there is a way to map Pauli operators into Fermionic operators, called the Jordan-Wigner transformation. The map looks a bit weird at first, but it will make sense in a second. It reads

$$\boxed{c_i = \left[\prod_{n=1}^{i-1} (-\sigma^n_z)\right] \sigma^i_-.} \tag{2.1}$$

Let me explain the logic. In terms of the typical tensor structure of Pauli operators, this would read explicitly something like

$$c_i = (-\sigma_z) \otimes (-\sigma_z) \otimes \ldots \otimes (-\sigma_z) \otimes \sigma_- \otimes 1 \otimes 1 \ldots \otimes 1.$$

The bunch of $(-\sigma_z)$'s is called a **Jordan-Wigner string**. The idea is that to convert a Pauli operator σ^i_- into a fermionic operator c_i, we must append to it a string of operators $(-\sigma^n_z)$ for all sites preceding site i. Notice also how all operators in the product (2.1) commute with each other. Thus, for instance, if I want to compute the adjoint, I can simply write

$$c^\dagger_i = \left[\prod_{n=1}^{i-1} (-\sigma^n_z)\right] \sigma^i_+.$$

In principle, I should have flipped the order around ($(AB)^\dagger = B^\dagger A^\dagger$). But since everybody commute, I don't care.

2.1 Mapping between algebras

Let us now actually check that the c_i are indeed fermionic operators. That is, that they satisfy

$$\boxed{\{c_i, c_j\} = 0, \qquad \{c_i, c_j^\dagger\} = \delta_{ij}.} \tag{2.2}$$

To do that, all we need to remember is that

$$(\sigma_z^i)^2 = 1. \tag{2.3}$$

Let us start with

$$c_i c_i^\dagger = \left[\prod_{n=1}^{i-1}(-\sigma_z^n)\right]\sigma_-^i\left[\prod_{m=1}^{i-1}(-\sigma_z^m)\right]\sigma_+^i.$$

We can move the σ_z's around. Each one will find its match and cancel out because of (2.3). We then get

$$c_i c_i^\dagger = \sigma_-^i\sigma_+^i. \tag{2.4}$$

By the exact same argument, we then also get

$$c_i^\dagger c_i = \sigma_+^i\sigma_-^i. \tag{2.5}$$

Thus, for operators in the same site, the Pauli algebra (1.15) yields

$$\{c_i, c_i^\dagger\} = \{\sigma_-^i, \sigma_+^i\} = 1,$$

as we hoped for.

Now let's analyze the case $i \neq j$, which is where the real problem is. The following analysis requires some thinking, so go through it slowly. If you understand the next steps, you will understand the Jordan-Wigner transformation. Consider a product such as

$$c_i c_j^\dagger = \left[\prod_{n=1}^{i-1}(-\sigma_z^n)\right]\sigma_-^i\left[\prod_{m=1}^{j-1}(-\sigma_z^m)\right]\sigma_+^j.$$

For concreteness, assume that $j > i$. As a general recommendation, let us adopt the procedure that we should always move the σ_z's to the left, as we did above in the case of $c_i c_i^\dagger$. In this case, however, the σ_z^m block cannot slide to the left through σ_-^i because in this block there will be one bloody σ_z^i which does not commute with σ_-^i. Here is where the *magic* comes in. Are you ready? The Pauli operators satisfy the following relations:

$$\begin{aligned} \sigma_+(-\sigma_z) &= \sigma_+ & \qquad \sigma_-(-\sigma_z) &= -\sigma_-, \\ (-\sigma_z)\sigma_+ &= -\sigma_+ & \qquad (-\sigma_z)\sigma_- &= \sigma_-, \end{aligned} \tag{2.6}$$

which you can verify by simply playing with the 2×2 matrices (1.12). Going back to $c_i c_j^\dagger$, we can therefore move the block of σ_z^m to the left, across σ_-^i. The only thing that is going to happen is that one of them, the σ_z^i, will yield a minus sign

$$\sigma_-^i(-\sigma_z^i) = -(-\sigma_z^i)\sigma_-^i.$$

As a result, we get

$$c_i c_j^\dagger = -\left[\prod_{n=i}^{j-1}(-\sigma_z^n)\right]\sigma_-^i\sigma_+^j. \tag{2.7}$$

To finish, we compare this with

$$c_j^\dagger c_i = \left[\prod_{m=1}^{j-1}(-\sigma_z^m)\right]\sigma_+^j\left[\prod_{n=1}^{i-1}(-\sigma_z^n)\right]\sigma_-^i.$$

In this case we have no problems sliding the σ_z^n to the left because $j > i$. As a result we simply get

$$c_j^\dagger c_i = \left[\prod_{n=i}^{j-1}(-\sigma_z^n)\right]\sigma_+^j\sigma_-^i. \tag{2.8}$$

The key point is the minus sign in Eq. (2.7), which is not present here. As a result, if we combine the two results as an anti-commutator, we get

$$\{c_i, c_j^\dagger\} = \left[\prod_{n=i}^{j-1}(-\sigma_z^n)\right](-\sigma_-^i\sigma_+^j - \sigma_+^j\sigma_-^i).$$

That minus sign converts the anti-commutator into a commutator. Now Eq. (1.14) applies and we get $\{c_i, c_j^\dagger\} = 0$ when $j \neq i$. Of course, we focused on $j > i$. But the calculations for $j < i$ are identical. I invite you to try them out.

Before we move on, I just want to briefly comment that the terms $(-\sigma_z^i)$ in Eq. (2.1) can also be written in a bunch of different ways, which are useful depending on the context. Using Eq. (1.11) and the fact that $(\sigma_+\sigma_-)^2 = \sigma_+\sigma_-$ one can verify that

$$(-\sigma_z^i) = e^{i\pi\sigma_+^i\sigma_-^i}. \tag{2.9}$$

This means that we can also rewrite (2.1) as

$$c_i = \left[\prod_{n=1}^{i-1} e^{i\pi\sigma_+^n\sigma_-^n}\right]\sigma_-^i. \tag{2.10}$$

Not only is this slightly prettier, but the nice thing about this formula is that it can be easily inverted because $(e^{i\pi\sigma_+\sigma_-})^2 = 1$. Moreover, as we saw in (2.5), $\sigma_+^i\sigma_-^i = c_i^\dagger c_i$. Whence, the inverse relation is simply

$$\sigma_-^i = \left[\prod_{n=1}^{i-1} e^{i\pi c_n^\dagger c_n}\right]c_i. \tag{2.11}$$

2.2 Mapping between states

We have learned how the Jordan-Wigner transformation (2.1) can be used to map spin operators into fermionic operators. Let us now see how this translates into a mapping of states. The usual Pauli basis has the form

$$|\boldsymbol{\sigma}\rangle = |\sigma_1 \ldots \sigma_L\rangle, \qquad \sigma_i = \pm 1, \tag{2.12}$$

where the σ_i are the eigenvalues of σ_z^i. What I want to understand is how these spin states look like in the fermionic language. For instance, which of these spin configurations play the role of the vacuum, $|0\rangle$? In the fermionic language, the vacuum is defined as the state for which $c_i|0\rangle = 0$ for all i. Looking at Eq. (2.1) and recalling that σ_- annihilates the state $|\sigma = -1\rangle$, we then conclude that

$$|0\rangle = |-1, -1, \ldots -1\rangle. \tag{2.13}$$

Within the Jordan-Wigner mapping, therefore, the state with no fermions corresponds to the state with all spins down. Fermionic excitations will then naturally be mapped into states with spin up.

This correspondence becomes more evident if we use Eq. (1.11) and (2.5) to write

$$\sigma_z^i = 2\sigma_+^i\sigma_-^i - 1 = 2c_i^\dagger c_i - 1. \tag{2.14}$$

The eigenvalues $n_i = 0, 1$ of $c_i^\dagger c_i$ are therefore related to the σ_i according to

$$\boxed{n_i = \frac{1+\sigma_i}{2} \qquad \text{or} \qquad \sigma_i = 2n_i - 1.} \tag{2.15}$$

The Pauli basis (2.12) is therefore equivalent to the Fock basis of the n_i:

$$\boxed{|n_1, \ldots, n_L\rangle = |\sigma_1, \ldots, \sigma_L\rangle.} \tag{2.16}$$

3 Fermionic representation of the spin Hamiltonian

Let us now go back to the XY model in Eq. (1.13) and let us express it in terms of the fermionic operators using the Jordan-Wigner transformation (2.1). As we have seen in Eq. (1.11), we have that $\sigma_+^i\sigma_-^i = c_i^\dagger c_i$. Moreover, in Eq. (2.8) we saw how to deal with $\sigma_+^j\sigma_-^i$. In our case, setting $j = i + 1$ we get only one $(-\sigma_z)$ left:

$$c_{i+1}^\dagger c_i = (-\sigma_z^i)\sigma_+^{i+1}\sigma_-^i.$$

This σ_z^i goes through σ_+^{i+1} and combines with σ_-^i to give $(-\sigma_z^i)\sigma_-^i\sigma_-^i$ [Eq. (2.6)]. Whence

$$c_{i+1}^\dagger c_i = \sigma_+^{i+1}\sigma_-^i. \tag{3.1}$$

Taking the adjoint also yields $c_i^\dagger c_{i+1} = \sigma_+^i\sigma_-^{i+1}$. This solves the issue for the first two terms in Eq. (1.13).

Next we have to deal with terms like $\sigma_+^i\sigma_+^{i+1}$. Using the Jordan-Wigner definition (2.1) again, we find

$$\begin{aligned} c_{i+1}^\dagger c_i^\dagger &= \left[\prod_{n=1}^{i}(-\sigma_z^n)\right]\sigma_+^{i+1}\left[\prod_{m=1}^{i-1}(-\sigma_z^m)\right]\sigma_+^i \\ &= \sigma_+^{i+1}(-\sigma_z^i)\sigma_+^i \\ &= -\sigma_+^{i+1}\sigma_+^i, \end{aligned} \tag{3.2}$$

Thus

$$\sigma_+^{i+1}\sigma_+^i = -c_{i+1}^\dagger c_i^\dagger.$$

The two operators on the left commute, whereas the two on the right anti-commute. Yeah, I know this may seem a bit weird at first. But if you think about it, there is nothing wrong with it. Thus, to avoid the minus sign, it is simpler write

$$\sigma_+^{i+1}\sigma_+^i = c_i^\dagger c_{i+1}^\dagger. \tag{3.3}$$

Taking the adjoint then yields $\sigma_-^i\sigma_-^{i+1} = c_{i+1}c_i$.

$$H = -\sum_{i=1}^{L}\Big\{J(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + J\gamma(c_i^\dagger c_{i+1}^\dagger + c_{i+1}c_i) + 2gc_i^\dagger c_i\Big\}. \tag{3.4}$$

If $\gamma = 0$, the Hamiltonian becomes *exactly* the tight-binding Hamiltonian. This is why all this effort to move to a fermionic representation is "worth it": we arrive at a familiar Hamiltonian, which we now know how to deal with.

3.1 Periodic boundary conditions

The Hamiltonian (3.4) is not 100% correct, however. We forgot to talk about periodic boundary conditions. That is, about the very last term in the sum (1.13):

$$H_{\text{PBC}} = -J(\sigma_+^L\sigma_-^1 + \sigma_-^L\sigma_+^1) - J\gamma(\sigma_+^L\sigma_+^1 + \sigma_-^L\sigma_-^1). \tag{3.5}$$

When I wrote Eq. (3.4) I just blindly assumed that this term transformed as all others. Well, it doesn't. So Eq. (3.4) will need some fixing. In many textbooks this detail is overlooked. The reason is because it will turn out to be irrelevant in the thermodynamic limit. But I think it is nice to see the full picture, so I wanna go through it in some detail.

The important point one should bear in mind is that *the Jordan-Wigner mapping is useful for spin chains having nearest-neighbor interactions.* The reason for this can be seen, for instance, in Eq. (3.2). When we take the product of two fermionic operators which are nearest-neighbor operators, such as $c_i^\dagger$ and $c_{i+1}^\dagger$, the σ_z-string cancels out and we obtain a product of only two Pauli operators, like $\sigma_+^{i+1}\sigma_+^i$. But if the fermionic operators are not nearest-neighbors, we will end up with something having more than two Pauli operators. For instance, using Eq. (2.1), we have

$$c_L^\dagger c_1 = \left[\prod_{n=1}^{L-1}(-\sigma_z^n)\right]\sigma_+^L\sigma_-^1. \tag{3.6}$$

This big σ_z-string just stays there. There is nothing we can do about it. This is a bit annoying.

Luckily, it is still possible to keep going. The trick is as follows. The σ_z-string in Eq. (3.6) contains almost the entire lattice, except L. Let us then use Eq. (2.6) to write $\sigma_+^L = -(-\sigma_z^L)\sigma_+^L$, which yields

$$c_L^\dagger c_1 = -\left[\prod_{n=1}^{L}(-\sigma_z^n)\right]\sigma_+^L\sigma_-^1.$$

We can now invert the relation and also use the same logic as in Eq. (2.11) to express the result in terms of $e^{i\pi c_n^\dagger c_n}$; viz.,

$$\sigma_+^L\sigma_-^1 = -\left[\prod_{n=1}^{L}e^{i\pi c_n^\dagger c_n}\right]c_L^\dagger c_1. \tag{3.7}$$

Lastly, we can rewrite this in a neat way in terms of the number operator

$$\hat{\mathcal{N}} = \sum_{n=1}^{L} c_n^\dagger c_n = \sum_{n=1}^{L} \sigma_+^n \sigma_-^n = \sum_{n=1}^{L} \frac{1+\sigma_z^n}{2}. \tag{3.8}$$

Notice how the number operator, in the spin language, is proportional to the magnetization operator. In terms of it we can write

$$\prod_{n=1}^{L} e^{i\pi c_n^\dagger c_n} = e^{i\pi \sum_{n=1}^{L} c_n^\dagger c_n} = e^{i\pi \hat{\mathcal{N}}}.$$

We can also write this in a nice, although a bit strange, way, by noticing that $e^{i\pi} = -1$. We then get

$$\prod_{n=1}^{L} e^{i\pi c_n^\dagger c_n} = e^{i\pi \hat{\mathcal{N}}} = (-1)^{\hat{\mathcal{N}}}. \tag{3.9}$$

As a result, Eq. (3.7) may finally be written as

$$\sigma_+^L \sigma_-^1 = -(-1)^{\hat{\mathcal{N}}} c_L^\dagger c_1. \tag{3.10}$$

The expressions for the three other terms in Eq. (3.5) are analogous.

Thus, we find that the full Hamiltonian in the fermionic representation is actually

$$H = -\sum_{i=1}^{L-1} \Big\{ J(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + J\gamma(c_i^\dagger c_{i+1}^\dagger + c_{i+1} c_i) \Big\} - \sum_{i=1}^{L} 2g c_i^\dagger c_i \tag{3.11}$$
$$+(-1)^{\hat{\mathcal{N}}} \Big\{ J(c_L^\dagger c_1 + c_1^\dagger c_L) + J\gamma(c_L^\dagger c_1^\dagger + c_1 c_L) \Big\}$$

The last term is quite complicated because $\hat{\mathcal{N}}$ is an operator involving all fermions. It therefore corresponds to a kind of global interaction. Luckily, however, since the eigenvalues of $\hat{\mathcal{N}}$ are integers, the eigenvalues of the operator $(-1)^{\hat{\mathcal{N}}}$ can only take on two distinct values, $+1$ or -1. This operator is called the **parity operator**: it gives $+1$ when the number of "Fermions" (i.e., spin excitations) is even and -1 when it is odd.

Before we move on to diagonalize the full Hamiltonian (3.11), I just want to mention an alternative; namely, using **open boundary conditions**. In this case the Hamiltonian becomes

$$H = -\sum_{i=1}^{L-1} \Big\{ J(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + J\gamma(c_i^\dagger c_{i+1}^\dagger + c_{i+1} c_i) \Big\} - \sum_{i=1}^{L} 2g c_i^\dagger c_i, \tag{3.12}$$

where the difference is now that the first sum only goes up to $L-1$. This Hamiltonian does not contain any of the weird $(-1)^{\hat{\mathcal{N}}}$ terms. Notwithstanding, unlike (3.11), it is not translationally invariant, which makes it a bit more difficult to diagonalize. Thus, even though the factor of $(-1)^{\hat{\mathcal{N}}}$ introduces some complications, it is still easier to deal with than (3.12).

3.2 Even and odd parity sectors

Let us now focus on the Hamiltonian (3.11). The last term, containing $(-1)^{\hat{N}}$ is a complication. But it is not insurmountable. The key observation is that the Hamiltonian actually commutes with the parity operator

$$[H, (-1)^{\hat{N}}] = 0. \tag{3.13}$$

This is a bit tricky, so let's go step-by-step. The first thing we need to realize is that $[H, \hat{N}] \neq 0$; the commutation only holds with $(-1)^{\hat{N}}$. The tight-binding terms in (3.11) do commute with $\hat{N}$

$$[c_i^\dagger c_{i+1}, \hat{N}] = 0,$$

since $c_i^\dagger c_{i+1}$ is creating one particle but destroying another, so that the total number of particles is conserved. It then follows that this term will also commute with $(-1)^{\hat{N}}$. But the terms proportional to γ in Eq. (3.11) do not commute with $\hat{N}$:

$$[c_i^\dagger c_{i+1}^\dagger, \hat{N}] \neq 0.$$

So, overall, H does not preserve the number of particles.

What matters for us, however is the parity $(-1)^{\hat{N}}$, not the number of particles. And the parity is "simpler" because it only cares if the number of particles is even or odd. A term like $c_i^\dagger c_{i+1}^\dagger$ creates *pairs* of particles; hence, it preserves the parity:

$$[c_i^\dagger c_{i+1}^\dagger, (-1)^{\hat{N}}] = 0. \tag{3.14}$$

If you want, you can verify this by hand. It suffices to convince yourself that

$$[c_i^\dagger c_{i+1}^\dagger, (-1)^{c_i^\dagger c_i}(-1)^{c_{i+1}^\dagger c_{i+1}}] = 0.$$

The best way to carry out this computation is to notice that since $(c_i^\dagger c_i)^2 = c_i^\dagger c_i$, we can write $(-1)^{c_i^\dagger c_i} = 1 - 2c_i^\dagger c_i$. I will leave for you the fun exercise of opening up this commutator.

Since H commutes with $(-1)^{\hat{N}}$, they can both be diagonalized in the same basis. The parity operator $(-1)^{\hat{N}}$ has only two eigenvalues, $+1$ and -1. Hence, H will be **block diagonal** with two big blocks corresponding to these two eigenvalues,

$$H = \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix}. \tag{3.15}$$

We can make this more formal by defining projection operators

$$P_\pm = \frac{1 \pm (-1)^{\hat{N}}}{2}. \tag{3.16}$$

These operators project onto the subspaces containing an even and odd number of particles respectively. They satisfy

$$P_+ + P_- = 1, \tag{3.17}$$

$$(P_\pm)^2 = P_\pm \tag{3.18}$$

$$P_+ P_- = P_- P_+ = 0. \tag{3.19}$$

The first say that the two subspaces add up to the full Hilbert space. The second says that if you project twice, you get nothing extra. And the third says that the two subspaces are orthogonal, so if you first project onto one and then onto another, you get zero.

The block-diagonal structure in Eq. (3.15) is then manifested by looking at

$$P_+HP_- = \left(\frac{1+(-1)^{\hat{N}}}{2}\right)H\left(\frac{1-(-1)^{\hat{N}}}{2}\right) = \frac{1}{2}\Big\{H + (-1)^{\hat{N}}H - H(-1)^{\hat{N}} - (-1)^{\hat{N}}H(-1)^{\hat{N}}\Big\}.$$

But since $[H,(-1)^{\hat{N}}] = 0$, the two terms in the middle cancel out. Moreover, since $((-1)^{\hat{N}})^2 = 1$, the first and fourth term also cancel out. Hence $P_+HP_- = 0$. This explains why there are no connections between the even and odd subspaces in Eq. (3.15). Using $P_+ + P_- = 1$ we can then write

$$H = 1H1 = (P_+ + P_-)H(P_+ + P_-).$$

The cross terms vanish and we are left with

$$H = P_+HP_+ + P_-HP_- := P_+H_+P_+ + P_-H_-P_-. \tag{3.20}$$

To see how the Hamiltonians $H_\pm$ look like, we refer back to Eq. (3.11). The first line is not affected by $P_\pm$. The only thing that is affect is the second line. In H_+ we replace $(-1)^{\hat{N}}$ with $+1$ and in H_- we replace $(-1)^{\hat{N}}$ with -1. That is

$$\begin{aligned} H_\pm = &-\sum_{i=1}^{L-1}\Big\{J(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + J\gamma(c_i^\dagger c_{i+1}^\dagger + c_{i+1}c_i)\Big\} - \sum_{i=1}^{L} 2gc_i^\dagger c_i \\ &\pm\Big\{J(c_L^\dagger c_1 + c_1^\dagger c_L) + J\gamma(c_L^\dagger c_1^\dagger + c_1 c_L)\Big\} \end{aligned}$$

We can make these formulas more compact by agreeing that $c_{L+1} = -c_1$ (anti-periodic BC) in H_+ and $c_{L+1} = c_1$ in H_- (periodic BC). We can then append the last term to the sum, leading to

$$H_\pm = -\sum_{i=1}^{L}\Big\{J(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + J\gamma(c_i^\dagger c_{i+1}^\dagger + c_{i+1}c_i) + 2gc_i^\dagger c_i\Big\}, \tag{3.21}$$

Looking at Eq. (3.20), you may notice that I wrote $P_+H_+P_+$ in the right-hand side, and not only H_+. The reason is because H_+ and H_- are still "big Hamiltonians", in the sense that they live on the full Hilbert space of the L spins (of dimensions 2^L). Thus, H_+ will have2^L eigenvalues/eigenvector pairs. And the same for H_-. What we are interested, however, is to find the 2^L eigenpairs of H. So it seems we have more pairs than we need. This is where the $P_+(\ldots)P_+$ comes in. Out of the 2^L eigenvectors of H_+, half will have even parity and half will have odd parity. Then $P_+H_+P_+$ will pick up only the eigenvalues with even parity. Similarly, $P_-H_-P_-$ will only pick the eigenvectors of H_- with odd parity. Thus, to summarize, we can from now on work with $H_\pm$. But once we diagonalize them, in order to get the full Hamiltonian H, we have to pick only half of the eigenpairs of H_+ (those with even parity) and half from H_- (those

with odd parity). The eigenpairs of H_+ with odd parity and the eigenpairs of H_- with even parity have no physical meaning.

3.3 Fourier space

We are now ready to diagonalize Eq. (3.21). The first step is to go to Fourier space by defining a new set of operators c_k according to [1]

$$\boxed{c_n = \frac{e^{-i\pi/4}}{\sqrt{L}} \sum_k e^{ikn} c_k,} \tag{3.22}$$

where the factor of $e^{-i\pi/4}$ is placed only for convenience. The allowed values of k are determined by the periodic or anti-periodic boundary conditions. In the case of H_+ we should have $c_{L+1} = -c_1$ (anti-periodic) so we must have $e^{ikL} = -1$. For concreteness, *we will assume L is even*. In Eq. (3.22) we need a total of L operators c_k. A set of L distinct k values satisfying $e^{ikL} = -1$ is, for instance,

$$K^+ = \left\{ k = \frac{\pm(2\ell+1)\pi}{L}, \qquad \ell = 0, 1, \ldots, \frac{L}{2} - 1 \right\}. \tag{3.23}$$

Similarly, in the case of H_- we should have $c_{L+1} = c_1$, which implies $e^{ikL} = 1$. A set of L distinct k values satisfying to this condition is

$$K^- = \left\{ k = 0, \frac{\pm 2\ell\pi}{L}, \pi, \qquad \ell = 1, \ldots, \frac{L}{2} - 1 \right\}. \tag{3.24}$$

The only reason why I single out the cases $k = 0$ and $k = \pi$ is because they will turn out to play a special role in what follows.

For either set, the sum in Eq. (3.22) then satisfies the usual Fourier orthogonality relation:

$$\frac{1}{L} \sum_{k \in K^\pm} e^{ik(n-n')} = \delta_{n,n'}, \qquad \frac{1}{L} \sum_{n=1}^{L} e^{i(k-q)n} = \delta_{k,q}. \tag{3.25}$$

Using this we then get, for instance,

$$\begin{aligned} \sum_n c_n^\dagger c_{n+j} &= \frac{1}{L} \sum_{n,k,q} e^{-ikn} e^{iq(n+j)} c_k^\dagger c_q \\ &= \sum_{k,q} e^{iqj} \left[\frac{1}{L} \sum_n e^{i(q-k)n} \right] c_k^\dagger c_q \\ &= \sum_k e^{ikj} c_k^\dagger c_k. \end{aligned}$$

This illustrates well the beauty of translation invariance. The right-hand side is diagonal ($c_k^\dagger c_k$), with a phase e^{ikj} which depends only on the distance between $c_n^\dagger$ and c_{n+j}.

[1] I am abusing the notation a bit by using c_k for this new set. I should have written them with a different letter, like d_k, to emphasize that this is a different set as the $\{c_n\}$ (or $\{c_i\}$). But physicists are environmentally conscious, so we like to save up letters. The two sets are differentiated by the indices: Fourier operators are always denoted as c_k or c_q, whereas real space operators are denoted by c_i, c_j, c_n, etc.

With this result, the first term in Eq. (3.21) becomes

$$\sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) = \sum_{k\in K^\pm} (e^{ik} + e^{-ik}) c_k^\dagger c_k = \sum_{k\in K^\pm} (2\cos k) c_k^\dagger c_k,$$

whereas the last term is simply

$$\sum_i 2g c_i^\dagger c_i = \sum_{k\in K^\pm} 2g c_k^\dagger c_k.$$

Lastly, we look at the terms in the middle, proportional to γ. In terms of the c_k, we have

$$\begin{aligned}
\sum_n c_n^\dagger c_{n+j}^\dagger &= \frac{e^{i\pi/2}}{L} \sum_{n,k,q} e^{-ikn} e^{-iq(n+j)} c_k^\dagger c_q^\dagger \\
&= i \sum_{k,q} e^{-iqj} \left[\frac{1}{L} \sum_n e^{-i(k+q)n} \right] c_k^\dagger c_q^\dagger \\
&= i \sum_k e^{ikj} c_k^\dagger c_{-k}^\dagger.
\end{aligned}$$

Thus, the terms proportional to γ in Eq. (3.21) becomes

$$\sum_i J\gamma c_i^\dagger c_{i+1}^\dagger = \sum_k iJ\gamma e^{ik} c_k^\dagger c_{-k}^\dagger.$$

The other term will simply be the adjoint of this one.

Combining everything, we finally arrive at the expression for the Hamiltonian (3.21) in Fourier space:

$$H_\pm = -\sum_{k\in K^\pm} \Big\{ 2(g + J\cos k) c_k^\dagger c_k + iJ\gamma (e^{ik} c_k^\dagger c_{-k}^\dagger - e^{-ik} c_{-k} c_k) \Big\}. \tag{3.26}$$

It is very interesting how the γ terms mix k with $-k$. But notice how, besides that, k never mixes with other k'. So it indeed feels like we are a step closer towards diagonalization: we started with a Hamiltonian where each site interacts with its neighbor, so that in the end everyone is indirectly interacting with everyone. Once we move to Fourier space, however, we split this into *pairwise interactions* between k and $-k$.

We can also write (3.26) in a slightly more symmetric way if we wish. Let us first consider the case of H_+. In H_- there will be a subtlety for us to handle. We can split, for instance,

$$\sum_{k\in K^+} 2(g + J\cos k) c_k^\dagger c_k = \sum_{k\in K^+, k>0} 2(g + J\cos k)(c_k^\dagger c_k + c_{-k}^\dagger c_{-k}).$$

Similarly,

$$\begin{aligned}
\sum_{k\in K^+} e^{ik} c_k^\dagger c_{-k}^\dagger &= \sum_{k\in K^+, k>0} \left(e^{ik} c_k^\dagger c_{-k}^\dagger + e^{-ik} c_{-k}^\dagger c_k^\dagger \right) \\
&= \sum_{k\in K^+, k>0} (e^{ik} - e^{-ik}) c_k^\dagger c_{-k}^\dagger
\end{aligned}$$

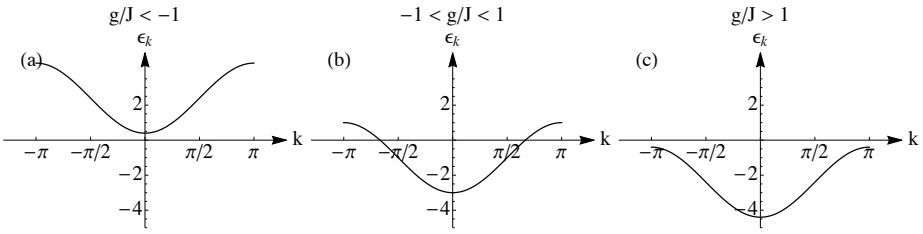

Figure 1: Dispersion relation ϵ_k [Eq. (4.2)] for the XX model.

where I used the fact that $c^\dagger_{-k}c^\dagger_k = -c^\dagger_k c^\dagger_{-k}$. With these changes, we can write H_+ in Eq. (3.26) as

$$\boxed{H_+ = -2\sum_{k\in K^+,k>0}\Big\{(g+J\cos k)(c^\dagger_k c_k + c^\dagger_{-k}c_{-k}) - J\gamma\sin k(c^\dagger_k c^\dagger_{-k} + c_{-k}c_k)\Big\}.} \tag{3.27}$$

This is pretty nice: we decomposed H_+ as a sum of *independent Hamiltonians* (for each $k > 0$), where in each term one has only the interactions between the pairs $(k, -k)$.

The situation for H_- is analogous, with only one subtlety. Namely, the states with $k = 0, \pi$ (see Eq. (3.24)). For these states $-k = k$: this is evident for $k = 0$, but is also true for $k = \pi$ because $e^{i\pi} = e^{-i\pi}$. Thus, for these states $c^\dagger_k c^\dagger_{-k} = (c^\dagger_k)^2 = 0$, which means that the γ terms are not present for these two states. As a result, we then find, instead of (3.27),

$$H_- = -2\sum_{k\in K^-,k\neq 0,\pi,k>0}\Big\{(g+J\cos k)(c^\dagger_k c_k + c^\dagger_{-k}c_{-k}) - J\gamma\sin k(c^\dagger_k c^\dagger_{-k} + c_{-k}c_k)\Big\} \tag{3.28}$$
$$-2(g+J)c^\dagger_0 c_0 - 2(g-J)c^\dagger_\pi c_\pi.$$

4 The XX model

Before we continue with the general solution, it is interesting to discuss the physics behind the particular case of the XX model; that is, when $\gamma = 0$. In this case Eq. (3.26) becomes

$$\boxed{H_\pm = -2\sum_{k\in K^\pm}(g+J\cos k)c^\dagger_k c_k.} \tag{4.1}$$

This Hamiltonian is already diagonal, with a dispersion relation

$$\epsilon_k = -2(g+J\cos k). \tag{4.2}$$

This dispersion relation is shown in Fig. 1 for multiple values of g. In the case of the XX model the fermionic Hamiltonian is *exactly* the tight-binding Hamiltonian [c.f. Eq. (3.21)]. Thus, it is no surprise that the dispersion relation is exactly the one we find on the tight-binding model.

The physics, however, is different. In the tight-binding model the number of particles was either fixed or adjusted with a chemical potential. Here there is no such thing

as "particles": we are still talking about a spin Hamiltonian. The fermionic particles are merely the spin excitations. And we can have as many of them as we want.

For instance, let us think about the ground-state. By definition, the ground-state is the state with the smallest possible energy. Suppose first that $g/J < -1$, as in Fig. 1(a). In this case all $\epsilon_k > 0$, so that putting fermions is never a good deal (it always increases the energy). The ground-state will therefore be a state with no excitations:

$$g/J < -1 : \qquad |\psi_{\rm gs}\rangle = |-1, -1, \ldots, -1\rangle = |0\rangle, \tag{4.3}$$

i.e., the fermionic vacuum [see Eq. (2.13)]. This is a state belonging to H_+ (because we are assuming L is even). The corresponding ground-state energy is $E_{\rm gs} = 0$. Similarly, suppose we have $g/J > 1$, as in Fig. 1(d). In this case all states have $\epsilon_k < 0$, so that it is advantageous to put excitations in all of them. As a consequence

$$g/J > 1 : \qquad |\psi_{\rm gs}\rangle = |1, 1, \ldots, 1\rangle = \Big[\prod_{k\in K^+} c_k^\dagger\Big]|0\rangle. \tag{4.4}$$

It is not immediately obvious that the state with all spins up is actually the state with all k states occupied. I will leave this as an exercise for you to check. This state also belongs to H_+. The corresponding ground-state energy is

$$E_{\rm gs} = \sum_{k\in K^+} \epsilon_k. \tag{4.5}$$

The interesting part is for $-1 < g/J < 1$ (Figs. 1(b)). In this case there will be some values of k for which $\epsilon_k < 0$, so that adding an excitation to that state is energetically advantageous. The ground-state in this case will therefore be a state where all k states with $\epsilon_k < 0$ filled. We can define a "Fermi momentum" k_F as the value for which $\epsilon_k = 0$:

$$\epsilon_{k_F} = 0 \qquad \rightarrow \qquad k_F = \arccos(-g/J). \tag{4.6}$$

The ground-state will then be

$$|\psi_{\rm gs}\rangle = \Big[\prod_{|k|<k_F} c_k^\dagger\Big]|0\rangle, \tag{4.7}$$

and the ground-state energy will be

$$E_{\rm gs} = \sum_{|k|<k_F} \epsilon_k. \tag{4.8}$$

In this case, however, it is more complicated to know to which parity subspace the ground-state will belong to. It will depend on the value of k_F and how many fermions we have with $|k| < k_F$. The situation will thus be rather complicated. However, the difference will be minuscular because the values in K^+ are very close to those in K^-. This is why we can pretend that the distinction between H_+ and H_- doesn't even exist. In order to gain some insight into the physics, this is what we shall henceforth assume.

4.1 Magnetization

Now that we have the ground-state, Eqs. (4.3), (4.4) and (4.7), let us compute the magnetization. Recall from Eq. (3.8) that the magnetization is related to the number of particles:

$$\langle\hat{N}\rangle = \frac{L}{2} + \frac{1}{2}\sum_{i=1}^{L}\langle\sigma_z^i\rangle.$$

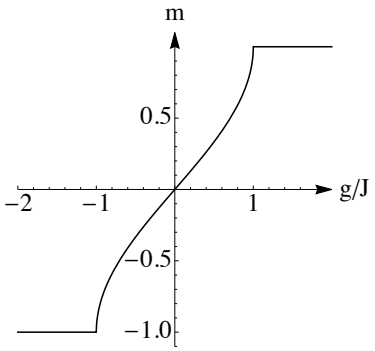

Figure 2: The magnetization of the XX model in the ground-state, Eq. (4.13), as a function of the transverse field g/J.

Thus,

$$m := \frac{1}{L}\sum_{i=1}^{L}\langle\sigma_z^i\rangle = \frac{2\langle\hat{\mathcal{N}}\rangle}{L} - 1. \tag{4.9}$$

From what we just discussed it is quite clear that

$$\langle\hat{\mathcal{N}}\rangle = \begin{cases} 0 & g/J < -1, \\ 1 & g/J > 1 \end{cases}. \tag{4.10}$$

For $g/J \in [-1, 1]$ we get, instead

$$\langle\hat{\mathcal{N}}\rangle = \sum_{|k|<k_F} 1 \tag{4.11}$$

Converting the sum to an integral we find

$$\langle\hat{\mathcal{N}}\rangle = \frac{L}{2\pi}\int_{-k_F}^{k_F} \mathrm{d}k = \frac{L}{\pi}k_F = \frac{L}{\pi}\arccos(-g/J). \tag{4.12}$$

Plugging this in Eq. (4.9) then yields for the magnetization:

$$\boxed{m = \begin{cases} -1 & g/J < -1, \\ \frac{2}{\pi}\arccos(-g/J) - 1 & -1 < g/J < 1, \\ 1 & g/J > 1. \end{cases}} \tag{4.13}$$

This result is plotted in Fig. 2.

As can be seen, at

$$g = g_c = \pm J, \tag{4.14}$$

the magnetization has a kink. This defines the critical point of the model. The derivative

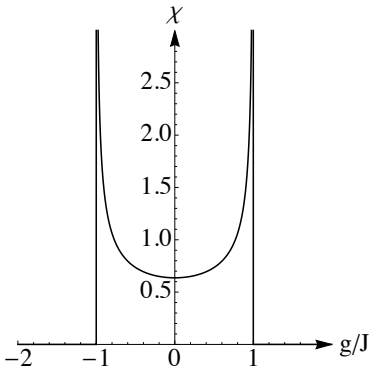

Figure 3: The susceptibility in Eq. (4.15).

of the magnetization, which is the susceptibility, behaves as

$$\chi = \frac{\partial m}{\partial g} = \begin{cases} 0 & g/J < -1, \\ \frac{2/\pi}{\sqrt{J^2 - g^2}} & -1 < g/J < 1, \\ 0 & g/J > 1. \end{cases} \tag{4.15}$$

which diverges as $g \to g_c$, as shown in Fig. 3.

4.2 Entanglement in the ground-state

This is the quantum phase transition in the XX model. It occurs due to a competition between the J and g terms: the former pushes the magnetization to the xy plane, whereas the latter pushes it towards the z direction. For $g/J > 1$ the latter wins. The key point about a quantum phase transition is that there is a fundamental reconfiguration of the ground-state $|\psi_{\rm gs}\rangle$. This, in fact, can already be seen in Eqs. (4.3), (4.4) and (4.7). For $g/J > 1$ or $g/J < -1$ the ground-state is a **product state** (either of all spins up or of all spins down); there is no entanglement. Conversely, for $g/J \in [-1, 1]$, however, the ground-state will be *highly* entangled. In fact, we can see that if we express the c_k in terms of the position operators as

$$c_k = \frac{e^{i\pi/4}}{\sqrt{L}} \sum_{n=1}^{L} e^{-ikn} c_n.$$

If we try to substitute this in the ground-state (4.7), we see that the result will be quite messy.

In fact, just to give you an idea of how messy it is, suppose we are just a tiny bit above $g/J = -1$, so that $k_F = 0$; that is, the only populated state is $k = 0$. In this case the ground-state will be

$$|\psi_{\rm gs}\rangle = c^\dagger_{k=0}|0\rangle = \frac{e^{-i\pi/4}}{\sqrt{L}} \sum_{n=1}^{L} c^\dagger_n |0\rangle. \tag{4.16}$$

In the language of spins,

$$c^\dagger_n|0\rangle = |\downarrow, \downarrow, \ldots, \uparrow, \ldots, \downarrow, \downarrow\rangle.$$

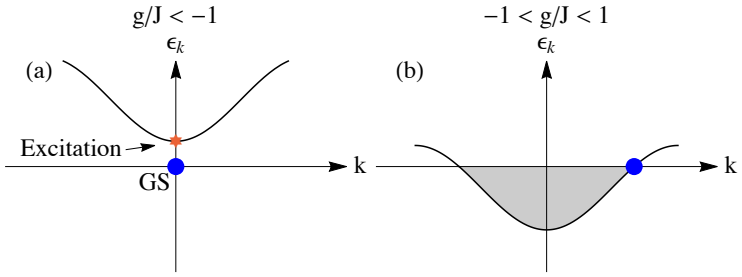

Figure 4: Illustration of the energy gap in the XX model. When $|g|/J > 1$ there is an energy gap to create an excitation, whereas for $|g|/J < 1$ this gap vanishes.

where the spin up is only at site n. The ground-state will therefore be a linear combination of these states, which is *highly entangled*. This is quite remarkable: for $g/J < -1$ we have a state with no entanglement at all, whereas for g/J only slightly above -1, we get an insanely entangled state. This is what I mean when I say that a quantum phase transition is marked by an *abrupt* reconfiguration of the ground-state.

4.3 Energy gap

Another important property of quantum phase transitions is the energy gap that exists between the ground-state and the first excited state. When $g/J < -1$ there are no fermions in the ground-state, so the first excited state will be a state where we put a single fermion with $k = 0$ (the smallest energy). The energy gap in this phase is therefore

$$(g/J < -1) \qquad \Delta = \epsilon_{k=0} = -g - J. \tag{4.17}$$

The situation is like that depicted in Fig. 4(a). The case of $g/J > 1$ is analogous.

On the other hand, let us see what happens when $|g|/J < 1$. In this case the ground state is obtained by filling all states up to k_F, leaving all states above it, empty. An excitation is then constructed by adding a fermion to one of these empty states. The situation is like that depicted in Fig. 4(b): we take a state which lies at k_F and give it a tiny kick, promoting to a state with a slightly higher k. But the ϵ_k are all packed very close together, so that the energy cost for doing this is vanishingly small; in fact, it becomes zero in the thermodynamic limit.

We therefore conclude that the phase for $|g|/J > 1$ is *gapped*, whereas the phase for $|g|/J < 1$ is *gapless*. The closing of an energy gap is a distinguishing feature of quantum phase transitions: **the gap always closes at the critical point**. In some systems the gap closes and remains closed (like here). In others, it closes and then opens again (as will be the case of the XY model below).

5 The XY model

5.1 Bogoliubov transformation

Now let us turn to the full XY model in Eqs. (3.27) or (3.28). As we have seen, the Hamiltonian factors into a product of $L/2$ independent Hamiltonians involving only pairs $(k, -k)$ of fermions. The Hamiltonian, however, is not yet diagonal. To finish the

job, we must diagonalize each pair independently. Let us call $c_k \to a$ and $c_{-k} \to b$. Getting rid of all the complicated indices, each Hamiltonian has the form

$$H_2 = \Omega(a^\dagger a + b^\dagger b) + \lambda(a^\dagger b^\dagger + ba). \tag{5.1}$$

This kind of Hamiltonian can be diagonalized by a Bogoliubov transformation. We introduce two new operators α and β according to

$$\begin{aligned} a &= u\alpha - v\beta^\dagger, \\ b &= u\beta + v\alpha^\dagger, \end{aligned} \tag{5.2}$$

where u and v are complex numbers. This is a more unusual kind of transformation, in that it mixes up creation and annihilation operators. We demand that α and β are also fermionic operators. This (as I leave for you to verify) imposes that u and v must satisfy

$$|u|^2 + |v|^2 = 1. \tag{5.3}$$

In our case it will suffice to choose them real, se we parametrize

$$u = \cos\theta/2, \qquad v = \sin\theta/2. \tag{5.4}$$

The idea behind the Bogoliubov transformation is that we will try to choose the value of θ so that the Hamiltonian (5.1) becomes diagonal.

To do that, we insert Eq. (5.2) in Eq. (5.1). We get the following terms

$$a^\dagger a = \cos^2(\theta/2)\alpha^\dagger\alpha + \sin^2(\theta/2)\beta\beta^\dagger - \sin(\theta/2)\cos(\theta/2)(\alpha^\dagger\beta^\dagger + \beta\alpha), \tag{5.5}$$

$$b^\dagger b = \sin^2(\theta/2)\alpha\alpha^\dagger + \cos^2(\theta/2)\beta^\dagger\beta - \sin(\theta/2)\cos(\theta/2)(\alpha^\dagger\beta^\dagger + \beta\alpha), \tag{5.6}$$

$$a^\dagger b^\dagger = \sin(\theta/2)\cos(\theta/2)(\alpha^\dagger\alpha - \beta\beta^\dagger) + \cos^2(\theta/2)\alpha^\dagger\beta^\dagger - \sin^2(\theta/2)\beta\alpha, \tag{5.7}$$

$$ba = \sin(\theta/2)\cos(\theta/2)(\alpha^\dagger\alpha - \beta\beta^\dagger) + \cos^2(\theta/2)\beta\alpha - \sin^2(\theta/2)\alpha^\dagger\beta^\dagger. \tag{5.8}$$

Plugging this in (5.1) and using the fermionic algebra to write, e.g., $\alpha\alpha^\dagger = \alpha^\dagger\alpha + 1$, we then find

$$\begin{aligned} H = {} & 2\Omega\sin^2(\theta/2) - \lambda\sin\theta + (\Omega\cos\theta + \lambda\sin\theta)(\alpha^\dagger\alpha + \beta^\dagger\beta) \\ & + (-\Omega\sin\theta + \lambda\cos\theta)(\alpha^\dagger\beta^\dagger + \beta\alpha). \end{aligned} \tag{5.9}$$

We now choose the angle θ to make the Hamiltonian diagonal; that is, to kill the last term. This means we must choose

$$\tan\theta = \lambda/\Omega.$$

To summarize, a fermionic Hamiltonian of the form

$$H_2 = \Omega(a^\dagger a + b^\dagger b) + \lambda(a^\dagger b^\dagger + ba). \tag{5.10}$$

can be diagonalized by introducing two new operators α and β according to a **Bogoliubov transformation**

$$\begin{aligned} a &= \cos(\theta/2)\alpha - \sin(\theta/2)\beta^\dagger, \\ b &= \cos(\theta/2)\beta + \sin(\theta/2)\alpha^\dagger, \end{aligned} \tag{5.11}$$

with

$$\tan\theta = \lambda/\Omega. \tag{5.12}$$

The Hamiltonian then becomes

$$H_2 = \left(\Omega - \sqrt{\Omega^2+\lambda^2}\right) + \sqrt{\Omega^2+\lambda^2}(\alpha^\dagger\alpha + \beta^\dagger\beta). \tag{5.13}$$

5.2 Diagonalization of the XY model

Let us now focus on H_+ in Eq. (3.27). We are going to apply the Bogoliubov transformation to each term in the sum. We therefore define, in analogy with (5.11),

$$\begin{aligned} c_k &= \cos(\theta_k/2)\eta_k - \sin(\theta_k/2)\eta^\dagger_{-k}, \\ c_{-k} &= \cos(\theta_k/2)\eta_{-k} + \sin(\theta_k/2)\eta^\dagger_k, \end{aligned} \tag{5.14}$$

with

$$\tan\theta_k = \frac{J\gamma\sin k}{-(g+J\cos k)}. \tag{5.15}$$

Copying and pasting Eq. (5.13), the Hamiltonian (3.27) will then become

$$H_+ = 2\sum_{k\in K^+,k>0}\Big\{(-g-J\cos k-\epsilon_k) + \epsilon_k(\eta^\dagger_k\eta_k + \eta^\dagger_{-k}\eta_{-k})\Big\},$$

where we defined

$$\boxed{\epsilon_k = \sqrt{(g+J\cos k)^2 + J^2\gamma^2\sin^2 k}.} \tag{5.16}$$

Sanity check: if $\gamma = 0$ we recover the XX case in Eq. (4.2).

The first term in H_+ is just a constant,

$$\mathcal{E}_0^+ = 2\sum_{k\in K^+,k>0}(-g-J\cos k-\epsilon_k). \tag{5.17}$$

As for the second term, we can write

$$\sum_{k\in K^+,k>0}\epsilon_k(\eta^\dagger_k\eta_k + \eta^\dagger_{-k}\eta_{-k}) = \sum_{k\in K^+,k>0}\epsilon_k\eta^\dagger_k\eta_k + \sum_{k\in K^+,k<0}\epsilon_{-k}\eta^\dagger_k\eta_k.$$

Since $\epsilon_{-k} = \epsilon_k$, we can actually combine the two terms and go back to a sum over all k. We then finally get

$$\boxed{H_+ = \mathcal{E}_0^+ + 2\sum_{k\in K^+}\epsilon_k\eta^\dagger_k\eta_k.} \tag{5.18}$$

The calculation for H_- in Eq. (3.28) is identical and leads to

$$H_- = \mathcal{E}_0^- + 2\sum_{k\in K^-,k\neq 0,\pi}\epsilon_k\eta^\dagger_k\eta_k - 2(g+J)c^\dagger_0c_0 - 2(g-J)c^\dagger_\pi c_\pi,$$

where $\mathcal{E}_0^-$ is defined as in Eq. (5.17), but with the sum being over K^- instead.

5.3 Ground-state

The interpretation of the XY Hamiltonian turns out to be different from the XX model due to the Bogoliubov transformation. Notice, for instance, how the dispersion relation (5.16) is always non-negative, unlike the XX case (4.2), which can be positive or negative. This is not a problem nor a mistake. It is just a peculiarity of the Bogoliubov transformation. Thus, to find the ground-state, we don't need to do any bookkeeping on how many fermions to populate. The ground-state is *always* a state with zero η_k fermions:

$$|\psi_{\text{gs}}\rangle = |0_\eta\rangle. \tag{5.19}$$

Now, this may seem fishy to you. How can it be that in the XX model the ground-state was not necessarily the vacuum, but in the XY model it is always the vacuum? After all, the XX model should be a particular case of this.

This is the fun point, which I wanted to highlight from this discussion: when you Bogoliubov stuff, **the vacuum is not unique**. The vacuum $|0_\eta\rangle$ in Eq. (5.19) is the vacuum of the η_k operators. But this is *not* the vacuum of the original c_k operators. We can see this as follows. By definition $|0_\eta\rangle$ is such that

$$\eta_k|0_\eta\rangle = 0. \tag{5.20}$$

With Eq. (5.14) at hand, let us now look at the *population of c-fermions in the η-vacuum*:

$$\langle 0_\eta|c_k^\dagger c_k|0_\eta\rangle = \langle 0_\eta|\Big[\cos(\theta_k/2)\eta_k^\dagger - \sin(\theta_k/2)\eta_{-k}\Big]\Big[\cos(\theta_k/2)\eta_k - \sin(\theta_k/2)\eta_{-k}^\dagger\Big]|0_\eta\rangle.$$

We then find

$$\langle 0_\eta|c_k^\dagger c_k|0_\eta\rangle = \sin^2\theta_k/2 = \frac{1-\cos\theta_k}{2} = \frac{1}{2}\Big(1 + \frac{g + J\cos k}{\epsilon_k}\Big). \tag{5.21}$$

We therefore see that in general the population is not zero.

As a sanity check, let us now look at the limiting case of the XX model ($\gamma = 0$). In this case we get $\epsilon_k = |g + J\cos k|$ so that

$$\langle 0_\eta|c_k^\dagger c_k|0_\eta\rangle = \frac{1}{2}\Big(1 + \frac{g + J\cos k}{|g + J\cos k|}\Big) = \begin{cases} 0 & g + J\cos k < 0, \\ 1 & g + J\cos k > 0. \end{cases} \tag{5.22}$$

This is exactly the rule we used in the XX model, of occupying states for which the energy $-g - J\cos k$ was negative.

5.4 Energy gap

Since the ground-state is always the η-vacuum, the first excited state will be a state populated by a single η-fermion. The energy gap will then be the smallest of all the ϵ_k:

$$\Delta = \min_k \epsilon_k. \tag{5.23}$$

For simplicity, let us focus on the TFIM case $\gamma = 1$. The dispersion relation then simplifies to

$$\epsilon_k = \sqrt{g^2 + J^2 + 2gJ\cos k}$$

so

$$\frac{\partial \epsilon_k}{\partial k} = -\frac{gJ \sin k}{\epsilon_k} = 0,$$

which means the extrema of ϵ_k will always take place at $k = 0$ or $k = \pi$. When $g > 0$ the minimum is at $k = \pi$, whereas for $g < 0$ it is at $k = 0$. The value of the dispersion relation at these points is

$$\epsilon_{k=0} = |g + J|, \qquad \epsilon_{k=\pi} = |g - J|. \tag{5.24}$$

Let us focus on $g > 0$. We see that the gap will close at

$$g_c = J. \tag{5.25}$$

This therefore shows that the TFIM also has a phase transition at the same g_c as the XX model. At the critical point the gap closes. Unlike the XX model, however, in this case the gap opens up again after we cross g_c.