Quantum spin chains

In these notes I want to talk about a topic I think is really cool: a family of exactly solvable 1D spin 1/2 chains. The basic Hamiltonian has the form

$$\boxed{H = -\frac{h}{2}\sum_{i=1}^{L} \sigma_z^i - \frac{1}{2}\sum_{i=1}^{L-1} \left(J_x \sigma_x^i \sigma_x^{i+1} + J_y \sigma_y^i \sigma_y^{i+1} \right)} \tag{1}$$

this goes by the name of <u>XY model</u>. If $J_x = J_y$ it is called the <u>XX model</u>:

$$H = -\frac{h}{2}\sum_{i=1}^{L} \sigma_z^i - \frac{J}{2}\sum_{i=1}^{L-1} \left(\sigma_x^i \sigma_x^{i+1} + \sigma_y^i \sigma_y^{i+1} \right) \tag{2}$$

this situation is special as the system has rotation invariance around the z axis (think about the last term as the dot product of 2 vectors in the XY plane).

Instead, if $J_y = 0$ in Eq (1) we obtain the <u>transverse field Ising model</u> (<u>TFIM</u>)

$$H = -\frac{h}{2}\sum_{i=1}^{L} \sigma_z^i - \frac{J}{2}\sum_{i=1}^{L-1} \sigma_x^i \sigma_x^{i+1} \tag{3}$$

this is perhaps one of the most famous models in statistical physics. We will also see that this is equivalent to a model by Kitaev for <u>topological superconductors</u>.

Oh, and I forgot to say, in (1) - (3) I am assuming open boundary conditions (OBC). But in these notes we will consider both OBC and periodic boundary conditions (PBC).

The Jordan - Wigner transformation

Let us change from σ_x^i, σ_y^i to $\sigma_\pm^i$:

$$\sigma_x^i = \sigma_+^i + \sigma_-^i \qquad\qquad \sigma_\pm^i = \frac{\sigma_x^i \pm i\,\sigma_y^i}{2} \tag{4}$$

$$\sigma_y^i = \frac{\sigma_+^i - \sigma_-^i}{i}$$

then

$$\begin{aligned} \sigma_x^i \sigma_x^{i+1} &= (\sigma_+^i + \sigma_-^i)(\sigma_+^{i+1} + \sigma_-^{i+1}) \\ &= \sigma_+^i \sigma_+^{i+1} + \sigma_-^i \sigma_-^{i+1} + \sigma_+^i \sigma_-^{i+1} + \sigma_-^i \sigma_+^{i+1} \end{aligned} \tag{5a}$$

$$\begin{aligned} \sigma_y^i \sigma_y^{i+1} &= -(\sigma_+^i - \sigma_-^i)(\sigma_+^{i+1} - \sigma_-^{i+1}) \\ &= -\sigma_+^i \sigma_+^{i+1} - \sigma_-^i \sigma_-^{i+1} + \sigma_+^i \sigma_-^{i+1} + \sigma_-^i \sigma_+^{i+1} \end{aligned} \tag{5b}$$

Thus

$$\begin{aligned} J_x \sigma_x^i \sigma_x^{i+1} + J_y \sigma_y^i \sigma_y^{i+1} &= (J_x - J_y)(\sigma_+^i \sigma_+^{i+1} + \sigma_-^i \sigma_-^{i+1}) \\ &+ (J_x + J_y)(\sigma_+^i \sigma_-^{i+1} + \sigma_-^i \sigma_+^{i+1}) \end{aligned} \tag{5c}$$

It is convenient to parametrize

$$J_x = J\frac{(1+\gamma)}{2} \qquad \gamma = 0 \rightarrow \text{XX model}$$

$$J_y = J\frac{(1-\gamma)}{2} \qquad \gamma = 1 \rightarrow \text{TFIM} \tag{6}$$

We then get $J_x - J_y = J\gamma$ and $J_x + J_y = J$, so that (5c) becomes

$$J_x \sigma_x^i \sigma_x^{i+1} + J_y \sigma_y^i \sigma_y^{i+1} = J \Big\{ \sigma_+^i \sigma_-^{i+1} + \sigma_-^i \sigma_+^{i+1} + \gamma \left(\sigma_+^i \sigma_+^{i+1} + \sigma_-^i \sigma_-^{i+1} \right) \Big\} \tag{7}$$

We also get rid of σ_z:

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

$$\hookrightarrow \sigma_+ \sigma_- = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{8a}$$

thus

$$\sigma_z = 2 \sigma_+ \sigma_- - 1 \tag{8b}$$

Hence, we may finally write the Hamiltonian (1) as

$$\boxed{H = - h \sum_{i=1}^{L} \sigma_+^i \sigma_-^i - \frac{J}{2} \sum_{i=1}^{L-1} \Big\{ \sigma_+^i \sigma_-^{i+1} + \sigma_-^i \sigma_+^{i+1} + \gamma \left(\sigma_+^i \sigma_+^{i+1} + \sigma_-^i \sigma_-^{i+1} \right) \Big\}} \tag{9}$$

where I neglected the constant that comes from the "1" in Eq (8)

Notice how, at least the term without γ, look a bit like a tight-binding chain. It essentially flips a spin at site i and then does the opposite flip on $i+1$. (the term with γ makes things a bit weirder, I admit).

However, there is one fundamental difference which distinguishes this from a tight-binding model: the spin algebra is messed up! Bosons and Fermions are clean

$$[a_i, a_j^\dagger] = \delta_{ij} \tag{10}$$

$$\{c_i, c_j^\dagger\} = \delta_{ij} \tag{11}$$

But for Pauli matrices we get something mixed. Recall that

$$\sigma_+^i = 1 \otimes \ldots \otimes \sigma_+ \otimes \ldots \otimes 1 \tag{12}$$

thus if $i \neq j$ then the $\sigma_\pm$ commute

$$\boxed{(i \neq j) \qquad [\sigma_+^i, \sigma_-^j] = [\sigma_+^i, \sigma_+^j] = 0} \tag{13}$$

But if $i = j$ then they satisfy the same algebra of the 2×2 matrices in Eq (8a), which is an anti-commutation relation

$$\boxed{\{\sigma_+^i, \sigma_-^i\} = 1} \tag{14}$$

Isn't this awkward? they behave like bosons when $i \neq j$ but like fermions when $i = j$. this messes up everything. At first we could be tempted to think about $\sigma_\pm^i$ as fermionic operators $c_i^\dagger$ and c_i, since both only have 2 levels. But they are not fermionic, as they commute for $i \neq j$ (whereas fermionic operators should anti-commute).

A day may come when there is nothing we can do to move forward. But it is not this day! This day we use an idea developed by Jordan and Wigner to map Pauli operators into fermionic operators:

> Jordan-Wigner: exact mapping between spin 1/2 Pauli operators and fermionic operators

The map looks like this

$$\boxed{c_i = \left[\prod_{m=1}^{i-1} (-\sigma_z^m)\right] \sigma_-^i} \qquad \text{Jordan-Wigner} \tag{15}$$

Yeah, it's weird I know. Let me explain. Recall the tensor structure of the Pauli operators [Eq (12)]. What (15) means is

$$c_i = (-\sigma_z) \otimes (-\sigma_z) \otimes \dots \otimes (-\sigma_z) \otimes \sigma_- \otimes 1 \otimes 1 \dots \otimes 1 \tag{16}$$

we get the operator σ_- and we multiply it by a <u>string</u> of $(-\sigma_z)$ operators on all sites to the left.

The operator c_i^+ is just the adjoint of (15). Since Pauli operators for different sites commute we can write

$$c_i^+ = \left[\prod_{m=1}^{i-1} (-\sigma_z^m)\right] \sigma_+^i \tag{17}$$

Let's now check that these guys satisfy the fermionic algebra (11) and in doing so we will understand why this transformation works.

The only thing we need to remember is that

$$(\sigma_z)^2 = 1 \tag{18}$$

We then get, for the same site $(i=j)$

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

Note how we can move the right-most block of σ_z's accross σ_-^i, as the block acts only on $1, \dots, i-1$. This block will then match up with the other block and give 1 due to (18)

$$\left[\prod_{M=1}^{i-1} (-\sigma_z^m) \right] \left[\prod_{m=1}^{i-1} (-\sigma_z^m) \right] = 1 \tag{19}$$

Thus we get simply

$$c_i c_i^+ = \sigma_-^i \sigma_+^i \tag{20a}$$

And, by the same arguments

$$c_i^+ c_i = \sigma_+^i \sigma_-^i \tag{20b}$$

Thus, the "same-site" algebra remains perfect

$$\boxed{\{ \sigma_-^i, \sigma_+^i \} = \{ c_i, c_i^+ \} = 1} \tag{21}$$

Next, let us talk about different sites, which is where the problem is. Suppose, for concreteness, that $j > i$. Then we get

$$c_i c_j^\dagger = \left[\prod_{m=1}^{i-1} (-\sigma_z^m)\, \sigma_-^i \right] \left[\prod_{m=1}^{j-1} (-\sigma_z^m)\, \sigma_+^j \right] \tag{22}$$

Now the σ_z block cannot go through the σ_-^i because there will be a $(-\sigma_z^i)$ in the right block. But now comes the magic. Are you ready? Using only the 2×2 matrices in Eq (8a), one may check that

$$\boxed{\begin{aligned} \sigma_+ (-\sigma_z) &= \sigma_+ & \sigma_- (-\sigma_z) &= -\sigma_- \\ (-\sigma_z)\, \sigma_+ &= -\sigma_+ & (-\sigma_z)\, \sigma_- &= \sigma_- \end{aligned}} \tag{23}$$

Thus, going back to (22) we <u>can</u>, in the end, take the right-most σ_z block through σ_-^i. But all we need to know is that, when $(-\sigma_z^i)$ crosses σ_-^i, we will get a -1:

$$\boxed{\sigma_-^i (-\sigma_z^i) = -(-\sigma_z^i)\, \sigma_-^i} \tag{24}$$

As a result, we will cancel most σ_z's, except those between i and j

$$(j>i) \qquad c_i c_j^\dagger = -\left[\prod_{m=i}^{j-1} (-\sigma_z^m) \right] \sigma_-^i \sigma_+^j \tag{25}$$

Next we do it the other way around

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

But now we have no problems moving the σ_z's to the left because $j > i$. Thus we get

$$c_j^\dagger c_i = \left[\prod_{m=i}^{j-1} (-\sigma_z^m) \right] \sigma_+^j \sigma_-^i \qquad (26)$$

Note how the key is the minus sign in (25). It converts a anti-commutator into a commutator

$$\{ c_i, c_j^\dagger \} = \left[\prod_{m=1}^{i-1} (-\sigma_z^m) \right] \underbrace{\left(-\sigma_-^i \sigma_+^j + \sigma_+^j \sigma_-^i \right)}_{0 \text{ because } \sigma\text{'s commute.}} = 0 \qquad (27)$$

Thus, as our big conclusion, we find that the Jordan-Wigner transformation (15) indeed produces fermionic operators from Pauli matrices

In terms of states, we can also map the computational basis $|\sigma_1 \dots \sigma_L\rangle$ into a fermionic Fock basis. From (15) it is quite clear that the vacuum corresponds to

$$|0\rangle = |\downarrow \dots \downarrow\rangle \tag{28}$$

as the σ_-^i annihilate any $\downarrow$ state. This motivates us to try a correspondence of the form

$$|0\rangle = |\downarrow\rangle \qquad |1\rangle = |\uparrow\rangle \tag{29}$$

Let's see if this works. Recall that Fermionic operators should be anti-symmetric under sign exchange. Thus

$$c_i |m_1, \dots, m_i, \dots, m_L\rangle = (-1)^{\Sigma_\ell} m_i |m_1 \dots, m_i - 1, \dots, m_L\rangle \tag{30}$$

where

$$\Sigma_\ell = \sum_{i=1}^{\ell-1} m_i \tag{31}$$

In words, every time we jump a c_i over each state, we get a (-1). Now it becomes even more evident why the factors of $(-\sigma_z^m)$ in (15) are so important: recall that

$$\sigma_z |\sigma\rangle = \sigma|\sigma\rangle \qquad \sigma = \pm 1 \tag{32}$$

In terms of $m = 0, 1$ we then have

$$\sigma = 2m - 1 \qquad m = 0 \leftrightarrow \sigma = -1$$
$$m = \frac{\sigma + 1}{2} \qquad m = 1 \leftrightarrow \sigma = 1 \tag{33}$$

Thus when $(-\sigma_z)$ acts on $|m\rangle$ it gives $1-2m$. But since $m = 0, 1$, we have

$$1 - 2m = (-1)^m \tag{34}$$

To summarize: the Jordan-Wigner transformation (15) works perfectly and it is awesome!

Before we move on, there is only one comment I would like to make. Namely that, as you may check by playing with the 2×2 Pauli matrices, it follows that

$$(-\sigma_z) = e^{i\pi \sigma_+ \sigma_-} \tag{35}$$

Thus Eq (15) is also sometimes written as

$$c_i = \prod_{m=1}^{i-1} e^{i\pi \sigma_+^m \sigma_-^m} \sigma_-^i \tag{36}$$

this formula can be easily inverted because $(e^{i\pi\sigma_+^m\sigma_-^m})^2 = 1$. Thus

$$\sigma_-^i = \left[\prod_{m=1}^{i-1} e^{i\pi\sigma_+^m\sigma_-^m}\right] c_i$$

But we already saw in Eq (20b) that $\sigma_+^m\sigma_-^m = c_m^\dagger c_m$. Thus we get

$$\boxed{\sigma_-^i = \left[\prod_{m=1}^{i-1} e^{i\pi c_m^\dagger c_m}\right] c_i} \tag{37}$$

Fermionic representation of the spin Hamiltonian

Let's now return to the Hamiltonian (9) and try to express it in terms of the fermionic operators c_i in Eq (15). We already saw that $\sigma_i^+ \sigma_i^- = c_i^\dagger c_i$, so the first part of (15) is done. Next, for $\sigma_+^i \sigma_-^{i+1}$ we use the result in Eq (26).

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

Setting $j = i+1$ we get only one term in the z-string

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

But $(-\sigma_z^i)\sigma_-^i = \sigma_-^i$ (Eq (23)). Thus

$$c_{i+1}^\dagger c_i = \sigma_+^{i+1} \sigma_-^i \tag{38}$$

Taking the adjoint, we get

$$c_i^\dagger c_{i+1} = \sigma_+^i \sigma_-^{i+1} \tag{39}$$

Finally, we study the terms $\sigma_+^i \sigma_+^{i+1}$. May be in this case we can just use the definition (17) again

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

$$= \sigma_+^{i+1} (-\sigma_z^i) \sigma_+^i$$

$$= - \sigma_+^{i+1} \sigma_+^i$$

Thus

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

Note: the left guys commute, $\sigma_+^i \sigma_+^{i+1} = \sigma_+^{i+1} \sigma_+^i$. But the guys on the right anti-commute, $c_{i+1}^\dagger c_i^\dagger = - c_i^\dagger c_{i+1}^\dagger$. Thus, to avoid minus signs let us write

$$\sigma_+^i \sigma_+^{i+1} = c_i^\dagger c_{i+1}^\dagger \tag{40}$$

Taking the adjoint we also find

$$\sigma_-^i \sigma_-^{i+1} = c_{i+1} c_i \tag{41}$$

We now have all ingredients required to write the Hamiltonian (9):

$$\boxed{H = -h \sum_{i=1}^{L} c_i^\dagger c_i - \frac{J}{2} \sum_{i=1}^{L-1} \left\{ c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i + \gamma \left(c_i^\dagger c_{i+1}^\dagger + c_{i+1} c_i \right) \right\}} \tag{42}$$

This is the <u>fermionic</u> <u>representation</u> <u>of</u> <u>the</u> <u>XY</u> <u>model</u>. We see that this is now really close to the tight-binding model. In fact if $\gamma = 0$ (XX model) we get exactly the tight-binding. This is therefore the reason why moving to a fermionic picture is "worth it": it allows us to use tools we are already familiar with

Annoying features of periodic boundary conditions

Periodic BCs are usually a blessing, as they reintroduce translation invariance. This is also true in this particular case. However, here they come with an annoying feature. Going back all the way to the Hamiltonian (9), in order to add PBCs we simply need to add an extra term

$$H_{PBC} = H_{OBC} - \frac{J}{2}\left\{ \sigma_+^N \sigma_-^1 + \sigma_-^N \sigma_+^1 + \gamma\left(\sigma_+^N \sigma_+^1 + \sigma_-^N \sigma_-^1\right)\right\} \quad (43)$$

where H_{OBC} is the expression in (9) [OBC = open boundary conditions].

Now let's see how these boundary terms behave when we use the Jordan-Wigner transformation (15). We get

$$c_N^\dagger c_1 = \left[\prod_{m=1}^{N-1} (-\sigma_z^m)\right] \sigma_+^N \sigma_-^1$$

Using (23) we can also write $\sigma_+^N = -(-\sigma_z^N)\sigma_+^N$, just so we can include an extra $(-\sigma_z^N)$ into the z-string. We then get

$$c_N^\dagger c_1 = -\left[\prod_{m=1}^{N} (-\sigma_z^N)\right] \sigma_+^N \sigma_-^1$$

Inverting, as we did in going from (36) to (37), we get

$$\sigma_+^N \sigma_-^1 = -\left[\prod_{m=1}^{N} e^{i\pi c_m^\dagger c_m}\right] c_N^\dagger c_1 \quad (44)$$

this remaining string can also be written in a fancy way as follows. Since $e^{i\pi} = -1$,

$$e^{i\pi c_m^\dagger c_m} = (-1)^{c_m^\dagger c_m}$$

thus

$$\prod_{m=1}^{N} e^{i\pi c_m^\dagger c_m} = \prod_{m=1}^{N} (-1)^{c_m^\dagger c_m}$$

$$= (-1)^{\sum_{m=1}^{N} c_m^\dagger c_m}$$

thus, we see here the appearance of the Number operator

$$\boxed{\hat{N} = \sum_{m=1}^{N} c_m^\dagger c_m} \tag{45}$$

with which, Eq (44) may be written as

$$\sigma_+^N \sigma_-^1 = -(-1)^{\hat{N}} c_N^\dagger c_1 \tag{46}$$

the expressions for the other terms in (43) are analogous. First, taking the adjoint of (46) we get

$$\sigma_-^N \sigma_+^1 = -(-1)^{\hat{N}} c_1^\dagger c_N \tag{47}$$

and so on for $\sigma_+^N \sigma_+^1$ and $\sigma_-^N \sigma_-^1$

Hence, Eq (43) becomes

$$\boxed{H_{PBC} = H_{OBC} - \frac{J}{2}(-1)^{\hat{N}}\left\{ c_N^\dagger c_1 + c_1^\dagger c_N + \gamma\,(c_N^\dagger c_1^\dagger + c_1 c_N)\right\}} \tag{48}$$

I know this formula may seem innocent. But it is not: $(-1)^{\hat{N}}$ is an operator and a fairly complicated one for that matter. Thus, we see that, quite annoyingly, using periodic boundary conditions is not as simple as in the standard tight-binding.

Notwithstanding, not all hope is lost. The operator $(-1)^{\hat{N}}$ can only take two values. Within those Fock states for which N is even, it will always be $+1$ and within odd N, it will be -1. So we can split out our Fock space into even and odd sectors and work on each one sepparately. Or we can also pretend this problem doesn't exist! Sometimes that works! We will get back to this later on.

Secondly

$$\sum_{i=1}^{N} c_i^\dagger c_{i+1} = \frac{1}{L} \sum_i \sum_{kq} e^{-i(k-q)x_i} e^{iq} b_k^\dagger b_q$$

$$= \sum_{k,q} e^{iq} \underbrace{\left[\frac{1}{L} \sum_i e^{-i(k-q)x_i} \right]}_{\delta_{kq}} b_k^\dagger b_q$$

$$= \sum_k e^{ik} b_k^\dagger b_k$$

thus (49) becomes

$$\boxed{\begin{aligned} H &= \sum_k \epsilon_k b_k^\dagger b_k \\ \epsilon_k &= -h - J\cos k \end{aligned}} \qquad \begin{matrix}(53)\\ \\ (54)\end{matrix}$$

this is a result we are already quite familiar with. However, the interpretation is now different because these are not actual fermions. We still have a spin model below all of this. So, for instance, the number of fermions is not fixed (they are not real!).

To understand what the number of fermions means in this case, recall that $c_i^\dagger c_i = \sigma_i^+ \sigma_i^- = (\sigma_z^i + 1)/2$, which is the operator measuring if the spin at site i is flipped or not. Thus the number of fermions $\sum_i c_i^\dagger c_i$ represents the number of spins that are flipped. It is really cool to see, in this sense, how the field h in Eq (49) plays the role of a chemical potential

The XX model

As our first investigation of the Hamiltonian (42), let us consider the XX model, which corresponds to $\gamma = 0$. In this case we get exactly a tight-binding chain. For simplicity, I will consider here the clumsy approach and use PBC without worrying about the extra term in (48). Thus, we will consider simply the model described by

$$\boxed{H = -h\sum_{i=1}^{L} c_i^\dagger c_i - \frac{J}{2}\sum_{i=1}^{L}(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i)} \tag{49}$$

with $c_{N+1} = c_1$. We already know that this model can be diagonalized by a Fourier transform

$$c_i = \frac{1}{\sqrt{L}}\sum_k e^{ikx_i} b_k \tag{50}$$

where $x_i = i$ (just so we don't confuse the i's) and

$$k = \frac{2\pi \ell}{L}, \quad \ell = 0, \pm 1, \pm 2, \ldots, \pm \frac{N}{2} \tag{51}$$

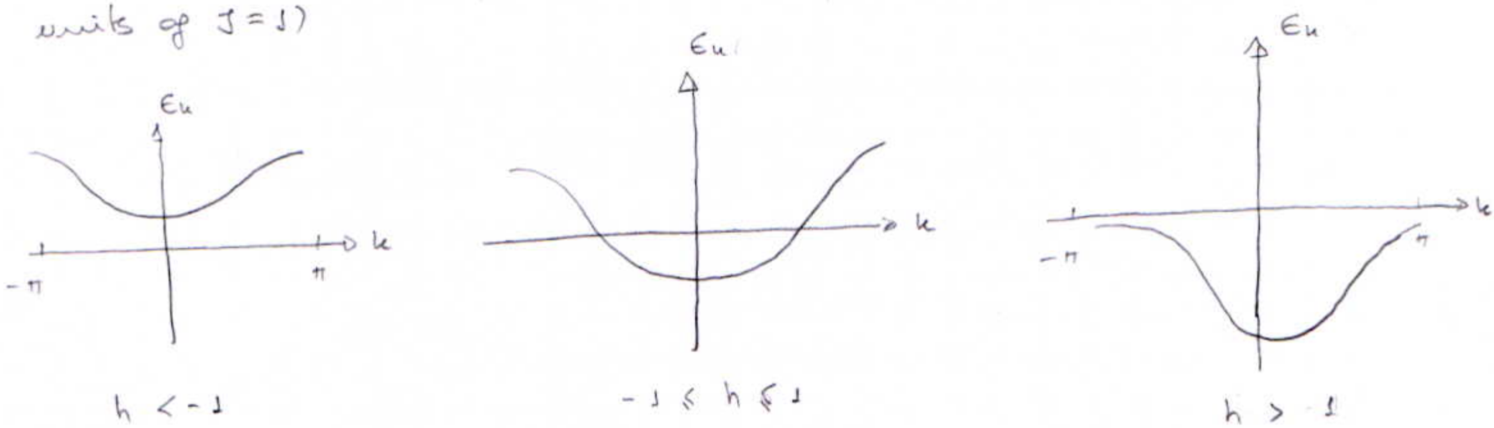
We also know that the b_k in (50) will also be fermionic operators (I got tired of using d_k. "d" is an ugly letter for an annihilation operator. "b" is much prettier). Let's review how (50) diagonalizes (49).

First,

$$\sum_{i=1}^{L} c_i^\dagger c_i = \sum_k b_k^\dagger b_k \tag{52}$$

Ground-state of the XX model

To start, let us try to figure out what is the ground-state of (53). Although it may seem obvious, to find the GS we just need to remember that the GS is the state with the smallest possible energy. the energies ϵ_k in (54) have the following form (all in units of $J=1$)



Now comes the fun part. Suppose $h<-1$. then $\epsilon_k > 0$ always so if we add a fermion to any mode k, it will always contribute with a positive energy. Hence, if what we want is the GS, we should not add any fermions. that is

$$\boxed{\begin{aligned} &\text{If } h<-1: \quad |\psi_{gs}\rangle = |0\rangle = |\downarrow\downarrow\cdots\downarrow\rangle \quad \text{see Eq (28)} \\ &\mathcal{E}_{gs} = 0 \end{aligned}}$$ (55a) (55b)

Next suppose $h \in [-1, 1]$. Then there are some values of k for which $\epsilon_k < 0$. For these states, adding a fermion is worth it, as it reduces the energy. Thus, the GS in this case will have all states with $\epsilon_k < 0$ filled and the others empty.

$-1 < h < 1$: GS has all k with $\epsilon_k < 0$ filled and the rest empty

We can make this more formal as follows. Define a "Fermi momentum" k_F as the value of k for which $\epsilon_k = 0$. That is

$$\boxed{k_F = \operatorname{acos}(-h/J)} \tag{56}$$

Then the GS can be written as

$$-1 < h < 1: \quad |\psi_{gs}\rangle = \left[\prod_{|k| < k_F} b_k^\dagger\right] |0\rangle \tag{57a}$$

$$\mathcal{E}_{gs} = \sum_{|k| < k_F} \epsilon_k \tag{57b}$$

Finally, if $h > 1$ then $\epsilon_k < 0$ for all values of k, so the GS will be the state with all spins up

$$h > 1: \quad |\psi_{gs}\rangle = \left[\prod_k b_k^\dagger\right] |0\rangle = |\uparrow\uparrow \ldots \uparrow\rangle \tag{58a}$$

$$\mathcal{E}_{gs} = \sum_k \epsilon_k \tag{58b}$$

(It is not immediately obvious that (58a) is indeed the state with all spins $\uparrow$. But I will leave this for you to check as an exercise).

The results in (55) - (58) are, in my opinion, really really cool.

Let's first compute the <u>magnetization</u>

$$m = \frac{1}{L}\sum_{i=1}^{L}\langle\sigma_z^i\rangle = \frac{1}{L}\sum_{i=1}^{L}\langle 2\sigma_+^i\sigma_-^i - 1\rangle$$
$$= \frac{2}{L}\sum_{i=1}^{N}\langle c_i^\dagger c_i\rangle - 1$$

this sum is nothing but the average number of fermions, so

$$m = \frac{2}{L}\langle\hat{N}\rangle - 1 \qquad (59)$$

the intuition about $\langle\hat{N}\rangle$ is already quite clear from what we just discussed:

$$\langle\hat{N}\rangle = \begin{cases} 0 & h < -1 \\ L & h > 1 \end{cases} \qquad (60)$$

for the interesting part, $h \in [-1, 1]$, we get instead

$$\langle\hat{N}\rangle = \sum_{|k|<k_F} 1 \qquad (61)$$

that is, we put 1 particle on all states with $|k|<k_F$

We can now convert the sum to an integral using our old trick:

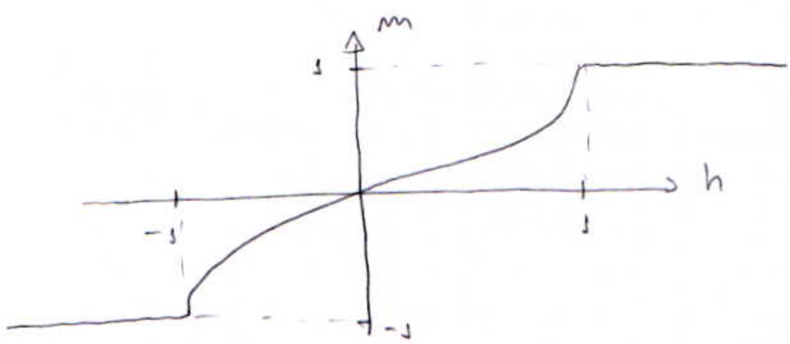
$$\langle \hat{N} \rangle = \frac{L}{2\pi} \int_{-k_F}^{k_F} dk = \frac{L}{\pi} k_F = \frac{L}{\pi} \operatorname{acos}(-h/J) \qquad (62)$$

Thus (59) reduces to

$$\boxed{m = \begin{cases} -1 & h < -1 \\ \frac{2}{\pi} \operatorname{acos}(-h) - 1 & -1 < h < 1 \\ 1 & h > 1 \end{cases}} \qquad (63)$$

← I put $J = 1$ because I am lazy

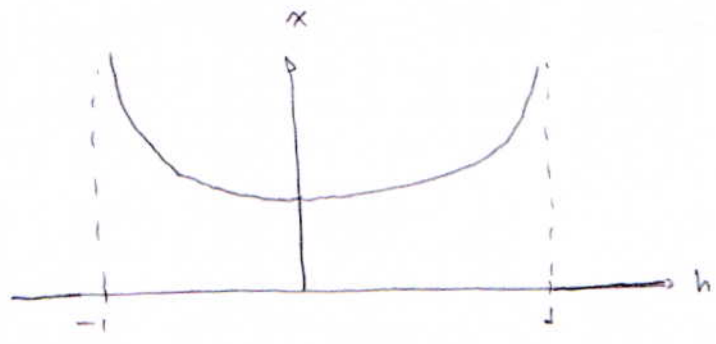
this result looks like this



At $h = \pm 1$ there is a sharp kink in m. It's derivative is discontinuous at this point. In fact, if we define the susceptibility

$$\chi = \frac{\partial m}{\partial h} = \begin{cases} 0 & h < -1 \\ \frac{2/\pi}{\sqrt{1 - h^2}} & -1 < h < 1 \\ 0 & h > 1 \end{cases}$$

We see that χ diverges at $h = \pm 1$ (the derivative of a kink diverges)



What we are looking at here is a quantum phase transition. These kinds of transitions occur due to a competition between two terms in the Hamiltonian: the J and h terms in Eq (49) (or Eq (2)). The J terms induce the spins to lie in the xy plane, whereas the h term induces them to point in the z direction.

As a consequence of this competition, there are two special values of the field (or, more generally, of h/J) which are

$$|h| = h_c = 1 = \text{critical field} \tag{64}$$

At these points there is a fundamental change in the ground state $|\psi_{gs}\rangle$. This is the key point of a quantum phase transition: the ground state changes in a dramatic way at the critical point.

To better understand what this change means, let us compare (55a) with (57a). In the $h<-1$ phase [Eq (55a)] the ground-state is a product state. There is no entanglement

$$\begin{aligned} |\psi_{gs}\rangle &= |\downarrow\downarrow \cdots \downarrow\rangle \\ &= |\downarrow\rangle \otimes |\downarrow\rangle \otimes \cdots \otimes |\downarrow\rangle \end{aligned} \tag{65}$$

Conversely, when $h \in [-1,1]$ the state will be highly entangled. To see this more clearly, let us write (57a) in terms of the c_i operators.

$$|\psi_{GS}\rangle = \left[\prod_{|k|<k_F} b_k^\dagger \right] |0\rangle \qquad (66)$$

$$b_k = \frac{1}{\sqrt{L}} \sum_{i=1}^{L} e^{-ikx_i} c_i \qquad (67)$$

If we stop for a second, we will see that substituting (67) in (66) will lead to a quite messy formula because it's a product of sums.

So, for simplicity, let us suppose that we are just above $h=-1$, in such a way that $k_F = 0$. That is, the only populated state is $b_{k=0}$. (see the middle fig in page 21). Then (66) becomes

$$\begin{aligned} |\psi_{gs}\rangle &= b_{k=0}^\dagger |0\rangle \\ &= \frac{1}{\sqrt{L}} \sum_{i=1}^{L} c_i^\dagger |0\rangle \end{aligned} \qquad (68)$$

But

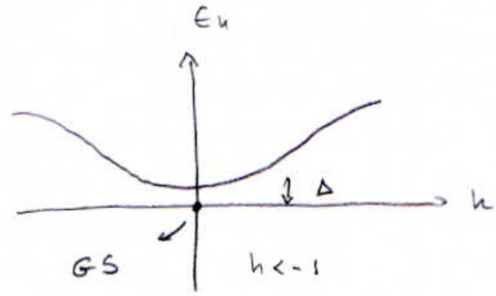
$$c_i^\dagger |0\rangle = |\downarrow\downarrow \ldots \underset{\substack{\uparrow \\ \text{position } i}}{\uparrow} \ldots \downarrow\rangle \qquad (69)$$

Thus the GS will be a superposition of all states with one spin ↑ and all others down. This state is highly entangled.

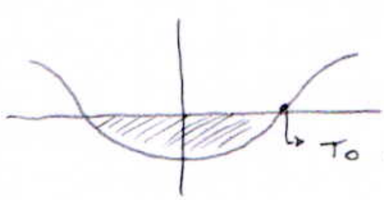
Another key property of quantum phase transitions is the energy gap between the GS and the first excited state. $h < -1$ there are no fermions [Eq (53a)] so the first excited state will be a state with a single fermion at $k=0$ (because this has the smallest energy). Thus, the energy gap is

$$\boxed{\begin{aligned}\Delta = \epsilon_0 &= -h-J \\ &= -h-1\end{aligned}} \qquad h < -J \qquad (70)$$

We now see that when we reach the critical point $h=-1$, the gap closes



Next, when we enter the phase with $|h|<1$, the GS will already have some fermions on it, so the first excited state will simply be that with 1 extra fermion, which has practically no energy cost to produce



We therefore see that another distinguishing feature of this model is that we have two phases, a gapped phase for $|h| > h_c$ and a gapless phase for $|h| < h_c$

$$\boxed{\begin{array}{l} |h| > h_c \ : \ \text{gapped phase} \\ |h| < h_c \ : \ \text{gapless phase} \end{array}} \tag{71}$$

The closing of the energy gap is a signature of a quantum critical point. However, in some models it remains closed at one of the phases, whereas in others it closes and then opens again.

The XX model at finite temperature

It is really easy to extend the previous results to $T \neq 0$. Once we have the Hamiltonian in diagonal form, as in Eq (53), then we already know that the thermal occupations will be described by the Fermi-Dirac distribution

$$\langle b_k^\dagger b_k \rangle := f_k = \frac{1}{e^{\beta \epsilon_k} + 1} \qquad (72)$$

From this we can compute anything we want. For instance

$$\boxed{\langle \hat{N} \rangle = \sum_k \langle b_k^\dagger b_k \rangle = \frac{L}{2\pi} \int_{-\pi}^{\pi} dk \, \frac{1}{e^{\beta \epsilon_k} + 1}} \qquad (73)$$

and the internal energy is

$$\boxed{\langle H \rangle = \sum_k \epsilon_k \langle b_k^\dagger b_k \rangle = \frac{L}{2\pi} \int_{-\pi}^{\pi} dk \, \frac{\epsilon_k}{e^{\beta \epsilon_k} + 1}} \qquad (74)$$

the magnetization is given by (59)

$$m = \frac{2}{L} \langle \hat{N} \rangle - 1 = \frac{1}{\pi} \int_{-\pi}^{\pi} dk \, \frac{1}{e^{\beta \epsilon_k} + 1} - 1$$

writing

$$1 = \int_{-\pi}^{\pi} dk \, \frac{1}{2\pi}$$

we get

$$m = \frac{1}{\pi}\int_{-\pi}^{\pi} dk \left[\frac{1}{e^{\beta\epsilon_k}+1} - \frac{1}{2} \right]$$

$$= \frac{1}{\pi}\int_{-\pi}^{\pi} dk \left\{ \frac{2 - e^{\beta\epsilon_k} - 1}{2(e^{\beta\epsilon_k}+1)} \right\}$$

$$= \frac{1}{2\pi}\int_{-\pi}^{\pi} dk \left\{ \frac{1 - e^{\beta\epsilon_k}}{1 + e^{\beta\epsilon_k}} \right\}$$

Finally we can write this as

$$m = -\frac{1}{2\pi}\int_{-\pi}^{\pi} dk \tanh\left(\frac{\beta\epsilon_k}{2} \right)$$

or

$$\boxed{m = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk \tanh\left\{ \frac{\beta(h + J\cos k)}{2} \right\}} \tag{75}$$

Other thermodynamic quantities follow a similar spirit.

For instance, the specific heat is

$$\boxed{c = \frac{1}{L}\frac{\partial \langle H\rangle}{\partial T} = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk \frac{(\epsilon_k/T)^2 \, e^{\beta\epsilon_k}}{(e^{\beta\epsilon_k}+1)^2}} \tag{76}$$

and the susceptibility is

$$\boxed{\chi = \frac{\partial m}{\partial h} = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk \frac{\beta}{2} \operatorname{sech}^2\left\{ \frac{\beta(h + J\cos k)}{2} \right\}} \tag{77}$$

XY model

We now turn to the diagonalization of the full XY model in Eq (1). Or, in the fermionic representation, Eq (42):

$$H = -h \sum_{i=1}^{L} c_i^\dagger c_i - \frac{J}{2} \sum_{i=1}^{L} \left\{ c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i + \gamma \left(c_i^\dagger c_{i+1}^\dagger - c_{i+1} c_i \right) \right\} \tag{78}$$

As before, we will be sloppy with the periodic boundary conditions.

Proceeding as we did in (49), the first thing we do is to move to Fourier space using Eq (50). The only new thing we need to compute are the γ terms in (78):

$$\sum_{i=1}^{L} c_i^\dagger c_{i+1}^\dagger = \sum_{i=1}^{L} \frac{1}{L} \sum_{k,q} e^{-ikx_i} e^{-iqx_{i+1}} b_k^\dagger b_q^\dagger$$

$$= \sum_{k,q} e^{-iq} \underbrace{\left[\frac{1}{L} \sum_{i=1}^{L} e^{-i(k+q)x_i} \right]}_{\delta_{k,-q}} b_k^\dagger b_q^\dagger$$

thus

$$\sum_{i=1}^{L} c_i^\dagger c_{i+1}^\dagger = \sum_{k} e^{ik} b_k^\dagger b_{-k}^\dagger \tag{79}$$

The Hamiltonian (78) thus becomes

$$H = \sum_k \left\{ -h - J\cos k \right\} b_k^\dagger b_k - \frac{J\gamma}{2} \sum_k \left\{ e^{ik} b_k^\dagger b_{-k}^\dagger + e^{-ik} b_{-k} b_k \right\} \tag{80}$$

this new form is not yet diagonal because it mixes k with $-k$. We can write this in a slightly better way by focusing only on $k>0$: for instance, using again $\epsilon_k = -h - J\cos k$, we can write

$$\sum_k \epsilon_k b_k^\dagger b_k = \sum_{k>0} \left(\epsilon_k b_k^\dagger b_k + \epsilon_{-k} b_{-k}^\dagger b_{-k} \right)$$

$$= \sum_{k>0} \epsilon_k \left(b_k^\dagger b_k + b_{-k}^\dagger b_{-k} \right)$$

since $\epsilon_{-k} = \epsilon_k$. Similarly

$$\sum_k e^{ik} b_k^\dagger b_{-k}^\dagger = \sum_{k>0} \left(e^{ik} b_k^\dagger b_{-k}^\dagger + e^{-ik} b_{-k}^\dagger b_k^\dagger \right)$$

$$= \sum_{k>0} \left(e^{ik} - e^{-ik} \right) b_k^\dagger b_{-k}^\dagger$$

because $b_{-k}^\dagger b_k^\dagger = b_k^\dagger b_{-k}^\dagger$. Thus,

$$\sum_k e^{ik} b_k^\dagger b_{-k}^\dagger = 2i \sum_{k>0} (\sin k) b_k^\dagger b_{-k}^\dagger$$

and taking the adjoint we get

$$\sum_k e^{-ik} b_{-k} b_k = -2i \sum_{k>0} (\sin k)\, b_{-k} b_k$$

Thus, Eq (80) becomes

$$\boxed{H = \sum_{k>0} \Big\{ \epsilon_k \left(b_k^+ b_k + b_{-k}^+ b_{-k} \right) + \\ - i J_x \sin k \left(b_k^+ b_{-k}^+ - b_{-k} b_k \right) \Big\}} \tag{81}$$

This Hamiltonian is still not diagonal. But it is now greatly simplified since it only involves the pairs $(k,-k)$ for a given k. That is, there is nothing here mixing k with some other k'.

The Hamiltonian (81) can be diagonalized by a technique known as a <u>Bogoliubov</u> <u>transformation</u>. The idea is to introduce two new operators α_k and β_k as

$$\boxed{\begin{aligned} b_k &= u_k \alpha_k - i v_k \beta_k^+ \\ b_{-k} &= i v_k \alpha_k^+ + u_k \beta_k \end{aligned}} \tag{82}$$

where u_k and v_k are numbers that we will try to adjust to put (81) in diagonal form.

But before we do so, let us see what are the restrictions imposed on u_k and v_k in order for α_k and β_k to be fermionic operators as well. That is, we want

$$\{\alpha_k, \alpha_k^+\} = \{\beta_k, \beta_k^+\} = 1 \qquad \{\alpha_k, \beta_k^+\} = 0$$
$$\{\alpha_k, \beta_k\} = 0 \tag{83}$$

We have

$$0 = \{ b_k, b_{-k} \} = \{ u_k \alpha_k - i v_k \beta_k^\dagger, i v_k \alpha_k^\dagger + u_k \beta_k \}$$

$$= i u_k v_k \{ \alpha_k, \alpha_k^\dagger \} - i u_k v_k \{ \beta_k^\dagger, \beta_k \}$$

$$+ u_k^2 \{ \alpha_k, \beta_k \} + v_k^2 \{ \beta_k^\dagger, \alpha_k^\dagger \}$$

Imposing (83), this looks naturally satisfied. Next

$$\{ b_k, b_k^\dagger \} = \{ u_k \alpha_k - i v_k \beta_k^\dagger, u_k \alpha_k^\dagger + i v_k \beta_k \}$$

$$= u_k^2 \underbrace{\{ \alpha_k, \alpha_k^\dagger \}}_{1} + v_k^2 \underbrace{\{ \beta_k^\dagger, \beta_k \}}_{1}$$

$$= 1$$

Thus we see that we must have

$$u_k^2 + v_k^2 = 1 \qquad (84)$$

It is therefore convenient to parametrize

$$u_k = \cos \phi_k/2 \qquad v_k = \sin \phi_k/2 \qquad (85)$$

where ϕ_k is a parameter to be determined

Now all we have to do is substitute (82) in (81), and pray for God that something useful happens. Here we go!

$$b_k^\dagger b_k = (u_k \alpha_k^\dagger + i v_k \beta_k)(u_k \alpha_k - i v_k \beta_k^\dagger)$$

$$= u_k^2 \alpha_k^\dagger \alpha_k + v_k^2 \beta_k \beta_k^\dagger - i u_k v_k (\alpha_k^\dagger \beta_k^\dagger - \beta_k \alpha_k)$$

$$b_{-k}^\dagger b_{-k} = (-i v_k \alpha_k + u_k \beta_k^\dagger)(i v_k \alpha_k^\dagger + u_k \beta_k)$$

$$= v_k^2 \alpha_k \alpha_k^\dagger + u_k^2 \beta_k^\dagger \beta_k - i u_k v_k (\alpha_k \beta_k - \beta_k^\dagger \alpha_k^\dagger)$$

Using, for instance, $\alpha_k \alpha_k^\dagger = 1 - \alpha_k^\dagger \alpha_k$, we get

$$b_k^\dagger b_k + b_{-k}^\dagger b_{-k} = (u_k^2 - v_k^2)(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k) +$$

$$- 2 i u_k v_k (\alpha_k^\dagger \beta_k^\dagger - \beta_k \alpha_k) + 2 v_k^2$$

Or, in terms of ϕ_k in (85)

$$u_k^2 - v_k^2 = \cos \phi_k \qquad (86)$$

$$2 u_k v_k = \sin \phi_k$$

so

$$b_k^\dagger b_k + b_{-k}^\dagger b_{-k} = \cos \phi_k \,(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k) - i \sin\phi_k \,(\alpha_k^\dagger \beta_k^\dagger - \beta_k \alpha_k)$$

$$+ 2 \sin^2 \phi_k / 2 \qquad (87)$$

Next:

$$b_k^+ b_{-k}^+ = (u_k \alpha_k^+ + i v_k \beta_k)(-i v_k \alpha_k + u_k \beta_k^+)$$

$$= -i u_k v_k (\alpha_k^+ \alpha_k - \beta_k \beta_k^+) + u_k^2 \alpha_k^+ \beta_k^+ + v_k^2 \beta_k \alpha_k$$

and taking the adjoint

$$b_{-k} b_k = i u_k v_k (\alpha_k^+ \alpha_k - \beta_k \beta_k^+) + u_k^2 \beta_k \alpha_k + v_k^2 \alpha_k^+ \beta_k$$

so

$$b_k^+ b_{-k}^+ - b_{-k} b_k = -2 i u_k v_k (\alpha_k^+ \alpha_k - \beta_k \beta_k^+)$$

$$+ (u_k^2 - v_k^2)(\alpha_k^+ \beta_k^+ - \beta_k \alpha_k)$$

or, in terms of ϕ_k (and writing $\beta_k \beta_k^+ = -\beta_k^+ \beta_k + 1$)

$$b_k^+ b_{-k}^+ - b_{-k} b_k = -i \sin\phi_k (\alpha_k^+ \alpha_k + \beta_k^+ \beta_k) \qquad (88)$$

$$+ \cos\phi_k (\alpha_k^+ \beta_k^+ - \beta_k \alpha_k) + i \sin\phi_k$$

Plugging (87) and (88) in (81) we then get

$$H = \sum_{k>0} \Big\{ \epsilon_k \cos\phi_k \,(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k) - i\epsilon_k \sin\phi_k \,(\alpha_k^\dagger \beta_k^\dagger - \beta_k \alpha_k) + 2\epsilon_k \sin^2\phi_k/2$$

$$- iJg\sin k \Big[(-i\sin\phi_k)(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k) + \cos\phi_k \,(\alpha_k^\dagger \beta_k^\dagger - \beta_k \alpha_k) + (i\sin\phi_k) \Big] \Big\}$$

collecting the terms yields

$$H = \sum_{k>0} \Big\{ (\epsilon_k \cos\phi_k - Jg\sin k \sin\phi_k)(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k) + \Big[-i\epsilon_k \sin\phi_k - iJg\sin k \cos\phi_k \Big] (\alpha_k^\dagger \beta_k^\dagger - \beta_k \alpha_k) + 2\epsilon_k \sin^2\frac{\phi_k}{2} + Jg\sin k \sin\phi_k \Big\} \tag{89}$$

At first it seems we just made everything worse. But now we can try to choose the angle ϕ_k so as to put this guy in diagonal form. The key is in the 2^{nd} line. That's the annoying term. If we can get rid of it, then we are done.

We therefore choose

$$- \epsilon_k \sin\phi_k - J\gamma \sin k \cos\phi_k = 0$$

or

$$\boxed{\tan\phi_k = -\frac{J\gamma \sin k}{\epsilon_k} = \frac{J\gamma \sin k}{h + J\cos k}} \tag{90}$$

the 2^{nd} line in (89) is now gone. Let us simplify what remains. We write

$$\cos\phi_k = \frac{\epsilon_k}{\sqrt{(J\gamma \sin k)^2 + \epsilon_k^2}} \tag{91}$$

$$\sin\phi_k = \frac{-J\gamma \sin k}{\sqrt{(J\gamma \sin k)^2 + \epsilon_k^2}} \tag{92}$$

The 1^{st} line in (89) then becomes

$$\epsilon_k \cos\phi_k - J\chi \sin k \sin\phi_k = \frac{\epsilon_k^2 + (J\chi \sin k)^2}{\sqrt{(J\chi \sin k)^2 + \epsilon_k^2}}$$

$$= \sqrt{(J\chi \sin k)^2 + \epsilon_k^2}$$

This incites us to define

$$\boxed{\Omega_k = \sqrt{(J\chi \sin k)^2 + \epsilon_k^2}} \qquad (92)$$

The last term in (89) can also be simplified as

$$2\epsilon_k \sin^2\phi_k/2 + J\chi \sin k \sin\phi_k = \epsilon_k(1-\cos\phi_k) + J\chi \sin k \sin\phi_k$$

$$= \epsilon_k - \Omega_k$$

Thus, we finally arrive at

$$H = \sum_{k>0}\left\{\Omega_k(\alpha_k^\dagger\alpha_k + \beta_k^\dagger\beta_k) + (\epsilon_k - \Omega_k)\right\} \qquad (93)$$

As a final twist we may go back to a sum over $k>0$ and $k<0$. Recall that α_k and β_k were defined only for $k>0$. So what we can do is keep α_k as is, but define a new operator α_{-k} as

$$\alpha_{-k} = \beta_k$$

Then, since $\Omega_{-k} = \Omega_k$, we finally arrive at

$$\boxed{H = \mathcal{E}_0 + \sum_k \Omega_k \alpha_k^\dagger \alpha_k} \qquad (94)$$

where

$$\boxed{\mathcal{E}_0 = \sum_k \frac{\epsilon_k - \Omega_k}{2}} \qquad (95)$$

Now let's try to interpret our results. Interestingly, in this case the interpretation is different from the XX model. Note that the dispersion relation (92) is always non-negative $\Omega_k \geq 0$. Thus, to look for the ground state, we don't have to do any bookkeeping on how many fermions to populate. The GS is always the state with no α_k fermions.

$$|\psi_{gs}\rangle = |0_\alpha\rangle \qquad (96)$$

where $|0_\alpha\rangle$ is the vacuum of the α_k. That is, it is the state which satisfies

$$\alpha_k |0_\alpha\rangle = 0 \qquad \forall k \qquad (97)$$

the energy of the GS is thus precisely E_0 in Eq (95).

It may seem strange at first that in the XX we had a phase with fermions and a phase without them, whereas here we always have a vacuum. But this is a very important, which is related to the Bogoliubov transformation (82). In our notation, since $\beta_k = \alpha_{-k}$, we can write

$$\boxed{\begin{aligned} b_k &= u_k \alpha_k - i v_k \alpha_{-k}^{+} \\ b_{-k} &= i v_k \alpha_k^{+} + u_k \alpha_{-k} \end{aligned}} \qquad (98)$$

Taking the adjoint of the 2nd we get

$$b_k = u_k \alpha_k - i v_k \alpha_{-k}^{+}$$
$$b_{-k}^{+} = -i v_k \alpha_k + u_k \alpha_{-k}^{+}$$

which can be written as

$$\begin{pmatrix} b_k \\ b_{-k}^{+} \end{pmatrix} = \begin{pmatrix} u_k & -i v_k \\ -i v_k & u_k \end{pmatrix} \begin{pmatrix} \alpha_k \\ \alpha_{-k}^{+} \end{pmatrix} \rightsquigarrow \begin{pmatrix} \alpha_k \\ \alpha_{-k}^{+} \end{pmatrix} = \begin{pmatrix} u_k & i v_k \\ i v_k & u_k \end{pmatrix} \begin{pmatrix} b_k \\ b_{-k}^{+} \end{pmatrix}$$

thus

$$\boxed{\begin{aligned} \alpha_k &= u_k b_k + i v_k b_{-k}^{+} \\ \alpha_{-k}^{+} &= i v_k b_k + u_k b_{-k}^{+} \end{aligned}} \qquad (99)$$

Now comes the key point, which I think is really cool: the vacuum of α_k is not the same as the vacuum of b_k. A state with 0 α- fermions is not necessarily a state with zero b- fermions. We can simply see that this is true: from (97) we get

$$\langle 0_\alpha | b_k^\dagger b_k | 0_\alpha \rangle = \langle 0_\alpha | (u_k \alpha_k^\dagger + i v_k \alpha_{-k})(u_k \alpha_k - i v_k \alpha_{-k}^\dagger) | 0_\alpha \rangle$$

Recalling that $\alpha_k |0_\alpha\rangle = \alpha_{-k} |0_\alpha\rangle = 0$ and $\langle 0_\alpha | \alpha_k^\dagger = \langle 0_\alpha | \alpha_{-k}^\dagger$, we get

$$\langle 0_\alpha | b_k^\dagger b_k | 0_\alpha \rangle = v_k^2 \langle 0_\alpha | \underbrace{\alpha_{-k} \alpha_{-k}^\dagger}_{1 - \alpha_{-k}^\dagger \alpha_{-k}} | 0_\alpha \rangle = v_k^2$$

Thus

$$\langle 0_\alpha | b_k^\dagger b_k | 0_\alpha \rangle = v_k^2 = \sin^2 \phi_k / 2 \qquad (100)$$

Or, using (91) and (92) and $\sin^2 \phi/2 = (1 - \cos\phi)/2$, we get

$$\boxed{\langle 0_\alpha | b_\alpha^\dagger b_\alpha | 0_\alpha \rangle = v_k^2 = \frac{1}{2}\left(1 - \frac{\epsilon_k}{\Omega_k}\right)} \qquad (101)$$

this number will in general be non-zero. Isn't this awesome? The vacuum is not unique! There is an infinite number of vacua

As a sanity check suppose first $\gamma = 0$, so that we recover the XX model. Then $\Omega_k = |\epsilon_k|$ and we get

$$\langle 0_\alpha | b_k^\dagger b_k | 0_\alpha \rangle = \frac{1}{2}\left(1 - \frac{\epsilon_k}{|\epsilon_k|}\right) = \begin{cases} 0 & \epsilon_k > 0 \\ 1 & \epsilon_k < 0 \end{cases} \tag{102}$$

This is exactly what we had in the XX model: put a fermion on all states with $\epsilon_k < 0$.

The total number of b-fermions, $\hat{N} = \sum_k b_k^\dagger b_k$, will then be given by

$$\begin{aligned} \langle \hat{N} \rangle &= \sum_k \langle 0_\alpha | b_k^\dagger b_k | 0_\alpha \rangle \\ &= \frac{1}{2} \sum_k \left(1 - \frac{\epsilon_k}{\Omega_k}\right) \end{aligned} \tag{103}$$

The magnetization is then $m = \frac{2\langle \hat{N} \rangle}{L} - 1$ [Eq (59)], or

$$m = \frac{1}{L} \sum_k \left(1 - \frac{\epsilon_k}{\Omega_k}\right) - 1$$

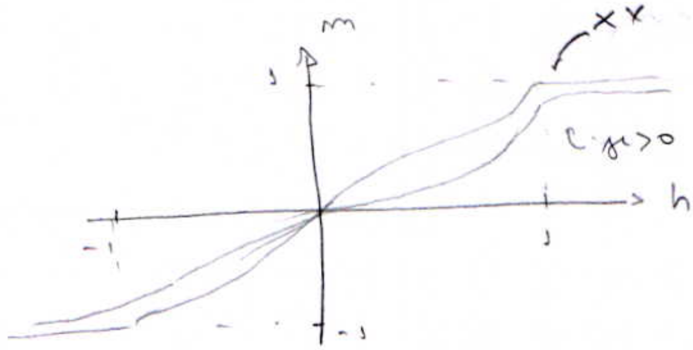
which gives

$$m = -\frac{1}{L} \sum_k \frac{\epsilon_k}{\Omega_k} \tag{104}$$

Converting the sum to an integral, we get

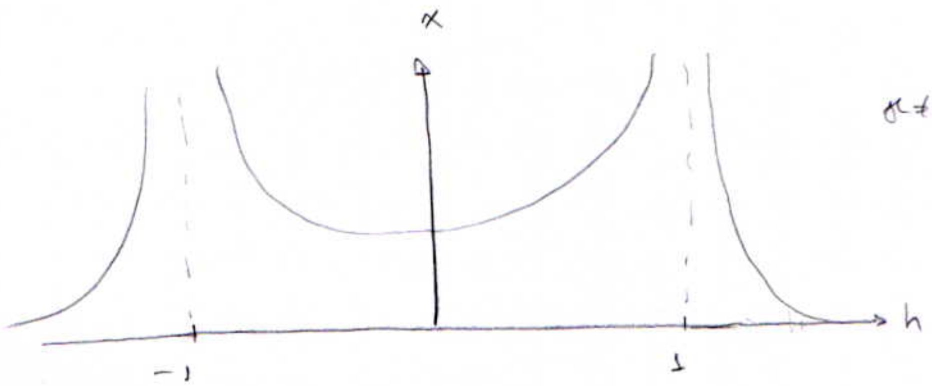
$$\boxed{m = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \, \frac{(h + J\cos k)}{\sqrt{(J\gamma \sin k)^2 + (h + J\cos k)^2}}} \qquad (105)$$

The guy now looks like this



← this is terrible! See Mathematica notebook.

It may seem from this that there is no transition at $h = h_c = 1$. But there is. That can be seen more clearly from the susceptibility



We see that the difference from the XX model is that the susceptibility remains finite for $h > 1$ or $h < -1$

But perhaps the clearest signature of a transition can be found by looking at the energy gap. Since the GS is always a state with 0 α-fermions, the first excited state is always a state with a single α-fermion. Thus, the gap can always be defined as

$$\boxed{\Delta = \min_k \Omega_k} \tag{106}$$

Let's find this minimum: for simplicity, let us focus on $\gamma = 1$ (TFIM). Then Ω_k simplifies to

$$\boxed{\Omega_k = \sqrt{h^2 + J^2 + 2hJ\cos k}} \tag{107}$$

so

$$\frac{\partial \Omega_k}{\partial k} = \frac{-hJ\sin k}{\Omega_k} = 0$$

Thus, we find that Ω_k will be a minimum when $k = 0$ or $k = \pm\pi$. At these points we have

$$\begin{aligned} \Omega_0 &= |h + J| \\ \Omega_{\pm\pi} &= |h - J| \end{aligned} \tag{108}$$

Thus, we see that the gap will close ($\Delta = 0$) when $h = \pm 1$.
But unlike in the XX model, in the TFIM it opens up again afterwards.