

Tutorial 3: The Transverse Ising Model

In this tutorial we are going to study a particular quantum spin system. So far, we have been considering classical spin systems, particularly the Ising model. The reason why we call the Ising model the “classical Ising model” is that a given spin degree of freedom, σ , has only two states, $\sigma = 1$ and $\sigma = -1$. There is no concept of a quantum superposition of those two states. In a quantum Ising model, in the other hand, a single spin could take up any of an infinite array of states containing quantum superpositions of the spin up state and the spin down state. Such a quantum spin, whose states are quantum superpositions of two basis states, is called a qubit. Each spin in a quantum Ising model is a qubit.

In the quantum Ising model, the spin is an operator which has eigenvalues $+1$ and -1 . We can write this operator for one of the spins in a basis where it is diagonal as

$$\sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (1)$$

In this basis the eigenvalues are just the unit vectors

$$\sigma^3 \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \sigma^3 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (2)$$

States in the two-dimensional Hilbert space if this single qubit have the generic form

$$\psi = \psi_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \psi_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \quad (3)$$

where ψ_1 and ψ_2 are two complex numbers obeying $|\psi_1|^2 + |\psi_2|^2 = 1$.

We could also call the state of a single spin a complex vector ψ_a and the operation of the spin operator σ^3 could be defined as

$$[\sigma^3 \psi]_a \equiv \sum_{b=1}^2 \sigma_{ab}^3 \psi_b \equiv \sigma_{ab}^3 \psi_b$$

where we will use the summation convention where repeated indices are automatically assumed to be summed over their range. The eigenvectors of σ^3 in this notation are just the unit vectors

$$\hat{e}_a^1 = \delta_a^1 \text{ corresponds to } \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \hat{e}_a^2 = \delta_a^2 \text{ corresponds to } \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

We shall consider an assembly of a large number of qubits, each of which reside at a particular position. We will focus on the case where they lie equally spaced along a one dimensional chain whose sites we shall label by the numbers $n = 1, 2, \dots, N$. As usual, we will take the limit where N is large. The quantum state of this assembly of qubits must have the form

$$\psi_{a_1 a_2 \dots a_N}$$

with one index for each individual qubit in the chain.

The spin operator for the qubit that is located at point n in the chain is the 2×2 matrix which we denote by σ_n^3 . It is the matrix whose eigenvalues are $+1$ and -1 corresponding to the two spin states of that n 'th qubit. There is an independent matrix for each value of n . Its action on the quantum state is as

$$[\sigma_n^3 \psi]_{a_1 a_2 \dots a_N} \equiv (\sigma^3)_{a_n b_n} \psi_{a_1 a_2 \dots b_n \dots a_N}$$

1. *Confirm that the spin operators for different qubits commute with each other, that is, that*

$$[\sigma_m^3 \sigma_n^3 \psi]_{a_1 a_2 \dots a_N} - [\sigma_n^3 \sigma_m^3 \psi]_{a_1 a_2 \dots a_N} = 0$$

Since the indices a_1, \dots, a_N each take on 2 values, the array $\psi_{a_1 a_2 \dots a_N}$ contains 2^N complex numbers and it is natural to think of it as a vector in a 2^N -dimensional complex vector space, the finite dimensional Hilbert space of the quantum spin chain. This vector space has a natural inner product which, for two state vectors, $\psi_{a_1 a_2 \dots a_N}$ and $\tilde{\psi}_{a_1 a_2 \dots a_N}$, is given by the complex number

$$(\tilde{\psi}|\psi) \equiv \tilde{\psi}_{a_1 a_2 \dots a_N}^* \psi_{a_1 a_2 \dots a_N}$$

This inner product can be used to normalize the states so that

$$\psi_{a_1 a_2 \dots a_N}^* \psi_{a_1 a_2 \dots a_N} = 1$$

We could also introduce the Ising model Hamiltonian for the spin chain (without the magnetic field)

$$H_I = -J \sum_{n=1}^{N-1} \sigma_n^3 \sigma_{n+1}^3 \tag{4}$$

This Hamiltonian is now an operator which operates on quantum states by virtue of the fact that the σ_n^3 's that it is constructed from are operators.

$$[H_I\psi]_{a_1\dots a_N} = -J \sum_{n=1}^{N-1} (\sigma^3)_{a_n b_n} (\sigma^3)_{a_{n+1} b_{n+1}} \psi_{a_1\dots b_n b_{n+1}\dots a_N}$$

It is also clear that it has the same eigenvalues as the classical Ising model Hamiltonian has energies, one for each set of eigenvalues of the σ_n^3 's, which are in one-to-one correspondence with the set of all classical spin configurations. Thus the quantum Ising Hamiltonian in equation (4) has precisely the same eigenvalues with the same multiplicities as the energy states of the classical Ising model Hamiltonian.

2. Show that the two ground states of the Hamiltonian in equation (4) are

$$\psi_{a_1 a_2 \dots a_N}^{0+} = e_{a_1}^1 e_{a_2}^1 \dots e_{a_N}^1 \quad (5)$$

and

$$\psi_{a_1 a_2 \dots a_N}^{0-} = e_{a_1}^2 e_{a_2}^2 \dots e_{a_N}^2 \quad (6)$$

and that the ground state energy is

$$U = -(N - 1)J$$

in each case.

3. Show that the magnetization, defined as the quantum expectation value in the ground state,

$$M \equiv \langle \Psi | \sum_{n=1}^N \sigma_n^3 | \Psi \rangle$$

is given by

$$M = N \quad \text{and} \quad M = -N$$

for each of two states, respectively

The degeneracy of the two ground states is due to the fact that they transform into each other under a symmetry of the Ising model Hamiltonian called Z_2 symmetry. This symmetry maps each spin into its negative,

$$Z_2 : \quad \sigma_n^3 \rightarrow -\sigma_n^3 \quad , \quad \forall n$$

In the quantum Ising model, there exists a unitary operator U (an operator obeying $UU^\dagger = 1$) which implements this symmetry transformation,

$$U\sigma_n^3U^\dagger = -\sigma_n^3, \quad \forall n \quad (7)$$

and the Hamiltonian is invariant

$$UH_IU^\dagger = H_I \quad (8)$$

4. *Find a unitary operator U which has the properties given in equations (7) and (8).* As a note of caution, there is more than one solution to this problem. At this point, U is not unique.

So far, the classical and the quantum Ising models are very similar. In fact, if we constructed the thermodynamic partition function by summing over all of the classical spin states as we usually do, we would get exactly the same answer as if we found the quantum Ising model partition function by taking a trace of the Boltzmann distribution

$$Z[T, B, N] = \text{Tr}e^{-H_I/k_B T} \quad (9)$$

The reason for this is that the trace of a Hermitian matrix can be taken to be the sum over its eigenvalues and as we have already noted, the eigenvalues of the Hamiltonian are exactly the same, with the same multiplicities as the classical energies, the values of the classical Hamiltonian for each configuration of the spins. The free energy of the quantum system would therefore also be identical to the one that we have studied for the classical model. This helps us for the one-dimensional case since we had an exact solution for the classical model. We saw that that classical model had a single critical point. It exhibited a first order phase transition at zero temperature, that is at the critical point $(T, B) = (0, 0)$.

Even though it has this similarity with the classical Ising model, there are some very big differences between the quantum and the classical models. This is due to the fact that, in the quantum theory, one can take superpositions of quantum states to find other quantum states which have no analog in the classical theory. One consequence would be Schrödinger cat states which are superpositions of the two ground states (5) and (6),

$$\psi_{a_1 a_2 \dots a_N}^0(\alpha, \beta) = \alpha \psi_{a_1 a_2 \dots a_N}^{0+} + \beta \psi_{a_1 a_2 \dots a_N}^{0-}, \quad |\alpha|^2 + |\beta|^2 = 1$$

Any of these states is a logical possibility. However, any measurement of any one of the N observables σ_n^3 that we have studied so far will collapse the wavefunction to one or the other of the ground states, $psi_{a_1 a_2 \dots a_N}^{0+}$ or $psi_{a_1 a_2 \dots a_N}^{0-}$ in equations (5) and (6).

One other interesting fact about the quantum Ising model ground state that we have found is that, both of the states $psi_{a_1 a_2 \dots a_N}^{0+}$ or $psi_{a_1 a_2 \dots a_N}^{0-}$ are simple products of the states of each spin. In the quantum parlance, in these states, the individual spins in the spin chain are not entangled. On the other hand, in either ground state, the spins are highly correlated. If one knows that the system is in its ground state and if one measures the polarization of any one of the spins, say the first one in the chain, σ_1^3 , and finds the value $+1$ then one knows with certainty that a subsequent measurement of the polarization of any other spin will also yield $+1$. We would therefore call this a “strongly correlated state”.

Another big difference between the classical and the quantum models is the presence of additional observables. To find some additional observables, consider the 2×2 Hermitian matrices,

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (10)$$

We can think of these as operators which operate on the state of a single spin. One of them, σ^3 , already has been used above. The others are also possible observables.

The matrices, $\sigma^1, \sigma^2, \sigma^3$ are called the Pauli matrices. They are often used to describe the spin degree of freedom of the electron, for example. They obey the commutator algebra

$$[\sigma^i, \sigma^j] = \sum_{k=1}^3 2i\epsilon^{ijk}\sigma^k \quad (11)$$

and the anti-commutator algebra

$$\{\sigma^i, \sigma^j\} = 2\delta^{ij} \quad (12)$$

We will think of them as operators in that they act on two-component state vectors $|\psi\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ by matrix multiplication.

If we use the Pauli matrices as operators which can act on any of the spins in the spin chain, we should add a label n to the matrices which act on the n 'th spin, so that they are now denoted σ_n^i . This label tells us which spin they act on. The action of σ_n^i on a quantum state is defined by

$$[\sigma_n^i \psi]_{a_1 a_2 \dots a_N} \equiv \sigma_{a_n b_n}^i \psi_{a_1 a_2 \dots b_n \dots a_N}$$

5. *Show that the spin operators obey the algebra*

$$[\sigma_m^i, \sigma_n^j] = \sum_{k=1}^3 2i \epsilon^{ijk} \sigma_n^k \delta_{mn} \quad (13)$$

To see how we can make use of these additional operators, let us consider an alternative but very simple model of a spin chain where the Hamiltonian is

$$H_h = -h \sum_{n=1}^N \sigma_n^1 \quad (14)$$

This Hamiltonian simply serves to polarize each spin so that it is oriented in the same direction as $\vec{h} = (h, 0, 0)$.

6. *Show that the lowest energy eigenstate of the Hamiltonian in equation (14) is given by*

$$\Psi_{a_1 a_2 \dots a_N}^{0 \rightarrow} = \frac{1}{2^{N/2}} (e^1 + e^2)_{a_1} (e^1 + e^2)_{a_2} \dots (e^1 + e^2)_{a_N} \quad (15)$$

if $h > 0$ and

$$\Psi_{a_1 a_2 \dots a_N}^{0 \leftarrow} = \frac{1}{2^{N/2}} (e^1 - e^2)_{a_1} (e^1 - e^2)_{a_2} \dots (e^1 - e^2)_{a_N} \quad (16)$$

if $h < 0$ and that the ground state energy is

$$U = -N|h|$$

We see that the ground state energy is a singular function of h . If this were a free energy – and in fact when referring to the ground state of the system the internal energy U is the zero temperature limit of the free energy – we would say that this singular behaviour of the free energy is indicative of a first order phase transition occurring at $h = 0$. This is probably the simplest possible

example of a “quantum phase transition”. The term quantum phase transition is defined as the phenomenon where a major re-structuring of the ground state wave-function of a quantum mechanical system which occurs as a parameter of the Hamiltonian of the system is varied. In this case the parameter is h and, as h is increased from negative to positive values, when it passes through zero the ground state of the system changes from $\Psi_{a_1 a_2 \dots a_N}^{0\leftarrow}$ to $\Psi_{a_1 a_2 \dots a_N}^{0\rightarrow}$ given in equations (16) and (15).

Now, let us construct a more sophisticated model with the Hamiltonian

$$\begin{aligned} H &= H_I + H_h \\ &= -J \sum_{n=1}^{N-1} \sigma_n^3 \sigma_{n+1}^3 - h \sum_{n=1}^N \sigma_n^1 \end{aligned} \quad (17)$$

The first term is just the usual Ising model Hamiltonian, but with quantum spins replacing the classical spins. The second term is called the “transverse coupling”. Sometimes the model with both of these terms is called the “transverse Ising model”. We will be able to find an exact solution of this model. However, first, it is illuminating to study it in some limits.

The limit $h \gg J$:

In the following we will assume that both h and J are positive real numbers. Let us consider the limit where $h \gg J$, where its ground state should be approximately that of H_h , that is, the state $\psi_{a_1 a_2 \dots a_N}^{0\rightarrow}$ that is given in equation (15). We could then estimate the effects of the H_I -term in the Hamiltonian using perturbation theory.

7. Use Rayleigh-Schrödinger (time-independent quantum mechanical) perturbation theory to show that the ground state energy density $u = U/N$ becomes

$$u = -h \left(1 + \frac{J^2}{4h^2} + \dots \right) \quad (18)$$

where we have assumed that $N \gg 1$. Here, the ellipses stand for terms of order J^4/h^4 and higher.

8. Show that the magnetization density M that is given by the expectation value

$$M \equiv \left\langle \sum_{n=1}^N \sigma_n^3 \right\rangle \quad (19)$$

vanishes, both in the zeroth order (its expectation value in the state $\psi_{a_1 a_2 \dots a_N}^{0 \rightarrow}$) and to the order J^2/h^2 of perturbation theory. Can you argue that it vanishes to all orders?

The limit $J \gg h$:

We can also study the ground state of the quantum spin chain governed by the Hamiltonian in equation (17) in the limit where $J \gg h$. In that case, it should be well approximated by the ground state of H_I which must be one of the two ordered states in equations (5) and (6). Then we could begin with either one of them, and we could study corrections due to the presence of the H_h term in the Hamiltonian using quantum mechanical perturbation theory.

9. Show that, if we consider the ordered ground state given in equation (5) as the leading contribution, the finding the the ground state to the leading order in an expansion in the small parameter h/J , the leading correction to the ground state energy density is

$$u = -J \left(1 + \frac{h^2}{4J^2} + \dots \right) \quad (20)$$

and the leading correction to the magnetization density is

$$m = 1 - \frac{h^2}{4J^2} + \dots \quad (21)$$

Can you argue that, if we had begun with the other state, given in equation (6), the energy density would have the same expression as in equation (20) and the magnetization would differ from the one quoted in equation (21) by an overall minus sign.

Between these limits, $h \ll J$ and $h \gg J$, the nature of the ground state must change. When $J \gg h$ there are two ground states, with opposite signs of magnetization. When $h \gg J$ there is a single ground state with zero magnetization. The transverse Ising model is interesting because it exhibits a second order “quantum phase transition” at a critical value of h/J which we will find by solving the model exactly. Here, a doublet of degenerate ground states, each with nonzero spontaneous magnetization must merge to form a unique ground state with zero magnetization. The quantum phase transition is of “second order” because the ground state energy, as a function of the parameter which is being varied to find the phase transition, has a discontinuous second derivative.

There is a Z_2 symmetry which is spontaneously broken by the ordered states (5) and (6). It is associated with a unitary (and Hermitian) matrix which we can write explicitly as

$$K \equiv \prod_{n=1}^N \sigma_n^1, \quad K = K^\dagger, \quad K^2 = \mathcal{I} \quad (22)$$

Since

$$K \sigma_n^3 K = -\sigma_n^3, \quad \forall n \quad (23)$$

$$K \sigma_n^1 K = \sigma_n^1, \quad \forall n \quad (24)$$

the K matrix implements a symmetry transformation in that it commutes with the Hamiltonian

$$K H K = H \quad (25)$$

This tells us that, if a state vector $\psi_{a_1 a_1 \dots a_N}$ is an eigenstate of the Hamiltonian with eigenvalue E ,

$$H \psi = E \psi$$

then

$$[K \psi]_{a_1 a_1 \dots a_N} = K_{a_1 a_2 \dots a_n; b_1 b_2 \dots b_N} \psi_{b_1 b_2 \dots b_N} = \sigma_{a_1 b_1}^1 \sigma_{a_2 b_2}^2 \dots \sigma_{a_N b_N}^1 \psi_{b_1 b_2 \dots b_N}$$

is also an eigenstate of the Hamiltonian with the same eigenvalue E

$$H K \psi = E K \psi$$

Then, since $K^2 = 1$, there are two possibilities:

- $K \psi = \psi$ or $K \psi = -\psi$. The ground state is a singlet under the Z_2 transformation.
- $K \psi$ is not proportional to ψ and the set of two vector $\{\psi, K \psi\}$ forms a doublet of two degenerate eigenstates, both having the same energy E .

In the solutions that we have been discussing for limits of the transverse Ising model, both of these behaviours occur. In the limit $J \gg h$, there was a pair of degenerate ground states (5) and (6). It is easy to check that they transform into each other under Z_2 and they therefore form a Z_2 doublet. This is the

case of spontaneously broken Z_2 symmetry and the appearance of ferromagnetic order.

On the other hand, in the $h \gg J$ limit, we found that there was a single ground state $\psi^{0\rightarrow}$ given in equation (15). It is easy to check that the ground state there is invariant under the Z_2 transformation, $K\psi^{0\rightarrow} = \Psi^{0\rightarrow}$, that is, it is indeed a singlet.

This means that, in this transverse Ising model, if we begin with $h = 0$, and we then turn on h and increase it from the $h \ll J$ regime the ground state must change from a doublet of Z_2 at small h/J to a singlet of Z_2 at large h/J . This transition is a phase transition and the value of h/J at which it happens is a critical point.

In order to solve the transverse Ising model, we have to begin by examining the spin algebra. Let us look at the spins on a single site, $\vec{\sigma}_n$. For simplicity of notation, for the moment, we will omit the subscript n . This is a set of three two-by-two matrices. Let us consider the following linear combinations of them

$$\begin{aligned}\sigma^+ &= \frac{1}{2} [\sigma^2 + i\sigma^3] \\ \sigma^- &= \frac{1}{2} [\sigma^2 - i\sigma^3]\end{aligned}$$

10. *Show that the matrices σ^\pm obey*

$$\begin{aligned}\sigma^+ \sigma^+ &= 0 \\ \sigma^- \sigma^- &= 0 \\ \{\sigma^+, \sigma^-\} &\equiv \sigma^+ \sigma^- + \sigma^- \sigma^+ = 1 \\ \sigma^1 &= 2\sigma^+ \sigma^- - 1 = [\sigma^+, \sigma^-]\end{aligned}$$

Let us now rename these spins as the symbols

$$a^\dagger \equiv \sigma^+ \quad , \quad a \equiv \sigma^- \tag{26}$$

The reason for this renaming is that the operators $a^\dagger = \sigma^+$ and $a = \sigma^-$ behave like the creation and annihilation operators of a Fermionic oscillator. We call it “fermionic” since their algebra is anti-commuting rather than commuting. They obey the algebraic identities

$$a^2 = 0 \quad , \quad a^{\dagger 2} = 0 \quad , \quad \{a, a^\dagger\} = 1 \tag{27}$$

We have also shown that $\sigma^1 = 2a^\dagger a - 1 = [a^\dagger, a]$ is related to the number operator for the fermionic oscillator, $a^\dagger a$.

The states upon which these fermion operators operate on are easy to construct. (Of course, there are identical to the states that the spin operators for the qubit operate on. This is just a different notation for them.) We begin with a “vacuum”, $|0\rangle$, which is annihilated by the annihilation operator,

$$a|0\rangle = 0 \quad , \quad \langle 0|a^\dagger = 0 \quad , \quad \langle 0|0\rangle = 1$$

Then, we create an excited state by operating the creation operator on the vacuum state,

$$|1\rangle = a^\dagger|0\rangle$$

We note that, since $a^{\dagger 2} = 0$, there are no more excited states. We can annihilate the excitation with the annihilation operator

$$a|1\rangle = |0\rangle$$

The basis for the Hilbert space is then the set of vectors two

$$\{|0\rangle, |1\rangle\}$$

and a generic state is a superposition of them,¹

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \quad , \quad |\alpha|^2 + |\beta|^2 = 1$$

The Fermionic re-labeling of the spin variables is interesting. It is called the fermion representation of a single qubit. However, we are eventually interested in a multi-qubit system and, so far, the fermionic description is incomplete. If we restore the site indices, we see that the fermions with the same site labels anticommute, $\{a_n^\dagger, a_n\} = 1$, as fermion oscillator variables should do. On the other hand, when the site labels are different, if $m \neq n$ the operators that

¹Here the complex numbers α and β parameterize the generic quantum state. If we use the fact that the overall phase of the state is arbitrary to make α a real number, we can solve the normalization constraint by setting

$$\alpha = \cos \theta \quad , \quad \beta = \sin \theta e^{i\phi} \quad , \quad 0 \leq \theta \leq \pi \quad -\pi < \phi \leq \pi$$

where one can think of (θ, ϕ) as coordinates of the unit 2-sphere, the Bloch sphere which parameterizes the states of a single qubit.

we have constructed commute with each other, $[a_m^\dagger, a_n] = 0$ rather than anti-commute. This means that they are not really fermions yet. Fermion operators associated with different sites should anti-commute with each other. So the question is, can they be further re-defined so that they are really fermions?

The answer to this question is yes. In order to do this, we will consider an open spin chain with open boundary conditions – we do not fix the states of the qubits at the ends of the chain. Then, consider the following operators

$$a_1 = \sigma_1^- \quad , \quad a_n = \sigma_1^1 \sigma_2^1 \dots \sigma_{n-1}^1 \sigma_n^- \quad (28)$$

$$a_1^\dagger = \sigma_1^+ \quad , \quad a_n^\dagger = \sigma_1^1 \sigma_2^1 \dots \sigma_{n-1}^1 \sigma_n^+ \quad (29)$$

$$\forall n = 2, 3, \dots, N$$

This is called a Jordan-Wigner transformation. It is commonly used in quantum information theory as a transformation which turns qubits into fermions or fermions into qubits.

11. *Show that, with the above definition,*

$$\{a_m, a_n\} = 0 \quad , \quad \forall m, n$$

$$\{a_m^\dagger, a_n^\dagger\} = 0 \quad , \quad \forall m, n$$

$$\{a_m, a_n^\dagger\} = \delta_{mn} \quad , \quad \forall m, n$$

Now, a_m^\dagger and a_n have the correct anti-commutation relations to be the creation and annihilation operators for a fermionic excitation at site m and n , respectively. The correct anti-commutation relations guarantee that the wave function

$$a_{n_1}^\dagger a_{n_2}^\dagger \dots a_{n_k}^\dagger |0\rangle$$

is totally antisymmetric in the positions n_1, n_2, \dots, n_k , as it should be to be a wave-function of a system of identical and indistinguishable fermions.

12. *Show that the inverse of the Jordan-Winger transformation is*

$$\sigma_1^- = a_1, \quad \sigma_1^+ = a_1^\dagger \quad (30)$$

$$\sigma_n^1 = [a_n^\dagger, a_n] \quad (31)$$

and, for $n > 1$,

$$\sigma_n^- = [a_1^\dagger, a_1] \dots [a_{n-1}^\dagger, a_{n-1}] a_n \quad (32)$$

$$\sigma_n^+ = [a_1^\dagger, a_1] \dots [a_{n-1}^\dagger, a_{n-1}] a_n^\dagger \quad (33)$$

13. *By plugging the Jordan-Wigner transformed spins into the Hamiltonian, show that, in terms of the Fermion creation and annihilation operators, the Hamiltonian takes the form*

$$H = J \sum_{n=1}^{N-1} (a_n^\dagger + a_n)(a_{n+1}^\dagger - a_{n+1}) + h \sum_{n=1}^N [a_n^\dagger, a_n] \quad (34)$$

Let us begin by solving the limit where $h \gg J$. In that limit, the Hamiltonian is approximately equal to

$$h \gg J : \quad H = -Nh + 2h \sum_{n=1}^N a_n^\dagger a_n \quad (35)$$

which is already diagonal. The fermion vacuum, defined by

$$a_n |0\rangle = 0, \quad \langle 0|a_n^\dagger = 0 \quad \forall n, \quad \langle 0|0\rangle = 1 \quad (36)$$

is the ground state with the ground state energy $U = -Nh$ and the excited states

$$a_{n_1}^\dagger a_{n_2}^\dagger \dots a_{n_k}^\dagger |0\rangle$$

which have k excited fermions. There excited states have energy equal to $2hk - Nh$ there are $N!/k!(N-k)!$ states with this energy.

Now, let us consider the other limit, where $J \gg h$ and the Ising model dominates. There, it is convenient to re-define the fermion variables once again, This Hamiltonian is quadratic in the Fermion operators. It has an interesting presentation using Majorana Fermions. Let us define the basic Majorana fermion variables as

$$\beta_n = a_n + a_n^\dagger, \quad \gamma_n = -i(a_n - a_n^\dagger) \quad (37)$$

14. *Show that the Majorana fermions obey the equations*

$$\begin{aligned} \beta_n^\dagger &= \beta_n, \quad \gamma_n^2 = 1 \\ \{\gamma_m, \gamma_n\} &= 2\delta_{m,n}, \quad \{\beta_m, \beta_n\} = 2\delta_{m,n}, \quad \{\gamma_m, \beta_n\} = 0 \end{aligned} \quad (38)$$

In terms of these ‘‘Majorana fermions’’, the Hamiltonian has a very simple form

$$H = -J \sum_{n=1}^{N-1} i\beta_n \gamma_{n+1} + h \sum_{n=1}^N i\beta_n \gamma_n \quad (39)$$

In the $J \gg \hbar$ limit, properties of the system must be governed by the first term in the Hamiltonian in equation (40),

$$H_I = -J \sum_{n=1}^{N-1} i\beta_n \gamma_{n+1} = -iJ\beta_2\gamma_3 - iJ\beta_3\gamma_4 + \dots - iJ\beta_{N-1}\gamma_N \quad (40)$$

The first thing to note is the interesting fact that β_N and α_1 do not appear in H_I at all. These “edge modes” therefore commute with H_I and we will see shortly that their presence indicates a degeneracy of the energy spectrum.² Also, we note that each combination of β_n and γ_{n+1} appear only once in the operator $i\beta_n \gamma_{n+1}$ that corresponds to the link of the chain that connects site n and site $n + 1$. To make this term really simple, we could replace equation (37) with

$$\beta_n = \tilde{a}_n + \tilde{a}_n^\dagger, \quad \gamma_{n+1} = i(\tilde{a}_n - \tilde{a}_n^\dagger) \quad (41)$$

where we can confirm that

$$\{\tilde{a}_m, \tilde{a}_n^\dagger\} = \delta_{mn} \quad \{\tilde{a}_m, \tilde{a}_n\} = 0 \quad \{\tilde{a}_m^\dagger, \tilde{a}_n^\dagger\} = \delta_{mn} \quad (42)$$

15. Show that, with this replacement,

$$-i\beta_n \gamma_{n+1} = (\tilde{a}_n + \tilde{a}_n^\dagger)(\tilde{a}_n - \tilde{a}_n^\dagger) = 2\tilde{a}_n^\dagger \tilde{a}_n - 1 \quad (43)$$

and the H_I is

$$H_I = -J(N-1) + 2J \sum_{n=1}^{N-1} \tilde{a}_n^\dagger \tilde{a}_n \quad (44)$$

There are also the left-over operators γ_1 and β_N which commute with H_I and with which we could combine to make the operators

$$\beta_N = \tilde{a}_0 + \tilde{a}_0^\dagger, \quad \gamma_1 = i(\tilde{a}_0 - \tilde{a}_0^\dagger) \quad (45)$$

which also commute with H_I .

The eigenstates of H_I begin with a vacuum state $|\tilde{0}\rangle$ with the properties

$$\tilde{a}_n |\tilde{0}\rangle = 0, \quad \langle 0 | \tilde{a}_n^\dagger = 0, \quad \langle \tilde{0} | \tilde{0}\rangle = 1, \quad n = 0, 1, 2, \dots, N-1 \quad (46)$$

²This is the degeneracy due to the fact that the ground state in this limit should be a doublet under the Z_2 transformation.

and two towers of excited states

$$\tilde{\alpha}_{n_1}^\dagger \tilde{\alpha}_{n_2}^\dagger \dots \tilde{\alpha}_{n_k}^\dagger |0\rangle \qquad \tilde{\alpha}_{n_1}^\dagger \tilde{\alpha}_{n_2}^\dagger \dots \tilde{\alpha}_{n_k}^\dagger \tilde{\alpha}_0^\dagger |\tilde{0}\rangle \qquad (47)$$

which both have energy $-J(N-1) + 2Jk$.

Generally the ground states $|\tilde{0}\rangle$ and $\tilde{\alpha}_0^\dagger |\tilde{0}\rangle$ are Schrödinger cat-like superpositions of the ferromagnetic states. To see this, we can reconstruct the spin operator σ_1^3 for the first spin in the spin chain. It is given by $\sigma_1^3 = \tilde{\alpha}_0 + \tilde{\alpha}_0^\dagger$ which has eigenstates

$$\sigma_1^3 \frac{1}{\sqrt{2}}(1 + \tilde{\alpha}_0^\dagger) |\tilde{0}\rangle = \frac{1}{\sqrt{2}}(1 + \tilde{\alpha}_0^\dagger) |\tilde{0}\rangle \quad , \quad \sigma_1^3 \frac{1}{\sqrt{2}}(1 - \tilde{\alpha}_0^\dagger) |\tilde{0}\rangle = -\frac{1}{\sqrt{2}}(1 - \tilde{\alpha}_0^\dagger) |\tilde{0}\rangle$$

A measurement of the orientation of the first spin in the spin chain will collapse the state of the entire spin system to one of these two ferromagnetic states which are, in this language, $\frac{1}{\sqrt{2}}(1 + \tilde{\alpha}_0^\dagger) |\tilde{0}\rangle$ corresponding to ψ^{0+} in equation (5) and $\frac{1}{\sqrt{2}}(1 - \tilde{\alpha}_0^\dagger) |\tilde{0}\rangle$ which is identical to ψ^{0-} in equation (6).

Now, let us restore the transverse coupling and return to the full Hamiltonian (39). The general solution for the spectrum of this Hamiltonian can be found, however, imposing the boundary conditions is somewhat complicated. The problem simplifies in the limit where the number of spins, N , is taken to infinity. In the spirit of focusing on behaviour of spins that are far from either of the boundaries, we put both ends of the chain to infinity so that the Hamiltonian becomes

$$H = -J \sum_{n=-\infty}^{\infty} i\beta_n \gamma_{n+1} + h \sum_{n=-\infty}^{\infty} i\beta_n \gamma_n \qquad (48)$$

Before we discuss how one might solve this problem, let us observe that it exhibits a version of Krammers-Wannier duality.

16. *Show that, if we relabel the fermion variables as*

$$\beta_n = \hat{\gamma}_n \quad , \quad \gamma_n = \hat{\beta}_{n-1} \qquad (49)$$

the Hamiltonian becomes

$$H = -h \sum_{n=-\infty}^{\infty} i\hat{\beta}_n \hat{\gamma}_{n+1} + J \sum_{n=-\infty}^{\infty} i\hat{\beta}_n \hat{\gamma}_n \qquad (50)$$

Since the change of variables in equation (49) is a canonical transformation³ the new Hamiltonian (50) is identical in structure to the old Hamiltonian (48), if we also interchange the two parameters, $J \leftrightarrow h$.

This is Krammers-Wannier duality for this model. It means that the $J \gg h$ and the $J \ll h$ solutions will be identical in structure. There is a one-to-one mapping of all of the states and their energies in one case to all of the states and energies in the other case. In particular, we might expect that the ground state energy is invariant under the duality transformation, that is, that

$$U(J, h) = U(h, J) \quad (51)$$

Moreover, the duality tells us that the phase transition between the ferromagnetic and the paramagnetic phases of this model must happen at the self-dual point, that is, the critical point occurs as $J = h$. We will see that these features are indeed there shortly when we solve the model exactly.

We can solve for the spectrum of the Hamiltonian in equation (48) by writing down the Hamilton equations of motion for the Majorana variables,

$$i\hbar\dot{\beta}_n = [\beta_n, H] = -2iJ\gamma_{n+1} + 2ih\gamma_n \quad (52)$$

$$i\hbar\dot{\gamma}_n = [\gamma_n, H] = 2iJ\gamma_{n-1} - 2ih\gamma_n \quad (53)$$

We can solve these equations using the ansatz

$$\begin{pmatrix} \beta_n \\ \gamma_n \end{pmatrix} = \begin{pmatrix} \beta(k) \\ \gamma(k) \end{pmatrix} e^{ikn - iE(k)t/\hbar} \quad (54)$$

where $k \in (-\pi, \pi]$, the Brillouin zone of the one-dimensional lattice. Then the equations become

$$\begin{pmatrix} E(k) & 2iJe^{ik} - 2ih \\ -2iJe^{-ik} + 2ih & E(k) \end{pmatrix} \begin{pmatrix} \beta(k) \\ \gamma(k) \end{pmatrix} = 0 \quad (55)$$

17. Show that the energy spectrum $E(k)$ consists of two bands and that the energies and wave-functions of each band are given by

$$E_+(k) = \omega(k) \quad , \quad \omega(k) = 2\sqrt{(J-h)^2 + 4Jh \sin^2(k/2)} \quad (56)$$

$$\begin{pmatrix} \beta(k) \\ \gamma(k) \end{pmatrix} = \frac{1}{\sqrt{4\pi}} \begin{pmatrix} 1 \\ \frac{2iJe^{-ik} - 2ih}{\omega(k)} \end{pmatrix} \quad (57)$$

³The reader might want to confirm that the anti-commutator algebra of the new operators is identical to the anti-commutator algebra of the old operators.

and

$$E(k) = -\omega(k) \quad (58)$$

$$\begin{pmatrix} \beta(k) \\ \gamma(k) \end{pmatrix} = \frac{1}{\sqrt{4\pi}} \begin{pmatrix} 1 \\ -\frac{2iJ e^{-ik} - 2ih}{\omega(k)} \end{pmatrix} \quad (59)$$

Using this solution, we can write

$$\begin{aligned} \beta_n(t) &= \int_{-\pi}^{\pi} \frac{dk}{\sqrt{4\pi}} \left\{ e^{ikn-i\omega(k)t/\hbar} b(k) + e^{-ikn+i\omega(k)t/\hbar} b^\dagger(k) \right\} \\ \gamma_n(t) &= \int_{-\pi}^{\pi} \frac{dk}{\sqrt{\pi}} \left\{ \frac{iJ e^{-ik} - ih}{\omega(k)} e^{ikn-i\omega(k)t/\hbar} b(k) - \frac{iJ e^{ik} - ih}{\omega(k)} e^{-ipn+i\omega(k)t/\hbar} b^\dagger(k) \right\} \end{aligned}$$

It is straightforward if tedious to confirm that the variables $b(k)$ and $b^\dagger(k)$ have the anti-commutator algebra

$$\{b(k), b^\dagger(\ell)\} = \delta(k - \ell), \quad \{b(k), b(\ell)\} = 0, \quad \{b^\dagger(k), b^\dagger(\ell)\} = 0 \quad (60)$$

and the Hamiltonian takes the form

$$H = U + \int_{-\pi}^{\pi} dk \, 2\sqrt{(J-h)^2 + 4Jh \sin^2(k/2)} \, b^\dagger(k)b(k) \quad (61)$$

$$U = -N \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sqrt{(J-h)^2 + 4Jh \sin^2(k/2)} \quad (62)$$

where U is the ground state energy and we can think of it as the zero temperature limit of the thermodynamic energy. The ground state of this system is the one without any fermion excitations, $|0\rangle$ which obeys

$$b(k)|0\rangle = 0, \quad \langle 0|b^\dagger(k) = 0 \quad \forall k, \quad \langle 0|0\rangle = 1$$

and

$$H|0\rangle = U|0\rangle$$

The excited states

$$b^\dagger(k_1) \dots b^\dagger(k_q)|0\rangle$$

have energy

$$E = \sum_i 2\sqrt{(J-h)^2 + 4Jh \sin^2(k_i/2)}$$

Now, there is a gap in the spectrum between the energy of the ground state and the energy of the first excited state which is $b^\dagger(k=0)|0\rangle$. That gap is $\Delta E = 2|J - h|$. This gap closes at the phase transition where $J \rightarrow h$. The fact that the gap closes is the source of non-analyticity there. For $J \sim h$

$$u \sim (J - h)^2 \ln |J - h|$$

It is easy to check that Taylor expanding $U(J, h)$ in either h or J reproduces the internal energies and the corrections to the internal energies of the $J \gg h$ and the $h \gg J$ limits that we have already examined.

The behaviour of the internal energy in the vicinity of the phase transition can be used to extract the critical exponent for the specific heat, which turns out to be identical to mean field theory. The scaling of the magnetization and the magnetic susceptibility in the critical regime are much more difficult to find as the magnetization density is a complicated object in the fermionic language. These have been studied in sufficient detail to extract their critical exponents and the exponents turn out to differ significantly from mean field theory. In fact they are the critical exponents of the two dimensional Ising model which must therefore be in the same universality class as this transverse one-dimensional Ising model. A summary of the critical exponents is:

$$\alpha = 0, \beta = \frac{1}{8}, \gamma = \frac{7}{4}, \delta = 15, \eta = \frac{1}{4}, \nu = 1 \quad (63)$$