# Transverse Field Ising Model with different boundary conditions

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**Abstract**
The one dimensional Transverse Field Ising Model is diagonalized for periodic and open boundary conditions. A third boundary condition imposed by fixing the spin in a arbitrary direction on one end of the one-dimensional Ising-chain is defined and diagonalized. Some similarities between the models are noted and a selection of properties are given.

## 1 Introduction

The systems we consider are chains of spin 1/2 particles that interact with uniform strenght with nearest neighbours as well as with a transverse field, namely one-dimensional Transverse Field Ising Models (TFIM). The Hamiltonian whose exact definition will be given later is without additional constraints given by

$$H = -\sum_n \sigma_n^x \sigma_{n+1}^x - \sum_n h\sigma_n^z. \tag{1}$$

The first sum describes the nearest neighbour interaction and the second sum characterises the interaction with the external field. The strength of the external field is captured by the variable $h$. The two sums in the Hamiltonian work against each other, the first sum preferring to align the spins in the plus or minus x-direction and the second sum preferring the z-direction.

We look at three different boundary conditions, periodic, open and what we will call fixed. Although similar systems have been considered[7], treatments of the fixed TFIM model is not readily found in the literature. On the other hand the periodic and open models were solved and analyzed as early as 1970 by Pfeuty[1] using the techniques introduced by Lieb, Schultz and Mattis[5]. The periodic and open TFIM are thus well known but we

will spend some time exploring these systems for completeness and to introduce techniques useful for diagonalizing the fixed TFIM. The key will be to write the Hamiltonian in terms of suitably defined fermionic operators, the spectrum can then be extracted straightforwardly.

As expected from the argument in part I of the book Quantum Phase Transitions by Sachdev[2] and the results by Pfeuty[1], we find in later sections that the periodic TFIM exhibits a phase transition in the thermodynamic limit. As a natural extension of the periodic and open TFIM family of systems we consider the same model but impose a boundary condition by choosing a fixed spin direction for one end of the chain, hence the name fixed TFIM.

# 2 Periodic Transverse Field Ising Model

## 2.1 Model description and diagonalization

We start by considering a Periodic Transverse Field Ising Model in one dimension, this is a chain of spin 1/2 particles with the ends connected. In this section we first find formulas that give the energy levels of the periodic TFIM and then show a selection of properties when the number of particles gets large. The formulas for the periodic TFIM will inspire some of the steps used to solve the open TFIM as will become clear in section 3. As a simplification we normalize the interaction strenght between the spins to be one, the Hamiltionian is then

$$H = -\sum_{n=1}^{N-1} \sigma_n^x \sigma_{n+1}^x - \sigma_N^x \sigma_1^x - \sum_{n=1}^{N} h\sigma_n^z. \tag{2}$$

Where $h$ is a number representing the strength of interaction with the transverse field, $N$ is the number of sites (particles) in the chain and $\sigma_n^x$ and $\sigma_n^z$ are the $x$ and $z$ Pauli matrices acting on site n. Two Pauli matrices acting on different sites are assumed to commute, i.e. $[\sigma_n^\rho, \sigma_m^\delta] = 0$ for all $n \neq m$ and $\rho, \delta \in \{x, y, z\}$. On any given site $n$ and $\rho, \delta, \tau \in \{x, y, z\}$, the $\sigma_n^\rho$ operators satisfy the ordinary Pauli matrix relations $(\sigma_n^\rho)^\dagger = \sigma_n^\rho$, $(\sigma_n^\rho)^2 = 1$, $\{\sigma_n^\rho, \sigma_n^\delta\} = 0$ for $\rho \neq \delta$. And $[\sigma_n^\rho, \sigma_n^\delta] = 2i\epsilon_{\rho\delta\tau}\sigma_n^\tau$ where $\epsilon_{\rho\delta\tau}$ is the Levi-Civita symbol, $\epsilon_{xyz} = 1$ and totally antisymmetric.

Without any further manipulations we consider two limiting cases in the parameter $h$. When the parameter $h$ is set to zero, the energy is lowered by setting the spins in the same x-direction, anti aligning the spins at one or more sites raises the energy. So the ground state is degenerate and has all

spins in the plus or minus x-direction. In the limit as $h \to +\infty$, the energy is lowered by aligning the spins in the up z-direction. So in this case the ground state is non degenerate and has all spins pointing in the up z-direction.

We proceed to diagonalize the Hamiltonian (2) by following section II in the paper by Dutta, Divakaran, Sen, Chakrabarti, Rosenbaum and Aeppli[3], the first step is to do a Jordan-Wigner transformation[4] by rewriting it in terms of the fermionic operators $c_n$ defined by

$$\begin{aligned} \sigma_n^z &= 2c_n^\dagger c_n - 1 \\ \frac{1}{2}(\sigma_n^x - i\sigma_n^y) &= c_n \exp\,(i\pi \sum_{j=1}^{n-1} c_j^\dagger c_j). \end{aligned} \tag{3}$$

The exponential in the definition (3) links different sites, so although the Pauli matrices commute on different sites the operators $c_n$ obey the fermionic anti commutation relations $\{c_n, c_m^\dagger\} = \delta_{n,m}$ and $\{c_n, c_m\} = 0$. After the transformation the Hamiltonian takes the following form

$$\begin{aligned} H = \sum_{n=1}^{N-1} [-(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) + (c_{n+1}^\dagger c_n^\dagger + c_n c_{n+1})] \\ -(-1)^{N_f}[-(c_N^\dagger c_1 + c_1^\dagger c_N) + (c_1^\dagger c_N^\dagger + c_N c_1)] - \sum_{n=1}^{N} h(2c_n^\dagger c_n - 1). \end{aligned} \tag{4}$$

The symbol $N_f$ counts the number of fermions and is given by $N_f = \sum_{j=1}^{N} c_j^\dagger c_j$ and $(-1)^{N_f} = \exp\,(i\pi N_f)$. We note that $(-1)^{N_f}$ commutes with the Hamiltonian $[H, (-1)^{N_f}] = 0$, so the spectrum of (4) can be separated into two sectors $N_f = \mathit{even}$ and $N_f = \mathit{odd}$. If we impose the periodicity condition $c_{N+1} = c_1$ if $N_f = \mathit{odd}$ and $c_{N+1} = -c_1$ if $N_f = \mathit{even}$, the Hamiltonian can be written on the form

$$\begin{aligned} H = \sum_{n=1}^{N} [-(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) + (c_{n+1}^\dagger c_n^\dagger + c_n c_{n+1})] \\ - \sum_{n=1}^{N} h(2c_n^\dagger c_n - 1). \end{aligned} \tag{5}$$

To make further progress we introduce the Fourier transform of the operators $c_n$

$$\tilde{c}_k = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} c_n \exp\,(-i2\pi kn/N). \tag{6}$$

The periodicity condition $c_{N+1} = c_1$ if $N_f = odd$ and $c_{N+1} = -c_1$ if $N_f = even$ imply that

$$\begin{aligned} k = -\frac{N-1}{2}, -\frac{N-1}{2}+1, ..., \frac{N-1}{2} \quad if \quad N = even, N_f = even \\ k = -\frac{N-1}{2}, -\frac{N-1}{2}+1, ..., \frac{N-1}{2} \quad if \quad N = odd, N_f = odd \\ k = -\frac{N}{2}, -\frac{N}{2}+1, ..., \frac{N}{2}-1 \quad if \quad N = even, N_f = odd \\ k = -\frac{N}{2}, -\frac{N}{2}+1, ..., \frac{N}{2}-1 \quad if \quad N = odd, N_f = even. \end{aligned} \tag{7}$$

The Fourier transform of the Hamiltonian can be written as

$$H = \sum_k [-2(\cos\frac{2\pi k}{N} + h)\tilde{c}_k^\dagger \tilde{c}_k + i\sin\frac{2\pi k}{N}(\tilde{c}_{-k}^\dagger \tilde{c}_k^\dagger + \tilde{c}_{-k}\tilde{c}_k) + h]. \tag{8}$$

Next we introduce the following matrix

$$H_k = 2\begin{bmatrix} -\cos\frac{2\pi k}{N} - h & -i\sin\frac{2\pi k}{N} \\ i\sin\frac{2\pi k}{N} & \cos\frac{2\pi k}{N} + h \end{bmatrix}. \tag{9}$$

Equation (8) can then be written on the form

$$\begin{gathered} H = \sum_{k>0} [\tilde{c}_k^\dagger \quad \tilde{c}_{-k}] H_k \begin{bmatrix} \tilde{c}_k \\ \tilde{c}_{-k}^\dagger \end{bmatrix} \\ N = even, N_f = even \end{gathered} \tag{10}$$

$$\begin{gathered} H = \sum_{k>0} [\tilde{c}_k^\dagger \quad \tilde{c}_{-k}] H_k \begin{bmatrix} \tilde{c}_k \\ \tilde{c}_{-k}^\dagger \end{bmatrix} - 2(1+h)\tilde{c}_0^\dagger \tilde{c}_0 + 2(1-h)\tilde{c}_{-N/2}^\dagger \tilde{c}_{-N/2} + 2h \\ N = even, N_f = odd. \end{gathered} \tag{11}$$

And similarly for the remaining two cases. In (10) and (11) the $k$ values are given by (7) and we dropped a term $\sum_{k>0}\cos\frac{2\pi k}{N}$ that sums to zero for these cases. In (11) the $k = -\frac{N}{2}, 0$ terms have been separated out from the sum since they are in diagonal form.The next step is to do a fermionic Bogoliubov transformation defined for $k > 0$

$$\begin{aligned} d_k^\dagger &= \sin\theta_k \tilde{c}_k + i\cos\theta_k \tilde{c}_{-k}^\dagger \\ d_{-k}^\dagger &= \sin\theta_k \tilde{c}_{-k} - i\cos\theta_k \tilde{c}_k^\dagger. \end{aligned} \tag{12}$$

By constraining the parameter $\theta_k$ with the equation

$$\tan 2\theta_k = \frac{\sin\frac{2\pi k}{N}}{\cos\frac{2\pi k}{N} + h} \tag{13}$$

we have the diagonal expression

$$[\tilde{c}_k^\dagger \quad \tilde{c}_{-k}] H_k \begin{bmatrix} \tilde{c}_k \\ \tilde{c}_{-k}^\dagger \end{bmatrix} = \epsilon_k (d_k^\dagger d_k + d_{-k}^\dagger d_{-k} - 1). \tag{14}$$

Where $\pm\epsilon_k$ are the eigenvalues of $H_k$ for $k \neq -\frac{N}{2}, 0$

$$\epsilon_k = 2\sqrt{1 + h^2 + 2h\cos(\frac{2\pi k}{N})}. \tag{15}$$

Note that the operators $d_k$ are also fermionic. Combining expression (14) with (10) and (11) we have after simplification the Hamiltonian (2) in diagonal form

$$\begin{gathered} H = \sum_k \epsilon_k (d_k^\dagger d_k - \frac{1}{2}) \\ N = even, N_f = even \\ k = -\frac{N-1}{2}, -\frac{N-1}{2} + 1, ..., \frac{N-1}{2} \end{gathered} \tag{16}$$

$$\begin{gathered} H = \sum_{k \neq -\frac{N}{2}, 0} \epsilon_k (d_k^\dagger d_k - \frac{1}{2}) - 2(1+h)(\tilde{c}_0^\dagger \tilde{c}_0 - \frac{1}{2}) + 2(1-h)(\tilde{c}_{-N/2}^\dagger \tilde{c}_{-N/2} - \frac{1}{2}) \\ N = even, N_f = odd \\ k = -\frac{N}{2}, -\frac{N}{2} + 1, ..., \frac{N}{2} - 1. \end{gathered} \tag{17}$$

The expressions for the remaining two cases $N = odd$, $N_f = even$ and $N = odd$, $N_f = odd$ are obtained similarly but are not stated here. We note that our results differ from those of Dutta, Divakaran, Sen, Chakrabarti,

Rosenbaum and Aeppli[3], it appears that $k = -\frac{N}{2}, 0$ terms are handled differently in their stated results.

## 2.2 Asymptotic behaviour

In this subsection we analyze the properties of the periodic TFIM. For systems with an even number of sites and $h > 0$, the lowest energies of (16) and (17) are respectively

$$\begin{gathered} E_0(N_f = even) = -\frac{1}{2}\sum_k \epsilon_k \\ N = even, N_f = even \\ k = -\frac{N-1}{2}, -\frac{N-1}{2}+1, ..., \frac{N-1}{2} \end{gathered} \tag{18}$$

$$\begin{gathered} E_0(N_f = odd) = -\frac{1}{2}(\sum_{k\neq -\frac{N}{2},0} \epsilon_k) - 2 \\ N = even, N_f = odd, \quad h > 0 \\ k = -\frac{N}{2}, -\frac{N}{2}+1, ..., \frac{N}{2}-1. \end{gathered} \tag{19}$$

The first excited state in the respective $N_f$ sectors have energies $E_1(N_f = even)$ and $E_1(N_f = odd)$ given by

$$\begin{gathered} E_1(N_f = even) = -\frac{1}{2}\sum_k \epsilon_k + \epsilon_{(-\frac{N-1}{2})} + \epsilon_{(\frac{N-1}{2})} \\ N = even, N_f = even \\ k = -\frac{N-1}{2}, -\frac{N-1}{2}+1, ..., \frac{N-1}{2} \end{gathered} \tag{20}$$

$$\begin{gathered} E_1(N_f = odd) = -\frac{1}{2}\sum_{k\neq -\frac{N}{2},0} \epsilon_k + \epsilon_{(-\frac{N}{2}+1)} - 2h \\ N = even, N_f = odd, \quad h > 0 \\ k = -\frac{N}{2}, -\frac{N}{2}+1, ..., \frac{N}{2}-1. \end{gathered} \tag{21}$$

These four energy levels are guaranteed to contain the ground state energy $E_0$ and the first excited energy level $E_1$ of the system. From numerical calculations we see that $E_1 - E_0$ aproach zero as $\sim \frac{1}{N}$ when $h = 1$. For other values of $h$ the behaviour is exponential as can be seen from figure 1 where the difference $E_1 - E_0$ is logarithmically plotted against $N$ for $h = 0.9$ and $h = 1.1$.

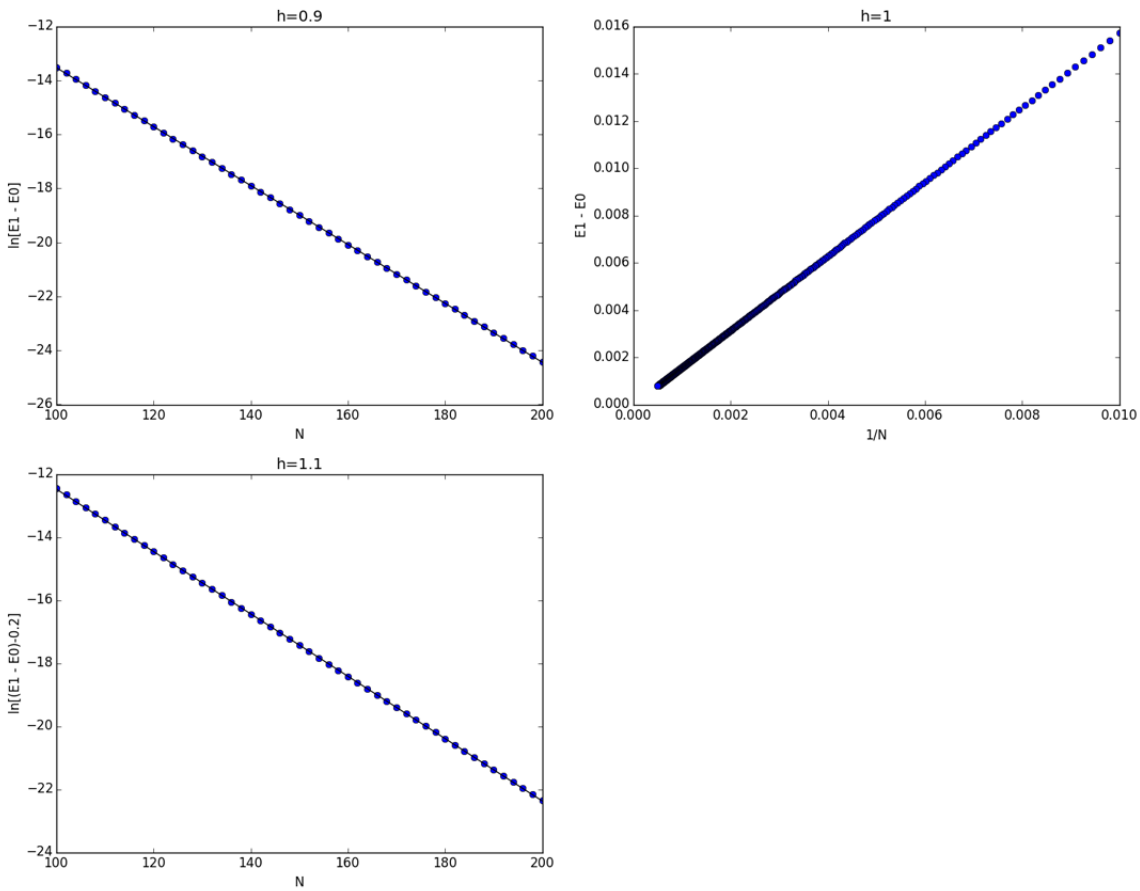


Figure 1: Periodic-TFIM with even number of sites ($N = even$). The difference $E_1 - E_0$ is plotted against $\frac{1}{N}$ for $h = 1$ in the upper right plot. In the upper left plot the natural logarithm of the difference $E_1 - E_0$ is plotted against $N$ for $h = 0.9$. The natural logarithm of the difference $(E_1 - E_0) - 0.2$ is plotted against $N$ for $h = 1.1$ in the lower plot. The solid line in the plot for $h = 0.9$ is the function $\alpha + \beta N$ with parameters $\alpha = -2.6315$ and $\beta = -0.1090$. The solid line in the plot for $h = 1.1$ is the function $\alpha + \beta N$ with $\alpha = -2.5897$ and $\beta = -0.0989$.

When $N \gg 1$ using a power expansion in terms of $\frac{1}{N}$ of $\epsilon_{(N/2+\alpha)}$ where $\alpha$ is some constant we see that in the $N = even, N_f = even$ sector the difference of the two lowest energies $E_1(N_f = even) - E_0(N_f = even)$ aproaches an $h$ dependent constant as $\sim \frac{1}{N}$ when $h = 1$ and as $\sim \frac{1}{N^2}$ when $h \neq 1, h > 0$. A similar behaviour is also seen in the $N = even$, $N_f = odd$ sector.

If we also write down the third energy level in each sector

$$\begin{gathered} E_2(N_f = even) = -\frac{1}{2}\sum_k \epsilon_k + \epsilon_{(-\frac{N-1}{2})} + \epsilon_{(\frac{N-1}{2})} + \epsilon_{(-\frac{N-1}{2}+1)} + \epsilon_{(\frac{N-1}{2}-1)} \\ N = even, N_f = even \\ k = -\frac{N-1}{2}, -\frac{N-1}{2}+1, ..., \frac{N-1}{2} \end{gathered} \tag{22}$$

$$\begin{gathered} E_2(N_f = odd) = -\frac{1}{2}\sum_{k \neq -\frac{N}{2}, 0} \epsilon_k + 2 \\ N = even, N_f = odd, \quad h > 0 \\ k = -\frac{N}{2}, -\frac{N}{2}+1, ..., \frac{N}{2}-1, \end{gathered} \tag{23}$$

we are guaranteed to find the second excited energy level $E_2$ of the system. In figure 2 the difference of the second excited energy level and the ground state energy $E_2 - E_0$ is plotted for values of $h = 0.9$, $h = 1$ and $h = 1.1$.

From the plots we find that unlike $E_1 - E_0$ the bahaviour is no longer exponential for $h = 0.9$ and $h = 1.1$, instead we have that $E_2 - E_0 \sim \frac{1}{N^2}$. If $h = 1$ we still have that the difference falls of like $\sim \frac{1}{N}$.

Note that when $h = 0.9$ the gap between $E_1$ and $E_0$ approaches zero. But the gap between $E_2$ and $E_0$ is non zero. Thus the ground state energy is degenerate up to a exponentially small error when $N >> 1$. But finite energy is required to excite the system to $E_2$. When $h = 1.1$ the difference $E_1 - E_0$ is unlike before non zero meaning that energy is required to excite the system. With $h = 1$ the energy levels $E_0$, $E_1$ and $E_2$ aproach the same value. Numerically this structure apears to hold for $0 < h < 1$, $h = 1$ and $h > 1$ pointing to $h = 1$ separating two phases.

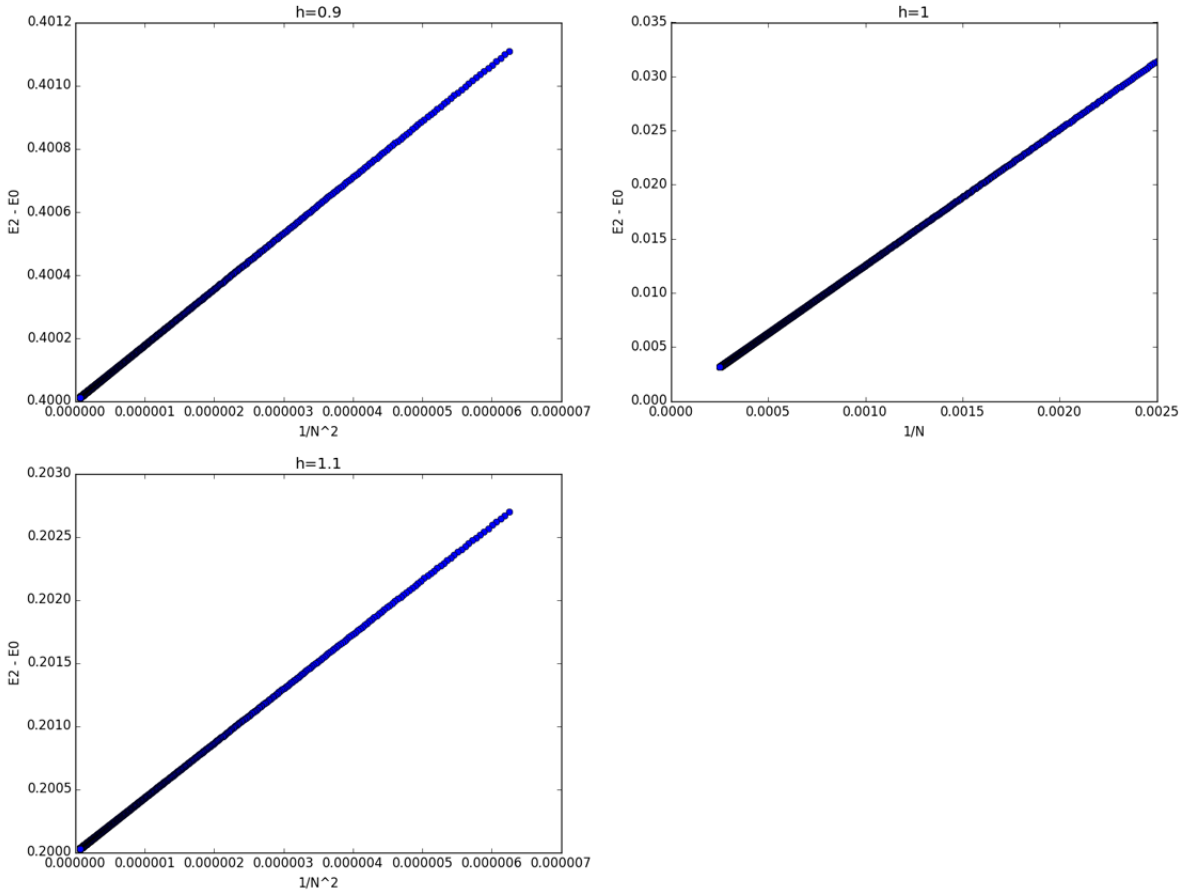


Figure 2: Periodic-TFIM with even number of sites ($N = even$). In the upper and lower left plots the difference of the second excited energy level and the ground state energy $E_2 - E_0$ is plotted against $\frac{1}{N^2}$ for values of $h = 0.9$ and $h = 1.1$. In the upper right plot the difference is plotted against $\frac{1}{N}$ for $h = 1$.

In the thermodynamic limit $N \to \infty$, the summation in the formulas (18) and (19) for the ground state energy is replaced by an integral and we have

$$\begin{gathered} E_0(N_f = even) = -\frac{N}{\pi}\int_0^{\pi} \sqrt{(h^2 + 1 + 2h\cos x)}dx \\ N = even, N_f = even \end{gathered} \tag{24}$$

$$
\begin{gathered}
E_0(N_f = odd) = -\frac{N}{\pi}\int_0^{\pi}\sqrt{(h^2+1+2h\cos x)}dx + g \\
g = 0 \quad if \quad 0 < h \leq 1, \quad g = 2(h-1) \quad if \quad h > 1 \\
N = even, N_f = odd.
\end{gathered}
\tag{25}
$$

The first derivative with respect to $h$ of the integral in (24) and (25) is finite but the second derivative with respect to $h$ of the integral shows a divergent behaviour when $h = \pm 1$, in figure 3 the second derivative is plotted against $h$ and the divergent behaviour can be seen. Note that the expressions (24) and (25) have the same value when $0 < h \leq 1$.

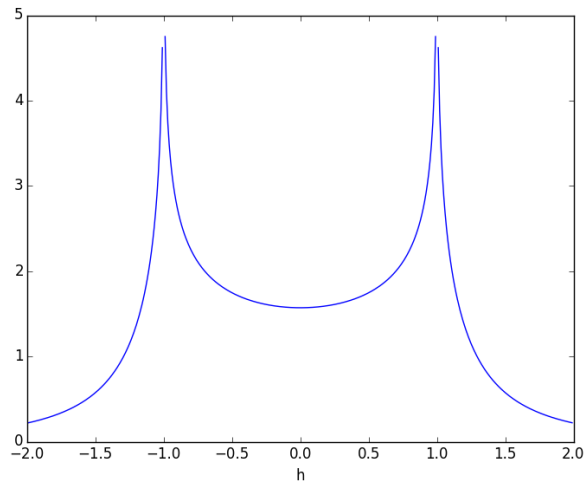


Figure 3: Periodic-TFIM, The second derivative with respect to $h$ of the integral in (24) plotted as a function of $h$. The behaviour is divergent for $h = \pm 1$.

# 3 Open Transverse Field Ising Model

## 3.1 Model description and diagonalization

In this section we look at the open TFIM. It is a model consisting of a one dimensional chain of spin 1/2 particles that interact with nearest neighbours and with a transverse field. The chain is open in the sence that the spins at the two endpoints do not interact with each other. The Hamiltonian is given by

$$H = -\sum_{n=1}^{N-1} \sigma_n^x \sigma_{n+1}^x - \sum_{n=1}^{N} h\sigma_n^z. \tag{26}$$

The operator $U = \sigma_1^x \sigma_2^x ... \sigma_N^x$ with inverse $U^{-1} = U$ acts on the hamiltonian by conjugation without changing the eigenvalues but the sign of $h$ is inverted

$$U^{-1}HU = -\sum_{n=1}^{N-1} \sigma_n^x \sigma_{n+1}^x - \sum_{n=1}^{N} (-h)\sigma_n^z. \tag{27}$$

Since the sign of $h$ is irrelevant for the spectrum of the system we can restrict ourself to $h \geq 0$. In section 2 we saw that $h = 1$ is of special interest, presumably this is still the case for the open TFIM. In this section we only consider the case $h = 1$, we first diagonalize the model and then give some of the properties.

The Hamiltonian (26) is algebraically nicer if we write it in terms of the fermionic operators (3) previously defined

$$\begin{aligned} H = \sum_{n=1}^{N-1} [-(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) + (c_{n+1}^\dagger c_n^\dagger + c_n c_{n+1})] \\ - \sum_{n=1}^{N} (2c_n^\dagger c_n - 1). \end{aligned} \tag{28}$$

To diagonalize the open chain we follow a method from Lieb, Schultz and Mattis[5], we use the method as it is given by Mahyaeh and Ardonne[6]. The first step is to realize that up to some constant, the Hamiltonian (28) is written on the form

$$H = \sum_{i,j=1}^{N} [c_i^\dagger A_{ij} c_j + \frac{1}{2}(c_i^\dagger B_{ij} c_j^\dagger + h.c.)]. \tag{29}$$

Where $A_{ij}$ and $B_{ij}$ are numbers determined by (28). These numbers form the elements of a hermitian matrix $A$ and an antisymmetric matrix $B$ respectively. The hermiticity of $A$ and the antisymmetry of $B$ ensures that $H$ is hermitian. We then define the operators

$$\eta_\alpha = \sum_{i=1}^{N} (g_{\alpha,i} c_i + h_{\alpha,i} c_i^\dagger). \tag{30}$$

Where $g_{\alpha,i}$ and $h_{\alpha,i}$ are real functions to be determined. The antisymmetry of the matrix $B$ together with the hermiticity of $A$ ensures that the $\eta_\alpha$ are fermionic as is explained in appendix A of the paper by Lieb, Schultz and Mattis[5]. Introducing the numbers $\Lambda_\alpha$ the Hamiltonian (29) can up to some constant be diagonalized as

$$H = \sum_\alpha \Lambda_\alpha \eta_\alpha^\dagger \eta_\alpha. \tag{31}$$

Here $\alpha$ runs over $N$ values. To determine the values of $\Lambda_\alpha$ we first define the linear combinations

$$\phi_{\alpha,i} = g_{\alpha,i} + h_{\alpha,i} \tag{32}$$

$$\psi_{\alpha,i} = g_{\alpha,i} - h_{\alpha,i}. \tag{33}$$

Then treating $\phi_{\alpha,i}$ and $\psi_{\alpha,i}$ as the elements of two vectors $\phi_\alpha$ and $\psi_\alpha$ we use the commutation relation $[H, \eta_\alpha] = -\Lambda_\alpha \eta_\alpha$, (29) and (30) to arrive at a pair of coupled matrix equations for $\Lambda_\alpha$, $\phi_\alpha$ and $\psi_\alpha$

$$\begin{aligned} \phi_\alpha(A - B) &= \Lambda_\alpha \psi_\alpha \\ \psi_\alpha(A + B) &= \Lambda_\alpha \phi_\alpha. \end{aligned} \tag{34}$$

These equations can be decoupled by multiplication from the right by $(A+B)$ and $(A-B)$ respectively. Since $\phi_\alpha$ and $\psi_\alpha$ mutually determine each other, it is sufficient to only consider $\phi_\alpha$. The decoupled equation for $\phi_\alpha$ is given by

$$\phi_\alpha(A - B)(A + B) = \Lambda_\alpha^2 \phi_\alpha. \tag{35}$$

This introduces an aparent but resolvable ambiguity of the sign of $\Lambda_\alpha$. Changing the sign of $\Lambda_\alpha$ leaves $\phi_\alpha$ unchanged but flips the sign of $\psi_\alpha$. This in turn changes $\eta_\alpha$ into $\eta_\alpha^\dagger$, which does not affect the energy gaps of the system. We may therefore assume that $\Lambda_\alpha$ is positive. In order to reproduce (28), the matrices $A$ and $B$ are given by

$$A - B = (-2) \begin{bmatrix} 1 & & & & & & \\ 1 & 1 & & & & & \\ & 1 & 1 & & & & \\ & & & \cdot & & & \\ & & & & \cdot & & \\ & & & & & \cdot & \\ & & & & 1 & 1 & \\ & & & & & 1 & 1 \end{bmatrix} \tag{36}$$

$$A + B = (-2)\begin{bmatrix} 1 & 1 & & & & & \\ & 1 & 1 & & & & \\ & & 1 & 1 & & & \\ & & & \cdot & & & \\ & & & & \cdot & & \\ & & & & & \cdot & \\ & & & & & 1 & 1 \\ & & & & & & 1 \end{bmatrix}. \tag{37}$$

The omitted entries are zero. From equation (35) we note that the effect of the multiplicative constant $(-2)$ is to scale $\Lambda_\alpha^2$ with a factor of 4. In the following calculations we simply drop the $(-2)$ terms to simplify the expressions, they can be reintroduced later if needed. Substituting into (35) leads to the equations for the boundary

$$\phi_{\alpha,1} + \phi_{\alpha,2} = \Lambda_\alpha^2 \phi_{\alpha,1} \tag{38}$$

$$\phi_{\alpha,(N-1)} + 2\phi_{\alpha,N} = \Lambda_\alpha^2 \phi_{\alpha,N}, \tag{39}$$

as well as the bulk equations for the interior

$$\begin{gathered} \phi_{\alpha,(n-1)} + 2\phi_{\alpha,n} + \phi_{\alpha,(n+1)} = \Lambda_\alpha^2 \phi_{\alpha,n} \\ n = 2, 3, ..., N-1. \end{gathered} \tag{40}$$

Inspired by the periodic-TFIM we make the anzats $\Lambda_\alpha^2 = 2(1+\cos\alpha)$ and to solve (40) we further assume that $\phi_{\alpha,n} \sim x_\alpha^n$. Under these assumptions the solution of (40) is given by

$$\phi_{\alpha,n} = A_1 e^{in\alpha} + A_2 e^{-in\alpha}. \tag{41}$$

Here $A_1$ and $A_2$ are some numbers not yet determined. Using this solution we write the boundary equations (38) and (39) as a matrix equation for $A_1$ and $A_2$.

$$\begin{bmatrix} e^{i\alpha}+1 & e^{-i\alpha}+1 \\ e^{i(N+1)\alpha} & e^{-i(N+1)\alpha} \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{42}$$

To avoid the zero vector we are only interested in nontrivial solutions for $\phi_{\alpha,n}$. We thus require that

$$0 = det \begin{bmatrix} e^{i\alpha}+1 & e^{-i\alpha}+1 \\ e^{i(N+1)\alpha} & e^{-i(N+1)\alpha} \end{bmatrix}. \tag{43}$$

The values of $\alpha$ then become constrained by the equation

$$0 = \sin(N\alpha) + \sin((N+1)\alpha). \tag{44}$$

To avoid any remaining trivial solutions for $\phi_{\alpha,n}$ and not overcounting $\Lambda_\alpha$, we need to choose a subset of the solutions to (44)

$$\begin{aligned} \alpha &= \frac{2\pi}{(2N+1)} j \\ j &= 1, 2, ..., N. \end{aligned} \tag{45}$$

We note that this result holds for $h = 1$ and hence also for $h = -1$. In section 4 we will derive equation (65), an analog to equation (44) that with the appropriate identifications can be used when $h \neq 1$. With arbitrary $h$ determining the possible values of $\alpha$ requires numerical methods.

## 3.2 Asymptotic behaviour

Because the operators $\eta_\alpha$ are fermionic, the energy gaps are determined by specifying the occupation number $n_\alpha \in \{0, 1\}$ for each $\alpha$. Choosing $\Lambda_\alpha$ to be positive, we have from (31)

$$E(n_\alpha) - E_0 = \sum_\alpha \Lambda_\alpha n_\alpha. \tag{46}$$

In (46) we omit any overall multiplicative constant that may differ from (28).

Since each $\alpha$ is determined by some integer (45), we might as well use the label $j$ instead of $\alpha$ and write $\Lambda_j = \sqrt{2}(1 + \cos[\frac{2\pi}{(2N+1)}(N+1-j)])^{1/2}$ . For very large systems we aproximate $\Lambda_j$ as a function of $\frac{1}{2N}$. The function then takes the simple form

$$\begin{aligned} \Lambda_j &= C(j - \frac{1}{2}) \\ j &= 1, 2, ..., N. \end{aligned} \tag{47}$$

Where $C$ is a $O(\frac{1}{N})$ constant for any given N. Using (46) and (47) we have an expression for the energy levels of large systems

$$E(n_j) - E_0 = C \sum_{j=1,2,...,N} (j - \frac{1}{2}) n_j. \tag{48}$$

The energy levels come in even steps. So there are $\sim N^2$ energy levels and $2^N$ energy eigenstates. We estimate the average degeneracy to be $\frac{2^N}{N^2}$.

For large systems, expression (48) enables us to write the partition function $Z$ on the form

$$Z = e^{-\beta E_0} \prod_{j=1,2,\ldots,N} [1 + e^{-\beta C(j-\frac{1}{2})}]. \tag{49}$$

# 4 Fixed Transverse Field Ising Model

## 4.1 Model description and diagonalization

In this section we consider systems goverened by the same interactions as the open TFIM but with the spin of one of the endpoints held fixed. We first define the system and diagonalize it, we then consider a few special cases and give two explicit examples of the model.

Fixing the spin on one of the ends reduces the number of states available and the Hamiltonian for the system will differ from the periodic and open TFIM. To be more precise we first note that the open TFIM (26) is equipped with a Hilbert-space $\mathcal{H}$. Specifying the $z$-direction of the spin at each site gives a natural basis for $\mathcal{H}$. We write such states as $|n >= |n_1 n_2 ... n_N >$ where $n_i$ is 1 if the spin on site $i$ is up and $-1$ if the spin is down. Taking $\{|n >\}$ to mean the set over all possible $n$ we have $\mathcal{H} = span\{|n_1 n_2 ... n_N >\}$. For a given choice of constants $\alpha_1$, $\alpha_2$ obeying $|\alpha_1|^2 + |\alpha_2|^2 = 1$, the fixed TFIM as we define it is given by the subset $\mathcal{H}' \subset \mathcal{H}$

$$\mathcal{H}' = span\{\alpha_1 |1 n_2 ... n_N > + \alpha_2 |(-1) n_2 ... n_N >\}. \tag{50}$$

And the Hamiltonian $H'$ given by

$$\begin{gathered} H' : \mathcal{H}' \to \mathcal{H}' \\ < \psi | H' | \phi >=< \psi | H | \phi > \\ \forall \quad |\psi >, |\phi > \in \mathcal{H}'. \end{gathered} \tag{51}$$

Here $H$ is the Hamiltonian for the open TFIM (26). To determine (51) it is sufficient to consider the action of the Hamiltonian on the basis vectors. For any pair of basis-vectors $|\psi >$, $|\phi >$ of (50) we have

$$< \psi|H'|\phi >=< \psi|H|\phi >=< \psi| - \sum_{i=1}^{N-1} \sigma_i^x \sigma_{i+1}^x - h \sum_{i=1}^{N} \sigma_i^z |\phi >=$$
$$=< \psi| - \sum_{i=2}^{N-1} \sigma_i^x \sigma_{i+1}^x - h \sum_{i=2}^{N} \sigma_i^z - (\alpha_1^* \alpha_2 + \alpha_2^* \alpha_1)\sigma_2^x - h(|\alpha_1|^2 - |\alpha_2|^2)|\phi > . \tag{52}$$

Since (52) holds for all pairs of basis vectors in $\mathcal{H}'$ we conclude that

$$\begin{gathered} H' = - \sum_{i=2}^{N-1} \sigma_i^x \sigma_{i+1}^x - h \sum_{i=2}^{N} \sigma_i^z - a\sigma_2^x - r \\ a = \alpha_1^* \alpha_2 + \alpha_2^* \alpha_1 \\ r = h(|\alpha_1|^2 - |\alpha_2|^2). \end{gathered} \tag{53}$$

For the special case $a = 0$ the fixed TFIM with $N$ sites is reduced to diagonalizing $[-\sum_{i=2}^{N-1} \sigma_i^x \sigma_{i+1}^x - h \sum_{i=2}^{N} \sigma_i^z]$, which we identify as the open TFIM with $(N-1)$ sites. The energy-gaps for a system with $h = 1$ would then be given by (46) with the appropriate number of sites. The set of solutions to $a = 0$ contain $\alpha_1 = 1, \alpha_2 = 0$ (the first spin fixed in the z-direction) and is thus nontrivial.

Before solving the general case $a \neq 0$ we consider the operator $R = \sigma_2^z \sigma_3^z ... \sigma_N^z$ with inverse $R^{-1} = R$. Letting this operator act by conjugation on (53) we obtain the useful relation

$$R^{-1} H' R = - \sum_{i=2}^{N-1} \sigma_i^x \sigma_{i+1}^x - h \sum_{i=2}^{N} \sigma_i^z + a\sigma_2^x - r. \tag{54}$$

Note that the sign of $a$ is inverted while the other terms stay the same. Since we just showed that $H'$ is similar to $R^{-1}H'R$, both (53) and (54) have the same eigenvalues, this will be important when we determine the spectrum. Similarly the operator $U = \sigma_2^x \sigma_3^x ... \sigma_N^x$ shows that inverting the sign of the parameter $h$ gives the same eigenvalues.

For systems with $a \neq 0$ the method used in section 3 is not directly applicable. However, adapting the methods introduced by Campostrini, Palissetto and Vicari[7], it is possible to find analytic expressions for the eigenvalues of (53). The first step is to introduce the extended hamiltonian

$$H_e = -\sum_{i=2}^{N-1} \sigma_i^x \sigma_{i+1}^x - h \sum_{i=2}^{N} \sigma_i^z - a\sigma_1^x \sigma_2^x - r. \tag{55}$$

Since $H_e$ and $\sigma_1^x$ commute they have simultaneous eigenvectors. So the eigenvalues $\{\lambda\}$ with corresponding eigenvectors such that $\sigma_1^x = 1$ give the spectrum for (53). And similarly the eigenvalues $\{\delta\}$ of $H_e$ with corresponding eigenvectors such that $\sigma_1^x = -1$ give the spectrum for (54). As was shown previously (53) and (54) have the same eigenvalues, it follows that $\{\lambda\} = \{\delta\}$. This means that we can unambiguously extract the spectrum of $H'$ given the spectrum of $H_e$.

Reusing the methods introduced in section 3, $H_e$ can be diagonalized and up to some constant be written on the form $H_e = \sum_\alpha \Lambda_\alpha \eta_\alpha^\dagger \eta_\alpha$. As before the first step is to write it in terms of fermionic operators (3)

$$\begin{aligned} H_e = &\sum_{n=2}^{N-1} [-(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) + (c_{n+1}^\dagger c_n^\dagger + c_n c_{n+1})] \\ -h &\sum_{n=2}^{N} (2c_n^\dagger c_n - 1) + a[-(c_1^\dagger c_2 + c_2^\dagger c_1) + (c_2^\dagger c_1^\dagger + c_1 c_2)] - r. \end{aligned} \tag{56}$$

The analogous matrices $A$ and $B$ in (29) are for this hamiltonian given by

$$A - B = (-2) \begin{bmatrix} 0 & 0 & & & & & & \\ a & h & & & & & & \\ & 1 & h & & & & & \\ & & 1 & h & & & & \\ & & & & . & & & \\ & & & & & . & & \\ & & & & & & . & \\ & & & & & & 1 & h & \\ & & & & & & & 1 & h \end{bmatrix} \tag{57}$$

$$A + B = (-2) \begin{bmatrix} 0 & a & & & & & & \\ & h & 1 & & & & & \\ & & h & 1 & & & & \\ & & & . & & & & \\ & & & & . & & & \\ & & & & & . & & \\ & & & & & & h & 1 \\ & & & & & & & h \end{bmatrix}. \tag{58}$$

Just as in section 3 we will drop the $(-2)$ terms in the following calculations, without them we have

$$C = (A-B)(A+B) = \begin{bmatrix} 0 & 0 & & & & & \\ & a^2+h^2 & h & & & & \\ & h & 1+h^2 & h & & & \\ & & & \cdot & & & \\ & & & & \cdot & & \\ & & & & & \cdot & \\ & & & & h & 1+h^2 & h \\ & & & & & h & 1+h^2 \end{bmatrix}. \tag{59}$$

Equation (35) then gives us the eigenvalue equation

$$\begin{aligned} C\phi^t_\alpha &= \Lambda^2_\alpha \phi^t_\alpha \\ C &= (A-B)(A+B). \end{aligned} \tag{60}$$

We would like to calculate the eigenvalues $\Lambda^2_\alpha$ since they together with (31) give us the spectrum of (55). They are given by the condition $det(C-\Lambda^2_\alpha) = 0$, directly from $C$ we find the eigenvalue 0 belonging to the eigenvector $(1,0,0,...,0)$, we should thus always find one zero eigenvalue. The zero eigenvalue can be explained by the degeneracy due to $[H_e, \sigma^x_1] = 0$. The form of $C-\Lambda^2_\alpha$ suggests the ansatz $\Lambda^2_\alpha = 1+h^2-2h\cos\alpha$. To calculate $det(C-\Lambda^2_\alpha)$ we first introduce the $n\times n$ matrix $D_n$ and define $d_n = det(D_n)$

$$D_n = \begin{bmatrix} 2\cos\alpha & 1 & & & & & \\ 1 & 2\cos\alpha & 1 & & & & \\ & 1 & 2\cos\alpha & 1 & & & \\ & & & \cdot & & & \\ & & & & \cdot & & \\ & & & & & \cdot & \\ & & & & 1 & 2\cos\alpha & 1 \\ & & & & & 1 & 2\cos\alpha \end{bmatrix}. \tag{61}$$

With the above ansatz and definitions we expand the determinant to find

$$det(C-\Lambda^2_\alpha) = -\Lambda^2_\alpha[(a^2-1+2h\cos\alpha)h^{N-2}d_{N-2} - h^{N-1}d_{N-3}]. \tag{62}$$

Expanding the determinants $d_n$ we find the recursion relation $d_n = 2(\cos\alpha)d_{n-1} - d_{n-2}$. Solutions can be found by setting $d_n \sim x^n$, we obtain $d_n = F_1 e^{i\alpha n} + F_2 e^{-i\alpha n}$ for some constants $F_1$ and $F_2$. From an explicit calculation we find $d_1 = 2\cos\alpha$ and $d_2 = 4\cos\alpha^2 - 1$. This is enough to fix

the constants to $F_1 = -i\frac{e^{i\alpha}}{2\sin\alpha}$, $F_2 = i\frac{e^{-i\alpha}}{2\sin\alpha}$, and the determinants are given by

$$d_n = \frac{\sin[\alpha(n+1)]}{\sin\alpha}. \tag{63}$$

The eigenvalues $\Lambda_\alpha^2 = 1 + h^2 - 2h\cos\alpha$ are thus given by the equation

$$\begin{gathered} 0 = det(C - \Lambda_\alpha^2) = -(1 + h^2 - 2h\cos\alpha)h^{N-2} \\ [(a^2 - 1 + 2h\cos\alpha)\frac{\sin[\alpha(N-1)]}{\sin\alpha} - h\frac{\sin[\alpha(N-2)]}{\sin\alpha}]. \end{gathered} \tag{64}$$

Or more compactly

$$\begin{gathered} 0 = det(C - \Lambda_\alpha^2) = -(1 + h^2 - 2h\cos\alpha)h^{N-2} \\ [(a^2 - 1)\frac{\sin[\alpha(N-1)]}{\sin\alpha} + h\frac{\sin[\alpha N]}{\sin\alpha}]. \end{gathered} \tag{65}$$

Note that we should always have a zero eigenvalue, depending on the value of $h$ this is not always possible if we restrict $\alpha$ to be real. With $a = 0$ we previously identified the fixed TFIM with the open TFIM, equation (65) can thus be used to find the spectrum of the open TFIM (26) with arbitrary $h$. In general we need to use numerical methods to find the possible values of $\alpha$.

## 4.2 Special cases and examples

Adapting the methods by Campostrini, Palissetto and Vicari[7] we obtained equations for the eigenvalues that we now solve for two cases.

First we note that if $a^2 = 1$, equation (65) reduces to $0 = (1 + h^2 - 2h\cos\alpha)\frac{\sin[\alpha N]}{\sin\alpha} = \Lambda_\alpha^2\frac{\sin[\alpha N]}{\sin\alpha}$, the solutions are

$$\alpha = \frac{\pi}{N}k \quad k = 0, 1, ..., N-1 \quad h = 1 \tag{66}$$

$$\alpha = \frac{\pi}{N}k \quad k = 1, 2, ..., N \quad h = -1 \tag{67}$$

$$\begin{gathered} \alpha = \frac{\pi}{N}k \quad k = 1, 2, ..., N-1 \\ \alpha_1 \quad s.t. \quad \Lambda_{\alpha_1}^2 = 0 \\ |h| \neq 1. \end{gathered} \tag{68}$$

We can combine these cases into one and write

$$H_e = -2\sum_{k=1}^{N-1}\sqrt{(1+h^2-2h\cos(\pi k/N))}\eta^\dagger_{\alpha(k)}\eta_{\alpha(k)} + (constant) \qquad (69)$$
$$a^2 = 1.$$

Above the zero eigenvector is not explicitly summed over but it is important to remember that $\alpha$ runs over $N$ values. Note also the factor of $-2$ that we have reintroduced after dropping it earlier. The identifications between the spectrum of (53), (54) and (55) given earlier determine the spectrum of (53).

We showed earlier that inverting the sign of the parameter $h$ gives the same spectrum. Therefore if we invert the sign of $h$ in $\Lambda^2_\alpha$ the same eigenvalues are also given by

$$0 = (1+h^2+2h\cos\alpha)h^{N-2}$$
$$[(a^2-1)\frac{\sin[\alpha(N-1)]}{\sin\alpha} - h\frac{\sin[\alpha N]}{\sin\alpha}]. \qquad (70)$$

If the parameters obey $a^2-1=\pm h$, we can if necessary invert the sign of $h$ and determine the non zero eigenvalues from the the equation

$$0 = \frac{\sin[\alpha(N-1)]}{\sin\alpha} + \frac{\sin[\alpha N]}{\sin\alpha}. \qquad (71)$$

This also requires the appropriate change of sign in $\Lambda^2_\alpha$. The non redundant solutions are given by

$$\alpha = \frac{2\pi}{2N-1}k, \quad k = 1,2,...,N-1$$
$$\alpha_1 \quad s.t. \quad \Lambda^2_{\alpha_1} = 0. \qquad (72)$$

Note the similarity with the solutions for the open TFIM with $h=1$ (45).

We will now validate the conclusions drawn earlier in this section with two explicit examples. The first example corresponds to $a=0$ (53), the second example similarly corresponds to $a=1$. We start with the open TFIM (26)

with 3 sites and $h = 1$, as a matrix in the z-basis

$$H = -\sum_{n=1}^{2} \sigma_n^x \sigma_{n+1}^x - \sum_{n=1}^{3} \sigma_n^z =$$
$$= \begin{bmatrix} -3 & 0 & 0 & -1 & 0 & 0 & -1 & 0 \\ 0 & -1 & -1 & 0 & 0 & 0 & 0 & -1 \\ 0 & -1 & -1 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & -1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & 1 & -1 & 0 \\ -1 & 0 & 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 0 & -1 & 0 & 0 & 3 \end{bmatrix}. \tag{73}$$

Fixing the spin in the z-direction on site one give us $\mathcal{H}' = span\{|1n_2n_3>\}$. The hamiltonian $H'$ is then in matrix form given by the upper left quarter of (73).

$$H' = \begin{bmatrix} -3 & 0 & 0 & -1 \\ 0 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \tag{74}$$

The matrix for the open TFIM with 2 sites is in the z-basis given by

$$H = \begin{bmatrix} -2 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 2 \end{bmatrix} =$$
$$= \begin{bmatrix} -3 & 0 & 0 & -1 \\ 0 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = H' + 1, \tag{75}$$

as expected from (53) for a systems with $a = 0$.

Next we consider fixing the first spin in the x-direction. This is the case $a = 1$ in (53). It is now convenient to use the x-basis, the starting point is still the open TFIM Hamiltonian (26) with 3 sites and $h$ set to one. As a matrix in the x-basis we have

$$H = -\sum_{n=1}^{2} \sigma_n^x \sigma_{n+1}^x - \sum_{n=1}^{3} \sigma_n^z =$$
$$= \begin{bmatrix} -2 & -1 & -1 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & -1 & 0 & -1 & 0 & 0 \\ -1 & 0 & 2 & -1 & 0 & 0 & -1 & 0 \\ 0 & -1 & -1 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & -1 & -1 & 0 \\ 0 & -1 & 0 & 0 & -1 & 2 & 0 & -1 \\ 0 & 0 & -1 & 0 & -1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & -1 & -1 & -2 \end{bmatrix}. \tag{76}$$

Writing the x-basis in a similar fashion as the z-basis, we have for a system with the first spin fixed in the x-direction $\mathcal{H}' = span\{|1n_2n_3>\}$. So the associated Hamiltonian $H'$ is given by the upper left quarter of (76).

$$H' = \begin{bmatrix} -2 & -1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ -1 & 0 & 2 & -1 \\ 0 & -1 & -1 & 0 \end{bmatrix} \tag{77}$$

We then introduce

$$H_e = -\sum_{i=2}^{2} \sigma_i^x \sigma_{i+1}^x - \sum_{i=2}^{3} \sigma_i^z - \sigma_1^x \sigma_2^x. \tag{78}$$

In the x-basis it is given by

$$H_e = \begin{bmatrix} -2 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & -1 & -2 \end{bmatrix}. \tag{79}$$

The upper left quarter of (79) is the same as the Hamiltonian (77) we want to diagonalize. The two $4 \times 4$ blocks on the diagonal of (79) do not mix, so the eigenvalues of (79) are given by the eigenvalues for the matrix constituting the upper left quarter together with the aigenvalues for the matrix constituting the lower right quarter. The spectrum of the Hamiltonian (79) thus contains the spectrum of (77). Note also that the spectrum of (79)

is doubly degenerate.

# 5 Summary

After diagonalizing the periodic TFIM we analyzed it both numerically and analytically. In the thermodynamic limit we found that the second derivative of the ground state energy with respect to the transverse field strengh $h$ is divergent for $h = 1$, signifying a phase transition. The first few excited energy levels fall of towards the ground state energy as $\sim \frac{1}{N}$ when $h = 1$. For other $h$ we found that the falloff can be exponential or $\sim \frac{1}{N^2}$ depending on the energy level under consideration.

The open TFIM was diagonalized for $h = 1$ and we saw that in the limit of large systems $N >> 1$ the energy levels are highly structured. The structure of the spectrum enabled us to write the partition function on a simple form for $N >> 1$.

The fixed TFIM proved after defining it to share similarities with the open TFIM, under certain circumstances they give rise to essentially the same system. We also found 'rotational' symmetries that were important when determining the spectrum of the fixed TFIM.

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