

Simulating the Ising Model with a Quantum Computer

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This work is based on replicating the results achieved in the paper "Exact Ising Model Simulation on a quantum computer" by Alba Cervera-Lierta et al. (2018) and comparing them with the ones given by current quantum machines. First, we present a way to analytically diagonalize the one-dimensional Ising Hamiltonian. Next, we create a quantum circuit that diagonalizes the Hamiltonian and simulates its eigenstates. Furthermore, thanks to the Ising model being solvable, the circuit can serve as a benchmark for evaluating the reliability of quantum machines. Through the application of this circuit, we have obtained the energy spectrum and ground state magnetization of the one-dimensional Ising Model.

I. INTRODUCTION

The physical world is filled with phase transitions, such as water freezing into ice, or less common ones, such as some metals turning superconductive in low temperatures. The most fascinating characteristic of this type of phenomenon is the abrupt change in the macroscopic properties of a system after the variation of an external parameter of the system, for example, the temperature [1]. A specific type of phase transitions are Quantum Phase Transitions which happen at $T = 0$ K and are due to quantum fluctuations of the system that are governed by Heisenberg's uncertainty principle [2].

One of the most relevant models in the study of phase transitions is the Ising Model. Even though this model was first developed to describe classically the phase transition of ferromagnetism, currently, its resolution extends to diverse fields of science like, for instance, the prediction of protein folding [3], or error mitigation algorithms [4], among others. However, our focus is on the Quantum Ising Model. This model has recently gained relevance with the rise of quantum computation as it is one of the few many-body quantum models that can be solved exactly, which means if simulated in a quantum computer, it can be used as a benchmark for quantum hardware. Furthermore, it also motivates the search of algorithms to simulate more complex N-body quantum models, such as the Kitaev honeycomb model, among others [5].

In this paper, we replicate the results of Ref. [6] using newer quantum hardware to show how much it has improved since 2018. The referenced paper proposes a quantum circuit for the simulation of the one-dimensional Ising Model with a transverse magnetic field with four sites following the analytical solutions for the Hamiltonian developed in Ref. [7, 8].

This paper is structured as follows: Section II we introduce the Ising model, the Hamiltonian, and the properties of the model. In Section III, we follow the analytical solution for the 1D Ising Hamiltonian with a Transverse Magnetic field developed in Ref. [7, 8]. In Section IV, we develop the quantum gates needed for the quantum circuits that diagonalize and simulate the Ising Hamil-

tonian. In Section V, we present the specific circuit for a chain with four sites using the gates developed in the former section. Both of these sections will follow the methods first introduced in Ref. [5] and then further developed and implemented in Ref. [6]. Section VI displays the results achieved for the energy spectrum of the Ising Model and the magnetization of the ground state for the Ising state using the quantum circuits proposed in the prior section. Finally, in Section VII, we present the conclusions of our paper.

II. THE ONE DIMENSIONAL ISING MODEL

This paper focuses on solving and simulating the one-dimensional Ising Model with a transverse magnetic field. The Hamiltonian for this model is

$$\mathcal{H} = \sum_{i=1}^n \sigma_i^x \sigma_{i+1}^x + \lambda \sum_{i=1}^n \sigma_i^z, \quad (1)$$

where σ_i^z, σ_i^x are the corresponding Pauli matrices and λ represents the strength of the polarizing magnetic field. We also impose periodic boundary conditions $\sigma_{n+1} = \sigma_1$.

If we study the expression of the Hamiltonian, the first term describes a near-neighbor interaction for a one-dimensional chain, and the second term is a polarization term. In this case, the strength of the magnetic field (λ) characterizes the quantum phase transition with a critical λ value, which separates the polarized phase for a strong magnetic field ($\lambda \gg 1$) from the non-polarized phase for a weak one ($\lambda \sim 0$).

III. SOLVING THE 1D ISING HAMILTONIAN

To solve the Hamiltonian described in the prior section, we will follow the resolutions developed in Ref. [7, 8], and more detailed resolutions were also consulted in Ref. [9–12].

We explain each step needed to analytically diagonalize the 1D Ising Hamiltonian with a transverse magnetic field.

A. Jordan-Wigner transformation

The first step to diagonalize the Ising Hamiltonian is to perform a Jordan-Wigner transformation. This transformation allows us to map $\frac{1}{2}$ -spin operators into spinless fermionic annihilation/creation operators that satisfy anticommutation relations [13]. The new annihilation operator reads as

$$a_j = \bigotimes_{l=1}^{j-1} \sigma_j^z \otimes (|0\rangle_j \langle 1|_j) = \bigotimes_{l=1}^{j-1} \sigma_j^z \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_j \quad (2)$$

where the basis used is $|0\rangle_j = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|1\rangle_j = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. These new operators are combined to express the Pauli matrices present in the Ising Hamiltonian with annihilation and destruction operators.

Consequently, after Jordan-Wigner, the Hamiltonian becomes [7, 11]

$$\begin{aligned} \mathcal{H} = & \sum_{j=1}^n (a_j^\dagger a_{j+1}^\dagger + a_j^\dagger a_{j+1} + a_{j+1} a_j + a_{j+1}^\dagger a_j) \\ & - \left[1 + \prod_{j=1}^n (1 - 2\hat{n}_j) \right] (a_n^\dagger a_1^\dagger + a_n^\dagger a_1 + a_1 a_n + a_1^\dagger a_n) \\ & + \lambda \sum_{j=1}^n (1 - 2\hat{n}_j) \end{aligned} \quad (3)$$

It is important to note that the Hamiltonian after Jordan-Wigner has different boundary conditions depending on the parity of the state applied. When the number of occupied states is odd the boundary terms are periodic ($a_{n+1} = a_1$), and when its even then it is antiperiodic ($a_{n+1} = -a_1$). This means that we essentially have two different Hamiltonians depending on the parity of the state we work with.

In the thermodynamic limit, the boundary term can be neglected and so, the Hamiltonian becomes

$$\begin{aligned} \mathcal{H} = & \sum_{j=1}^n (a_j^\dagger a_{j+1}^\dagger + a_j^\dagger a_{j+1} + a_{j+1} a_j + a_{j+1}^\dagger a_j) \\ & + \lambda \sum_{j=1}^n (1 - 2\hat{n}_j) \end{aligned} \quad (4)$$

which it is the Hamiltonian we use for the rest of this section.

B. Fourier transformation

The next step to diagonalize the Hamiltonian is to perform a Fourier transformation. A transformation that allows us to go from the position space to the momentum one. In our case, we use the discrete quantum Fourier

transformation, and we take advantage of the translational invariance of the Ising Hamiltonian so the momentums can be defined in the set $k \in (-\frac{n}{2}, \frac{n}{2}]$ [9, 11].

The expression for the Discrete Fourier Transformation (DFT) is

$$b_k = \frac{1}{\sqrt{n}} \sum_{j=1}^n e^{-i\frac{2\pi}{n}jk} a_j, \quad k = -\frac{n}{2} + 1, \dots, \frac{n}{2}, \quad (5)$$

where k is the momentum and n is the number of sites.

Applying the Fourier transform to Eq. (4), gives us

$$\begin{aligned} \mathcal{H} = & \sum_{k=-\frac{n}{2}+1}^{\frac{n}{2}} \left\{ 2 \left[\cos\left(\frac{2\pi}{n}k\right) - \lambda \right] b_k^\dagger b_k \right. \\ & \left. + e^{i\frac{2\pi k}{n}} \left(b_k b_{-k} + b_k^\dagger b_{-k}^\dagger \right) \right\} + \lambda n, \end{aligned} \quad (6)$$

allowing us to get rid of the first-neighbor interaction, and instead, it now is between opposite sign momenta. This type of Hamiltonian is called the Quadratic Hamiltonian.

C. Bogoliubov transformation

The final step for our diagonalization is performing a Bogoliubov transformation, which allows us to get a Hamiltonian without interaction. This transformation proposes a new set of operators that are a linear combination of the original ones

$$\begin{cases} c_k = A_k b_k + B_k b_{-k}^\dagger \\ c_{-k} = C_k b_{-k} + D_k b_k^\dagger \end{cases} \quad (7)$$

$$|A_k|^2 + |B_k|^2 = 1 \quad A_k C_k + B_k D_k = 0,$$

where the conditions of the coefficients are imposed by the fermionic anticommutation relations.

The development of this transformation in detail can be consulted in [11, 12]. The new operators for the Bogoliubov transformation are

$$\begin{cases} c_k = \cos\left(\frac{\theta_k}{2}\right) b_k + i \sin\left(\frac{\theta_k}{2}\right) b_{-k}^\dagger \\ c_{-k} = \cos\left(\frac{\theta_k}{2}\right) b_{-k} - i \sin\left(\frac{\theta_k}{2}\right) b_k^\dagger \end{cases} \quad (8)$$

Where the angle is given by $\theta_k = \arctan\left[\frac{\sin\left(\frac{2\pi k}{n}\right)}{\cos\left(\frac{2\pi k}{n}\right) - \lambda}\right]$

As a result of this transformation, we achieve a non-interacting fermionic Hamiltonian

$$\mathcal{H} = \sum_{k=-\frac{n}{2}+1}^{\frac{n}{2}} 2\epsilon_k \left(c_k^\dagger c_k - \frac{1}{2} \right), \quad (9)$$

where $\epsilon_k = \pm \sqrt{[\cos(k_n) - \lambda]^2 + \sin^2(k_n)}$ are the monoparticular eigenenergies.

IV. SOLVING THE ISING HAMILTONIAN WITH A QUANTUM COMPUTER

After explaining the analytical resolution on the Hamiltonian we now explain how to find a unitary operator U_{dis} , made up of quantum gates, that can disentangle the Ising Hamiltonian $\mathcal{H}_{\text{diag}} = U_{\text{dis}}^\dagger \mathcal{H} U_{\text{dis}}$, where $\mathcal{H}_{\text{diag}}$ is the non-interacting fermionic Hamiltonian.

To construct this operator, we follow the development explained in the previous section and create quantum gates for each of the necessary transformations for the diagonalization of the Hamiltonian. After finding these gates, we can construct a circuit to diagonalize the Hamiltonian with a quantum computer.

A. Gate for Jordan-Wigner transformation

The first step for our diagonalization is the Jordan-Wigner transformation, but this transformation does not change any of the coefficients of the wave function. It just changes from a $\frac{1}{2}$ -spin basis

$$|\Psi\rangle = \sum_{n_{\sigma_i} = -\frac{1}{2}, \frac{1}{2}} \psi_{1, \dots, m} |n_{\sigma_1}, n_{\sigma_2}, \dots, n_{\sigma_m}\rangle \quad (10)$$

to a spinless fermionic basis

$$|\Psi\rangle = \sum_{n_i=0,1} \psi_{1, \dots, m} (a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} \dots (a_m^\dagger)^{n_m} |\text{vac}\rangle, \quad (11)$$

for $i = 1, \dots, m$ and where $|\text{vac}\rangle$ is the vacuum state. Thus, we do not need a gate for this step of the diagonalization.

The only important change when applying Jordan-Wigner is that the system now is fermionic, so it must comply with the anticommutation relations of fermions. Consequently, when performing any SWAP between qubits, we take these relations into account and use a modified SWAP gate, which we call "fSWAP", and it reads as

$$\text{fSWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (12)$$

As we can observe, the only difference from a standard SWAP gate is that when applying it to a fully occupied 2-qubit state, we get a negative sign because of anticommutation.

B. Gate for Fourier transformation

The next step is the Fourier transformation, for the quantum circuit application we perform a Fast Fourier transformation, which consists of separating the original

transformation Eq. (5) into two sums, one with the even sites and the other with the odd ones [14].

With this method, when working with 2^m sites for the Ising Hamiltonian, we can decompose the 2^m Fourier transformation into a combination of several of the following 2-qubit gates

$$F_k^n = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -e^{-i\frac{2\pi}{n}k} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{e^{-i\frac{2\pi}{n}k}}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & -e^{-i\frac{2\pi}{n}k} \end{pmatrix}, \quad (13)$$

where k is the momentum, and n is the number of sites of our system. The method of getting the matrix and the algorithm is explained in further detail in Ref. [5, 15]

C. Gate for Bogoliubov transformation

The final step is the Bogoliubov transformation, which only mixes qubits with opposite momenta see Eq. (8). Thus, only a 2-qubit gate acting on the corresponding qubits is needed to perform it. The transformation ends up being characterized by the matrix [5, 6]

$$B_k^n = \begin{pmatrix} \cos\left(\frac{\theta_k}{2}\right) & 0 & 0 & i \sin\left(\frac{\theta_k}{2}\right) \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ i \sin\left(\frac{\theta_k}{2}\right) & 0 & 0 & \cos\left(\frac{\theta_k}{2}\right) \end{pmatrix}, \quad (14)$$

where $\theta_k = \arctan\left[\frac{\sin\left(\frac{2\pi}{n}k\right)}{\cos\left(\frac{2\pi}{n}k\right) - \lambda}\right]$ and k is the momentum and n is the number of sites.

V. QUANTUM CIRCUIT FOR $n = 4$ CHAIN

Now that we have established the gates needed to solve the Ising Hamiltonian with a quantum computer, we introduce the circuit that allows us to go from states in the Ising basis to the diagonal basis [6]. Specifically, for this work, we present how the quantum gates developed in the previous section let us build a circuit for the $n = 4$ 1D Ising Hamiltonian.

Considering that we are working with only four sites, we are not in the Thermodynamic limit. To solve this without altering the resolution presented before, we modify the boundary term of the original Hamiltonian

$$\mathcal{H}_{\text{finite}} = \sum_{i=1}^{n-1} \sigma_i^x \sigma_{i+1}^x + \lambda \sum_{i=1}^n \sigma_i^z + \sigma_1^y \sigma_2^z \dots \sigma_{n-1}^z \sigma_n^y \equiv \mathcal{H}, \quad (15)$$

so that after Jordan-Wigner it becomes Eq. (4).

A. Diagonalization for $n = 4$ Chain

In Fig. 1 we present a diagram of the quantum circuit for the diagonalization of a 4-site Ising Model with

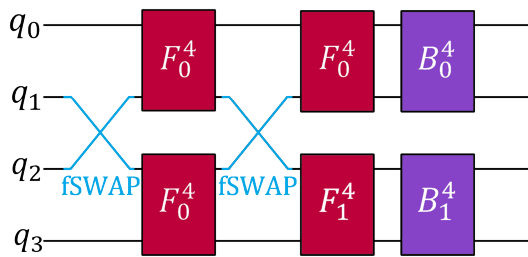


FIG. 1: Diagram of the quantum circuit proposed for a 4-qubit computer to diagonalize the modified Ising Hamiltonian Eq. (15) with $n = 4$.

a Transverse Magnetic Field. The gates necessary for its implementation have been described in Section IV. For their implementation the gates have been decomposed into more basic gates, they can be consulted in Ref. [6]. This circuit is the unitary operator (U_{dis}) that disentangles our Hamiltonian described in the previous section. If we apply this operator to the Hamiltonian's matrix, we obtain the diagonalized matrix and the eigenenergies of the system.

B. Simulation for $n = 4$ Chain

Having found a circuit that allows us to go from Ising states to the corresponding state in the computational basis we can do the inverse circuit to get the opposite. Performing the inverse circuit allows us to simulate Ising states in a quantum computer.

In particular, for this work, we are interested in simulating the ground state and observing the quantum phase transition characteristic of the one-dimensional Ising model with a transverse field. For this purpose, we need to find the ground state of the non-interacting Hamiltonian for different ranges of magnetic field strength (λ). We take advantage of the direct circuit and find the ground state for Eq. (9) in the computational basis

$$|\text{G.S.}\rangle = \begin{cases} |0000\rangle, & \text{if } \lambda \leq -1 \\ |0100\rangle, & \text{if } -1 < \lambda \leq 0 \\ |0111\rangle, & \text{if } 0 < \lambda \leq 1 \\ |1111\rangle, & \text{if } \lambda > 1 \end{cases} \quad (16)$$

To prepare these states for the simulation, we need to add additional "X-Pauli" gates for any qubit in the occupied state ($|1\rangle$).

VI. RESULTS

The circuit discussed before for the diagonalization of the Hamiltonian has been first performed with a classical approach, using the matrices described for the transformations and performing the tensorial products and

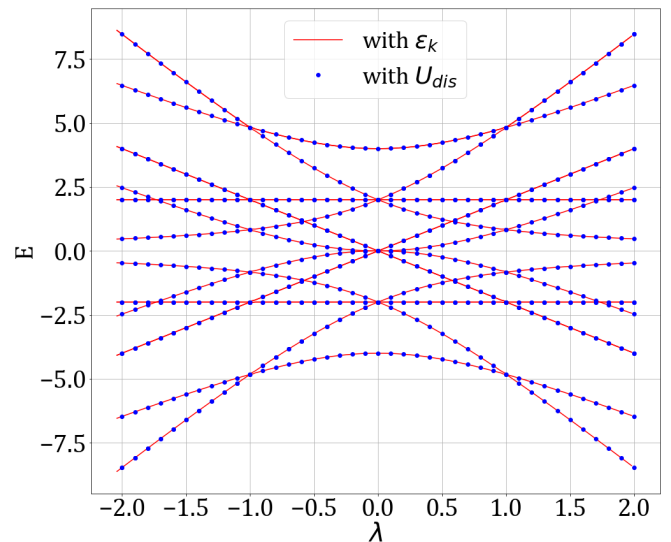


FIG. 2: Energies of all the eigenstates of an $n = 4$ Ising Chain with the Hamiltonian Eq. (15) as a function of the strength of the magnetic field (λ). The solid line represents the energies calculated with the monoparticular energies from Eq. (9), and the points are the energies found when diagonalizing the Hamiltonian with the operator U_{dis} using Python.

products of matrices to get the operator that defines the whole circuit U_{dis} and running it through the Hamiltonian's matrix. This first step's purpose was to, on the one hand, verify that the circuit proposed does diagonalize the Hamiltonian's matrix and, on the other hand, obtain the eigenenergies and compare them to the energies found with the non-interacting Hamiltonian with Eq. (9), Fig. 2 shows the results of this.

After checking that the direct circuit works correctly, we now perform the circuit for the simulation of the Ising Model, but this time the code is developed with qiskit so we run it with real quantum hardware. For this part, we will calculate the expected value of σ_z for each qubit, and normalize it. To achieve this, we must run the ground state in the computational basis, see Eq. (16), through the inverse quantum circuit to transform it into the Ising basis, and then measure the final state. This procedure must be repeated several times (N) to get the expected value, and it has a statistical error associated. This is the only error represented in Fig. 3, even though, for quantum machines, there are other sources of error.

In Fig. 3 we show our results for the transverse magnetization of the ground state of the Ising Hamiltonian. We can observe how the system goes through a quantum phase transition in $|\lambda| = 1$ where the ground state changes abruptly from a polarized phase to a non-polarized phase for $\lambda < 0$ and the opposite for $\lambda > 0$.

When observing Fig. 3 the results for the real machine are remarkable for the range $\lambda \in [-1, 1]$, where they match or are very close to the classically obtained results. For the other values of λ , the experimental values diverge more, but we are still able to distinguish where

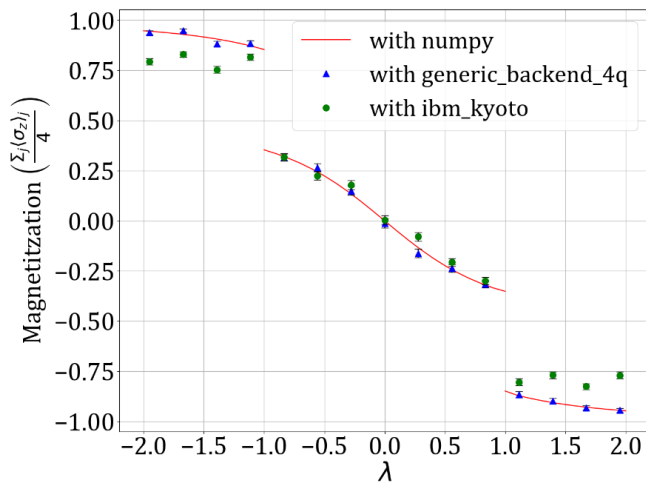


FIG. 3: Transverse magnetization of the Ising ground state as a function of the magnetic field strength (λ). The solid line represents the results when solving the Hamiltonian with a classical computer using Python, the blue triangles represent the values when using a quantum simulator, "generic_backend_4q", and the green dots represent the ones obtained using real quantum hardware "ibm_kyoto", in both cases we have performed 500 measurements. The error bars are represented for the quantum simulator and quantum machine and it is the statistical error associated to the measurements.

the phase transition takes place when $|\lambda| = 1$.

To finish up this section, all the code for both Fig.2 and Fig. 3 was developed with Python and qiskit and can be consulted in Ref. [16]. The qiskit code was developed in May 2024 and with the 1.1.0 qiskit version, any earlier or later versions might present compatibility issues.

VII. CONCLUSIONS AND DISCUSSION

In this paper, we have successfully solved the one-dimensional Hamiltonian with a transverse magnetic field,

following the resolutions developed originally in Ref. [7, 8]. Moreover, we have found quantum gates that allowed us to apply this exact resolution to create a quantum circuit, which when applied directly can diagonalize the Ising Hamiltonian and when we run the inverse circuit, we can simulate the Ising model by going from the eigenstates in the diagonal basis to the Ising basis [5, 6].

Specifically, we have used the circuit for $n = 4$, first proposed in Ref. [6], and we have successfully recovered the eigenenergies of the $n = 4$ Ising Hamiltonian, applying it numerically. Furthermore, we have run the inverse quantum circuit, simulated the ground state for the Ising Model, and calculated the expected value for the transverse magnetization with different methods: a classical computer, a simulation of a quantum computer, and a quantum machine ("ibm_kyoto").

If we use this as a benchmark for "ibm_kyoto", although the experimental results do not match up exactly with the classical ones, particularly in the polarized phase ($|\lambda| > 1$), the overall results have improved significantly when comparing them to the ones obtained in the original paper Ref. [6]. This shows us that the accuracy of IBM quantum machines has improved since 2018 when the paper was originally published.

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- [1] S. Sachdev, *Physics World* **12**, 33 (1999).
 - [2] S. Haravifard, Z. Yamani, and B. D. Gaulin, *Experimental Methods in the Physical Sciences* **48**, 43 (2015).
 - [3] V. Muñoz, *Current Opinion in Structural Biology* **11**, 212 (2001).
 - [4] E. Rosenberg, P. Ginsparg, and P. L. McMahon, *Quantum Science and Technology* **7**, 015024 (2022).
 - [5] F. Verstraete, J. I. Cirac, and J. I. Latorre, *Phys. Rev. A* **79**, 032316 (2009).
 - [6] A. Cervera-Lierta, *Quantum* **2**, 114 (2018).
 - [7] E. Lieb, T. Schultz, and D. Mattis, *Annals of Physics* **16**, 407 (1961).
 - [8] S. Katsura, *Phys. Rev.* **127**, 1508 (1962).
 - [9] E. Eriksson, Master's thesis (2008).
 - [10] A. De Pasquale and P. Facchi, *Phys. Rev. A* **80**, 032102 (2009).
 - [11] A. Cervera Lierta, Ph.D. thesis, Universitat de Barcelona (2019).
 - [12] P. Scholl and R. Orús, *Phys. Rev. B* **95**, 045112 (2017).
 - [13] M. A. Nielsen *et al.*, *School of Physical Sciences The University of Queensland* **59**, 75 (2005).
 - [14] W. H. Julian, *Computers Mathematics with Applications* **15**, 311 (1988).
 - [15] A. J. Ferris, *Phys. Rev. Lett.* **113**, 010401 (2014).
 - [16] M. Domínguez-Navarro, Github repository (2024), https://github.com/martadomin/IsingModel_TFG.

VIII. APPENDIX

A. Development of the Bogoliubov transformation

In this section we explain in more detail the Bogoliubov transformation proposed in Eq. (7) and how to get the final operators, Eq. (8) [12].

First we need to rewrite the Hamiltonian before Bogoliubov, Eq. (6)

$$\mathcal{H} = \sum_{k=-\frac{n}{2}+1}^{\frac{n}{2}} \left\{ \left[\cos\left(\frac{2\pi k}{n}\right) - \lambda \right] (b_k^\dagger b_k + b_{-k}^\dagger b_{-k}) + i \sin\left(\frac{2\pi k}{n}\right) (b_k b_{-k} + b_k^\dagger b_{-k}^\dagger) \right\} + \lambda n \quad (\text{A1})$$

taking advantage of the symmetries of the Hamiltonian and its periodic boundary condition.

As a result, now we can write this expression for the Hamiltonian in matrix form

$$\mathcal{H} = \sum_{k=-\frac{n}{2}+1}^{\frac{n}{2}} X_k^\dagger h X_k, \quad (\text{A2})$$

where $h = \begin{pmatrix} \cos\left(\frac{2\pi k}{n}\right) - \lambda & i \sin\left(\frac{2\pi k}{n}\right) \\ -i \sin\left(\frac{2\pi k}{n}\right) & -[\cos\left(\frac{2\pi k}{n}\right) - \lambda] \end{pmatrix}$ and $X_k = \begin{pmatrix} b_k \\ b_{-k}^\dagger \end{pmatrix}$.

With this new way of expressing the Hamiltonian, first, we can straight away get the eigenvalues of the h matrix, which correspond to the monoparticular energies for our future non-interacting Hamiltonian

$$\pm \epsilon_k = \pm \sqrt{[\cos(k_n) - \lambda]^2 + \sin^2(k_n)}. \quad (\text{A3})$$

Then, we can rework Eq. (A2) to get a diagonal matrix for the Hamiltonian with the new operators from Eq. (7)

$$\mathcal{H} = \sum_{k=-\frac{n}{2}+1}^{\frac{n}{2}} Y_k^\dagger U_k h U_k^\dagger Y_k = \sum_{k=-\frac{n}{2}+1}^{\frac{n}{2}} Y_k^\dagger h_{\text{diag}} Y_k \quad (\text{A4})$$

where $U_k = \begin{pmatrix} A_k & B_k \\ C_k^* & D_k^* \end{pmatrix}$, $h_{\text{diag}} = \begin{pmatrix} \epsilon_k & 0 \\ 0 & -\epsilon_k \end{pmatrix}$ and $Y_k = \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix}$.

Using the relations between coefficients written in Eq. (7) and imposing in Eq. (A4) that the non-diagonal terms of $U_k h U_k^\dagger$ are zero, we can obtain the values for the transformation matrix, and thus getting the new operators for our diagonal Hamiltonian, see Eq. (8).

B. Boundary term for the Modified Ising Hamiltonian

In this section we discuss the boundary term of the Modified Ising Hamiltonian, Eq. (15).

First, we apply the Jordan-Wigner transformation, Eq. (3), to this new boundary term

$$\sigma_1^y \sigma_2^z \dots \sigma_{n-1}^z \sigma_n^y = a_n^\dagger a_1^\dagger + a_n^\dagger a_1 + a_1 a_n + a_1^\dagger a_n. \quad (\text{A5})$$

We can see it gives us a periodic boundary condition ($a_{n+1} = a_1$) and we recover the Hamiltonian for the thermodynamic limit, Eq. (4).

Next we show a few examples on how this boundary term ($\sigma_1^y \sigma_2^z \sigma_3^z \sigma_4^y$), acts on some spin states for a system with $n = 4$ sites

$$\begin{aligned} \sigma_1^y \sigma_2^z \sigma_3^z \sigma_4^y | \uparrow \uparrow \uparrow \uparrow \rangle &= - | \downarrow \uparrow \uparrow \downarrow \rangle \\ \sigma_1^y \sigma_2^z \sigma_3^z \sigma_4^y | \uparrow \downarrow \uparrow \uparrow \rangle &= | \downarrow \uparrow \uparrow \uparrow \rangle \end{aligned} \quad (\text{1})$$

compared to the original boundary term ($\sigma_n^x \sigma_1^x$)

$$\begin{aligned} \sigma_n^x \sigma_1^x | \uparrow \uparrow \uparrow \uparrow \rangle &= | \downarrow \uparrow \uparrow \downarrow \rangle \\ \sigma_n^x \sigma_1^x | \uparrow \downarrow \uparrow \uparrow \rangle &= | \downarrow \uparrow \uparrow \uparrow \rangle \end{aligned} \quad (\text{2})$$

As we can see the modified boundary term gives us periodic boundary conditions for an odd number of up spins and antiperiodic for an even number of up spins.