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Quantum algorithms for 1D Ising and Glauber-Ising models

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1 Introduction

Quantum computing is little by little turning into a realistic technology. Huge advances started to take place toward the so-called quantum advantage in the 2000s, departing mainly from the first 5-qbit nuclear magnetic resonance computer [1], Shor's theorem proof using photonic qbits [2] and quantum entanglement [3], and the implementation of Deutsch's algorithm in a clustered quantum computer [4]. Today, there are quantum processors such as superconducting system Rigetti-19Q [5], with 19 qbits, capable of performing unsupervised learning [6]; superconducting chip Intel Tangle Lake [7], with 49 qbits; Bristlecone [8], from Google, with 72 qbits, which follows the physics of Google's previous 9 qbits linear array technology; 127-qbit quantum processor IBM Eagle [9]; or, from the University of Science and Technology of China (USTC), we find photonic quantum processor Jiuzhang [10], which reached quantum advantage by implementing gaussian boson sampling on 76 photons; later with Jiuzhang 2.0 [11] achieving 66 qbits, in which gaussian boson sampling is implemented to detect 113 photons from a 144-mode optical interferometer; or superconducting quantum processor Zuchongzi, with a system scale of up to 60 qbits [12], among others. We are nevertheless on the NISQ (noisy intermediate-scale quantum) era [13], in which one of the goals of the scientific community is to find algorithms which are realistic and show quantum advantage over classical schemes (the often called quantum supremacy [14] in some contexts), as well as to achieve experimental practicability. See, for instance, the paper [15] as a relevant step towards quantum advantage in training deep generative models by using quantum annealers.

Our main objects of analysis, algorithms, can be briefly defined as recipes for performing specific tasks, with its corresponding degree of complexity. Historically and formally, one of the fundamental models for them are the so-called Turing machines, due to Alan M. Turing, who proposed the famous question *Can Machines Think?* in his famous paper [16]. Some years before, in 1936, he published [17], responding the 1900 Hilbert problems. In such a paper he described the well known *universal computing machines*, later known as the aforementioned Turing machines. In 1980, P. Benioff [18] used Turing's work to analyze the theoretical feasibility of quantum computing. In the cited paper, we find the first attempt to demonstrate that reversible nature of quantum computing, as long as dissipated energy is arbitrarily small, is possible. In 1982, R. Feynman [19] proved that quantum mechanics cannot be simulated on classical computers. Soon after that, D. Deutsch [20] described a quantum Turing machine and created an algorithm thought to run on a quantum computer. Furthermore, it is reasonable to locate one of the main turning points of quantum computing history, as we know it today, in 1994, when Peter Shor provided an efficient quantum algorithm for primes factorization [21]. One year later, C. Monroe and D. Wineland, among others, published a work [22] which marked the first demostration of a quantum logic gate, namely the two-qbit *controlled-NOT* or *CNOT*. In 1996, L. Grover had a great contribution to the sub-field of search problems, with the design of the so-called *Grover's algorithm* [23]. In fact, after such a publication, a remarkable interest in fabricating a quantum computer was put into motion.

From all this background, quantum computing has matured, namely its sub-field of quantum algorithms, with direct applications in simulation, optimization and search, machine learning, and cryptography (see overview from [24]). For instance, today's algorithms have reached a high degree of implementation in the study of statics and dynamics of chemical and physical systems, e.g. by obtaining molecular energies via quantum phase estimation on a quantum computer [25], or through the construction of electronic Hamiltonians [26]. On the other hand, the field of machine learning has found a great advantage within the quantum algorithms, either supervised (e.g., quantum Kernel estimation [27], or supervised quantum learning without measurements [28]), unsupervised (e.g., for clustering [29] [30] or generative modelling [31]), reinforcement learning (e.g., Markov decision process [32]), or genetic algorithms [33]. With regard to statistical learning theory and quantum computing, there have been also remarkable advances in hybrid quantum-classical algorithms, such as quantum-assisted machine learning in near-term quantum computers [34], or generative modelling approachs [35]. Furthermore, we find relevant applications in singular value decomposition [36], or linear system solving [37]. In [38] and [39], deeper reviews of quantum algorithms and its applications are presented.

However, there is a need of realization and interpretation of new algorithms that provide new points of view, or even new algorithmic structures, for well-known physical systems whose dynamics, in or out of equilibrium, yields interesting properties, and from which new applications can be developed. In this context, we focus on quantum many-body physical algorithms, namely in open systems; and our goal is to provide a new and feasible algorithm which could be included in the aforementioned list [38].

Our approach links to a family of quantum algorithms based on the evolution in imaginary time. Imaginary time evolution is a powerful tool to study numerous systems, in particular quantum systems. In turn, in the context of quantum systems, it has been used to study finite temperature properties and dissipative dynamics [40, 41, 42], finding the ground state wavefunction [43], and for real time dynamics [44, 45]. On the other hand, it is a well known issue in quantum algorithms that only unitary operators can be implemented as quantum gates [46]. Once said that, note that for a quantum system with propagator $U_t = \exp[-iHt/\hbar]$ the corresponding propagator in imaginary time, $\tau = it$, is $U_\tau = \exp[-H\tau/\hbar]$. While the first one is unitary, the second one is not. As we have just pointed out, since the latter is non-unitary, it cannot be written in terms of unitary gates, and thus directly realized with a quantum circuit (see some strategies, like hybrid classical-quantum, e.g. [48, 47, 49, 50, 51, 53, 52, 54, 55]; and see also [56]). One option would be then to consider that the evolution takes place in imaginary time, and use the results for the dissipative system. This is not the path we follow in the rest of this work given that, instead, we will pursue to use quantum kinetic Ising models as in [57], as we discuss below.

On the other hand, our algorithm also links to a family of procedures related to the diagonalization of standard strongly correlated Hamiltonians, departing from previous works mainly related to Ising Hamiltonians [58] [59], in order to give a quantum extension, in terms of density matrices [57], of such a diagonalization setting. Here is where a relevant mathematical object, essential in our work, shows up: quantum Master's equation. This is the approach we study in this work.

As a central element of our study, Master equations are mathematical tools used to study out-of-equilibrium dynamics of stochastic systems [60]. They fulfill the so-called detailed balance condition, which provides us with a specific symmetry in terms of the transition probabilities of the corresponding states in the corresponding lattice sites. A traditional approach has been to write its quantum counterpart, known as quantum Master equations [61] [62], and to use them to study Markovian dynamics of open systems, mainly, in two directions: to model actual quantum systems; and as a trick to solve the associated classical out-of-equilibrium dynamics. Such quantum Master equations have turned into a guideline for the design of new open systems for quantum simulations and quantum state engineering. See [57] as an example.

In terms of implementation, we provide a simulation scheme of one-dimensional antiferromagnetic Ising model with transverse external magnetic field, providing a quantum circuit which performs Hamiltonian diagonalization based on [58]. Furthermore, we carry out the analytical development that drives us to diagonalization implementation from [58] or [59], but adapted to the scenario of Glauber Master equation [63]. With those objectives in mind and before implementation, we firstly focus the diagonalization approach on the classical 1D Glauber model, and then we extend it through [57], in order to provide the quantum simulation with the Master operator that results from one-dimensional Glauber's formulation and its density matrix version. In other words, we look for the quantum gates that disentangle Ising Hamiltonian from [59] and [58], Glauber Master operator from [63] and [64], and Master operator, extended through density matrices, from [57], finding at the end the whole energies spectra.

All in all, we have two objectives: on the one hand, to implement in a quantum algorithm two possible ways of diagonalizing an Ising Hamiltonian with two different contexts (with external magnetic field, like in [58], and with thermal out-of-equilibrium dynamics, like in [64]); and, on the other hand, to explore to which extent we are capable of using the aforementioned quantum kinetic model, with its corresponding algorithm, to solve out-of-equilibrium complex problems within a context of classical dynamics. This last point is the one which we intend to include in the list of NISQ algorithms implemented with current quantum computers.

The structure of the present work goes as follows: in section 2, we formulate 1D Glauber-Ising model, departing from the original formulation from Glauber [63] and considering later Pauli matrices algebra, in order to provide, in next subsections, an analytical diagonalization which drives us to a interpretation of the system states through fermionic occupation in the corresponding momentum modes, once we reached the diagonalized Hamiltonian; in section 3, with a similar approach with regard to the diagonalization procedure, we apply the extension of the previous model towards the description in terms of density matrices using a Lindblad formulation, so that we do not only study populations of the quantum system but also coherences; section 4 is devoted to the implementation of the diagonalization quantum circuit and the analysis of simulation results, with the focus on the Ising model from [58], in which external magnetic field is considered; and section 5 consists of a summary of the conclusions and the outlook from our work. At the end of the document, there are several appendices which include computations from the aforementioned analytical diagonalizations, quantum gates decomposition for the implemented quantum circuit, and a final appendix in which some relevant codes of our simulations and calculations are exposed.

We must mention that the present approach, as pointed out in [59], can be interpreted as an extension of the renormalization group method given by Wilson in 1975 [65]. In such an approach, simple effective Hamiltonians describing low energy states from a given model are obtained through several transformations in which high energy states are removed. In our case, on the other hand, we aim to find a unitary operator which transforms a given Hamiltonian into a diagonalized or non-interacting Hamiltonian, and from it we obtain the whole desired spectrum. As it is said in [59], with the approach we propose here:

(...) We do not loose the physics of the high energy modes in the way; (...) it can be implemented experimentally. Of course, our method only works exactly for the small set of integrable problems, but very similar approximate transformations can in principle be found for any system whose effective low energy physics is well described by quasi-particles.

More generally, strongly correlated quantum many-body systems in the context of quantum simulation are nowadays deeply studied since it is not hard to find immediate and practical benefit from it: finding the whole spectrum of certain correlated many-body models let us study arbitrary thermal states, at any temperature, as well as the dynamics of such states at any time instant. That is, it has physical relevance in its own right. Therefore, finding the quantum circuit which transforms the original Hamiltonian into a diagonalized Hamiltonian with non-interacting terms will lead us to such a desired situation in which we know the entire energy spectrum, in rather simple computational terms. We find references looking for this scheme with the transverse Ising model [58], as well as the Kitaev's Hamiltonian on the honey-comb lattices and the Hamiltonians corresponding to stabilizer states [59], among others. We go further, and extend their studies to non-equilibrium states, through the corresponding one-dimensional Glauber Master equation.

2 One-dimensional Glauber-Ising model

In this section we review the kinetic Ising model or Glauber-Ising model, following closely R. Glauber's seminal paper [63]. For that reason, let us consider a set of N particles arranged in a regularly spaced one dimensional array with periodic boundary conditions (PBC), i.e., an N-particle ring. We can assume that each i-th particle interacts with a reservoir at temperature T which causes its spin to flip randomly between two values, $\sigma_i = \pm 1$, at a known constant rate. Also it has a tendency to align with its neighbors. That is, each variable with two values, at each site i, is not statistically independent from the neighbors. This can be done assuming that the transition probabilities of the individual spins depend on the values of its neighbors spins, as we shall see below.

There are 2^N possible configurations of the system, $\sigma = (\sigma_1, \ldots, \sigma_N)$. Let us call $P(\sigma, t)$ the probability to find the system in configuration σ at time t. Let us call $\omega_i(\sigma_i)$ or $\omega_i(\sigma)$ the rate (probability per unit time) that spin i-th flips from ± 1 to ∓ 1 while the rest are fixed. Glauber dynamics only consider one-spin flip at a time. There are generalizations which consider multiple spin flips, but which we do not consider here. Anyhow, it will be interesting for future research, see e.g. [66] [67] [68]. To avoid misunderstanding, we emphasize already here that we are still not using Pauli matrices representation, but later on we will use the z-Pauli matrix as that which has as eigenvectors spin up or down, and x-Pauli matrix the one that flips from one to the other.

Only from considerations of stochastic processes, for this system one can write the Master equation for the evolution of the probability of the system to be at configuration σ at time t, $P(\sigma, t)$, as

$$\frac{d}{dt}P(\sigma, t) = -\left[\sum_i \omega_i(\sigma_i)\right] P(\sigma, t) + \sum_i \omega_i(-\sigma_i) P(\sigma_1, \ldots, -\sigma_i, \ldots, \sigma_N, t). \tag{2.1}$$

The assumption introduced above, i.e., that the spins have a tendency to align, is accomodated if the transitions rates are

$$\omega_i(\sigma_i) = \frac{1}{2}\alpha \left[1 - \frac{1}{2}\gamma\sigma_i(\sigma_{i-1} + \sigma_{i+1})\right]. \tag{2.2}$$

Then, this gives $\omega_i(\sigma_i) = \alpha/2$ if the neighbors are antiparallel, $\omega_i(\sigma_i) = \alpha(1-\gamma)/2$ if the neighbors are parallel and σ_i parallel to them two, and $\omega_i(\sigma_i) = \alpha(1+\gamma)/2$ if the neighbors are parallel and σ_i antiparallel to them two. For γ positive, parallel neighbors configurations, in turn antiparallel to σ_i, favour spin flips at i-th site. Here, α only gives a time scale.

The original classical Lenz-Ising Hamiltonian is [69, 70]:

$$H(\sigma) = -J\sum_{i=1}^{N} \sigma_i\sigma_{i+1}, \tag{2.3}$$

where J is an interaction parameter, which can be positive or negative. Notice that $H(\sigma)$ is simply a function which takes different values for each configuration, depending on such a parameter J. So far, σ_i are the same variables introduced above, i.e., components of a vector describing a N spins 1/2 ring.

As described in [63], one can establish a relationship between the dynamics described up to know and the Ising model in the following way. The equilibrium probabilities for the Ising model, when in contact with a large reservoir a temperature T, are given by the Maxwell-Boltzman distribution

$$P_{\text{eq}}(\sigma) = \exp[-H(\sigma)/kT]/Z_N(\beta), \tag{2.4}$$

with k Boltzman constant, $\beta = 1/kT$, and $Z_N(\beta)$ the partition function, given by

$$Z_N(\beta) = \sum_\sigma \exp[-H(\sigma)/kT]. \tag{2.5}$$

Now, we impose that the equilibrium final state is that given by the Ising model in equilibrium with a reservoir at temperature T. That justifies that such equilibrium final states in the studied Ising model are states $P_{\text{eq}}(\sigma)$ given in (2.4).

The equilibrium for the Glauber dynamics described by the Master equation (2.1) requires by definition that $\frac{d}{dt}P(\sigma,t)=0$. This implies that

$$P_{\text{eq}}(\sigma_1,\dots,-\sigma_i,\dots,\sigma_N)\omega(-\sigma_i)=P_{\text{eq}}(\sigma_1,\dots,\sigma_i,\dots,\sigma_N)\omega(\sigma_i), \tag{2.6}$$

or

$$\frac{P_{\text{eq}}(\sigma_1,\dots,-\sigma_i,\dots,\sigma_N)}{P_{\text{eq}}(\sigma_1,\dots,\sigma_i,\dots,\sigma_N)}=\frac{\omega(\sigma_i)}{\omega(-\sigma_i)}=\frac{1-\frac{1}{2}\gamma\sigma_i(\sigma_{i-1}+\sigma_{i+1})}{1+\frac{1}{2}\gamma\sigma_i(\sigma_{i-1}+\sigma_{i+1})}, \tag{2.7}$$

where we used (2.2). This is the detailed balance condition (DBC) in this system, which is central for out-of-equilibrium dynamics. On the other hand, note that ratios of probabilities of equilibrium configurations which differ only in one spin are

$$\frac{P_{\text{eq}}(\sigma_1,\dots,-\sigma_i,\dots,\sigma_N)}{P_{\text{eq}}(\sigma_1,\dots,\sigma_i,\dots,\sigma_N)}=\frac{\exp[-(J/kT)\sigma_i(\sigma_{i-1}+\sigma_{i+1})]}{\exp[(J/kT)\sigma_i(\sigma_{i-1}+\sigma_{i+1})]}. \tag{2.8}$$

Let us use that $\exp[\pm x]=\cosh(x)\pm\sinh(x)$ to write

$$\exp[\pm(J/kT)\sigma_i(\sigma_{i-1}+\sigma_{i+1})]=\cosh((J/kT)(\sigma_{i-1}+\sigma_{i+1}))\pm\sigma_i\sinh((J/kT)(\sigma_{i-1}+\sigma_{i+1})), \tag{2.9}$$

where we have taken into account that $\cosh(-x)=\cosh(x)$ and that $\sinh(-x)=-\sinh(x)$ for any $x\in\mathbb{C}$, and then, if σ_i is negative ($\sigma_i=-1$) the sign of the sinh has to change, while if it is possitive it does not change. Thus, we can write:

$$\exp[\pm(J/kT)\sigma_i(\sigma_{i-1}+\sigma_{i+1})]=\cosh((J/kT)(\sigma_{i-1}+\sigma_{i+1}))[1\pm\frac{1}{2}\sigma_i(\sigma_{i-1}+\sigma_{i+1})\tanh(J/kT)], \tag{2.10}$$

after noticing that $\sigma_{i-1}+\sigma_{i+1}$ can only be $+2$, -2 or 0, and using that $\tanh(-x)=-\tanh(x)$. To get the correspondence between the dynamics as described by Glauber and the equilibrium described by the Lenz-Ising model, it suffices to substitue expression (2.10) in (2.8), and take into consideration (2.7). Therefore, one should take $\gamma=\tanh(2J/kT)=\tanh(2\beta J)$ [63]. With all this we have established the relation between J, temperature T, and parameter γ, by just identifying gamma with the other two. To sum up, transition rates, and therefore the whole model, depend on parameters T and J through γ.

A note on following steps: Now we will consider equation (2.1) as an equation of motion. Before this we note the following: the diffusion equation which describes for example the probability density function associated with the position $\mathbf{x}$ of a single particle at time t is

$$\frac{\partial P(\mathbf{x},t)}{\partial t}=D\nabla^2P(\mathbf{x},t), \tag{2.11}$$

with D the diffusion constant and ∇^2 the Laplacian differential operator. This is a parabolic partial differential equation, similar to the heat equation. On the other hand, the Schrödinger equation for the wave function ψ can be written as

$$\frac{\partial\psi(\mathbf{x},t)}{\partial t}=\frac{i\hbar}{2M}\nabla^2\psi(\mathbf{x},t). \tag{2.12}$$

There is a well known and old formal analogy between both equations, with the identification $P\to\psi$ and $D\to\frac{i\hbar}{2M}$. Note that one can also observe this analogy $D\to\frac{\hbar}{2M}$ and $t\to it$, that is, the evolution occurs in imaginary time. As pointed out before, we do not follow this approach in the present work.

2.1 Kinetic Ising model

During this subsection, all considerations are made in a classical context, following [64]. In next section we will discuss a quantum Master equation which generalizes the classical kinetic models. Particularly they will have as stationary states the thermal (Boltzmann-Gibbs) states of the related classical model. These states are of the form

$$|\psi\rangle = \sum_{\sigma} P_{\text{eq}}(\sigma)|\sigma\rangle = \frac{1}{\mathcal{Z}} \sum_{\sigma} \exp[-\beta H(\sigma)]|\sigma\rangle, \tag{2.13}$$

with $|\sigma\rangle$ stands for a vector in the Hilbert space representing the configuration of N spins, $\sigma = (\sigma_1, \sigma_2, \cdots, \sigma_N)$. Here $H(\sigma)$ is the Ising (classical) Hamiltonian. These states are associated to a classical Kinetic Ising model, and describe the approach to a thermal equilibrium state obeying detailed balance, see equation (2.7).

Let us now rewrite the Master equation, equation (2.1), as a Schrödinger equation. To this end we write $P(\sigma, t) = \sqrt{P_{\text{eq}}(\sigma)}\phi(\sigma, t)$. Then equation (2.1) can be written as

$$\dot{\phi}(\sigma, t) = \sum_{i} P_{\text{eq}}(\sigma_i)^{-1/2}\omega(-\sigma_i)P_{\text{eq}}(-\sigma_i)^{1/2}\phi(-\sigma_i, t) - \omega(\sigma_i)\phi(\sigma_i, t). \tag{2.14}$$

We need then to compute, for an arbitrary $i \in \{1, \ldots, N\}$, the expression

$$\begin{aligned} P_{\text{eq}}(\sigma_i)^{-1/2}\omega(-\sigma_i)P_{\text{eq}}(-\sigma_i)^{1/2} &= \left[\frac{\exp(\beta J\sigma_i(\sigma_{i-1} + \sigma_{i+1}))}{Z_N(\beta)}\right]^{-1/2} \\ &\times \frac{\alpha}{2}(1 + \frac{\gamma}{2}\sigma_i(\sigma_{i-1} + \sigma_{i+1})) \left[\frac{\exp(-\beta J\sigma_i(\sigma_{i-1} + \sigma_{i+1}))}{Z_N(\beta)}\right]^{1/2}. \end{aligned} \tag{2.15}$$

Observe that, as discussed above,

$$\exp(\pm\beta J\sigma_i(\sigma_{i-1} + \sigma_{i+1})) = \cosh(\beta J(\sigma_{i-1} + \sigma_{i+1})) \pm \sigma_i \sinh(\beta J(\sigma_{i-1} + \sigma_{i+1})) \tag{2.16}$$

$$= \cosh(\beta J(\sigma_{i-1} + \sigma_{i+1}))[1 \pm \sigma_i \tanh(\beta J(\sigma_{i-1} + \sigma_{i+1}))], \tag{2.17}$$

where

$$1 \pm \sigma_i \tanh(\beta J(\sigma_{i-1} + \sigma_{i+1})) = 1 \pm \sigma_i \left(\frac{\sigma_{i-1} + \sigma_{i+1}}{2}\right) \tanh(2\beta J) = 1 \pm \frac{\gamma}{2}\sigma_i(\sigma_{i-1} + \sigma_{i+1}), \tag{2.18}$$

where we have used that $\gamma = \tanh(2\beta J)$. Therefore, from (2.15), we obtain that

$$P_{\text{eq}}(\sigma_i)^{-1/2}\omega(-\sigma_i)P_{\text{eq}}(-\sigma_i)^{1/2} = \frac{\alpha}{2}(1 - \frac{\gamma}{2}\sigma_i(\sigma_{i-1} + \sigma_{i+1}))^{1/2}(1 + \frac{\gamma}{2}\sigma_i(\sigma_{i-1} + \sigma_{i+1}))^{1/2} \tag{2.19}$$

$$\begin{aligned} &= \frac{\alpha}{2}\sqrt{1 - \frac{\gamma^2}{4}\sigma_i^2(\sigma_{i-1} + \sigma_{i+1})(\sigma_{i-1} + \sigma_{i+1})} = \frac{\alpha}{2}\sqrt{1 - \frac{\gamma^2}{4}(2 + 2\sigma_{i-1}\sigma_{i+1})} \\ &= \begin{cases} \frac{\alpha}{2} & if \quad \sigma_{i-1} = -\sigma_{i+1} \\ \frac{\alpha}{2}\sqrt{1 - \gamma^2} & if \quad \sigma_{i-1} = \sigma_{i+1}. \end{cases} \end{aligned} \tag{2.20}$$

Note that, since $\gamma = \tanh(2\beta J)$, and $\text{sech}^2(x) + \tanh^2(x) = 1$ for any $x \in \mathbb{R}$, we have that $\sqrt{1 - \gamma^2} = \text{sech}(2\beta J)$, just for not losing what are the involved constants about. For this reason, if we define the system constants

$$A = A(\gamma) = \frac{\sqrt{1 - \gamma^2} + 1}{2}, \quad B = B(\gamma) = 1 - A(\gamma), \tag{2.21}$$

thus, we can write Master's operator as

$$W_\beta = \frac{\alpha}{2}\sum_{i=1}^{N}\{[A - B\sigma_{i-1}\sigma_{i+1}]\sigma_i^x - [1-\frac{\gamma}{2}\sigma_i(\sigma_{i-1}+\sigma_{i+1})]\} = \frac{\alpha}{2}\sum_{i=1}^{N} W_{i,\beta}(\sigma), \tag{2.22}$$

where we included a σ_i^x in the first terms since (2.14) is described in terms of $\phi(-\sigma_i, t)$ with regard to such first term. At this point, such σ_i^x only means flipping from σ_i to $-\sigma_i$, and later, when entering quantum context, this reading will be natural in terms of the corresponding Pauli matrices. This Master operator can be understood as a *classical* Hamiltonian (σ^x and σ^z are not yet taken as Pauli matrices, where used notation so far for σ^z omits its superindex unless it is confusing), in which we already considered the symmetry given by the Detailed Balance condition. All in all, it yields the equation:

$$\dot{\phi}(\sigma, t) = W_\beta\phi(\sigma, t). \tag{2.23}$$

Notice that, according to this equation (2.23), diagonalization of this Hamiltonian is equivalent to solving the Master equation.

2.2 Analytical diagonalization of 1D Glauber's Master operator

The full diagonalization of the Ising Hamiltonian is possible. This was first introduced by B. U. Felderhof, and it is an important success on condensed matter physics. For that reason and for its usefulness in our approach, here we review such results from [64]. Moreover, we are also guided by work [71], in which practical techniques about diagonalizations of this kind are given.

In order to perform the desired diagonalization of W_β, we get into a quantum context. In other words, from now, σ_i^j in each lattice site i will be the corresponding j-Pauli matrix, for $j \in \{x, y, z\}$. We carry out such a diagonalization in three phases: Jordan-Wigner transformation to transform ladder Pauli operators into fermionic operators, Fourier transform to get into momentum space, and Bogoliubov rotation between opposite momenta operators in order to give a fully diagonalized Master operator.

2.2.1 Jordan-Wigner tranformation

Before proceeding, we express (2.22) in terms of raising and lowering spin-1/2 operators. Such raising and lowering spin operators at site j are

$$\sigma_j^\pm = \frac{\sigma_j^y \pm i\sigma_j^z}{2}, \tag{2.24}$$

from which

$$\sigma_j^y = \sigma_j^+ + \sigma_j^-, \quad \sigma_j^z = -i(\sigma_j^+ - \sigma_j^-), \tag{2.25}$$

$$\sigma_j^-\sigma_j^+ = \frac{1}{4}((\sigma_j^z)^2 + (\sigma_j^y)^2 + i[\sigma_j^y, \sigma_j^z]) = \frac{1}{4}(1 + 1 + i(2i)\sigma_j^x) = \frac{1}{2} - \frac{1}{2}\sigma_j^x \Longrightarrow \sigma_j^x = 1 - 2\sigma_j^-\sigma_j^+, \tag{2.26}$$

where we denote 1 as the identity operator (and we will use this notation, unless it is confusing), and where we used the well-known Pauli matrices commutation relation $[\sigma_j^y, \sigma_j^z] = 2i\sigma_j^x$. Note that, from this definition of ladder operators (2.24) before Jordan-Wigner transformation, the physical meaning is not standard: $\sigma_j^\pm$ refers to raising and lowering core boson modes (see [71] to get deep in such a nomenclature) in lattice site j, in X-spin direction.

Thus, we can now express (2.22) in terms of σ_j^+ and σ_j^-:

$$W_\beta = \frac{\alpha}{2}\sum_{j=1}^{N}\{A(1-2\sigma_j^-\sigma_j^+) + B(\sigma_{j-1}^+ - \sigma_{j-1}^-)(\sigma_{j+1}^+ - \sigma_{j+1}^-)(1-2\sigma_j^-\sigma_j^+)$$
$$-(1+\frac{\gamma}{2}(\sigma_j^+ - \sigma_j^-)(\sigma_{j+1}^+ + \sigma_{j-1}^+ - \sigma_{j+1}^- - \sigma_{j-1}^-))\}. \quad (2.27)$$

Now, we express Jordan-Wigner (JW) transformation, which establishes a direct link between spin-1/2 σ_j^+,σ_j^- and fermionic $c_j^\dagger$,c_j raising and lowering operators (once clarified Jordan-Wigner formulation we are using from [64], remaining calculations are standard JW computations):

$$c_j = -iK_j\sigma_j^+, \quad c_j^\dagger = iK_j\sigma_j^-, \quad (2.28)$$

where

$$K_j = \exp\left(i\pi\sum_{s=1}^{j-1}\sigma_s^-\sigma_s^+\right), \quad K_j^\dagger = \exp\left(-i\pi\sum_{s=1}^{j-1}\sigma_s^-\sigma_s^+\right) = K_j. \quad (2.29)$$

Last equality in (2.29) follows directly from operator K_j definition. Indeed,

$$K_j = K_j^\dagger \iff \exp\left(i\pi\sum_{s=1}^{j-1}\sigma_s^-\sigma_s^+\right)\exp\left(-i\pi(\sum_{s=1}^{j-1}\sigma_s^-\sigma_s^+)^\dagger\right) = 1$$
$$\iff \exp\left(i\pi\sum_{s=1}^{j-1}\sigma_s^-\sigma_s^+\right)\exp\left(i\pi\sum_{s=1}^{j-1}\sigma_s^-\sigma_s^+\right) = 1, \quad (2.30)$$

where we have used that $(\sigma_s^+)^\dagger = \sigma_s^-$ and $(\sigma_s^-)^\dagger = \sigma_s^+$ for any $s \in \{1,\ldots,N\}$. Moreover, last equality in (2.30) is straightforward. Some useful relations from (2.28) are:

1. Simplification of K_j operator in terms of n_s operators. Since $[n_i, n_k] = 0$ for any $i,k \in \{1,\ldots,N\}$, $i \neq k$; and $n_s^m = n_s$ for any $m \in \mathbb{N}$, it follows that

$$K_j = \prod_{s=1}^{j-1}\exp(i\pi\sigma_s^-\sigma_s^+) = \prod_{s=1}^{j-1}\sum_{m=0}^{\infty}\frac{(i\pi)^m}{m!}n_s^m = \prod_{s=1}^{j-1}\left[1+\left(\sum_{m=1}^{\infty}\frac{(i\pi)^m}{m!}\right)n_s\right] \quad (2.31)$$
$$= \prod_{s=1}^{j-1}[1+(e^{i\pi}-1)n_s] = \prod_{s=1}^{j-1}[1-2n_s]. \quad (2.32)$$

2. $\sigma_j^+ = iK_jc_j$ and $\sigma_j^- = -iK_jc_j^\dagger$ for any $j \in \{1,\ldots,N\}$. It is important to notice that $K_j = K_j^\dagger = K_j^{-1}$.

3. Occupation number operators are invariant against JW tranformation:

$$\sigma_j^-\sigma_j^+ = c_j^\dagger(K_j^\dagger K_j)c_j = c_j^\dagger c_j = n_j, \quad j \in \{1,\ldots,N\}. \quad (2.33)$$

Observe that, from PBC on $\sigma_j^\pm$'s, it follows PBC on c_j's. Moreover, from a general perspective of our setting, JW transformation procedure lies on the fact that, to pass from a tensor product of Hilbert spaces in terms of spin-1/2 states in each of them, to spinless fermion states which describe fermionic occupation, in one dimension we only need to have parity considerations, that is, we only need to take into account the lattice site of the corresponding fermionic spinless operator with respect to the origin lattice site, and regarding that fact, we must add the corresponding sign if necessary.

Moreover, it is relevant to express anti-commutation relations of fermionic raising and lowering operators, in order to use them in computations below:

$$\{c_i, c_{i'}\} = 0, \quad \{c_i^\dagger, c_{i'}^\dagger\} = 0, \quad \{c_i^\dagger, c_{i'}\} = \delta_{i,i'}, \quad i \in \{1, \dots, N\} \tag{2.34}$$

All in all, applying computations carried out in appendix (A) in terms of fermionic operators, we can express operator (2.27) in a way such that

$$W_\beta = \frac{\alpha}{2}\sum_{j=1}^{N} W_{j,\beta} = \frac{\alpha}{2}\sum_{j=1}^{N}\{A(1-2c_j^\dagger c_j) - B(c_{j-1}^\dagger - c_{j-1})(c_{j+1}^\dagger + c_{j+1}) - 1 + \gamma(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1})\}. \tag{2.35}$$

Now, we make boundary conditions considerations. Assume, by now, that N could be even or odd, and that boundary conditions are periodic. Therefore,

$$\begin{aligned}
&\sigma_N\sigma_{N+1} = \sigma_N\sigma_1 = -(\sigma_N^+ - \sigma_N^-)(\sigma_1^+ - \sigma_1^-) = -\sigma_N^+\sigma_1^+ + \sigma_N^+\sigma_1^- + \sigma_N^-\sigma_1^+ - \sigma_N^-\sigma_1^- \\
&= K_N[c_Nc_1 + c_Nc_1^\dagger + c_N^\dagger c_1 + c_N^\dagger c_1^\dagger] = -(-1)^{\mathcal{N}}[-c_Nc_1 - c_Nc_1^\dagger + c_N^\dagger c_1 + c_N^\dagger c_1^\dagger] \\
&= -(-1)^{\mathcal{N}}(c_N^\dagger - c_N)(c_1^\dagger + c_1),
\end{aligned} \tag{2.36}$$

where $\mathcal{N} = \sum_{j=1}^{N} c_j^\dagger c_j$ is the total fermionic number operator, and where we took into account properties such that

$$\begin{aligned}
&\sigma_N^+\sigma_1^+ = i^2K_Nc_Nc_1 = -K_Nc_Nc_1, \quad \sigma_N^+\sigma_1^- = -i^2K_Nc_Nc_1^\dagger = K_Nc_Nc_1^\dagger, \\
&K_Nc_N = \exp\left(i\pi\sum_{s=1}^{N-1}c_s^\dagger c_s\right)c_N = \exp\left(i\pi\sum_{s=1}^{N}c_s^\dagger c_s\right)c_N = (-1)^{\mathcal{N}}c_N, \\
&K_Nc_N^\dagger = \exp\left(i\pi\sum_{s=1}^{N-1}c_s^\dagger c_s\right)c_N^\dagger = -\exp\left(i\pi\sum_{s=1}^{N}c_s^\dagger c_s\right)c_N^\dagger = -(-1)^{\mathcal{N}}c_N^\dagger,
\end{aligned} \tag{2.37}$$

and relations (2.26). Similarly,

$$\begin{aligned}
&\sigma_{N-1}\sigma_{N+1} = \sigma_{N-1}\sigma_1 = -(\sigma_{N-1}^+ - \sigma_{N-1}^-)(\sigma_1^+ - \sigma_1^-) = -\sigma_{N-1}^+\sigma_1^+ + \sigma_{N-1}^+\sigma_1^- + \sigma_{N-1}^-\sigma_1^+ - \sigma_{N-1}^-\sigma_1^- \\
&= K_{N-1}[c_{N-1}^\dagger c_1^\dagger + c_{N-1}^\dagger c_1 + c_{N-1}c_1^\dagger + c_{N-1}c_1] = -K_N[c_{N-1}^\dagger c_1^\dagger + c_{N-1}^\dagger c_1 - c_{N-1}c_1^\dagger - c_{N-1}c_1] \\
&\Longrightarrow \sigma_{N-1}\sigma_N^x\sigma_{N+1} = -K_N(1-2c_N^\dagger c_N)(c_{N-1}^\dagger - c_{N-1})(c_1^\dagger + c_1) \\
&= -(-1)^{\mathcal{N}}(c_{N-1}^\dagger - c_{N-1})(c_1^\dagger + c_1),
\end{aligned} \tag{2.38}$$

where we used that $K_{N-1}c_{N-1}$ remains the same, that

$$K_{N-1}c_{N-1}^\dagger = -K_Nc_{N-1}^\dagger, \tag{2.39}$$

and the corresponding relation in (2.26) for σ_N^x. In a very similar way, we obtain

$$\sigma_N\sigma_1^x\sigma_2 = -(-1)^{\mathcal{N}}(c_N^\dagger - c_N)(c_2^\dagger - c_2), \tag{2.40}$$

where factor $1-2c_1^\dagger c_1$ disappearing through $(1-2c_1^\dagger c_1)^2 = 1$ from K_NK_2 in $\sigma_N\sigma_2$, reappears when considering σ_1^x, which is equal to $1-2c_1^\dagger c_1$. Then, master's operator turns into

$$\begin{aligned}
W_\beta &= \frac{\alpha}{2}\sum_{j=2}^{N-1}\{A(1-2c_j^\dagger c_j) - B(c_{j-1}^\dagger - c_{j-1})(c_{j+1}^\dagger + c_{j+1}) - 1 + \gamma(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1})\} \\
&+ \alpha A(1 - c_1^\dagger c_1 - c_N^\dagger c_N) - \alpha - \gamma\frac{\alpha}{2}(-1)^{\mathcal{N}}(c_N^\dagger - c_N)(c_1^\dagger + c_1) + \frac{\alpha}{2}B(-1)^{\mathcal{N}}(c_{N-1}^\dagger - c_{N-1})(c_1^\dagger + c_1) \\
&+ \frac{\alpha}{2}B(-1)^{\mathcal{N}}(c_N^\dagger - c_N)(c_2^\dagger + c_2) + \gamma\frac{\alpha}{2}(c_1^\dagger - c_1)(c_2^\dagger + c_2).
\end{aligned} \tag{2.41}$$

All in all, with this periodic boundary considerations, if we define, when $\mathcal{N}$ is an even operator

$$c_{N+1} = -c_1, \quad c_{N+2} = -c_2; \tag{2.42}$$

and, when $\mathcal{N}$ is odd,

$$c_{N+1} = c_1, \quad c_{N+2} = c_2; \tag{2.43}$$

therefore, we can express W_β as in (2.35), taking into consideration that the fact that $\mathcal{N}$ is an even or an odd operator determines c_{N+1} and c_{N+2}. Generalizing these statements, for an arbitrary $k \in \{1, \dots, N\}$, we will consider W_β as in (2.35) by considering

$$c_{N+k} = -c_k, \tag{2.44}$$

when $\mathcal{N}$ is an even operator; and

$$c_{N+k} = c_k, \tag{2.45}$$

when $\mathcal{N}$ is odd.

2.2.2 Fourier Transform

In order to continue with our diagonalization process of Master's operator (2.22), we pass our fermionic operators c_j to momentum space, denoting the new operators d_k, with adjoint counterparts $d_k^\dagger$. We assume that the number of spins N is even. Otherwise, when labelling momentum space fermionic operators, we must take a different range of values depending on N. Their inverse version, to directly make substitutions in (2.35), are

$$c_j = \frac{1}{\sqrt{N}} \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} e^{ijk} d_k, \quad c_j^\dagger = \frac{1}{\sqrt{N}} \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-ijk} d_k^\dagger, \quad j = 1, \dots, N. \tag{2.46}$$

If we assume periodic boundary conditions, we should take into account that, for any $j \in \{1, \dots, N\}$,

$$c_j = c_{N+j} \Longrightarrow \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} e^{ikj} d_k = \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} e^{ik(N+j)} d_k \Longrightarrow e^{ikN} = 1. \tag{2.47}$$

This implies that $k = 2\pi l/N$, for $l \in \{-N/2+1, \dots, N/2\}$, so $k = 0, \pm 2\pi/N, \pm 4\pi/N, \dots$ This consideration let us consider the same PBC on fermionic momentum-space operators, i.e., $d_{j+N} = d_j$ for any $j \in \{1, \dots, N\}$.
On the other hand, and just as a remark since so far **we are considering PBC**, if we assume antiperiodic boundary conditions (ABC), we would have, for any $j \in \{1, \dots, N\}$,

$$c_j = -c_{N+j} \Longrightarrow \sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} e^{ikj} d_k = -\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} e^{ik(N+j)} d_k \Longrightarrow e^{ikN} = -1, \tag{2.48}$$

that is, $k = (2l+1)\pi/N$, for $l \in \{-N/2+1, \dots, N/2\}$, so $k = \pm\pi/N, \pm 3\pi/N, \dots$

Then, we proceed with the computations on product terms in (2.35). For these calculations, we use that

$$\sum_{j=1}^{N} e^{ij(p-l)} = N\delta_{l,p}, \tag{2.49}$$

where $\delta_{l,p}$ is the Kronecker's Delta function. Exact computations of this transformation are included in appendix (B), where we have used the core equality (2.49). We define l-dependent constants $C_l = 2[-A - B\cos(2l) + \gamma\cos(l)]$, $D_l = Be^{2il} + \gamma e^{-il}$, and $E_l = A - 1 - 2\gamma\cos(l)$, for $l = 2\pi k/N$, $k \in \{-N/2+1, \ldots, N/2\}$, what implies $l = -\pi + 2\pi/N, \ldots, -2\pi/N, 0, 2\pi/N, \ldots, \pi - 2\pi/N, \pi$.

Now, we use the symmetry of this l-momenta domain, in order to express all undetermined coefficients in terms of real values. First of all, denote

$$W_\beta = \frac{\alpha}{2}(I_1 + I_2 + I_3), \tag{2.50}$$

for each of the three different sums that appear in (B.27), in the order expressed (the one with coefficients E_l, the one with coefficients C_l, and finally the one with coefficients D_l). We will employ indifferently index notation with k's or l's, in order to provide the reader with a not heavy reading. Observe that

$$\begin{aligned} I_2 = \sum_{k=-N/2+1}^{N/2} C_k d_k^\dagger d_k &= C_0 d_0^\dagger d_0 + C_\pi d_\pi^\dagger d_\pi + \sum_{k=-N/2+1}^{-1} C_k d_k^\dagger d_k + \sum_{k=1}^{N/2-1} C_k d_k^\dagger d_k \\ &= C_0 d_0^\dagger d_0 + C_\pi d_\pi^\dagger d_\pi + \sum_{k=1}^{N/2-1} C_{-k} d_{-k}^\dagger d_{-k} + \sum_{k=1}^{N/2-1} C_k d_k^\dagger d_k = \sum_{l=0}^{\pi} C_l (d_l^\dagger d_l + d_{-l}^\dagger d_{-l}), \end{aligned} \tag{2.51}$$

where we redefined $C_0 = -A - B + \gamma$, $C_\pi = -A - B - \gamma$, and considered $C_l = C_{-l}$, given the even condition of the cosine function. We used as well that the periodic boundary condition $d_{-\pi} = d_\pi$. On the other hand, taking into account such PBCs, and relations derived from fermionic anti-commutation relations which have the form $d_0 d_0 = 0$, $d_0^\dagger d_0^\dagger = 0$, $d_\pi^\dagger d_\pi^\dagger = 0$, $d_l^\dagger d_{-l}^\dagger = -d_{-l}^\dagger d_l^\dagger$, and $d_l d_{-l} = -d_{-l} d_l$, we have

$$\begin{aligned} I_3 = \sum_{k=-N/2+1}^{N/2} D_k (d_{-k}^\dagger d_k^\dagger + d_{-k} d_k) &= \sum_{k=-N/2+1}^{-1} D_k (d_{-k}^\dagger d_k^\dagger + d_{-k} d_k) + \sum_{k=1}^{N/2} D_k (d_{-k}^\dagger d_k^\dagger + d_{-k} d_k) \\ = \sum_{k=1}^{N/2} D_{-k} (d_k^\dagger d_{-k}^\dagger + d_k d_{-k}) + \sum_{k=1}^{N/2-1} D_k (d_{-k}^\dagger d_k^\dagger + d_{-k} d_k) &= \sum_{l=0}^{\pi} [d_l^\dagger d_{-l}^\dagger (D_{-l} - D_l) + d_l d_{-l} (D_{-l} - D_l)]. \end{aligned} \tag{2.52}$$

Given that

$$D_{-l} - D_l = i2(-B\sin(2l) + \gamma\sin(l)) = iF_l, \tag{2.53}$$

then

$$I_3 = \sum_{l=0}^{\pi} iF_l [d_l^\dagger d_{-l}^\dagger + d_l d_{-l}], \tag{2.54}$$

where we denoted $F_l = 2(\gamma\sin(l) - B\sin(2l))$. Regarding the first sum I_1, if we denote

$$\begin{aligned} E_0 &= A - 1 - 2\gamma, \quad E_\pi = A - 1 + 2\gamma, \\ E_l &= A - 1 - 2\gamma\cos(l) = E_{-l}, \end{aligned} \tag{2.55}$$

then,

$$I_1 = \sum_{l=0}^{\pi} G_l, \tag{2.56}$$

where $G_l = 2E_l$ for $l \neq 0, \pi$, and $G_0 = E_0$, $G_\pi = E_\pi$. All in all, one obtains

$$W_\beta = \frac{\alpha}{2}\sum_{l=0}^{\pi}[G_l + iF_l(d_l^\dagger d_{-l}^\dagger + d_l d_{-l}) + C_l(d_l^\dagger d_l + d_{-l}^\dagger d_{-l})]. \tag{2.57}$$

Note that W_β, as expressed in (2.57), is hermitian since G_l, F_l and C_l are real, and

$$\begin{aligned} W_\beta^\dagger &= \frac{\alpha}{2}\sum_{l=0}^{\pi}[G_l - iF_l(d_{-l}d_l + d_{-l}^\dagger d_l^\dagger) + C_l(d_l^\dagger d_l + d_{-l}^\dagger d_{-l})] \\ &= \frac{\alpha}{2}\sum_{l=0}^{\pi}[G_l + iF_l(d_l^\dagger d_{-l}^\dagger + d_l d_{-l}) + C_l(d_l^\dagger d_l + d_{-l}^\dagger d_{-l})] = W_\beta, \end{aligned} \tag{2.58}$$

where fermionic anti-commutation relations have been used.

2.2.3 Bogoliubov transformation

In this section, we aim to remove products from (2.58) of operators with opposite momenta such as $d_l d_{-l}$, in order to obtain a completely diagonalized Hamiltonian. With that purpose, we apply Bogoliubov transformation. It consists of a rotation of opposite momenta, exectuted in the momentum space, with a priori two degrees of freedom. This let us, by imposing some conditions on them, to remove non-diagonal terms from the Hamiltonian. In practical terms, following formulation from [64], we are going to express W_β as a sum of cross-products of operators ξ_s given by

$$\xi_s = u_s d_s + iv_s d_{-s}^\dagger, \quad \xi_{-s}^\dagger = iv_s d_s + u_s d_{-s}^\dagger, \quad s \in \{0, \dots, \pi\}, \tag{2.59}$$

where $u_s, v_s \in \mathbb{R}$ are coefficients to specify. Equivalently, their adjoint counterparts are

$$\xi_s^\dagger = u_s d_s^\dagger - iv_s d_{-s}, \quad \xi_{-s} = -iv_s d_s^\dagger + u_s d_{-s}, \quad s \in \{0, \dots, \pi\}. \tag{2.60}$$

To preserve anti-commutation relations, observe that

$$\{\xi_s^\dagger, \xi_s\} = \{u_s d_s^\dagger - iv_s d_{-s}, u_s d_s + iv_s d_{-s}^\dagger\} = u_s^2\{d_s^\dagger, d_s\} + v_s^2\{d_{-s}, d_{-s}^\dagger\} = u_s^2 + v_s^2, \tag{2.61}$$

for any $s \in \{0, \dots, \pi\}$, and where we used the established anti-commutation relations of operators d_s, d_{-s}. Then, we impose $u_s^2 + v_s^2 = 1$. Furthermore, from this observation we can infere that there is at least one $\theta_s \in (-3\pi/2, \pi/2]$ such that

$$u_s = \cos(\theta_s/2), \quad v_s = \sin(\theta_s/2), \tag{2.62}$$

from which it is straightforward that $u_{-s} = u_s$ and $v_{-s} = -v_s$. Apart from this, the other anti-commutation relations with these new operators are:

$$\begin{aligned} \{\xi_s^\dagger, \xi_t^\dagger\} &= \{u_s d_s^\dagger - iv_s d_{-s}, u_t d_t^\dagger - iv_t d_{-t}\} = 0, \\ \{\xi_{-s}, \xi_{-t}\} &= \{-iv_s d_s^\dagger + u_s d_{-s}, -iv_t d_t^\dagger + u_t d_{-t}\} = 0, \end{aligned} \tag{2.63}$$

where we have used the already known anti-commutation relations of d_s, d_t d_{-s} and d_{-t}, for any $s, t \in \{0, \dots, \pi\}$.

This Bogoliubov transformation is unitary (namely, it is a rotation), which can be expressed in the following way:

$$\begin{pmatrix} \xi_s \\ \xi_{-s}^\dagger \\ \xi_s^\dagger \\ \xi_{-s} \end{pmatrix} = \begin{pmatrix} u_s & iv_s & 0 & 0 \\ iv_s & u_s & 0 & 0 \\ 0 & 0 & u_s & -iv_s \\ 0 & 0 & -iv_s & u_s \end{pmatrix} \begin{pmatrix} d_s \\ d_{-s}^\dagger \\ d_s^\dagger \\ d_{-s} \end{pmatrix}. \tag{2.64}$$

Thus, in order to express d_s terms as linear combinations of ξ_s terms, we take the rotation's inverse, which from its unitary condition takes the following form:

$$\begin{pmatrix} d_s \\ d_{-s}^\dagger \\ d_s^\dagger \\ d_{-s} \end{pmatrix} = \begin{pmatrix} u_s & -iv_s & 0 & 0 \\ -iv_s & u_s & 0 & 0 \\ 0 & 0 & u_s & iv_s \\ 0 & 0 & iv_s & u_s \end{pmatrix} \begin{pmatrix} \xi_s \\ \xi_{-s}^\dagger \\ \xi_s^\dagger \\ \xi_{-s} \end{pmatrix}. \tag{2.65}$$

In order to not having cross-product terms with opposite momenta, using the computations provided in appendix (C), and since we have still one degree of freedom in our Bogoliubov rotation, we impose the following, for any l:

$$F_l \cos(\theta_l) + C_l \sin(\theta_l) = 0. \tag{2.66}$$

Therefore, we take the Bogoliubov coefficients as

$$\cos(\theta_l) = \frac{C_l}{\sqrt{C_l^2 + F_l^2}}, \quad \sin(\theta_l) = -\frac{F_l}{\sqrt{C_l^2 + F_l^2}}. \tag{2.67}$$

This implies that the coefficient of the final diagonalized Master operator of $\xi_l^\dagger \xi_l + \xi_{-l}^\dagger \xi_{-l}$ is, for any l,

$$-F_l \sin(\theta_l) + C_l \cos(\theta_l) = \frac{F_l^2}{\sqrt{C_l^2 + F_l^2}} + \frac{C_l^2}{\sqrt{C_l^2 + F_l^2}} = \sqrt{C_l^2 + F_l^2}. \tag{2.68}$$

For the independent terms in (C.4), using the equality $\sin^2(x/2) = (1 - \cos(x))/2$, we have

$$\begin{aligned} G_l + F_l \sin(\theta_l) + 2C_l \sin^2(\theta_l/2) = G_l + C_l + F_l \sin(\theta_l) - C_l \cos(\theta_l) = G_l + C_l - \frac{C_l^2}{\sqrt{C_l^2 + F_l^2}} \\ - \frac{F_l^2}{\sqrt{C_l^2 + F_l^2}} = G_l + C_l - \sqrt{C_l^2 + F_l^2}. \end{aligned} \tag{2.69}$$

Thus, for any l, we have that

$$W_{l,\beta} = G_l + C_l - \sqrt{C_l^2 + F_l^2} + \sqrt{C_l^2 + F_l^2}(\xi_l^\dagger \xi_l + \xi_{-l}^\dagger \xi_{-l}). \tag{2.70}$$

In fact, regarding implementation and to give one of the most relevant parts of the Bogoliubov transformation, we have that, for any momentum l:

$$\theta_l = -\arcsin \frac{F_l}{\sqrt{C_l^2 + F_l^2}}, \tag{2.71}$$

so, for $l \neq 0, \pi$,

$$\begin{aligned} \theta_l &= \arcsin \frac{2(B \sin(2l) - \gamma \sin(l))}{\sqrt{4(\gamma \sin(l) - B \sin(2l))^2 + 4(-A - B \cos(2l) + \gamma \cos(l))^2}} \\ &= \arcsin \frac{B \sin(2l) - \gamma \sin(l)}{\sqrt{(\gamma \sin(l) - B \sin(2l))^2 + (-A - B \cos(2l) + \gamma \cos(l))^2}} \end{aligned} \tag{2.72}$$

and, for $l = 0, \pi$,

$$\theta_0 = 0 = \theta_\pi. \tag{2.73}$$

Therefore, we express, in general for any $l = 2k\pi/N$, where $k = -N/2+1, \ldots, N/2$ (recall that we are considering PBCs),

$$\theta_k = \arcsin \frac{B\sin(4k\pi/N) - \gamma\sin(2k\pi/N)}{\sqrt{(\gamma\sin(2k\pi/N) - B\sin(4k\pi/N))^2 + (-A - B\cos(4k\pi/N) + \gamma\cos(2k\pi/N))^2}}. \quad (2.74)$$

We could carry out the simplification even further [64] in order to obtain, for any momentum $l \neq 0, \pi$,

$$W_{l,\beta} = -(1-\gamma\cos(l))(\xi_l^\dagger\xi_l + \xi_{-l}^\dagger\xi_{-l} - 1) - 1, \quad (2.75)$$

along with the direct expressions obtained from (2.70) ($F_0 = F_\pi = 0$):

$$\begin{aligned} W_{0,\beta} &= G_0 + 2C_0\xi_0^\dagger\xi_0 = A - 1 - 2\gamma - 2(A+B-\gamma)\xi_0^\dagger\xi_0, \\ W_{\pi,\beta} &= G_\pi + 2C_\pi\xi_\pi^\dagger\xi_\pi = A - 1 + 2\gamma - 2(A+B+\gamma)\xi_\pi^\dagger\xi_\pi. \end{aligned} \quad (2.76)$$

Following again formulation from [64], and once clarified simplification of Master's operator W_β, we can easily find the complete set of eigenvectors and eigenvalues. First of all, vacuum state $|0\rangle$ (i.e., no

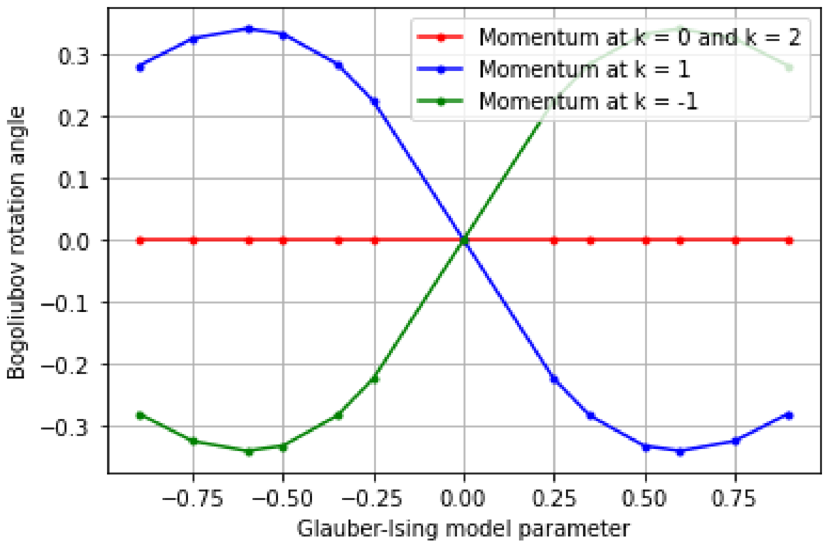

Figure 1: Bogoliubov rotation angles for the diagonalization of Master operator W_β given finally in terms of (2.70), considering momenta determined by $k = 0$, $k = 2$, $k = 1$ and $k = -1$, versus 1D Glauber-Ising model parameter γ.

fermionic occupation at any momentum mode) is an eigesntate of transformed W_β with eigenvalue 0. This can be determined through

$$\xi_l|0\rangle = 0, \text{ for any momentum } l. \quad (2.77)$$

In general, states with an even (odd) number of ξ-quasi-particles imply an even (odd) number of d-quasi-particles, which in turn imply an even (odd) number of c-quasi-particles. Then, ξ-quasi-particles are subject to fermionic modes algebra obtained after Jordan-Wigner transformation. Thus, eigenstates of W_β are

$$|q_1, \ldots, q_N\rangle = \xi_{q_1}^\dagger \ldots \xi_{q_N}^\dagger|0\rangle, \quad (2.78)$$

which for N even q-momenta are obtained from (2.47), and for N odd they are obtained from (2.48). Let's understand, by now, the q_i's ordered in a way such that ($q_1 < \cdots < q_N$), what is allowed given that permutation of q-values merely change the phase.

All in all, the complete set of eigenvectors of W_β are the $|q_1,\ldots,q_N\rangle$'s just described. In particular, this means that there are 2^N possible eigenstates of W_β, for N the number of spins considered. From all this algebra, the eigenvalue of W_β for eigenstate $|q_1,\ldots,q_N\rangle$ is determined by

$$W_\beta|q_1,\ldots,q_N\rangle = -\Lambda(q_1,\ldots,q_N)|q_1,\ldots,q_N\rangle, \tag{2.79}$$

where

$$\Lambda(q_1,\ldots,q_N) = \sum_{i=1}^{N}\lambda_{q_i}, \quad \lambda_q = 1-\gamma\cos(q), \tag{2.80}$$

also valid for $q=0,\pi$. This solves Master's equation explicitly, and concludes the analytical procedure through which we express the original Hamiltonian (i.e., the original Master operator (2.22)) in a diagonalized form, in terms of fermionic momentum modes which, under a Bogoliubov rotation, do not admit operators products with different momenta.

2.2.4 Example of energy eigenvalues computations

Following the just derived (2.80) and (2.78), we show now an example of eigenvalues computation for $N=4$ spins, that is, for 4 possible fermionic momentum modes. Since we are considering N even and PBC, we know that the exact momenta q_i defining our eigenstates are obtained from $q=2\pi k/N$, for $k\in\{-1,0,1,2\}$, that is, in increasing order, $q_1=-\pi/2$, $q_2=0$, $q_3=\pi/2$ and $q_4=\pi$.

Let $|r_{q_1},r_{q_2},r_{q_3},r_{q_4}\rangle$ be an arbitrary eigenstate of Master's operator defined in terms of (2.75), where r_{q_i} is 0 or 1 depending on whether there is a fermionic quasi-particle with momentum q_i or not. Unlike we did in the theoretical deduction, in order to write the corresponding eigenstates, we consider the order of momenta in which we later express the quantum circuit, in terms of qbits. Then, momenta order is $q_1=0$, $q_2=\pi$, $q_3=\pi/2$ and $q_4=-\pi/2$. In order to compute energy eigenvalues (2.80)

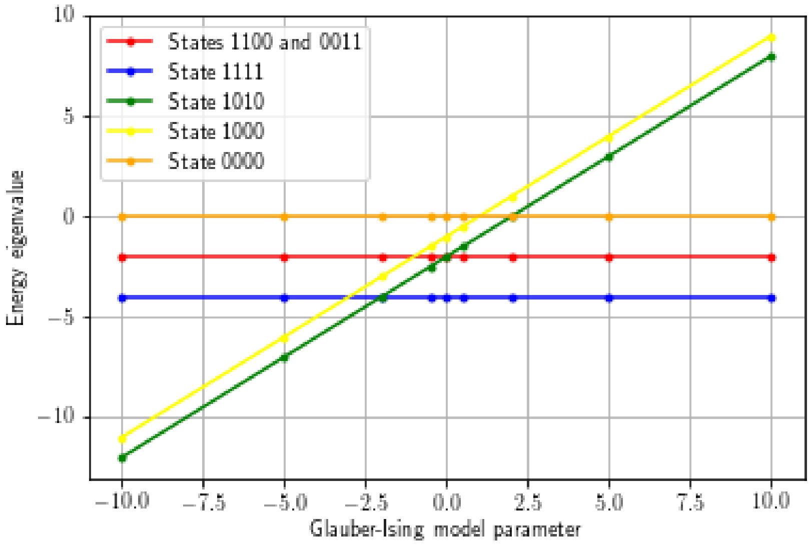

Figure 2: Energy eigenvalues for transformed Master operator W_β given in terms of (2.70), considering eigenstates $|1100\rangle$, $|0011\rangle$, $|1111\rangle$, $|1010\rangle$, $|1000\rangle$ and vacuum state $|0000\rangle$ (given in order of momenta determined by $k=0$, $k=2$, $k=1$ and $k=-1$), versus 1D Glauber-Ising model parameter γ.

from the general considered eigenstate, we first compute all λ_{q_i} from (2.80) for the cases in which

$r_{q_i} = 1$, and then we sum all the obtained values like in the first expression of (2.80), adding a minus sign at the end. This yields the energy eigenvalue of eigenstate $|r_{q_1}, r_{q_2}, r_{q_3}, r_{q_4}\rangle$. Note that, from this procedure, energy eigenvalue of vacuum state $|0000\rangle$ is 0. First of all, we compute all λ_{q_i} values:

$$\begin{aligned}
&\lambda_{q_1} = 1 - \gamma\cos(0) = 1 - \gamma, \quad \lambda_{q_2} = 1 - \gamma\cos(\pi) = 1 + \gamma, \\
&\lambda_{q_3} = 1 - \gamma\cos(\pi/2) = 1, \quad \lambda_{q_4} = 1 - \gamma\cos(-\pi/2) = 1.
\end{aligned} \tag{2.81}$$

Now, we select the eigenstates $|1100\rangle$, $|0011\rangle$, $|1111\rangle$, $|1010\rangle$ and $|1000\rangle$ to proceed with the example. With all we have exposed, it suffices to sum λ_{q_i} values taking into account which momentum modes are present in the state. For instance, energy eigenvalue of state $|1100\rangle$ is

$$E_{1100} = -(\lambda_{q_1} + \lambda_{q_2}) = -(1 - \gamma + 1 + \gamma) = -2. \tag{2.82}$$

Similarly,

$$\begin{aligned}
&E_{0011} = -(\lambda_{q_3} + \lambda_{q_4}) = -(1 + 1) = -2, \\
&E_{1111} = -(\lambda_{q_1} + \lambda_{q_2} + \lambda_{q_3} + \lambda_{q_4}) = -(1 + 1 + 1 - \gamma + 1 + \gamma) = -4, \\
&E_{1010} = -(\lambda_{q_1} + \lambda_{q_3}) = -(1 - \gamma + 1) = \gamma - 2, \\
&E_{1000} = -\lambda_{q_1} = -(1 - \gamma) = \gamma - 1;
\end{aligned} \tag{2.83}$$

and, as we said, $E_{0000} = 0$. In figure 2 we represent the obtained energies with respect to external field strength parameter γ. Note from $\gamma = \tanh(2\beta J)$ that, for the non-constant energies, parameter J from Ising Hamiltonian (2.3), and temperature T (which is inside the temperature parameter β) determine the slope of the corresponding eigenvalue as a function of γ. Recall that tanh is an increasing function. Thus, for E_{1000} and E_{1010}, the larger J or the lower T get, the larger slope is reached.

3 Open quantum dynamics

So far we have been concentrated on the diagonalization of the quantum version of the Hamiltonian (2.22) using standard techniques. However, equation (2.23) involves a dissipative dynamics. Therefore, in order to achieve a consistent description, we need to make use of the formalism of open quantum systems, so as to derive a fully quantum Master equation, in which the state of the system will be written in terms of a density operator. As we will show later, equation (2.23) just corresponds to the diagonal part (in the σ_z eigenstates basis) of this quantum Master equation. We base the upcoming work on the formulation from [57].

3.1 Lindblad formulation. Division into 2^N subsystems

First, we consider as basis the 2^N vectors $|\sigma\rangle = |\sigma_1\rangle|\sigma_2\rangle\cdots|\sigma_N\rangle$; these states belong to the Hilbert space $(\mathbb{C}^2)^{\otimes N}$. Each $|\sigma_i\rangle$ is an eigenstate of the operator σ^z. Notice that notation here has to be distinguished from previous sections: the state $|\sigma\rangle$ is a quantum state, though it shares notation with previous classical state; the quantum Pauli operators σ^z and σ^x shares notation with the objects σ^z and σ^x, used in the classical context above. With this notation we simply write the following Master equation:

$$\frac{\partial\rho(t)}{\partial t} = \sum_i \{\sigma_i^x[w_i(\sigma^z)]^{1/2}\rho(t)[w_i(\sigma^z)]^{1/2}\sigma_i^x - \frac{1}{2}\{w_i(\sigma^z),\rho(t)\}\}, \tag{3.1}$$

where $\{\cdot,\cdot\}$ is the anticommutator and $w_i(\sigma^z)$ are the transition rate operators obtained when in the classical transition rates on substitute the matrix σ^z by the corresponding operator (Ising variables replaced by σ^z). Note the operator w_i is diagonal in the basis we are using. Here the density operator is explicitly

$$\rho(t) = \sum_{\sigma,\tilde{\sigma}} [\rho(t)]_{\sigma,\tilde{\sigma}} |\sigma\rangle\langle\tilde{\sigma}|. \tag{3.2}$$

One can prove now that the diagonal part of this equation reproduces the Master equation (2.1), upon identification of states modulus with probabilities, as we will do later. Equation (3.1) can be written as a Master Linblad equation as

$$\frac{\partial\rho(t)}{\partial t} = \sum_i \{L_i\rho(t)L_i^\dagger - \frac{1}{2}\{L_i^\dagger L_i,\rho(t)\}\}, \tag{3.3}$$

with the Lindblad operator $L_i = \sigma_i^x[w_i(\sigma^z)]^{1/2}$.

We now proceed as follows. The density operator, given in equation (3.2), is a matrix of dimension $2^N\times 2^N$. The space of matrices of this dimension, $\mathbb{M}_{2^N}(\mathbb{C})$ can be mapped into the vector space $\mathbb{C}^{2^N}\otimes\mathbb{C}^{2^N}$, thus representing in this space the density operator as [57]

$$|\rho(t)\rangle = \sum_{\sigma,\tilde{\sigma}} [\rho(t)]_{\sigma,\tilde{\sigma}} |\sigma\rangle|\tilde{\sigma}\rangle. \tag{3.4}$$

Then we can write equation (3.3), again from [57], as

$$|\dot{\rho}(t)\rangle = \sum_i \{\sigma_i^x\tilde{\sigma}_i^x\,[w_i(\sigma^z)w_i(\tilde{\sigma}^z)]^{1/2} - \frac{1}{2}\,[w_i(\sigma^z)+w_i(\tilde{\sigma}^z)]\}|\rho(t)\rangle, \tag{3.5}$$

where bar operators act on bar kets and non-bar operators act on non-bar kets. The matrix on the right hand side is not Hermitian. To make it Hermitian we use the following transformation:

$$|\rho(t)\rangle = \exp\left[-\frac{\beta}{4}(H(\sigma^z)+H(\tilde{\sigma}^z))\right]|\psi(t)\rangle, \tag{3.6}$$

with $H(\sigma^z)$ the quantum version of the Ising Hamiltonian, equation (2.3). Now, passing the exponential operator from (3.6), corresponding to the derivative $|\dot{\rho}(t)\rangle$, to the right member, and using that, for each term in the right hand of (3.5), σ_i^x and $\tilde{\sigma}_i^x$ exchange 1's and -1's in the corresponding entries of the state $|\sigma_1^z, \dots, \sigma_n^z\rangle$, then, from the aforementioned (3.5), we have that

$$
\begin{aligned}
|\dot{\psi}(t)\rangle &= \exp\left[\frac{\beta}{4}(H(\sigma^z) + H(\tilde{\sigma}^z))\right] \sum_{i=1}^{N} \{\sigma_i^x \tilde{\sigma}_i^x [w_i(\sigma^z)]^{1/2} [w_i(\tilde{\sigma}_i^z)]^{1/2} \exp\left[-\frac{\beta}{4}(H(\sigma^z) + H(\tilde{\sigma}^z))\right] \\
&- \frac{1}{2}[w_i(\sigma_i^z) + w_i(\tilde{\sigma}_i^z)]\}|\psi(t)\rangle = \sum_{i=1}^{N} \{\sigma_i^x \tilde{\sigma}_i^x [w_i(\sigma^z) \exp[-\beta J \sigma_i^z(\sigma_{i+1}^z + \sigma_{i-1}^z))]]^{1/2} \\
&\times [w_i(\tilde{\sigma}_i^z) \exp[-\beta J \tilde{\sigma}_i^z(\tilde{\sigma}_{i+1}^z + \tilde{\sigma}_{i-1}^z))]]^{1/2} - \frac{1}{2}[w_i(\sigma_i^z) + w_i(\tilde{\sigma}_i^z)]\}|\psi(t)\rangle
\end{aligned} \tag{3.7}
$$

where we used that

$$
\exp\left[-\frac{\beta}{4}(H(\sigma^z) + H(\tilde{\sigma}^z))\right] \tag{3.8}
$$

and $w_i(\sigma_i^z)$ commute. With this, the final equation of motion reads

$$
|\dot{\psi}(t)\rangle = \sum_i \{\sigma_i^x \tilde{\sigma}_i^x \left[v_i(\sigma^z)\right]^{1/2} \left[v_i(\tilde{\sigma}^z)\right]^{1/2} - \frac{1}{2}\left[w_i(\sigma^z) + w_i(\tilde{\sigma}^z)\right]\}|\psi(t)\rangle, \tag{3.9}
$$

with $v_i(\sigma^z) = w_i(\sigma^z)\exp\left[-(\beta J)\sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z)\right]$. Now, σ_i^x and $v_i(\sigma^z)$ commute. This is because the action of σ_i^x operator on states given in σ_i^z-eigenstates basis is swapping from -1 to 1 and from 1 to -1 in each component. Therefore:

$$
\begin{aligned}
&\sigma_i^x v_i(\sigma^z) = \sigma_i^x [w_i(\sigma^z)\exp\left(-\beta J \sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z)\right)] = [w_i(-\sigma^z)\exp\left(\beta J \sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z)\right)]\sigma_i^x \\
&= [w_i(\sigma^z)\exp\left(-\beta J \sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z)\right)]\sigma_i^x.
\end{aligned} \tag{3.10}
$$

Thus, we have a Schrödinger equation for $2N$ spins. So far, we have obtained an Hermitian transformed Master operator W_β (which we will also call Hamiltonian when there is no confusion with Ising Hamiltonian (2.3)) given by

$$
W_\beta = \sum_i H_i, \tag{3.11}
$$

where

$$
H_i = \sigma_i^x \tilde{\sigma}_i^x \left[v_i(\sigma^z)\right]^{1/2} \left[v_i(\tilde{\sigma}^z)\right]^{1/2} - \frac{1}{2}\left[w_i(\sigma^z) + w_i(\tilde{\sigma}^z)\right]. \tag{3.12}
$$

This Master equation can be further simplified. In particular, if we identify operators that commute with Ising Hamiltonian H, we can split the equation to a series of 2^N Schrödinger equations. Notice that H commute with $\sigma_i^z\tilde{\sigma}_i^z$, for any $i \in \{1, \dots, N\}$. Then, we introduce new *spin* variables $\tau_i = \sigma_i^z\tilde{\sigma}_i^z$, which are constants of motion given the aforementioned commutation with W_β, and since their time derivatives are the zero operator. With that, we can split W_β into a group of 2^N Schrödinger equations by considering vectors of operators $\tau = (\tau_1, \dots, \tau_n)$ and $\tilde{\sigma}_i^z = \tau_i\sigma_i^z$, for any $i \in \{1, \dots, N\}$. Thus, we can write Hamiltonian W_β in terms of the 2^N Hamiltonians

$$
H_\tau = -\sum_i \{\sigma_i^x \tilde{\sigma}_i^x [v_i(\sigma^z)]^{1/2} [v_i(\tau\sigma^z)]^{1/2} - \frac{1}{2}[w_i(\sigma_z) + w_i(\tau\sigma_z)]\} = -\sum_i H_{\tau,i}, \tag{3.13}
$$

where $\tau\sigma^z$ denotes the vector with components $\tau_i\sigma_i^z$. This implies 2^N possible configurations for the τ's, i.e., 2^N Hamiltonians. We label them through natural numbers $\tau = 0, \dots, 2^N - 1$, with the convention of $\tau = 0$ for all τ-spins up (all equal eigenvalues and eigenvectors of σ and $\tilde{\sigma}$), and $\tau = 2^N - 1$

for all τ-spins down (all equal eigenvalues between σ and $\tilde{\sigma}$, with the eigenvectors exchanged).

From our equation (3.4), let's see now diagonal elements of the vector $|\rho(t)\rangle$, what in practice means equal eigenvalues for σ and $\tilde{\sigma}$ in (3.13) ($\tau = 0$ from our convention). Each of them is applied in a different space, i.e., although the operators act in the same way, the first ones act on the i-th quasi-particle corresponding to σ, and the second ones on the i-th quasi-particle corresponding to $\tilde{\sigma}$. That is:

$$
\begin{aligned}
H_{\tau=0} &= -\sum_{i=1}^{N}\{\sigma_i^x\sigma_i^x v_i(\sigma^z)^{1/2}v_i(\sigma^z)^{1/2} - \frac{1}{2}[w_i(\sigma^z)+w_i(\sigma^z)]\} \\
&= -\sum_{i=1}^{N}\{\sigma_i^x\sigma_i^x w_i(\sigma^z)^{1/2}\exp\big(-\beta J\sigma_i^z(\sigma_{i-1}^z+\sigma_{i+1}^z)/2\big)w_i(\sigma^z)^{1/2}\exp\big(-\beta J\sigma_i^z(\sigma_{i-1}^z+\sigma_{i+1}^z)/2\big) \\
&- \frac{1}{2}[w_i(\sigma^z)+w_i(\sigma^z)]\},
\end{aligned}
\tag{3.14}
$$

where it must be clear that, although the notation is the same (since they act in the same way), their spaces of action are different. Note that action of $H_{\tau=0}$ on the corresponding eigenstates are equivalent to the classical Master's equation when we take the latter with Pauli matrices instead of in classical terms, what makes this formulation a natural extension from the notions of previous sections. That is to say, expression (3.14) is exactly our Master equation given in terms of σ^z and σ^x matrices, recovering the kinetic equations (2.14). Going back to the general case, we have the following operator:

$$
W_\beta = -\sum_{\tau=0}^{2^N-1} H_\tau. \tag{3.15}
$$

To sum up, taking N operators that commute with Ising Hamiltonian H, we translate the solution of the extended Master equation (3.1) to the diagonalization of 2^N Hamiltonians which are $2^N \times 2^N$-dimensional.

Now, we take our particular transition rates:

$$
w_i(\sigma^z) = \frac{\alpha}{2}[1-\frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z+\sigma_{i+1}^z)]. \tag{3.16}
$$

From (3.13), (3.16) and the expression of $v_i(\sigma^z)$, we have that, for any $\tau \in \{0,\dots,2^N-1\}$, and omitting $\alpha/2$:

$$
\begin{aligned}
H_\tau &= -\sum_i\{\sigma_i^x\tilde{\sigma}_i^x[(1-\frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z+\sigma_{i+1}^z))\exp\big(-\beta J\sigma_i^z(\sigma_{i+1}^z+\sigma_{i-1}^z)\big)]^{1/2} \\
&\times[(1-\frac{\gamma}{2}\tilde{\sigma}_i^z(\tilde{\sigma}_{i-1}^z+\tilde{\sigma}_{i+1}^z))\exp\big(-\beta J\tilde{\sigma}_i^z(\tilde{\sigma}_{i+1}^z+\tilde{\sigma}_{i-1}^z)\big)]^{1/2} \\
&-\frac{1}{2}[1-\frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z+\sigma_{i+1}^z)+1-\frac{\gamma}{2}\tilde{\sigma}_i^z(\tilde{\sigma}i-1^z+\tilde{\sigma}_{i+1}^z)]\}.
\end{aligned}
\tag{3.17}
$$

To make the computations more clear, denote, for a fixed and arbitrary $i \in \{1,\dots,N\}$,

$$
\begin{aligned}
I_1 &= \sigma_i^x\tilde{\sigma}_i^x[(1-\frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z+\sigma_{i+1}^z))\exp\big(-\beta J\sigma_i^z(\sigma_{i+1}^z+\sigma_{i-1}^z)\big)]^{1/2} \\
&\times[(1-\frac{\gamma}{2}\tilde{\sigma}_i^z(\tilde{\sigma}_{i-1}^z+\tilde{\sigma}_{i+1}^z))\exp\big(-\beta J\tilde{\sigma}_i^z(\tilde{\sigma}_{i+1}^z+\tilde{\sigma}_{i-1}^z)\big)]^{1/2} = \sigma_i^x\tilde{\sigma}_i^x I_{11}^{1/2}I_{12}^{1/2},
\end{aligned}
\tag{3.18}
$$

$$
I_2 = \frac{1}{2}[1-\frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z+\sigma_{i+1}^z)+1-\frac{\gamma}{2}\tilde{\sigma}_i^z(\tilde{\sigma}_{i-1}^z+\tilde{\sigma}_{i+1}^z)]. \tag{3.19}
$$

Firstly, recalling that $\tilde{\sigma}_i^z = \tau_i \sigma_i^z$, by extending the expressions we obtain:

$$I_2 = 1 - \frac{\gamma}{4}\sigma_i^z[\sigma_{i-1}^z + \tau_i\tau_{i-1}\sigma_{i-1}^z + \sigma_{i+1}^z + \tau_i\tau_{i+1}\sigma_{i+1}^z]. \tag{3.20}$$

On the other hand, for I_1, let's first assume that $\tau_{i-1} = \tau_{i+1}$. Thus, since $\exp(x) = \sinh(x) + \cosh(x)$ for any $x \in \mathbb{C}$,

$$\begin{aligned} I_{11} &= (1 - \frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z)) \exp\big(-\beta J\sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z)\big) = (1 - \frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z))[\cosh\big(\beta J(\sigma_{i-1}^z + \sigma_{i+1}^z)\big) \\ &- \sigma_i^z \sinh\big(\beta J(\sigma_{i-1}^z + \sigma_{i+1}^z)\big)] = (1 - \frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z)) \cosh\big(\beta J(\sigma_{i-1}^z + \sigma_{i+1}^z)\big) \\ &\times (1 - \sigma_i^z \left(\frac{\sigma_{i-1}^z + \sigma_{i+1}^z}{2}\right) \tanh(2\beta J)) = \cosh\big(\beta J(\sigma_{i-1}^z + \sigma_{i+1}^z)\big)(1 - \frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z))^2, \end{aligned} \tag{3.21}$$

where we used the odd condition of sinh and tanh, the even condition of cosh, and the fact that $\tanh(2\beta J) = \gamma$, since detailed-balance condition remains the same. Analogously,

$$I_{12} = \cosh\big(\beta J(\tilde{\sigma}_{i-1}^z + \tilde{\sigma}_{i+1}^z)\big)(1 - \frac{\gamma}{2}\tilde{\sigma}_i^z(\tilde{\sigma}_{i-1}^z + \tilde{\sigma}_{i+1}^z))^2 \tag{3.22}$$

Therefore, given again that $\tilde{\sigma}_i^z = \tau_i\sigma_i^z$,

$$\begin{aligned} I_{11}^{1/2} I_{12}^{1/2} &= (1 - \frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z))(1 - \frac{\gamma}{2}\tilde{\sigma}_i^z(\tilde{\sigma}_{i-1}^z + \tilde{\sigma}_{i+1}^z)) \cosh^{1/2}(\beta J(\tilde{\sigma}_{i-1}^z + \tilde{\sigma}_{i+1}^z)) \cosh^{1/2}(\beta J(\sigma_{i-1}^z + \sigma_{i+1}^z)) \\ &= (1 - \frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z))(1 - \frac{\gamma}{2}\tilde{\sigma}_i^z(\tilde{\sigma}_{i-1}^z + \tilde{\sigma}_{i+1}^z)) \cosh\big(\beta J(\sigma_{i-1}^z + \sigma_{i+1}^z)\big), \end{aligned} \tag{3.23}$$

where we used $\tau_{i-1} = \tau_{i+1}$, and the even condition of cosh (what let us omit factors τ_{i-1} out of its argument). Note that

$$\cosh\big(\beta J(\sigma_{i-1}^z + \sigma_{i+1}^z)\big) = \left(\frac{1 + \sigma_{i-1}^z\sigma_{i+1}^z}{2}\right)(\cosh(2\beta J) - 1) + 1, \tag{3.24}$$

which implies that

$$\begin{aligned} I_{11}^{1/2} I_{12}^{1/2} &= (1 - \frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z))(1 - \tau_i\tau_{i-1}\frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z)) \cdot [\left(\frac{1 + \sigma_{i-1}^z\sigma_{i+1}^z}{2}\right)(\cosh(2\beta J) - 1) + 1] \\ &= [1 + \frac{\gamma^2\tau_i\tau_{i-1}}{2}(1 + \sigma_{i-1}^z\sigma_{i+1}^z) - \frac{\gamma(1 + \tau_i\tau_{i-1})}{2}\sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z)] \cdot [\left(\frac{1 + \sigma_{i-1}^z\sigma_{i+1}^z}{2}\right)(\cosh(2\beta J) - 1) + 1]. \end{aligned} \tag{3.25}$$

Recall that we are applying on the left of $I_{11}^{1/2} I_{12}^{1/2}$ the operators product $\sigma_i^x\tilde{\sigma}_i^x$. Furthermore, $1 + \tau_i\tau_{i-1} = 0$ or $1 + \tau_i\tau_{i-1} = 2$, so before or after applying $\tilde{\sigma}_i^x$ over the third term of the first bracket in the last expression of (3.25) , we obtain 0 in such a term, for any $i \in \{1, \dots, N\}$. Then, we restrict our analysis to

$$\begin{aligned} I_{11}^{1/2} I_{12}^{1/2} &= [1 + \frac{\gamma^2\tau_i\tau_{i-1}}{2}(1 + \sigma_{i-1}^z\sigma_{i+1}^z)] \cdot [1 + \frac{(\cosh(2\beta J) - 1)}{2}(1 + \sigma_{i-1}^z\sigma_{i+1}^z)] \\ &= 1 + (\gamma^2\tau_i\tau_{i-1} + \cosh(2\beta J) - 1)\left(\frac{1 + \sigma_{i-1}^z\sigma_{i+1}^z}{2}\right) + \gamma^2\tau_i\tau_{i-1}(\cosh(2\beta J) - 1)\left(\frac{1 + \sigma_{i-1}^z\sigma_{i+1}^z}{2}\right) \\ &= 1 + P_i\left(\frac{1 + \sigma_{i-1}^z\sigma_{i+1}^z}{2}\right) = \left(1 + \frac{P_i}{2}\right) + \frac{P_i}{2}\sigma_{i-1}^z\sigma_{i+1}^z \end{aligned} \tag{3.26}$$

where

$$P_i = \cosh(2\beta J)(1 + \gamma^2\tau_i\tau_{i-1}) - 1 = \frac{1 + \tau_i\tau_{i-1}\gamma^2}{\sqrt{1 - \gamma^2}} - 1, \tag{3.27}$$

where we used that $\cosh^2(x) = 1/(1-\tanh^2(x))$ for any $x \in \mathbb{C}$, and $\gamma = \tanh(2\beta J)$. Now, observe that applying $\tilde{\sigma}_i^x \sigma_i^x$ over states $|\sigma\rangle \otimes |\tilde{\sigma}\rangle$ is equivalent to applying σ_i^x to $|\sigma\rangle \otimes |\sigma\rangle$ including the corresponding τ_i's. Therefore, for $\tau_{i-1} = \tau_{i+1}$:

$$I_1 = \{\left[1 + \frac{P_i}{2}\right] - \left(-\frac{P_i}{2}\right)\sigma_{i-1}^z \sigma_{i+1}^z]\}\sigma_i^x. \tag{3.28}$$

Then, for this case $\tau_{i-1} = \tau_{i+1}$ we have already obtained a more treatable form of H_τ, including again parameter α:

$$H_\tau = -\frac{\alpha}{2}\sum_{i=1}^{N}\{[\tilde{A}_i(\gamma) - \tilde{B}_i(\gamma)\sigma_{i-1}^z\sigma_{i+1}^z]\sigma_i^x - 1 + \frac{\gamma}{4}[\sigma_{i-1}^z + \tau_{i-1}\tau_i\sigma_{i-1}^z + \sigma_{i+1}^z + \tau_i\tau_{i+1}\sigma_{i+1}^z]\sigma_i^z\}, \tag{3.29}$$

where

$$\begin{aligned}\tilde{A}_i(\gamma) &= \frac{1+\gamma^2\tau_i\tau_{i-1}}{2\sqrt{1-\gamma^2}} + \frac{1}{2},\\ \tilde{B}_i(\gamma) &= 1 - \tilde{A}_i(\gamma) = -\frac{1+\gamma^2\tau_i\tau_{i-1}}{2\sqrt{1-\gamma^2}} + \frac{1}{2}.\end{aligned} \tag{3.30}$$

Analogously, if we consider $\tau_{i-1} = -\tau_{i+1}$, following a similar procedure we have that

$$\begin{aligned}&I_{11}^{1/2}I_{12}^{1/2} = (1 - \frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z))(1 - \frac{\gamma}{2}\tau_i\tau_{i-1}\sigma_i^z(\sigma_{i-1}^z - \sigma_{i+1}^z))\cosh^{1/2}(\beta J(\sigma_{i-1}^z + \sigma_{i+1}^z))\\ &\times \cosh^{1/2}(\beta J(\sigma_{i-1}^z - \sigma_{i+1}^z)) = [1 + \frac{\gamma^2}{4}((\sigma_{i-1}^z)^2 - (\sigma_{i+1}^z)^2) - \frac{\gamma}{2}\sigma_i^z(\sigma_{i-1}^z + \sigma_{i+1}^z) - \frac{\gamma}{2}\tau_i\tau_{i-1}\sigma_i^z(\sigma_{i-1}^z - \sigma_{i+1}^z)]\\ &\times [(\cosh(\beta\sigma_{i-1}^z)\cosh(\beta\sigma_{i+1}^z) + \sinh(\beta\sigma_{i+1}^z)\sinh(\beta\sigma_{i-1}^z))\cdot(\cosh(\beta\sigma_{i-1}^z)\cosh(\beta\sigma_{i+1}^z)\\ &- \sinh(\beta\sigma_{i+1}^z)\sinh(\beta\sigma_{i-1}^z))]^{1/2} = \{1 - \frac{\gamma}{2}\sigma_i^z[\sigma_{i-1}^z(1+\tau_i\tau_{i-1}) + \sigma_{i+1}^z(1-\tau_i\tau_{i-1})]\}\sqrt{\cosh^4(\beta J) - \sinh^4(\beta J)},\end{aligned} \tag{3.31}$$

where we used even condition of cosh and odd condition of sinh. Now, through the same reasoning about the application of $\tilde{\sigma}_i^x\sigma_i^x$ and the fact that $1+\tau_i\tau_{i-1}$ and $1-\tau_i\tau_{i-1}$ take 0 values before or after its application, we can restrict to

$$\begin{aligned}I_{11}^{1/2}I_{12}^{1/2} &= \sqrt{1-\tanh^2(\beta J)}\sqrt{1+\tanh^2(\beta J)}\cosh^2(\beta J) = \cosh(\beta J)\sqrt{\frac{\sinh^2(\beta J)+\cosh^2(\beta J)}{\cosh^2(\beta J)}}\\ &= \sqrt{\frac{1}{\sqrt{1-\tanh^2(2\beta J)}}} = \frac{1}{(1-\gamma^2)^{1/4}},\end{aligned} \tag{3.32}$$

where we took advantage of hyperbolic cosine and sine standard relations. This implies that, for the case $\tau_{i-1} = -\tau_{i+1}$, we have (3.34) with

$$\tilde{A}_i(\gamma) = \frac{1}{(1-\gamma^2)^{1/4}}, \quad \tilde{B}_i(\gamma) = 0, \tag{3.33}$$

for any $i \in \{1, \ldots, N\}$.

Imitating their notation, this leads us to the following general quantum kinetic Hamiltonians from [57], taking $\delta = 0$ in their general model for each $\tau \in \{0, \ldots, 2^N - 1\}$ (see their equation (22)):

$$H_\tau = -\frac{\alpha}{2}\sum_{i=1}^{N}\{[\tilde{A}_i(\gamma,0) - \tilde{B}_i(\gamma,0)\sigma_{i-1}^z\sigma_{i+1}^z]\sigma_i^x - 1 + \frac{\gamma}{4}[\sigma_{i-1}^z + \tau_{i-1}\tau_i\sigma_{i-1}^z + \sigma_{i+1}^z + \tau_i\tau_{i+1}\sigma_{i+1}^z]\sigma_i^z\}. \tag{3.34}$$

3.2 Diagonalization of the 2^N Hamiltonians from our Quantum Kinetic Ising model

We proceed now to give the corresponding diagonalization, though the well-known three transformations (Jordan-Wigner transformation, discrete Fourier transformation, and Bogoliubov transformation) of each of the 2^N Hamiltonians (3.34), and considering N even and PBC when necessary. We fix $\tau \in \{0,1\}^{2^N}$. From the same development of the model above, recall that

$$\begin{aligned}
&\sigma^z_{j-1}\sigma^z_{j+1}\sigma^x_j = (c^\dagger_{j-1} - c_{j-1})(c^\dagger_{j+1} + c_{j+1}),\\
&\sigma^z_{j+1}\sigma^z_j = (c^\dagger_j - c_j)(c^\dagger_{j+1} + c_{j+1}),\\
&\sigma^z_{j-1}\sigma^z_j = \sigma^z_j\sigma^z_{j-1} = (c^\dagger_{j-1} - c_{j-1})(c^\dagger_j + c_j),
\end{aligned} \tag{3.35}$$

where $c_j = -iK_j\sigma^+_j$, and $c^\dagger_j = iK_j\sigma^-_j$, for $K_j = \exp\Big(i\pi\sum_{s=1}^{j-1}\sigma^-_s\sigma^+_s\Big)$. Then,

$$\begin{aligned}
H_\tau = &-\frac{\alpha}{2}\sum_{j=1}^{N}\{\tilde{A}_i(\gamma)(1-2c^\dagger_j c_j) - \tilde{B}_i(\gamma)(c^\dagger_{j-1} - c_{j-1})(c^\dagger_{j+1} + c_{j+1}) - 1\\
&+\frac{\gamma}{4}[1+\tau_{i-1}\tau_i](c^\dagger_{j-1} - c_{j-1})(c^\dagger_j + c_j) + \frac{\gamma}{4}[1+\tau_i\tau_{i+1}](c^\dagger_j - c_j)(c^\dagger_{j+1} + c_{j+1})\}.
\end{aligned} \tag{3.36}$$

Similarly with respect to previous computations, it is straightforward that

$$\begin{aligned}
&\frac{\gamma}{4}\sum_{j=1}^{n}(1+\tau_i\tau_{i+1})(c^\dagger_j - c_j)(c^\dagger_{j+1} + c_{j+1}) + \frac{\gamma}{4}\sum_{j=1}^{n}(1+\tau_{i-1}\tau_i)(c^\dagger_{j-1} - c_{j-1})(c^\dagger_j + c_j)\\
&= \frac{\gamma}{2}\sum_{j=1}^{n}(1+\tau_i\tau_{i+1})(c^\dagger_j - c_j)(c^\dagger_{j+1} + c_{j+1}).
\end{aligned} \tag{3.37}$$

Therefore, from (3.36),

$$\begin{aligned}
H_\tau = &-\frac{\alpha}{2}\sum_{j=1}^{N}\{\tilde{A}_j(\gamma)(1-2c^\dagger_j c_j) - \tilde{B}_j(\gamma)(c^\dagger_{j-1} - c_{j-1})(c^\dagger_{j+1} + c_{j+1}) - 1\\
&+\frac{\gamma}{2}(1+\tau_j\tau_{j+1})(c^\dagger_j - c_j)(c^\dagger_{j+1} + c_{j+1})\}.
\end{aligned} \tag{3.38}$$

Reached this point, it is straightforward that we can write $\tilde{A}_j(\gamma)$ and $\tilde{B}_j(\gamma)$ as

$$\begin{aligned}
\tilde{A}_j(\gamma) &= \left(\frac{1+\tau_{j-1}\tau_{j+1}}{2}\right)A_1 + \left(\frac{1-\tau_{j-1}\tau_{j+1}}{2}\right)A_2,\\
\tilde{B}_j(\gamma) &= \left(\frac{1+\tau_{j-1}\tau_{j+1}}{2}\right)B_1 + \left(\frac{1-\tau_{j-1}\tau_{j+1}}{2}\right)B_2,
\end{aligned} \tag{3.39}$$

where A_1 and B_1 are the values $\tilde{A}_j(\gamma)$ and $\tilde{B}_j(\gamma)$ take when $\tau_{i-1} = \tau_{i+1}$, and A_2 and B_2 the values it takes when $\tau_{i-1} = -\tau_{i+1}$ (see (3.30) and (3.33)).

In order to apply a Fourier transformation, we take the H_τ's by pairs, taking each τ and its opposite version $-\tau$, yielding operators such that $H_{|\tau|} = H_\tau + H_{-\tau}$. Reordering the terms so as to have all positive $\tau_{j+1}\tau_{j-1}$ and all negative $\tau_{j+1}\tau_{j-1}$ together, we obtain

$$
\begin{aligned}
H_{|\tau|} &= -\frac{\alpha}{2}\sum_{j=1}^{N}\{A_1\left(\frac{1+\tau_{j-1}\tau_{j+1}}{2}\right)(1-2c_j^\dagger c_j) - B_1\left(\frac{1+\tau_{j-1}\tau_{j+1}}{2}\right)(c_{j-1}^\dagger - c_{j-1})(c_{j+1}^\dagger + c_{j+1}) - 1\} \\
&- \frac{\alpha}{2}\sum_{j=1}^{N}\{A_2\left(\frac{1-\tau_{j-1}\tau_{j+1}}{2}\right)(1-2c_j^\dagger c_j) - B_2\left(\frac{1-\tau_{j-1}\tau_{j+1}}{2}\right)(c_{j-1}^\dagger - c_{j-1})(c_{j+1}^\dagger + c_{j+1}) - 1\} \\
&- \frac{\alpha}{2}\sum_{j=1}^{N}\{\frac{\gamma}{2}(1+\tau_j\tau_{j+1})(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1})\} - \frac{\alpha}{2}\sum_{j=1}^{N}\{\frac{\gamma}{2}(1+(-\tau_j)(-\tau_{j+1}))(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1})\} \\
&= -\frac{\alpha}{2}\sum_{j=1}^{N}\{A_1(1-2c_j^\dagger c_j) - B_1(c_{j-1}^\dagger - c_{j-1})(c_{j+1}^\dagger + c_{j+1}) - 1\} \\
&- \frac{\alpha}{2}\sum_{j=1}^{N}\{A_2(1-2c_j^\dagger c_j) - B_2(c_{j-1}^\dagger - c_{j-1})(c_{j+1}^\dagger + c_{j+1}) - 1\} \\
&- \frac{\alpha}{2}\sum_{j=1}^{N}\{\gamma(1+\tau_j\tau_{j+1})(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1})\} \\
&= -\frac{\alpha}{2}\sum_{j=1}^{N}\{(A_1+A_2)(1-2c_j^\dagger c_j) - (B_1+B_2)(c_{j-1}^\dagger - c_{j-1})(c_{j+1}^\dagger + c_{j+1}) - 2 \\
&+ \gamma(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1})\} - \frac{\alpha\gamma}{2}\sum_{j=1}^{N}\{\tau_j\tau_{j+1}(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1})\}. \qquad (3.40)
\end{aligned}
$$

Therefore, redefining $\tilde{c}_j = \tau_j c_j$, we must also apply DFT on these other spinless fermionic operators, because $H_{|\tau|}$ takes the form

$$
\begin{aligned}
H_{|\tau|} &= -\frac{\alpha}{2}\sum_{j=1}^{N}\{(A_1+A_2)(1-2c_j^\dagger c_j) - (B_1+B_2)(c_{j-1}^\dagger - c_{j-1})(c_{j+1}^\dagger + c_{j+1}) - 2 \\
&+ \gamma(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1})\} - \frac{\alpha\gamma}{2}\sum_{j=1}^{N}\{(\tilde{c}_j^\dagger - \tilde{c}_j)(\tilde{c}_{j+1}^\dagger + \tilde{c}_{j+1})\} \\
&= -\frac{\alpha}{2}\sum_{j=1}^{N}\{(A_1+A_2)(1-2c_j^\dagger c_j) - (B_1+B_2)(c_{j-1}^\dagger - c_{j-1})(c_{j+1}^\dagger + c_{j+1}) - 1 \\
&+ \gamma(c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1})\} - \frac{\alpha\gamma}{2}\sum_{j=1}^{N}\{(\tilde{c}_j^\dagger - \tilde{c}_j)(\tilde{c}_{j+1}^\dagger + \tilde{c}_{j+1})\} + \frac{\alpha N}{2}. \qquad (3.41)
\end{aligned}
$$

The first sum, which we denote h_1, has already been diagonalized in the studied 1D Glauber-Ising scenario, so we use the well-known result. Regarding the second sum, we denote it by $h_{|\tau|}$ and compute it with an analogous procedure. With respect to the constant term, we can omit it. Note that we are interested in energy eigenvalues differences, given that global phases will not play a relevant role in our setting.
We now apply the following discrete Fourier transformations, for N even, as in the already studied scheme:

$$
c_j = \frac{1}{\sqrt{N}}\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} e^{ijk} d_k, \quad c_j^\dagger = \frac{1}{\sqrt{N}}\sum_{k=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-ijk} d_k^\dagger, \quad j = 1, \ldots, N. \qquad (3.42)
$$

For the first sum, we obtain:

$$h_1 = -\frac{\alpha}{2}\sum_{l=0}^{\pi}[g_l + i f_l(d_l^\dagger d_{-l}^\dagger + d_l d_{-l}) + c_l(d_l^\dagger d_l + d_{-l}^\dagger d_{-l})], \tag{3.43}$$

where

$$\begin{aligned}
&g_l = 2(A_1 + A_2 - 1 - 2\gamma\cos(l)) \ \ (l \neq 0, \pi), \ \ g_0 = A_1 + A_2 - 1 - 2\gamma, \ \ g_\pi = A_1 + A_2 - 1 + 2\gamma, \\
&f_l = 2[\gamma\sin(l) - (B_1 + B_2)\sin(2l)], \ \text{for any } l, \\
&c_l = 2[-A_1 - A_2 - (B_1 + B_2)\cos(2l) + \gamma\cos(l)] \ \ (l \neq 0, \pi), \\
&c_0 = -A_1 - A_2 - B_1 - B_2 + \gamma, \ \ c_\pi = -A_1 - A_2 - B_1 - B_2 - \gamma.
\end{aligned} \tag{3.44}$$

Applying a Bogoliubov rotation analogous to (2.65), we obtain

$$h_1 = -\frac{\alpha}{2}\sum_{l=0}^{\pi}\{g_l + c_l - \sqrt{c_l^2 + f_l^2} + \sqrt{c_l^2 + f_l^2}(\xi_l^\dagger \xi_l + \xi_{-l}^\dagger \xi_{-l})\}. \tag{3.45}$$

Namely, Boliubov rotation angle, for $l = 0, \pi$, turns into

$$\theta_0 = 0 = \theta_\pi; \tag{3.46}$$

while, for any $l = 2k\pi/N$, where $k = -N/2 + 1, \ldots, N/2$, is

$$\begin{aligned}
&\theta_k = \arcsin\{[(B_1 + B_2)\sin(4\pi k/N) - \gamma\sin(2\pi k/N)] \\
&/[\sqrt{((B_1 + B_2)\sin(4\pi k/N) - \gamma\sin(2\pi k/N))^2 + (-A_1 - A_2 - (B_1 + B_2)\cos(4\pi k/N) + \gamma\cos(2\pi k/N))^2}]\},
\end{aligned} \tag{3.47}$$

where the whole expression inside the keys is the argument of function arcsin. Now, for $h_{|\tau|}$, we apply same transformations (3.42), but with fermionic operators in momentum space $\tilde{d}_l$. We obtain that

$$h_{|\tau|} = -\frac{\alpha\gamma}{2}\sum_l [2\cos(l)\tilde{d}_l^\dagger \tilde{d}_l - e^{-il}(\tilde{d}_l^\dagger \tilde{d}_{-l}^\dagger + \tilde{d}_l \tilde{d}_{-l}) - e^{il}]. \tag{3.48}$$

Now, recall that we consider PBC and N even. This implies that $l = 2\pi k/N$, for $k \in \{1 - N/2, \ldots, N/2\}$. Furthermore, given the even nature of the cosine and the equality $2\cos(x) = e^{ix} + e^{-ix}$ for any $x \in \mathbb{C}$, then, following a procedure very similar to the one carried out in the already studied kinetic Ising model:

$$\begin{aligned}
\star \sum_l 2\cos(l)\tilde{d}_l^\dagger \tilde{d}_l &= 2\tilde{d}_0^\dagger \tilde{d}_0 - 2\tilde{d}_\pi^\dagger \tilde{d}_\pi + \sum_{l=-\pi+\frac{2\pi}{N}}^{-\frac{2\pi}{N}} 2\cos(l)\tilde{d}_l^\dagger \tilde{d}_l + \sum_{l=\frac{2\pi}{N}}^{\pi-\frac{2\pi}{N}} 2\cos(l)\tilde{d}_l^\dagger \tilde{d}_l \\
&= 2\tilde{d}_0^\dagger \tilde{d}_0 - 2\tilde{d}_\pi^\dagger \tilde{d}_\pi + \sum_{l=\frac{2\pi}{N}}^{\pi-\frac{2\pi}{N}} 2\cos(l)(\tilde{d}_l^\dagger \tilde{d}_l + \tilde{d}_{-l}^\dagger \tilde{d}_{-l}).
\end{aligned} \tag{3.49}$$

$$\begin{aligned}
\star \sum_l e^{-il}(\tilde{d}_l^\dagger \tilde{d}_{-l}^\dagger + \tilde{d}_l \tilde{d}_{-l}) &= \sum_{l=-\pi+\frac{2\pi}{N}}^{-\frac{2\pi}{N}} e^{-il}(\tilde{d}_l^\dagger \tilde{d}_{-l}^\dagger + \tilde{d}_l \tilde{d}_{-l}) + \sum_{l=\frac{2\pi}{N}}^{\pi-\frac{2\pi}{N}} e^{-il}(\tilde{d}_l^\dagger \tilde{d}_{-l}^\dagger + \tilde{d}_l \tilde{d}_{-l}) + (\tilde{d}_0^\dagger \tilde{d}_0^\dagger + \tilde{d}_0 \tilde{d}_0) \\
&+ (\tilde{d}_\pi^\dagger \tilde{d}_{-\pi}^\dagger + \tilde{d}_\pi \tilde{d}_{-\pi}) = -2i\sum_{l=\frac{2\pi}{N}}^{\pi-\frac{2\pi}{N}} \sin(l)(\tilde{d}_l^\dagger \tilde{d}_{-l}^\dagger + \tilde{d}_l \tilde{d}_{-l}) = -2i\sum_{l=0}^{\pi} \sin(l)(\tilde{d}_l^\dagger \tilde{d}_{-l}^\dagger + \tilde{d}_l \tilde{d}_{-l}).
\end{aligned} \tag{3.50}$$

$$\star \sum_l e^{il} = 2\sum_{l=0}^{\pi}\cos(l). \tag{3.51}$$

In the first and second sums, we put together the sums with opposite momenta l and $-l$. In the second one, we used as well fermionic anti-commutation relations, in order to obtain $\tilde{d}_0\tilde{d}_0 = \tilde{d}_0^\dagger\tilde{d}_0^\dagger = 0$ and $\tilde{d}_\pi\tilde{d}_\pi = \tilde{d}_\pi^\dagger\tilde{d}_\pi^\dagger = 0$, using the boundary condition $\tilde{d}_\pi = \tilde{d}_{-\pi}$ for the latter. All in all, we obtain

$$h_{|\tau|} = -\frac{\alpha\gamma}{2}\sum_{l=0}^{\pi}\{2\cos(l)(\tilde{d}_l^\dagger\tilde{d}_l + \tilde{d}_{-l}^\dagger\tilde{d}_{-l}) - 2i\sin(l)(\tilde{d}_l^\dagger\tilde{d}_{-l}^\dagger + \tilde{d}_l\tilde{d}_{-l}) + 2\cos(l)\} - 2\tilde{d}_0^\dagger\tilde{d}_0 + 2\tilde{d}_\pi^\dagger\tilde{d}_\pi. \tag{3.52}$$

Now, we are in position of applying a Bogoliubov rotation of the form (2.65). From such expressions, and for each term of the sum in (3.52), we have, denoting by φ_l the angle of the Bogoliubov rotation:

$$\begin{aligned} &2\cos(l)(\tilde{d}_l^\dagger\tilde{d}_l + \tilde{d}_{-l}^\dagger\tilde{d}_{-l}) - 2i\sin(l)(\tilde{d}_l^\dagger\tilde{d}_{-l}^\dagger + \tilde{d}_l\tilde{d}_{-l}) + 2\cos(l) \\ &= 2(\tilde{\xi}^\dagger\tilde{\xi}_l + \xi_{-l}^\dagger\tilde{\xi}_{-l})[\cos(l)\cos(\varphi_l) + \sin(l)\sin(\varphi_l)] \\ &+ 2i(\tilde{\xi}_l^\dagger\xi_{-l}^\dagger + \tilde{\xi}_l\tilde{\xi}_{-l})[\cos(l)\sin(\varphi_l) - \sin(l)\cos(\varphi_l)] \\ &+ [4\cos(l)\sin^2(\varphi_l/2) - 2\sin(l)\sin(\varphi_l) + 2\cos(l)]. \end{aligned} \tag{3.53}$$

From the same transformation, terms $\tilde{d}_0^\dagger\tilde{d}_0$ and $\tilde{d}_\pi^\dagger\tilde{d}_\pi$ can be expressed as

$$\tilde{d}_0^\dagger\tilde{d}_0 = \cos(\varphi_0)\tilde{\xi}_0^\dagger\tilde{\xi}_0 + \sin^2(\varphi_0/2), \quad \tilde{d}_\pi^\dagger\tilde{d}_\pi = \cos(\varphi_\pi)\tilde{\xi}_\pi^\dagger\tilde{\xi}_\pi + \sin^2(\varphi_\pi/2), \tag{3.54}$$

where we used again $\tilde{d}_0\tilde{d}_0 = \tilde{d}_0^\dagger\tilde{d}_0^\dagger = 0$ and $\tilde{d}_\pi\tilde{d}_\pi = \tilde{d}_\pi^\dagger\tilde{d}_\pi^\dagger = 0$, PBC on $\xi_{-\pi} = \xi_\pi$, as well as (C.2) from appendix (C). Now, we select Bogoliubov angle in order to make zero terms with coupled opposite momenta. We select, for all l:

$$\sin(\varphi_l) = \sin(l), \quad \cos(\varphi_l) = \cos(l). \tag{3.55}$$

In other words, taking $\varphi_l = l$ for all l, we obtain

$$h_{|\tau|} = -\frac{\alpha\gamma}{2}\sum_{l=0}^{\pi}\{2(\tilde{\xi}^\dagger\tilde{\xi}_l + \xi_{-l}^\dagger\tilde{\xi}_{-l}) + 2(2\cos(l) - 1)\} - 2\tilde{\xi}_0^\dagger\tilde{\xi}_0 - 2\tilde{\xi}_\pi^\dagger\tilde{\xi}_\pi + 2, \tag{3.56}$$

where we used that, from (3.55),

$$\begin{aligned} &\star\, 4\cos(l)\sin^2(\varphi_l/2) - 2\sin(l)\sin(\varphi_l) + 2\cos(l) = 4\cos(l)\left(\frac{1-\cos(l)}{2}\right) - 2 + 2\cos^2(l) + 2\cos(l) \\ &= 2(2\cos(l) - 1), \end{aligned} \tag{3.57}$$

$$\begin{aligned} &\star\, \sin^2(\theta_0/2) = \frac{1-\cos(0)}{2} = 0, \quad \sin^2(\theta_\pi/2) = \frac{1-\cos(\pi)}{2} = 1, \\ &\star\, \cos(\varphi_0) = \cos(0) = 1, \quad \cos(\varphi_\pi) = \cos(\pi) = -1. \end{aligned} \tag{3.58}$$

Therefore, from (3.56), (3.45) and (3.41), we obtain, for each $\tau \in \{0, \ldots, 2^N - 1\}$,

$$\begin{aligned} H_{|\tau|} = &-\frac{\alpha}{2}\sum_{l=0}^{\pi}\{g_l + c_l - \sqrt{c_l^2 + f_l^2} + \sqrt{c_l^2 + f_l^2}(\xi_l^\dagger\xi_l + \xi_{-l}^\dagger\xi_{-l})\} \\ &- \frac{\alpha\gamma}{2}\sum_{s=0}^{\pi}\{2(\tilde{\xi}_s^\dagger\tilde{\xi}_s + \tilde{\xi}_{-s}^\dagger\tilde{\xi}_{-s}) + 2(2\cos(s) - 1)\} - 2\tilde{\xi}_0^\dagger\tilde{\xi}_0 - 2\tilde{\xi}_\pi^\dagger\tilde{\xi}_\pi + 2 + \frac{\alpha N}{2}, \end{aligned} \tag{3.59}$$

where we denote by s the momentum for the fermionic particles with occupation number operators $\tilde{\xi}_s^\dagger\tilde{\xi}_s$, so that we can distinguish both kinds of momentum: from operator h_1, and from operator $h_{|\tau|}$.

Omitting operator-independent terms from (3.59), we have the following quantum master operator:

$$H_{|\tau|} = -\frac{\alpha}{2}\sum_{l=0}^{\pi}\sqrt{c_l^2+f_l^2}(\xi_l^\dagger\xi_l+\xi_{-l}^\dagger\xi_{-l}) - \alpha\gamma\sum_{s=0}^{\pi}(\tilde{\xi}_s^\dagger\tilde{\xi}_s+\tilde{\xi}_{-s}^\dagger\tilde{\xi}_{-s}) - 2\tilde{\xi}_0^\dagger\tilde{\xi}_0 - 2\tilde{\xi}_\pi^\dagger\tilde{\xi}_\pi. \tag{3.60}$$

Therefore, we obtain the following eigenvalues, each corresponding to each element of the basis of Master's operator eigenstates expressed in terms of fermionic occupation after Bogoliubov rotation:

$$w_{l,s} = \begin{cases} -\frac{\alpha}{2}\sqrt{c_l^2+f_l^2} - \alpha\gamma & \text{if } s\neq 0,\pi \ \ (s\neq 0,\pi) \\ -\frac{\alpha}{2}\sqrt{c_l^2+f_l^2} - (2+\alpha\gamma) & \text{if } s=0 \ \ (k=0 \text{ and } k=N/2). \end{cases} \tag{3.61}$$

where l and s are momenta for the first (h_1) and the second ($h_{|\tau|}$) fermionic particles in $H_{|\tau|}$, respectively. Note that, since $c_l = c_{-l}$ and $f_l = -f_{-l}$, these eigenvalues are equal for each $l\neq 0,\pi$ and its counterpartner $-l$. This statement is also applicable to s and $-s$, for $s\neq 0,\pi$.

Following the approach from [57], we find a feasibly computational approach, as we are about to see, for this kind of analytical diagonalization: we could interpret $\xi_l^\dagger\xi_l$ and $\tilde{\xi}_s^\dagger\tilde{\xi}_s$ operators, respectively, as different kinds of quasi-particles occupation number operators. This is an important consideration when departing from specific initial states when applying our circuit, since we must take into account fermionic occupation of both types of quasi-particles.

4 Quantum simulation: implementation and numerical results

In this section, we provide the structure of the quantum circuit that yields a proper diagonalization for the studied Master equations, both from original Glauber-Ising model and for the extended quantum Master version, understanding W_β (after the corresponding *hermitization*) as the Hamiltonian whose eigenvalues and eigenstates we are interested in. Simulation and computations in this work are focused in a more simple operator: Ising Hamiltonian with external transverse magnetic field. We base the present implementation approach on the analytical diagonalization provided so far, following the same steps from [59] and [58]. Nevertheless, our ultimate objective regarding implementation is to diagonalize each of the $H_{|\tau|}$ from (3.41), varying $\tau\in\{0,\ldots,2^N-1\}$, although such calculations are not included in this work, but in its outlook.

Once the diagonalization circuit, represented by a unitary operator U_{dis}, is clear, we proceed to compute expectation value of a relevant physical property: spin along the z-direction. Such operator U_{dis} let us consider fermionic occupation of mometum modes in a first instance, in order to obtain the corresponding state expressed in the basis of eigenstates of z-Pauli matrices, which in turn let us compute the aforementioned expectation values more easily. The way we decompose quantum gates is summarized in appendix (D), and some highlighted codes for the following computations are included in appendix (E). In particular, the code we represent in the aforementioned appendix for the quantum circuit we use for diagonalization corresponds to Master's operators considered so far, and thus to its corresponding Bogoliubov angles, all of them given in similar terms. Note that, when applying such a circuit to a different Hamiltonian, all we need is changing the Bogoliubov angle to the one obtained after the corresponding diagonalization.

4.1 Implementation of U_{dis}

In this section, we give a brief exposure of how the quantum circuit is constructed following the same steps from [59]. That is, our immediate goal is to identify the quantum circuit that disentangles

(3.41) for each of the $\tau \in \{0, \dots, 2^N - 1\}$ or, as we will see explicitly, Hamiltonian (4.16). For N spins (which is going to correspond exactly to the number of qbits), from the aforementioned reference, we know that the circuit consists of a number of gates that scales as N^2 and a depth which scales as $N \log(N)$.

The analytical path which guides us to build such U_{dis} consists, as we saw, in three main parts: Jordan-Wigner map of spins into fermions, discrete Fourier transform to locate fermions in momentum space, and Bogoliubov rotations to express the operator in terms of free fermions.

According to the first part, it is all about relabeling the degrees of freedom of the physical system. Fermionic operators c_j, in each of the lattice sites $j \in \{1, \dots, N\}$, are useful for translating the degrees of freedom which, at the end, will pass through the filter of a Fourier transform. In more algebraic terms, we use the maps from (2.28), which are thought to transform spin operators into fermionic operators $c_i, c_i^\dagger$, i.e., fermionic annihilation and creation operators acting on the vacuum $|\Omega_c\rangle$ in a way such that

$$\{c_i, c_j\} = 0, \quad \{c_i, c_j^\dagger\} = \delta_{ij}, \quad c_i|\Omega_c\rangle = 0. \tag{4.1}$$

In short, Jordan-Wigner transform takes states of spin 1/2 particles, given by

$$|\psi\rangle = \sum_{i_1,\dots,i_N=0,1} \psi_{i_1,\dots,i_N} |i_1, \dots, i_N\rangle, \tag{4.2}$$

into fermionic states of the form

$$|\psi\rangle = \sum_{i_1,\dots,i_N=0,1} \psi_{i_1,\dots,i_n} (c_1^\dagger)^{i_1} \dots (c_N^\dagger)^{i_N} |\Omega_c\rangle. \tag{4.3}$$

It is straightforward that, during the transformation, there is no effect on the coefficients $\psi_{i_1,\dots,i_N}$. This means that, for Jordan-Wigner transformation, we do not have to include any explicit gate in the circuit, as long as we do not forget to swap the corresponding degrees of freedom with minus sign. In general terms, when performing $U_{dis}^\dagger$, Jordan-Wigner transformation let us depart from states which can be read as fermionic states, whose simplicity is due to Pauli exclusion principle. In computational terms, it thus does not need any intervention in the system, apart from the fermionic analogous version of SWAP gate (fSWAP), needed every time we swap qbits. Such an operator is given by

$$\text{fSWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{4.4}$$

Unlike Jordan-Wigner transformation, Fourier and Bogoliubov maps do act on the original spin σ degrees of freedom, giving to U_{dis} its main structure:

$$U_{\text{dis}} = U_{\text{Bog}} U_{\text{FT}}, \tag{4.5}$$

where U_{FT} and U_{Bog} refer to the unitary operators for Fourier transform and Bogoliubov rotation. The following scheme, extracted from [59], gives a clear image of what is happening in our diagonalization circuit, starting from an initial Hamiltonian H:

$$H = H_1[\sigma] \leftarrow H_1[c] \leftarrow H_2[d] \leftarrow H_4[\xi] = \tilde{H}, \tag{4.6}$$

where $H = H_1[\sigma]$, $H_1[c]$, $H_2[d]$, and $H_4[\xi] = \tilde{H}$ refer, respectively from left to right, to the original (Ising or Master operator in our study) Hamiltonian, and the Hamiltonian after Jordan-Wigner map, after Fourier transform, and after Bogoliubov rotation, with the corresponding degrees of freedom denoted between brackets (as it was denoted in previous sections). Namely, for N even and PBC, recall that the Fourier tranformation acting on the fermionic modes is given by

$$d_k = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{i\frac{2\pi jk}{N}} c_j, \quad k = -\frac{N}{2} + 1, \ldots, \frac{N}{2}. \tag{4.7}$$

From previous notation, when going from $H_2[c]$ to $H_3[d]$, we are getting profit of translational invariance and putting the Hamiltonian into momentum space. In particular, we limit the construction to a circuit given in terms of two-body local gates for $N = 2^p$, for some $p \in \mathbb{N}$, which is exactly the context in which classical fast Fourier transform can be performed. Note that for a matrix of dimension

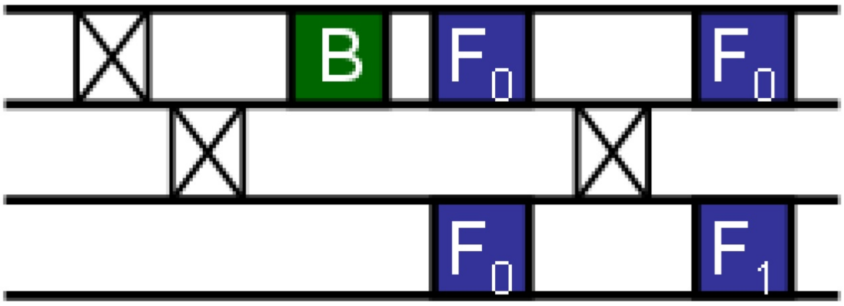

Figure 3: Quantum circuit which implements $U^\dagger_{dis}$ for Fourier tranform and Bogoliubov rotation, yielding both $U^\dagger_{FT}$ and $U^\dagger_{Bog}$ along with the necessary fSWAPS, for $N = 4$ spins. Image from [59]. Note that, for $N = 4$ spins, and apart from fSWAP gates, we only need 6 gates. In fact, we only need 5 gates, as we see in the figure, if we do no count the identity obtained from Bogoliubov rotation B^4_0 when departing from $|00\rangle$ or $|11\rangle$ in qbits corresponding to momenta $k = 0$ and $k = 2$. In such a context, $B = B^4_1$.

$d \in \mathbb{N}$, classical Fourier transform complexity scales as d^2, while, as we will see schematically, fast Fourier transform complexity scales as $d\log(d)$. This lies on the fact that the latter consists on two parallel Fourier transformations over $N/2$ lattices sites (for N the number of spins), the even and the odd sites, given in the form [72]:

$$\sum_{j=0}^{N-1} e^{\frac{2\pi ikj}{N}} c^\dagger_j = \sum_{j'=0}^{\frac{N}{2}-1} e^{\frac{2\pi ikj'}{N/2}} c^\dagger_{2j'} + e^{\frac{2\pi ik}{N}} e^{\frac{2\pi ikj'}{N/2}} c^\dagger_{2j'+1}. \tag{4.8}$$

To implement such an operation, we can understand it as a combination of a two-qbit gate, the so-called *beam splitter*, and one-qbit gate, the *phase-delay* w^k_N. The latter applies the so-called *twiddle-factor*. Namely,

$$F_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad w^k_N = \begin{pmatrix} 1 & 0 \\ 0 & e^{\frac{2\pi ik}{N}} \end{pmatrix}, \tag{4.9}$$

where fermionic anti-commutation has been considered in F_2 with its last entry. With all that in mind, the Fourier transform gate is

$$F_k^N = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{e^{\frac{2\pi i k}{N}}}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{e^{\frac{2\pi i k}{N}}}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & -e^{\frac{2\pi i k}{N}} \end{pmatrix}. \tag{4.10}$$

To illustrate the method in which we implement fast Fourier transform, let's consider the case of $N = 4$ spins (see figure 3). Modes are transformed into the momentum space, from (4.7), as

$$d_k = (c_0 + e^{2\pi i \frac{2k}{4}} c_2) + e^{2\pi i \frac{k}{4}} (c_1 + e^{2\pi i \frac{2k}{4}} c_3), \tag{4.11}$$

that is, firstly modes 0 and 2, and modes 1 and 3 are mixed in the same way, and then another mixing takes place. The first step of the method would be

$$\begin{aligned} c_0' &= c_0 + c_2, \quad c_1' = c_! + c_3, \\ c_2' &= c_0 + e^{i\pi} c_2, \quad c_3' = c_1 + e^{i\pi} c_3. \end{aligned} \tag{4.12}$$

As we can see in figure 3, there are two identical Fourier gates in the first part of $U_{FT}^\dagger$; and then, more mixtures take place along with some fermionic swaps. The explicit form of F_2 can be discovered by writing down the tranformation from, e.g., modes 0 and 2:

$$|\psi\rangle = \sum_{i,j=0,1} A'_{ij} (c_0'^\dagger)^i (c_2'^\dagger)^j |00\rangle = \sum_{i,j=0,1} A_{ij} (c_0^\dagger + c_2^\dagger)^i (c_0^\dagger + e^{-i\pi} c_2^\dagger)^j |00\rangle. \tag{4.13}$$

By expanding this last expression, the coefficients of the resulting state, in the basis $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$, can be obtained through the operation $A' = F_2 A$, what gives us (4.9).

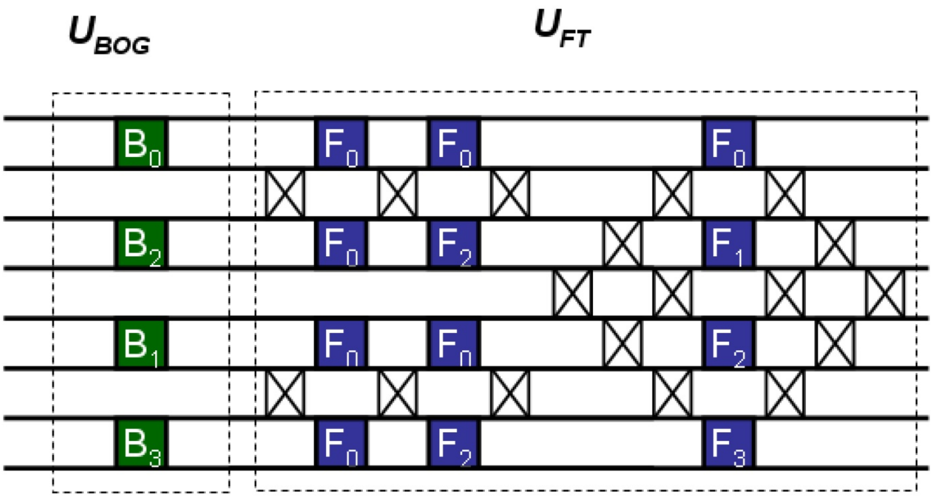

Figure 4: Quantum circuit of $U_{dis}^\dagger$ for Fourier tranform and Bogoliubov rotation, yielding both $U_{FT}^\dagger$ and $U_{Bog}^\dagger$ along with the necessary fSWAPS, for $N = 8$ spins. Image from [59]. We are denoting $B_k^8 = B_k$.

This fast Fourier transformation (4.10) has depth $N \log(N)$ for N spins and, along with the necessary fSWAPS, gates number scales as N^2 (see [59] to go further with this complexity analysis). For $N = 2^p$ spins, our circuit requires $2^{p-1}(2^p - 1)$ local quantum gates, for which pN are lattice site-dependent interacting gates. The rest consists of the aforementioned fSWAPS.

As we know, the final transformation of the diagonalization process is a Bogoliubov rotation given as (2.65), with the coefficients determined by the form of the Hamiltonian as a sum of operators defined on the momentum space, and obtained after Fourier transformation. In other words, the Bogoliubov angle θ_k that let us finish our disentanglement depends also on such Hamiltonian. The mixing of pairs of modes performed by this Bogoliugov rotation is given by an operator like

$$B_k^N = \begin{pmatrix} \cos(\theta_k/2) & 0 & 0 & i\sin(\theta_k/2) \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ i\sin(\theta_k/2) & 0 & 0 & \cos(\theta_k/2), \end{pmatrix} \tag{4.14}$$

where θ_k is the Bogoliubov angle of the pair of modes correspoding to $k, -k \in \{-N/2+1, \dots, N/2\}$.

All in all, this yields the Hamiltonian in the following diagonalized form:

$$H_4[\xi] = \sum_{k=-N/2+1}^{N/2} w_k \xi_k^\dagger \xi_k. \tag{4.15}$$

This $H_4[\xi]$ is equivalent to the original form of the Hamiltonian $H = \sum_i w_i \sigma_i^z$, for σ_i^z the z-Pauli matrix in the i-th lattice site, and w_i the corresponding eigenvalue when such a Pauli matrices eigenstates basis is selected. This is the analytical procedure whose operations we aim to reproduce in a quantum circuit. In appendix E we represent the code we use for the $U_{dis}^\dagger$ derived from the one-dimensional Glauber-Ising model whose analytical diagonalization we have developed in detail during the document. For that purposed, we use *Qiskit* (see `https://qiskit.org/documentation/`) library in programming language *Python* (see `https://www.python.org/downloads/release/python-397/` for the specific version we use).

4.2 Analysis of an Ising Hamiltonian

In this section, we provide the reader with some relevant and useful results and procedures in the quantum simulation from [58] and [59], which let us illustrate the described circuit directly on an Ising Hamiltonian, instead of a one-dimensional Master operator extracted from Glauber's model. The analytical diagonalization resolution is the same, apart from a determinant key: the operator to diagonalize is different, what is translated, in terms of circuit implementation, in a different Bogoliubov angle. The methodology for the computation of expectation values is based on [58] as well.

4.2.1 Diagonalization of an Ising Hamiltonian

We must note that here the entire diagonalization is based on an antiferromagnetic Hamiltonian with transverse external magnetic field, given by

$$H_a = \sum_{i=1}^{N} \sigma_i^x \sigma_{i+1}^x + \sigma_1^y \sigma_2^z \dots \sigma_{n-1}^z \sigma_n^y + \lambda \sum_{i=1}^{N} \sigma_i^z, \tag{4.16}$$

where λ is the transverse field strength. In the setting we have been studying so far, in terms of the Master's operator, we have always restricted the analysis to $\lambda = 0$, since we avoided external magnetic field considerations. Moreover, the second term let us cancel the periodic boundary term $\sigma_N^x \sigma_1^x$ after the corresponding Jordan-Wigner transformation. This, as it is pointed out in [58], let us solve the system as it was infinite, and has finite size effects that will become negligible for N

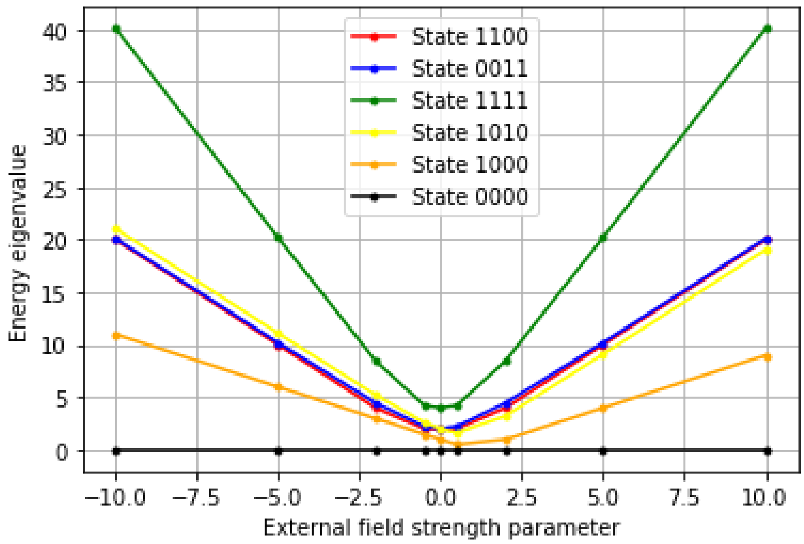

Figure 5: Energy eigenvalues for Hamiltonian (4.16) eigenstates $|1100\rangle$, $|0011\rangle$, $|1111\rangle$, $|1010\rangle$, $|1000\rangle$ and vacuum state $|0000\rangle$ (given in order of momenta determined by $k=0$, $k=2$, $k=1$ and $k=-1$), versus external field strength parameter λ.

large. We consider PBC and N even in the form $N=2^p$ for some $p\in\mathbb{N}$ (this let us perform fast Fourier transformation). In this context, we are in position of providing, from [58], the expression of H_a after the different stages of the diagonalization process:

$$\begin{aligned}
&\text{Jordan-Wigner: } H_a = \frac{1}{2}\sum_{i=1}^{N}(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i + c_i c_{i+1} + c_i^\dagger c_{i+1}^\dagger) + \lambda\sum_{i=1}^{N} c_i^\dagger c_i,\\
&\text{Fourier: } H_a = \sum_{k=-N/2+1}^{N/2}[2(\lambda-\cos(2\pi k/N)))b_k^\dagger b_k + i\sin(2\pi k/N)(b_{-k}^\dagger b_k^\dagger + b_{-k}b_k)],\\
&\text{Bogoliubov: } H_a = \sum_{k=-N/2+1}^{N/2} w_k a_k^\dagger a_k,
\end{aligned} \tag{4.17}$$

where $a_k^\dagger a_k$ are the corresponding number operators, for lattice site k in the momentum space, and with eigenvalue

$$w_k = \sqrt{(\lambda-\cos(2\pi k/N))^2 + \sin^2(2\pi k/N)}. \tag{4.18}$$

In figure 5 we represent the evolution of energy eigenvalues for different λ's and for several fixed Hamiltonian eigenstates, expressed with the same considerations and momenta order than section (2.2.4). Due to its key role in the circuit implementation, we represent the corresponding Bogoliubov rotation angle, recalling that such a rotation is implemented in the same way than (4.14):

$$\theta_k = \arccos\left(\frac{\lambda-\cos\left(\frac{2\pi k}{N}\right)}{\sqrt{(\lambda-\cos\left(\frac{2\pi k}{N}\right))^2+\sin^2\left(\frac{2\pi k}{N}\right)}}\right), \quad k=-\frac{N}{2}+1,\ldots,\frac{N}{2}. \tag{4.19}$$

In figure 6 we represent how Bogoliubov angle changes in this scheme with respect to external field strength λ for all possible momenta in the case of $N=4$ spins.

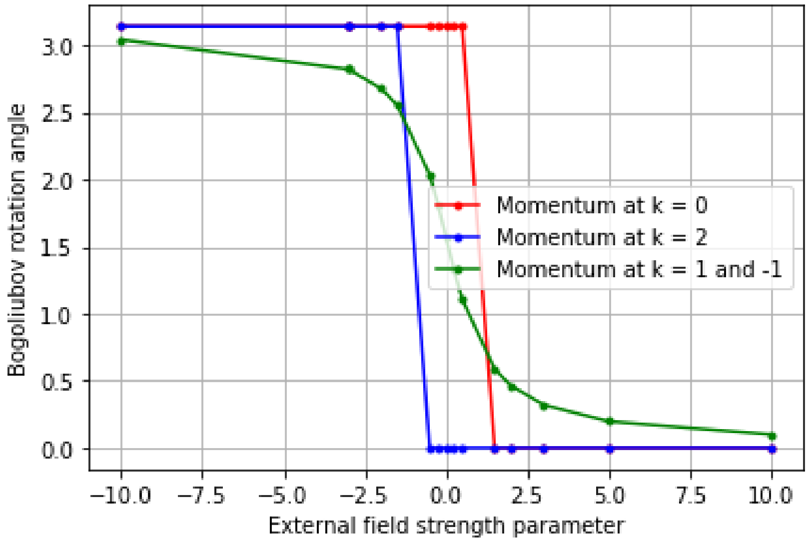

Figure 6: Bogoliubov rotation angles from (4.19) versus external field strength parameter λ, for each possible momentum, determined by $k = 0$, $k = 2$ and $k = 1$ or $k = -1$ ($N = 4$ spins). Note that red and blue lines ($k = 0$ and $k = 2$ respectively) coincide for, approximately, $|\lambda| > 1.5$.

4.2.2 Computation of $\langle \sigma_z \rangle$ with an antiferromagnetic Ising Hamiltonian

With regard to thermal simulation, we present two methods following the methodology in [58]. Firstly, note that the model we are now analyzing from such a paper responds to a Boltzmann thermal equilibrium. This means that we understand that model as a quantum system exposed to a heat bath through thermally distributed populations of states following a Boltzmann distribution, given by

$$\rho(\beta) = \frac{e^{-\beta H}}{Z_N(\beta)} = \frac{1}{Z_N(\beta)} \sum_i e^{-\beta E_i} |E_i\rangle\langle E_i|, \tag{4.20}$$

where $\beta = 1/(k_B T)$ (the so-called *temperature parameter*), T is the temperature, k_B the Boltzmann constant, N the number of spins, and $Z_N(\beta)$ is the partition function expressed as

$$Z_N(\beta) = \sum_i e^{-\beta E_i}. \tag{4.21}$$

This let us compute the expectation value of some observable O at finite temperature T as

$$\langle O(\beta)\rangle = \mathrm{Tr}[O\rho(\beta)] = \frac{1}{Z_N(\beta)} \sum_i e^{-i\beta E_i} \langle E_i|O|E_i\rangle. \tag{4.22}$$

Thermal simulation is direct through the operator U_{dis} we implement in a quantum circuit, given that the latter transforms states in the $H_4[\xi]$ into states in the σ_z-eigenstates basis. Since $|E_i\rangle$ are elements of the computational basis, expressed in terms of eigenstates of the Hamiltonian (namely, through fermionic occupation in momentum modes), qbits initialization in order to perform thermal simulation are not needed, apart from the necessary X gates.
With all this description of the present framework, thermal simulation in [58] is carried out through either exact simulation or sampling. The former consists of considering all possible initial states from the computational basis, compute the corresponding expectation value, and average the values obtained with their energies. The latter is performed by sampling among Hamiltonian eigenstates,

according to the aforementioned Boltzmann distribution (4.20), and then running the circuit and computing the expectation value from the randomly generated state, initially given in the Hamiltonian eigenstates basis, and finally in the σ_z eigenstates basis.

According to computational complexity (see [58]), we must make the following remark: the first method demands $K \times 2^N$ runs, for K the number of repetitions in order to do the average, since we are computing the expectation value for each element of the computational basis, with no statistical error. For the second method, maintaining notation, only K runs are needed, with a statistical error of $1/\sqrt{K}$.

We use only the second approach, since it let us take into account temperature considerations (Boltzmann distribution depends on the temperature parameter β). This would let us more easily establish the comparison with this setting and an out-of-equilibrium setting, which explicitly depends on the temperature. We implement, for $N = 4$ spins, the Boltzmann distribution sampling just described among all possible initial Hamiltonian eigenstates, given that we know the whole spectrum. We focus now on the analysis of $\langle \sigma_z \rangle$ versus λ and β, for fixed β's and λ's, respectively. To illustrate the computational procedure followed, in appendix E we represent the code used for a $\langle \sigma_z \rangle$ versus β simulation, for a specific fixed λ. In figures 7 and 8, we provide the plots of computed $\langle \sigma_z \rangle$ after

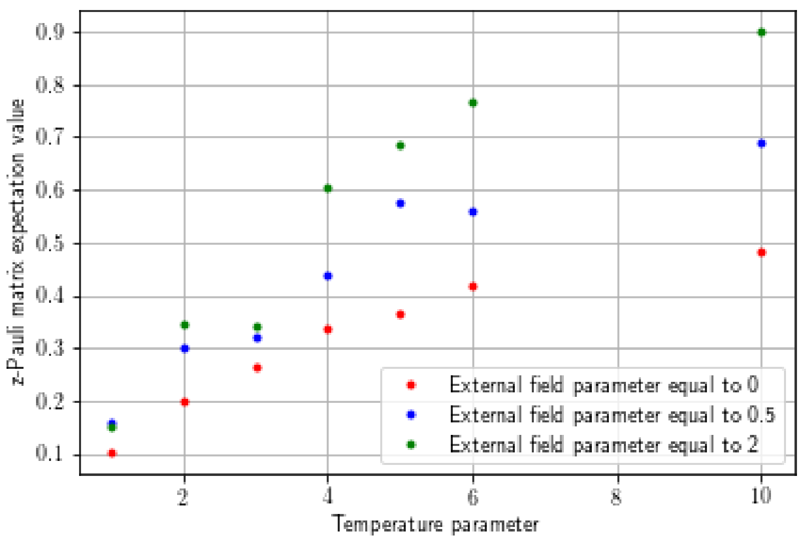

Figure 7: $\langle \sigma_z \rangle$ versus temperature parameter β, for fixed external field parameters $\lambda = 0, 0.5, 2$.

simulated diagonalization, versus β and λ, respectively. The implementation of these computations goes as follows: first of all, as mentioned above, we sample with Boltzmann distribution among all Hamiltonian eigenstates determined, as pointed out, through fermionic occupation in 4 momentum space modes; secondly, we perform circuit U_{dis} to pass from Hamiltonian eigenstates basis to σ_z eigenstates basis, in which computation of σ_z eigenvalues is straightforward through standard computations; then, we compute such eigenvalues, which in practice reduce to a product of 1's and -1's; and we repeat the approach just described as many times as desired (we carried out computations with 1000 samples), in order to provide a final estimation of $\langle \sigma_z \rangle$ with the corresponding average.

Note that physical implication [73] of the plots we have just mentioned serve us as sanity check for the computed simulation. On the one hand, dependence of $\langle \sigma_z \rangle$ with respect to temperature parameter β shows that for low temperatures ($\beta \to \infty$), the ground state, given by $\langle \sigma_z \rangle = 1$, tends to put on top of the other states; while for large temperatures ($\beta \to 0$), we find a probabilistically uniform situation in which, since all eigenstates are equally probable, $\langle \sigma_z \rangle$ tends to 0. Moreover, we

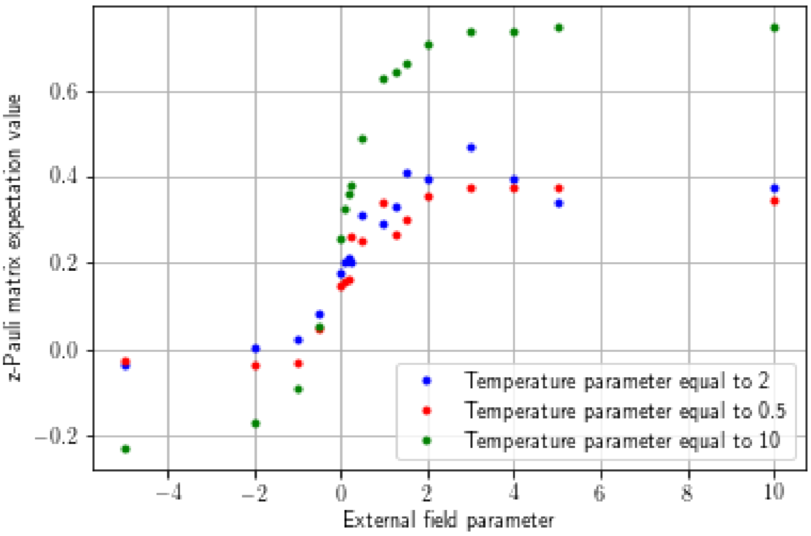

Figure 8: $\langle \sigma_z \rangle$ versus external field parameter λ, for fixed temperature parameters $\beta = 2, 0.5, 10$.

note that such a behaviour is more pronounced for higher values of λ.

On the other hand, regarding dependence of $\langle \sigma_z \rangle$ with respect to transverse external field strength λ, averaged spin (in z-direction) state transition around $\lambda = 1$ is visualized, going from -1 average spin for $\lambda < 1$, to 1 average spin for $\lambda > 1$, as it is expected for an antiferromangetic Ising model described by a Hamiltonian like (4.16).

5 Conclusions and outlook

We now summarize the most relevant points reached in the present document:

1. First of all, following [63] and [64], we carried out a formalization of Glauber-Ising model for a N-ring of spins 1/2, in terms of the corresponding Master equation, which permitted us to manage such an equation, primarily, through Pauli matrices. Then, we have developed three standard transformations (Jordan-Wigner, Fourier and Bogoliubov) in order to express the Master's operator that determines the aforementioned equation by free-fermion operators located in lattice sites of the momentum space. We have restricted the analysis to PBC and N even, when concreteness was required.

2. From the previous setting, following [57], we have extended the analytical diagonalization from populations to every entry of the corresponding density matrix of the system (populations and coherences) through a Lindblad formulation. Moreover, by performing some algebra over the operators, we have reached a very similar setting to the one obtained in the only-populations version, by dividing the original Master's operator into 2^N Hamiltonians. That allowed us to go ahead with an analogous analytical diagonalization, on each of the 2^N Hamiltonians, by considering two different kinds of fermionic quasi-particles.

3. In both procedures just described, indispensable parameters for quantum circuit implementation, which can only be obtained once the whole diagonalization process is considered, were determined: the Bogoliubov rotation angles. This is our first result.

4. Furthermore, we obtained, for all studied systems (quantum kinetic Glauber-Ising model, its extended version in terms of density matrices, and antiferromagnetic Ising model) the whole

energy spectrum, as well as the description of the corresponding eigenvectors. A computationally efficient and easy to interpret management of the latter algebra is essential for the implementation of the corresponding diagonalization quantum circuit.

5. Once established the theoretical approach for diagonalization, we set up a quantum circuit that let us pass states and operators from σ_z eigenstates basis, to the corresponding Hamiltonian eigenstates basis (included the case in which the Hamiltonian consists of a Master's operator); and in the other way round. This made necessary the study of quantum gate decompositions for the three aforementioned transformations. In particular, we provided such a quantum circuit for $N = 4$ spins and PBC. For such a quantum simulation, we must note that we did not implement it in any quantum computer, since given the computational level we reached, it made no remarkable difference. However, we implemented directly the circuit with *Qiskit* library in programming language *Python* in order to simulate our quantum circuit without taking considerations of circuit architectures.

6. Getting profit of the quantum circuit we implemented, we applied it to a more practical scheme: the computation of σ_z expectation values for the antiferromagnetic Hamiltonian studied in [58]. Indeed, we analyzed the behaviour of such $\langle\sigma_z\rangle$'s values against β and λ, which are the prefixed parameters of the considered Ising model. That served us as sanity checks for the diagonalization quantum circuit.

As outlook of this work, the logical immediate continuation could be, firstly, the repetition of the implemented quantum simulation for larger multiples of 2 (i.e., $N = 8, 16, \ldots$ spins); secondly, to simulate the diagonalization for the studied Master's operators, either from the original Glauber model or for the $H_{|\tau|}$ Hamiltonians obtained from the extended setting with density matrices; and thirdly, it would be highly interesting to implement all these algorithms in a quantum computer. All these points would let us, in terms of numerical simulations, properly compare both ways of diagonalizing an Ising Hamiltonian: with external magnetic field like in [58], and with thermal out-of-equilibrium dynamics through a Master equation. Furthermore, Master's operators computational diagonalization would also let us explore to which extent we are capable of using such a quantum kinetic model to solve out-of-equibilibrium complex problems, in a context of classical dynamics. As pointed out before, the latter is the point through which we intend to include an algorithm to the current list of NISQ algorithms.
In the future, we will study the possibility of using this or related strategies to Machine Learning problems. We notice that there is a close relationship between Ising models with arbitrary couplings and e.g. Boltzmann machines, which is well known in the traditional literature. See [74] [75] as examples of these approaches. Some techniques or physical contexts not studied in the present work may be necessary for this new perspective, such as the extension to more dimensions in the Ising models, or the use of variational quantum eigensolvers [76] [77].

A Jordan-Wigner computations

In this appendix, we show all necessary computations, with regard to the part based on the classical Glauber model (before extending its notion to the density matrix), related to the transformation from core-boson operators, given in terms of raising and lowering Pauli matrices, to spinless fermionic operators, and which did not fit, due to limited space, in the main part of this document. The Jordan-Wigner transformation acting on product terms of raising and lowering spin-1/2 operators appearing in W_β (see equation (2.27)) goes as we express below, for the crossed products in such a Master's operator. Given any $j \in \{1, \dots, N\}$, and recalling that, when not expressing superindex x, y or z, we assume superindex is z:

$$\star\sigma_j^x = (1 - 2c_j^\dagger c_j). \tag{A.1}$$

$$\begin{aligned}
&\star\, \sigma_{j-1}\sigma_{j+1} = -(\sigma_{j-1}^+ - \sigma_{j-1}^-)(\sigma_{j+1}^+ - \sigma_{j+1}^-) = -\sigma_{j-1}^+\sigma_{j+1}^+ + \sigma_{j-1}^+\sigma_{j+1}^- + \sigma_{j-1}^-\sigma_{j+1}^+ - \sigma_{j-1}^-\sigma_{j+1}^- \\
&= c_{j-1}(1-2n_{j-1})(1-2n_j)c_{j+1} + c_{j-1}(1-2n_{j-1})(1-2n_j)c_{j+1}^\dagger + c_{j-1}^\dagger(1-2n_{j-1})(1-2n_j)c_{j+1} \\
&+ c_{j-1}^\dagger(1-2n_{j-1})(1-2n_j)c_{j+1}^\dagger = -c_{j-1}c_{j+1}(1-2n_j) - c_{j-1}c_{j+1}^\dagger(1-2n_j) + c_{j-1}^\dagger c_{j+1}(1-2n_j) \\
&+ c_{j-1}^\dagger c_{j+1}^\dagger(1-2n_j).
\end{aligned} \tag{A.2}$$

where, to illustrate one of the calculations just developed, observe that, using anti-commutation relations:

$$c_{j-1}(1-2n_{j-1}) = c_{j-1}(1-2+2c_{j-1}c_{j-1}^\dagger) = -c_{j-1}. \tag{A.3}$$

Now, we use that, since $n_j^2 = n_j$, then $(1-2n_j)^2 = 1$. Therefore, regrouping terms,

$$\sigma_{j-1}\sigma_{j+1}\sigma_j^x = -c_{j-1}c_{j+1} - c_{j-1}c_{j+1}^\dagger + c_{j-1}^\dagger c_{j+1} + c_{j-1}^\dagger c_{j+1}^\dagger = (c_{j-1}^\dagger - c_{j-1})(c_{j+1}^\dagger + c_{j+1}). \tag{A.4}$$

On the other hand,

$$\begin{aligned}
\sigma_j\sigma_{j+1} &= -(\sigma_j^+ - \sigma_j^-)(\sigma_{j+1}^+ - \sigma_{j+1}^-) = -\sigma_j^+\sigma_{j+1}^+ + \sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+ - \sigma_j^-\sigma_{j+1}^- \\
&= c_j(1-2n_j)c_{j+1} + c_j(1-2n_j)c_{j+1}^\dagger + c_j^\dagger(1-2n_j)c_{j+1} + c_j^\dagger(1-2n_j)c_{j+1}^\dagger \\
&= -c_jc_{j+1} - c_jc_{j+1}^\dagger + c_j^\dagger c_{j+1} + c_j^\dagger c_{j+1}^\dagger = (c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1}).
\end{aligned} \tag{A.5}$$

Similarly, considering commutation relations and taking different indices in (A.5), we have

$$\sigma_j\sigma_{j-1} = \sigma_{j-1}\sigma_j = (c_{j-1}^\dagger - c_{j-1})(c_j^\dagger + c_j). \tag{A.6}$$

Observe that, assuming PBC conditions,

$$\frac{\gamma}{2}\sum_{j=1}^N (c_j^\dagger + c_j)(c_{j-1}^\dagger - c_{j-1}) + \frac{\gamma}{2}\sum_{j=1}^N (c_{j+1}^\dagger + c_{j+1})(c_j^\dagger - c_j) = \gamma\sum_{j=1}^N (c_{j+1}^\dagger + c_{j+1})(c_j^\dagger - c_j). \tag{A.7}$$

B Discrete Fourier Transform computations

In this section, we provide the reader with all computations related to discrete Fourier transformation that did not fit in the main part of the present document, regarding the part which goes before extending Glauber model's notion to the density matrix. We express the computations for all possible combinations of c_j, with and without dagger, and for all combinations of indices j appearing in W_β, although many of these computations are redundant, for two reasons: firstly, because there are operators which are adjoint counterparts of other ones already computed; and because rewriting indices j (e.g., taking $c_{j-1}c_j$ and summing 1 to their indices, we obtian c_jc_{j+1}), we directly obtain different combinations. Omitting the initial and the final values of the following sums we have that

$$\star\ c_{j-1}^\dagger c_j = \frac{1}{N}\sum_{l,p} e^{-i(j-1)p}e^{ijl}d_p^\dagger d_l \quad j\in\{1,\dots,N\} \tag{B.1}$$

$$\implies \sum_{j=1}^{N} c_{j-1}^\dagger c_j = \frac{1}{N}\sum_{l,p} e^{ip}d_p^\dagger d_l\left(\sum_{j=1}^{N} e^{ij(l-p)}\right) = \sum_{l=-\frac{N}{2}+1}^{\frac{N}{2}} e^{il}d_l^\dagger d_l. \tag{B.2}$$

$$\star\ c_{j-1}c_j^\dagger = \frac{1}{N}\sum_{l,p} e^{i(j-1)p}e^{-ijl}d_p d_l^\dagger \quad j\in\{1,\dots,N\} \tag{B.3}$$

$$\implies \sum_{j=1}^{N} c_{j-1}c_j^\dagger = \frac{1}{N}\sum_{l,p} e^{-ip}d_p d_l^\dagger\left(\sum_{j=1}^{N} e^{ij(p-l)}\right) = \sum_{l=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-il}d_l d_l^\dagger. \tag{B.4}$$

$$\star\ c_{j-1}^\dagger c_j^\dagger = \frac{1}{N}\sum_{l,p} e^{-i(j-1)p}e^{-ijl}d_p^\dagger d_l^\dagger \quad j\in\{1,\dots,N\} \tag{B.5}$$

$$\implies \sum_{j=1}^{N} c_{j-1}^\dagger c_j^\dagger = \frac{1}{N}\sum_{l,p} e^{ip}d_p^\dagger d_l^\dagger\left(\sum_{j=1}^{N} e^{-ij(p+l)}\right) = \sum_{l=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-il}d_{-l}^\dagger d_l^\dagger. \tag{B.6}$$

$$\star\ c_{j+1}c_j^\dagger = \frac{1}{N}\sum_{l,p} e^{i(j+1)p}e^{-ijl}d_p d_l^\dagger \quad j\in\{1,\dots,N\} \tag{B.7}$$

$$\implies \sum_{j=1}^{N} c_{j+1}c_j^\dagger = \frac{1}{N}\sum_{l,p} e^{ip}d_p d_l^\dagger\left(\sum_{j=1}^{N} e^{ij(p-l)}\right) = \sum_{l=-\frac{N}{2}+1}^{\frac{N}{2}} e^{il}d_l d_l^\dagger. \tag{B.8}$$

$$\star\ c_{j-1}c_j = \frac{1}{N}\sum_{l,p} e^{i(j-1)p}e^{ijl}d_p d_l = \sum_{l,p} e^{-ip}e^{ij(l+p)}d_p d_l \quad j\in\{1,\dots,N\} \tag{B.9}$$

$$\implies \sum_{j=1}^{N} c_{j-1}c_j = \frac{1}{N}\sum_{l,p} e^{-ip}d_p d_l\left(\sum_{j=1}^{N} e^{ij(p+l)}\right) = \sum_{l=-\frac{N}{2}+1}^{\frac{N}{2}} e^{il}d_{-l}d_l. \tag{B.10}$$

$$\star\ c_{j+1}c_j = \frac{1}{N}\sum_{l,p} e^{i(j+1)p}e^{ijl}d_p d_l = \sum_{l,p} e^{ip}e^{ij(l+p)}d_p d_l \quad j\in\{1,\dots,N\} \tag{B.11}$$

$$\implies \sum_{j=1}^{N} c_{j+1}c_j = \frac{1}{N}\sum_{l,p} e^{ip}d_p d_l\left(\sum_{j=1}^{N} e^{ij(p+l)}\right) = \sum_{l=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-il}d_{-l}d_l. \tag{B.12}$$

$$\star\ c_{j+1}^\dagger c_j = \frac{1}{N}\sum_{l,p} e^{-il(j+1)}e^{ipj}d_l^\dagger d_p = \sum_{l,p} e^{-il}e^{ij(p-l)}d_l^\dagger d_p \quad j\in\{1,\dots,N\} \tag{B.13}$$

$$\implies \sum_{j=1}^{N} c_{j+1}^\dagger c_j = \frac{1}{N}\sum_{l,p} e^{-il}d_l^\dagger d_p\left(\sum_{j=1}^{N} e^{ij(p-l)}\right) = \sum_{l=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-il}d_l^\dagger d_l. \tag{B.14}$$

$$\star\ c_{j+1}^\dagger c_j^\dagger = \frac{1}{N}\sum_{l,p} e^{-il(j+1)}e^{-ipj}d_l^\dagger d_p^\dagger = \sum_{l,p} e^{-il}e^{-ij(p+l)}d_l^\dagger d_p^\dagger \quad j\in\{1,\dots,N\} \tag{B.15}$$

$$\Longrightarrow \sum_{j=1}^{N} c_{j+1}^\dagger c_j^\dagger = \frac{1}{N}\sum_{l,p} e^{-il}d_l^\dagger d_p^\dagger\left(\sum_{j=1}^{N} e^{-ij(p+l)}\right) = \sum_{l=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-il}d_l^\dagger d_{-l}^\dagger. \tag{B.16}$$

$$\star\ c_{j+1}^\dagger c_{j-1}^\dagger = \frac{1}{N}\sum_{l,p} e^{-i(j+1)p}e^{-i(j-1)l}d_p^\dagger d_l^\dagger = \sum_{l,p} e^{i(l-p)}e^{-ij(l+p)}d_p^\dagger d_l^\dagger \quad j\in\{1,\dots,N\} \tag{B.17}$$

$$\Longrightarrow \sum_{j=1}^{N} c_{j+1}^\dagger c_{j-1}^\dagger = \frac{1}{N}\sum_{l,p} e^{i(l-p)}d_p^\dagger d_l^\dagger\left(\sum_{j=1}^{N} e^{-ij(p+l)}\right) = \sum_{l=-\frac{N}{2}+1}^{\frac{N}{2}} e^{2il}d_{-l}^\dagger d_l^\dagger. \tag{B.18}$$

$$\star\ c_{j+1}c_{j-1}^\dagger = \frac{1}{N}\sum_{l,p} e^{i(j+1)p}e^{-i(j-1)l}d_p d_l^\dagger = \sum_{l,p} e^{i(l+p)}e^{ij(p-l)}d_p d_l^\dagger \quad j\in\{1,\dots,N\} \tag{B.19}$$

$$\Longrightarrow \sum_{j=1}^{N} c_{j+1}c_{j-1}^\dagger = \frac{1}{N}\sum_{l,p} e^{i(l+p)}d_p d_l^\dagger\left(\sum_{j=1}^{N} e^{ij(p-l)}\right) = \sum_{l=-\frac{N}{2}+1}^{\frac{N}{2}} e^{2il}d_l d_l^\dagger. \tag{B.20}$$

$$\star\ c_{j+1}c_{j-1} = \frac{1}{N}\sum_{l,p} e^{i(j+1)p}e^{i(j-1)l}d_p d_l = \sum_{l,p} e^{i(p-l)}e^{ij(p+l)}d_p d_l \quad j\in\{1,\dots,N\} \tag{B.21}$$

$$\Longrightarrow \sum_{j=1}^{N} c_{j+1}c_{j-1} = \frac{1}{N}\sum_{l,p} e^{i(p-l)}d_p d_l\left(\sum_{j=1}^{N} e^{ij(p+l)}\right) = \sum_{l=-\frac{N}{2}+1}^{\frac{N}{2}} e^{2il}d_l d_{-l}. \tag{B.22}$$

$$\star\ c_{j+1}^\dagger c_{j-1} = \frac{1}{N}\sum_{l,p} e^{-i(j+1)p}e^{i(j-1)l}d_p^\dagger d_l = \sum_{l,p} e^{-i(l+p)}e^{ij(l-p)}d_p^\dagger d_l \quad j\in\{1,\dots,N\} \tag{B.23}$$

$$\Longrightarrow \sum_{j=1}^{N} c_{j+1}^\dagger c_{j-1} = \frac{1}{N}\sum_{l,p} e^{-i(l+p)}d_p^\dagger d_l\left(\sum_{j=1}^{N} e^{ij(l-p)}\right) = \sum_{l=-\frac{N}{2}+1}^{\frac{N}{2}} e^{-2il}d_l^\dagger d_l. \tag{B.24}$$

$$\star\ c_j^\dagger c_j = \frac{1}{N}\sum_{l,p} e^{-ijl}e^{ijp}d_l^\dagger d_p \tag{B.25}$$

$$\Longrightarrow \sum_{j=1}^{N} c_j^\dagger c_j = \frac{1}{N}\sum_{l,p} d_l^\dagger d_p\left(\sum_{j=1}^{N} e^{ij(p-l)}\right) = \sum_{l=-N/2+1}^{N/2} d_l^\dagger d_l. \tag{B.26}$$

Furthermore, these momentum space fermionic operators fulfill the same anti-commutation relations than c_l, $c_l^\dagger$. All in all, Hamiltonian (2.35) can be written as

$$\begin{aligned}
W_\beta &= \frac{\alpha}{2}\sum_l\{A(1-2d_l^\dagger d_l) + Be^{2il}d_{-l}^\dagger d_l^\dagger + Be^{2il}d_l d_l^\dagger - Be^{-2il}d_l^\dagger d_l - Be^{2il}d_l d_{-l} - 1 \\
&- \gamma e^{il}d_l d_l^\dagger - \gamma e^{-il}d_l^\dagger d_{-l}^\dagger + \gamma e^{-il}d_l^\dagger d_l + \gamma e^{-il}d_{-l}d_l\} = \frac{\alpha}{2}\sum_l\{[A-1+Be^{2il}-\gamma e^{il}-\gamma e^{-il}-Be^{2il}] \\
&+ d_l^\dagger d_l[-2A-2B\cos(2l)+2\gamma\cos(l)] + d_{-l}^\dagger d_l^\dagger[Be^{2il}+\gamma e^{-il}] + d_{-l}d_l[Be^{2il}+\gamma e^{-il}]\} = \frac{\alpha}{2}\sum_l\{[A-1 \\
&- 2\gamma\cos(l)] + 2d_l^\dagger d_l[-B\cos(2l)-A+\gamma\cos(l)] + d_{-l}^\dagger d_l^\dagger[Be^{2il}+\gamma e^{-il}] + d_{-l}d_l[Be^{2il}+\gamma e^{-il}]\} \\
&= \frac{\alpha}{2}\sum_l\{E_l + C_l d_l^\dagger d_l + D_l(d_{-l}^\dagger d_l^\dagger + d_{-l}d_l)\},
\end{aligned} \tag{B.27}$$

where $C_l = 2[-A - B\cos(2l) + \gamma\cos(l)]$, $D_l = Be^{2il} + \gamma e^{-il}$, and $E_l = A - 1 - 2\gamma\cos(l)$, for $l = 2\pi k/N$, for $k \in \{-N/2+1, \dots, N/2\}$, what implies $l = -\pi + 2\pi/N, \dots, -2\pi/N, 0, 2\pi/N, \dots, \pi - 2\pi/N, \pi$ (recall that we are considering PBC).

C Bogoliubov transformation computations

Now, we show the computations related to Bogoliugov rotations carried out throughout our exposure, regarding the original Glauber model. Expanding the corresponding sums from (2.65), we have that

$$\begin{aligned} d_s &= u_s\xi_s + iv_s\xi_{-s}^\dagger, \quad d_{-s}^\dagger = u_s\xi_{-s}^\dagger + iv_s\xi_s, \\ d_{-s} &= u_s\xi_{-s} - iv_s\xi_s^\dagger, \quad d_s^\dagger = u_s\xi_s^\dagger - iv_s\xi_{-s}. \end{aligned} \tag{C.1}$$

From the terms of the sum (B.27), we must compute the following in terms of the rotated operators, taking into account anti-commutation relations:

$$\begin{aligned} &\star\, d_l^\dagger d_l = (u_l\xi_l^\dagger - iv_l\xi_{-l})(u_l\xi_l + iv_l\xi_{-l}^\dagger) = \cos^2(\theta_l/2)\xi_l^\dagger\xi_l - \sin^2(\theta_l/2)\xi_{-l}^\dagger\xi_{-l} \\ &+ i\frac{\sin(\theta_l)}{2}\xi_l^\dagger\xi_{-l}^\dagger + i\frac{\sin(\theta_l)}{2}\xi_l\xi_{-l} + \sin^2(\theta_l/2). \\ &\star\, d_{-l}^\dagger d_{-l} = (u_l\xi_{-l}^\dagger + iv_l\xi_l)(u_l\xi_{-l} - iv_l\xi_l^\dagger) = \cos^2(\theta_l/2)\xi_{-l}^\dagger\xi_{-l} - \sin^2(\theta_l/2)\xi_l^\dagger\xi_l \\ &+ i\frac{\sin(\theta_l)}{2}\xi_l\xi_{-l} + i\frac{\sin(\theta_l)}{2}\xi_l^\dagger\xi_{-l}^\dagger + \sin^2(\theta_l/2) \\ &\star\, d_{-l}^\dagger d_l^\dagger = (u_l\xi_{-l}^\dagger + iv_l\xi_l)(u_l\xi_l^\dagger - iv_l\xi_{-l}) = -\cos^2(\theta_l/2)\xi_l^\dagger\xi_{-l}^\dagger + \sin^2(\theta_l/2)\xi_l\xi_{-l} \\ &- i\frac{\sin(\theta_l)}{2}\xi_l^\dagger\xi_l - i\frac{\sin(\theta_l)}{2}\xi_{-l}^\dagger\xi_{-l} + i\frac{\sin(\theta_l)}{2}, \\ &\star\, d_{-l}d_l = (u_l\xi_{-l} - iv_l\xi_l^\dagger)(u_l\xi_l + iv_l\xi_{-l}^\dagger) = -\cos^2(\theta_l/2)\xi_l\xi_{-l} + \sin^2(\theta_l/2)\xi_l^\dagger\xi_{-l}^\dagger \\ &- i\frac{\sin(\theta_l)}{2}\xi_{-l}^\dagger\xi_{-l} - i\frac{\sin(\theta_l)}{2}\xi_l^\dagger\xi_l + i\frac{\sin(\theta_l)}{2}. \end{aligned} \tag{C.2}$$

From (2.57), we need to express in terms of the new operators the following, using some elementary trigonometric equalities:

$$\begin{aligned} d_l^\dagger d_l + d_{-l}^\dagger d_{-l} &= \cos(\theta_l)\xi_l^\dagger\xi_l + \cos(\theta_l)\xi_{-l}^\dagger\xi_{-l} + i\sin(\theta_l)\xi_l^\dagger\xi_{-l}^\dagger + iW_l, \sin(\theta_l)\xi_l\xi_{-l} + 2\sin^2(\theta_l/2). \\ d_l^\dagger d_{-l}^\dagger + d_l d_{-l} &= \cos(\theta_l)(\xi_l\xi_{-l} + \xi_l^\dagger\xi_{-l}^\dagger) + i\sin(\theta_l)(\xi_l^\dagger\xi_l + \xi_{-l}^\dagger\xi_{-l}) - i\sin(\theta_l). \end{aligned} \tag{C.3}$$

Now, if we write $W_\beta = (\alpha/2)\sum_l W_{l,\beta}$, regrouping terms we obtain:

$$\begin{aligned} W_{l,\beta} &= G_l + iF_l[\cos(\theta_l)(\xi_l\xi_{-l} + \xi_l^\dagger\xi_{-l}^\dagger) + i\sin(\theta_l)(\xi_l^\dagger\xi_l + \xi_{-l}^\dagger\xi_{-l}) - i\sin(\theta_l)] \\ &+ C_l[\cos(\theta_l)(\xi_l^\dagger\xi_l + \xi_{-l}^\dagger\xi_{-l}) + i\sin(\theta_l)(\xi_l^\dagger\xi_{-l}^\dagger + \xi_l\xi_{-l}) + 2\sin^2(\theta_l/2)] \\ &= [G_l + F_l\sin(\theta_l) + 2C_l\sin^2(\theta_l/2)] + (\xi_l\xi_{-l} + \xi_l^\dagger\xi_{-l}^\dagger)[iF_l\cos(\theta_l) + iC_l\sin(\theta_l)] \\ &+ (\xi_l^\dagger\xi_l + \xi_{-l}^\dagger\xi_{-l})[-F_l\sin(\theta_l) + C_l\cos(\theta_l)]. \end{aligned} \tag{C.4}$$

D Gates decomposition for U_{dis} operators

Following [58] and [78], we briefly explain and represent gates decompositions for the transformations involved in our diagonalizations. Given that images represented come from [58], there is a slight change in notation in such figures: number of spins, in this appendix, is denoted by n instead of N.

D.1 Fermionic SWAP

As we know, Jordan-Wigner transformation, in which we go from spin operators in terms of Pauli matrices σ_j, to fermionic modes c_j, do not require specific operators, apart from a fermionic SWAP every time we exchange two occupied modes, since the latter should carry a minus sign. In figure 9 we express the way we implement such a special swap, from [58].

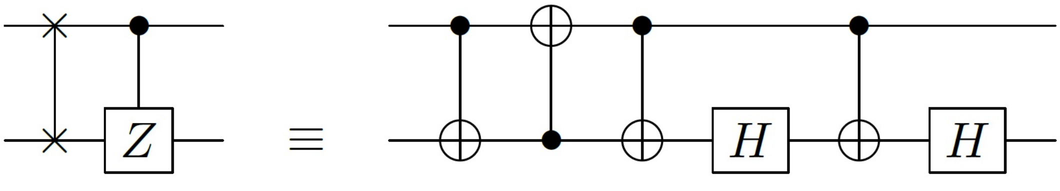

Figure 9: Quantum gates necessary to implement a fermionic SWAP, taking into account the fermionic anticommutativity. Image from [58].

D.2 Fourier transform

In (4.10) we express the general fast Fourier transformation gate which let us place the fermionic modes in the momentum space. Again from [58], we use the gates decomposition expressed in

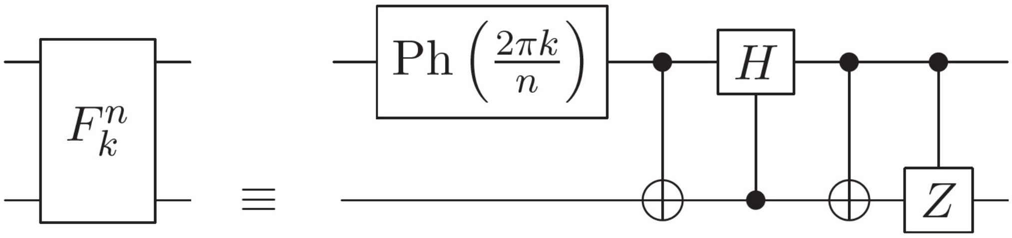

Figure 10: Quantum gates necessary to implement the fast Fourier transformation from (4.10). Image from [58].

figure 10. We start by adding $2\pi k/n$-phases in the first qbit, followed by controlled-NOT (CNOT), controlled-Hadamard gate, and again CNOT, to end up with a controlled-Z. All these operators locate its control qbit in the first qbit, apart from controlled-Hadamard, which locate it in the second one.

D.3 Bogoliubov rotation

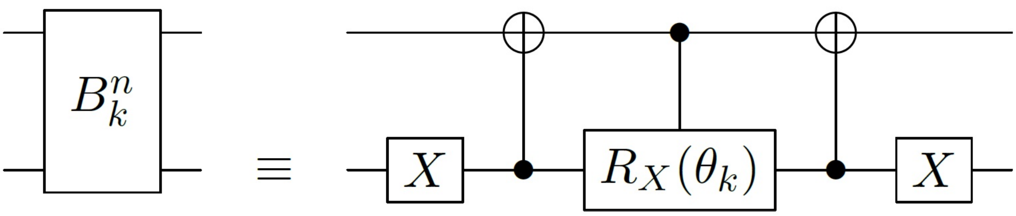

Figure 11: Quantum gates in which we decompose the Bogoliubov rotation from (4.14). Image from [58].

The last transformation consists of the operator B_k^n represented in (4.14). Following [78], we decompose these operations in the gates represented in figure 11. Operator $R_X(\theta_k)$ refers to a rotation, with respect to X-axis in the Bloch sphere, with an angle corresponding to the Bogoliubov

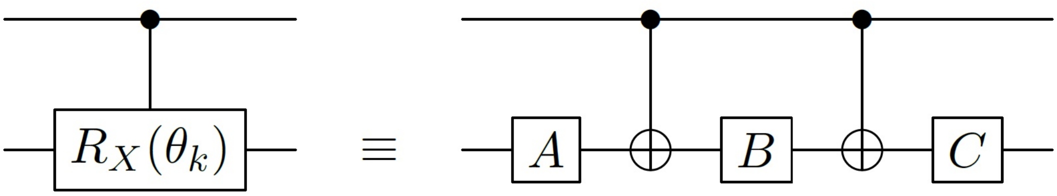

Figure 12: Quantum gates in which we decompose the controlled x-rotation needed for Bogoliubov rotation (4.14), where $A = R_Z(\pi/2)R_Y(\theta_k/2)$, $B = R_Y(-\theta_k/2)$, and $C = R_Z(-\pi/2)$. Image from [58].

angle θ_k. In figure 12 we show the exact decomposition of such a controlled rotation: we alternate $\pi/2$ and $-\pi/2$-rotations with respect to Z-axis with the corresponding Y-axis rotations with angles $\theta_k/2$ and $-\theta_k/2$, along with two CNOTs.

E Relevant codes

We summarize some important codes through which we implemented the diagonalization quantum circuit and performed some highlighted computations for our simulations.

E.1 Code for quantum circuit

We provide in this section the main codes used to implement the diagonalization quantum circuit for the Master's operator from original kinetic Ising model (2.22). As pointed out before, to implement this code for another Hamiltonian or Master's operator, it suffices to change the corresponding Bogoliubov angle properly. We use *Qiskit* in programming language *Python*. We limit our example here to $N = 4$ spins. Note that methodology here presented consists of departing from states in the eigenstates basis of σ_i^z's, in order to express them in terms of the Hamiltonian eigenstates basis. That is, in the notation used above, we are implementing $U_{dis}^\dagger$. Before giving the quantum circuit code, we need to compute constants A and B from the aforementioned model, as well as Bogoliubov rotation angles for the correpsonding momentum $2\pi k/N$:

```
from numpy import sqrt, sin, cos
def Agamma(gamma):
    return (sqrt(1-gamma**2)-1)/2
def Bgamma(gamma):
    return 1 - Agamma(gamma)

from numpy import arcsin, sin, cos, pi
def angbog_feld(k,gamma,N):
    A = Agamma(gamma)
    B = Bgamma(gamma)
    return arcsin( (B*sin(4*pi*k/N) - gamma*sin(2*pi*k/N)) /
                    (sqrt( (B*sin(4*pi*k/N) - gamma*sin(2*pi*k/N))**2 +
                    ( gamma*cos(2*pi*k/N) - A - B*cos(4*pi*k/N) )**2) ) )
```

Once we know Bogoliubov angle function, we are in position to write the described diagonalization circuit (i.e., unitary operator $U_{dis}^\dagger$) for the present setting:

```
import numpy as np
from numpy import arccos, cos, sqrt, sin
from math import pi
from qiskit import QuantumCircuit, QuantumRegister, ClassicalRegister
```

```
from qiskit import transpile, Aer, assemble
from qiskit.visualization import plot_histogram

def UdisM_inv(init,fswap,gamma):
    #init is a list of 4 float numbers lists
    #yielding initial state components
    #in sigma_z eigenstates basis.
    #fswap is 1 if we apply fswap gates
    #between inverse fourier trans,
    #and 0 otherwise.

    N=4
    qq = QuantumRegister(N)
    qa = QuantumCircuit(qq)

    # Apply initialization on all qbits:
    qa.initialize(init[0], 0)
    qa.initialize(init[1], 1)
    qa.initialize(init[2], 2)
    qa.initialize(init[3], 3)

    #Bogoliubov rotations:

    k=1
    ang_bog1 = angbog_feld(k,gamma,N)
    qa.x(1)
    qa.cx(1,0)
    #qa.crx(ang_bog,0,1)
    #We can be more specific for controlled x-rotations:
    qa.rz(pi/2,1)
    qa.cx(0,1)
    qa.ry(ang_bog1/2,1)
    qa.cx(0,1)
    qa.ry(-ang_bog1/2,1)
    qa.rz(-pi/2,1)
    #End of controlled x-rotation with Bog. angle
    qa.cx(1,0)
    qa.x(1)

    k=0
    ang_bog0 = angbog_feld(k,gamma,N)
    qa.x(3)
    qa.cx(3,2)
    #qa.crx(ang_bog,2,3)
    #We can be more specific for controlled x-rotations:
    qa.rz(pi/2,3)
    qa.cx(2,3)
    qa.ry(ang_bog0/2,3)
    qa.cx(2,3)
    qa.ry(-ang_bog0/2,3)
    qa.rz(-pi/2,3)
```

```
#End of controlled x-rotation with Bog. angle
qa.cx(3,2)
qa.x(3)

qa.barrier()

#Now, 4 inverse Fouriers:

k=1
qa.cz(0,1)
qa.cx(0,1)
qa.ch(1,0)
qa.cx(0,1)
qa.p(-2*pi*k/N,0)

k=0
qa.cz(2,3)
qa.cx(2,3)
qa.ch(3,2)
qa.cx(2,3)
qa.p(-2*pi*k/N,2)

if fswap == 1:
    qa.cz(1,2)
    qa.swap(1,2)

k=0
qa.cz(0,1)
qa.cx(0,1)
qa.ch(1,0)
qa.cx(0,1)
qa.p(-2*pi*k/N,0)

k=0
qa.cz(0,1)
qa.cx(0,1)
qa.ch(1,0)
qa.cx(0,1)
qa.p(-2*pi*k/N,0)

if fswap == 1:
    qa.cz(1,2)
    qa.swap(1,2)
return qa
```

To go deeper in *Qiskit* implementation, see https://qiskit.org/documentation/.

E.2 Code for some important simulations

Now, we provide the reader with the code used for simulation and computation of $\langle\sigma_z\rangle$ versus β for the Ising model with external magnetic field, with strength parameter λ. We only consider $\lambda = 0$

in the presented example, although computations have been carried out for different λ's. Output *expect0* is the corresponding list whose entries are σ_z estimated averages, one per β.

```
from math import exp
from numpy import argmax
from scipy.constants import k
import numpy as np
from numpy.random import multinomial
import matplotlib.pyplot as plt

fswap = 1
lamb = 0 #External field parameter
N = 4 #Number of fermions
Lbeta = [1,2,3,4,5,6,10] #beta's considered
Nsamples = 1000 #Number of samples to estimate average
expect0 = [] #List for computed expectation values
T = [] #List to store all temperatures

for beta in Lbeta:
    partition = 0
    T.append(1/(k*beta))
    for i in range(2**N-1):
        partition += exp(-beta*energies[i])
    probs = []
    for i in range(2**N-1):
        probs.append(exp(-beta*energies[i])/partition)
    expaux = 0
    for i in range(Nsamples-1):
            dist = multinomial(1,probs,size=1)
            ind = argmax(dist)
            init = states[ind]
            qa = Udis(init,fswap,lamb)
            [pp,amps] = isingstate(qa)
            expaux += sigmaz(pp,N)
    expect0.append(expaux/Nsamples)
print(expect0)
```

Function *isingstate* takes as input the corresponding diagonalization quantum circuit, and yields probabilities and amplitudes for each of the 2^N eigenstates of the Hamiltonian eigenstates basis, in the order expressed below. Such a function is given by:

```
from qiskit.quantum_info import Statevector, random_statevector
from qiskit import QuantumCircuit
from qiskit.visualization import plot_histogram, plot_bloch_multivector

def isingstate(qa):
    #We always initialize from label with 0000,
    #and do the corresponding proper change to real
    #initialization through the init argument
    #in our quantum circuit function.
    init = '0000'
    sv = Statevector.from_label(init)
    sv = sv.evolve(qa)
```

```
    sv_prob = sv.probabilities_dict([0,1,2,3])
    return sv_prob, sv
```

Note that energy spectrum is previously computed from (4.18), and that the states string list is also previously given, determined in terms of 0's and 1's, and in the order given by default in *Qiskit* for 4 qbits:

```
states = ['0000','0001','0010','0011','0100','0101','0110','0111','1000',
'1001','1010','1011','1100','1101','1110','1111'].
```

In turn, function σ_z performs the computation of the quantum-mechanical expectation value of σ_z for a certain state, given in *dict* format, expressed in σ_z eigenstates basis:

```
def sigmaz(state,N):
    sig = 0
    keys = list(state.keys())
    probs = list(state.values())
    for i in range(len(probs) - 1):
        sig += probs[i] * sigmazind(keys[i])
    return sig
```

where state is a *dict* object with the aforementioned basis elements as keys, and the probabilities as values; and *sigmazind* is the function yielding the direct calculus of averages for σ_z given an element of such a basis in *string* format.

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