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Real-time simulation of the Ising Model

Simon Williams[1]

[a] *Institute for Particle Physics Phenomenology, Department of Physics, Durham University, Durham DH1 3LE, U.K.*

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1 Introduction: The Ising Model Hamiltonian

The lattice Ising model Hamiltonian describes a system of spins on a lattice, where each spin interacts with its neighbours and possibly an external magnetic field. The Ising model on a d-dimensional lattice has the form

$$H = -\sum_{\langle i,j\rangle} J_{i,j}\,\sigma_i\sigma_j - \mu\sum_i h_i\,\sigma_i, \tag{1.1}$$

where $J_{i,j}$ is the interaction strength between neighbouring spins i and j, $\langle i,j\rangle$ denotes the sum over nearest-neighbour pairs of sites i and j, σ_i represents the spin at site i, where $\sigma_i = \pm 1$

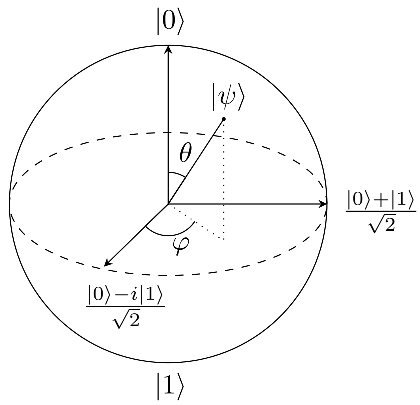


Figure 1. The Bloch Sphere

(i.e. spin up or spin down in the classical Ising model), and h is an external magnetic field applied uniformly across the lattice with magnetic moment μ. If $J > 0$ the interaction is *ferromagnetic* where neighbouring spins align; if $J < 0$ the interaction is *antiferromagnetic* where neighbouring spins anti-align.

The Hamiltonian can be split into two parts, $H = H_1 + H_2$, where

$$H_1 = -\sum_{\langle i,j\rangle} J_{i,j}\,\sigma_i\sigma_j \tag{1.2}$$

describes the spin-spin interactions between nearest-neighbours, and

$$H_2 = -\mu\sum_i h_i\,\sigma_i, \tag{1.3}$$

describes the interaction with an external field.

2 Quantum Mechanical Ising Model

To express the Ising Hamiltonian using a quantum mechanical description of spins, we must now replace the classical spin variables $\sigma = \pm 1$ with the respective Pauli matrices. Making the assumption that the interactions between neighbouring sites is equal for every i and j, and decomposing the magnetic field into transverse and longitudinal fields, the Hamiltonian becomes

$$H = -J\sum_{\langle i,j\rangle}\sigma_i^z\sigma_j^z - h\sum_i\sigma_i^z - \Gamma\sum_i\sigma_i^x. \tag{2.1}$$

where h is now the longitudinal field (oriented along the z direction) and Γ is the transverse field (oriented along the x direction).

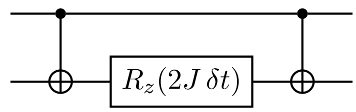


Figure 2. Pauli-ZZ gate

If the value of the transverse-field strength, Γ, is zero, then the system is purely classical. Therefore, at low values of Γ the system behaves similarly to the classical Ising model: The spins will tend to (anti-)align in the z-direction depending on the value of J, forming (anti-)ferromagnetic states. If the value f Γ is large, the transverse field dominates, and the spins are likely to be in a superposition of states due to the σ^x in the transverse term. In the limit $J \ll h$, the spins will all align in the x-direction, leading to a highly-disordered phase. At the point where the interactions between neighbouring spins and the transverse field become comparable, $J \sim \Gamma$, the Ising model can experience a phase transition between the ordered and disordered regime.

2.1 Ising model in 1D:

In one-dimension, the Ising model describes a one-dimensional chain of N-spins,

$$H = -J \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z - \Gamma \sum_{i=1}^{N} \sigma_i^x, \tag{2.2}$$

where here we have taken the value of the the longitudinal field $h = 0$.

We will use the one-dimensional Ising spin model in our example below where we will simulate the real-time evolution of the model using Hamiltonian simulation.

3 Hamiltonian Simulation - Real-time evolution of H

To simulate the real-time evolution of a quantum system, we use the Schrödinger time-evolution operator

$$U(t) = e^{-iHt}. \tag{3.1}$$

Using this method avoids costly sign-problems experienced by Monte-Carlo approaches to evolution of lattice modes in imaginary time. However, directly calculating the real-time evolution of a Hamiltonian is quickly unfeasible on a classical device, as the required resources grow exponentially with the number of lattice sites. Quantum computers have an exponentially growing Hilbert space, and therefore can feasibly simulate lattice models in real-time.

In this example, we wish to consider the real-time evolution of the Ising model with a transverse-field in one dimension, as shown in Equation (2.2). However, we see that the two terms in the Hamiltonian do not commute due to the Pauli-operator commutation relations,

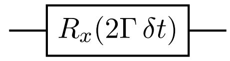


Figure 3. Pauli-X gate

$[\sigma_j, \sigma_k] = 2i\,\varepsilon_{ijk}\sigma_l$. We must therefore construct an approximation of the full Hamiltonian where the terms can be separated.

3.1 Trotter-Suzuki Decomposition

Expressing the Hamiltonian as a sum of non-commuting parts $H = \sum_i H_i$ and using the Zassenhaus formula, it is possible to separate the non-commuting terms in H by Trotter-Suzuki decomposition, such that the time-evolution operation from Equation (3.1) is approximated by

$$\mathcal{U}(t) = \left[\prod_i e^{-iH_i t/n}\right]^n, \tag{3.2}$$

up to an error $\mathcal{O}(t^2/n)$, where n is a positive integer. The operator $\mathcal{U}(t)$ defines the so-called *Trotterised time-evolution*, which divides the total evolution time, t, into n steps of time $\delta t = t/n$. The total time evolution is then achieved by applying n Trotter steps, such that the Trotterised time-evolution is exact in the limit $n \to \infty$.

A single Trotter step for the real-time evolution of the one-dimensional Ising model from Equation (2.2) is therefore

$$e^{iJ\delta t\,\sigma_i^z\sigma_{i+1}^z}\,e^{i\Gamma\delta t\,\sigma_i^x}. \tag{3.3}$$

4 Hamiltonian Simulation on Quantum Computers

Now that the model has been constructed and Trotterised, we are ready to implement the real-time evolution on a quantum device. To do so, we must first define a mapping to qubits.

4.1 Mapping to Qubits

In this example, we will us a qubit-based quantum computer to carry out the simulation. Qubits are the natural representation of spin-1/2 particles. The qubit is represented by the Bloch Sphere, as shown in Figure 1.

A suitable basis for qubits is constructed from the Pauli-operator basis, $(\sigma^0, \sigma^x, \sigma^y, \sigma^z)$. Exponentials of the Pauli-operators are rotations on the qubit, and can be visualised as rotations on the Bloch sphere around an axis. For example, the R_z gate corresponds to a rotation about the z-axis and is described by

$$R_z\left(\frac{\theta}{2}\right) = e^{-i\theta\sigma_z}. \tag{4.1}$$

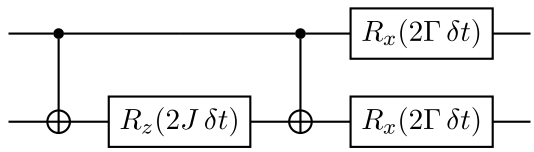


Figure 4. Trotter Step for n=2 sites

4.2 Circuit decomposition for the 1D Ising Model

Conveniently, the Ising model is already written in the Pauli basis, and the Trotter step from Equation (3.3) maps directly onto a qubit-based device. We will break this down into two steps:

4.2.1 Nearest Neighbour Interaction: $-J\sum_i \sigma_i^z\sigma_{i+1}^z$

The term describes the interaction between two qubits in the 1D chain and is described by the product of two Pauli-Z operators. This Pauli-ZZ operation, when exponentiated, corresponds to a *controlled-Z* operation. An entangling operation between the two qubits. This can be decomposed in a series of CNOT and R_z gates and is shown in Figure 2.

Notice that the argument of the R_z gate corresponds to the coefficient of the $\sigma_i^z\sigma_{i+1}^z$ term in the exponent. The operation is a two-qubit operation, acting on qubits i and $i+1$.

4.2.2 Transverse Field: $-\Gamma\sum_i \sigma_i^x$

The transverse-field term corresponds to a single-qubit R_x operation and is applied independently to each qubit. For each qubit, one applies the operation

$$R_x(2\Gamma\,\delta t) = e^{-i\Gamma\,\delta t\,\sigma_x}. \tag{4.2}$$

which can be expressed on a circuit as shown in Figure 3

5 Hamiltonian Simulation of the Ising Model on a Quantum Computer

We are now interested in the circuit decomposition of the 1D Ising model with a transverse field for a specific number of lattice sites. We now wish to study the model and examine the real-time evolution of different physical observables. In this section, we will use PennyLane to perform the Hamiltonian Simulation.

5.1 Quantum circuits for $n = 2$ sites

To begin we consider the $n = 2$ case. Putting all the above together, the circuit has the structure shown in Figure 4. The attached notebook takes you through the simulation using PennyLane, and we will discuss the evolution here. The model we build implements the circuit from Figure 4 and returns some measurements corresponding to the following values:

$$\langle\sigma_i^z\rangle, \quad \langle\sigma_1^z\sigma_2^z\rangle. \tag{5.1}$$

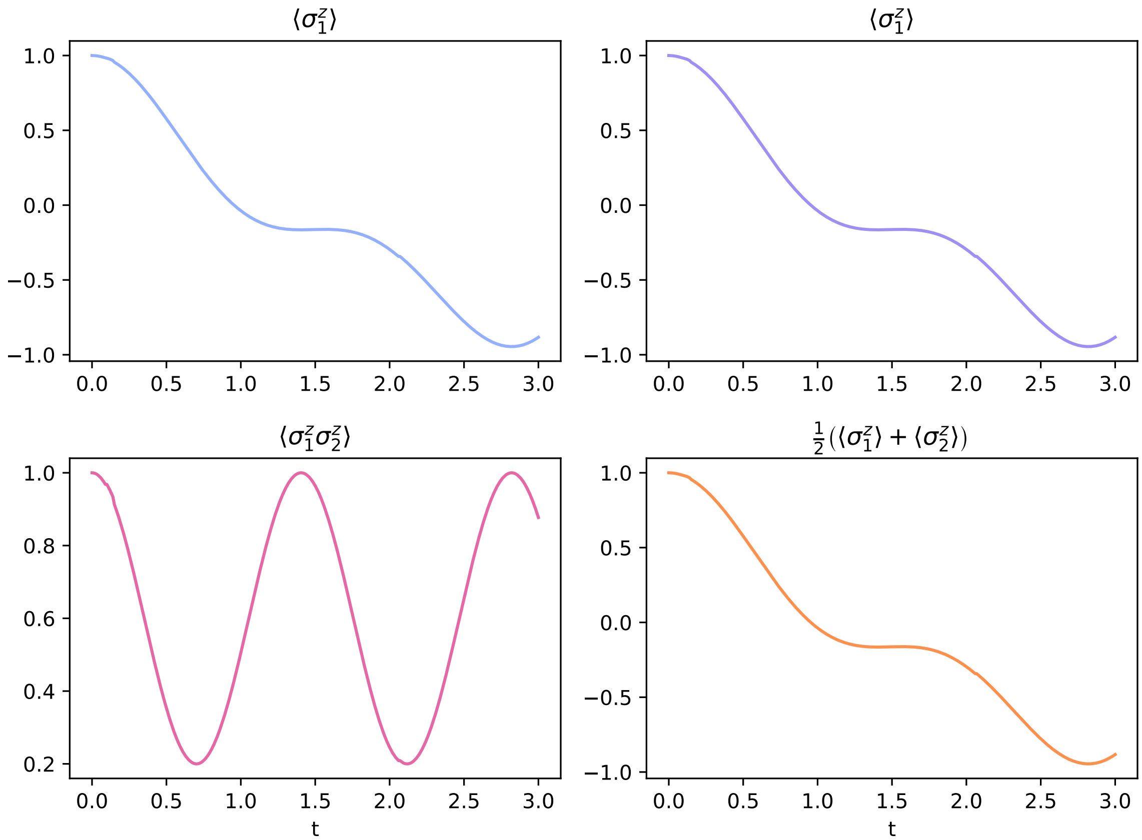


Figure 5. The time evolution of physical observables for the $n = 2$ site Ising model.

One can ask the question how these values are returned from the device. Since the qubit is defined in the computation basis, then a simple measurement on the qubit of the 0 or 1 state corresponds directly to the expectation values of σ_z, -1 and 1 respectively. Therefore, to return the values above from the quantum device, one simply applies a measurement to each qubit. This is not true for all observables, and this is discussed in Appendix B.

We can now run the circuit to simulate the time-evolution of the system for different nearest-neighbour couplings, J, and a transverse-field coupling, Γ. We will use the measurements to study the time-evolution of the two-point correlation function

$$C_{zz} = \langle\sigma_1^z\sigma_2^z\rangle, \tag{5.2}$$

and the total magnetisation along the z-axis

$$M_z = \frac{1}{2}\left(\langle\sigma_1^z\rangle + \langle\sigma_2^z\rangle\right). \tag{5.3}$$

Running the evolution for a total time of $t = 3$ with a Trotter-step of $\delta t = 0.01$, the time-evolution of the two-point correlation function between spin-one and spin-two, and the

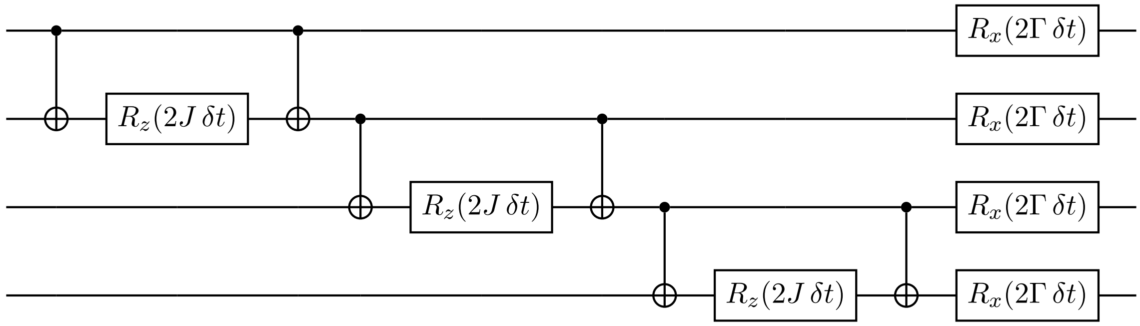


Figure 6. Circuit decomposition for the one-dimensional Ising model with $n = 4$ lattice sites and open boundary conditions.

time-evolution of the total magnetisation is shown in Figure 5. We see that the spins remain in aligned throughout the time-evolution, despite $J \sim \Gamma$. This is a consequence of the small system size of $n = 2$. While a two-site model can illustrate basic principles of the Ising model and quantum mechanics, it cannot capture the emergent phenomena associated with phase transitions. This is the case for several reasons, including:

- **Thermodynamic limit**: The system does not have a thermodynamic limit (i.e. $n \to \infty$). In a finite system, all thermodynamic quantities are smooth functions of the system parameters. Therefore, the system does not exhibit discontinuous changes, indicative of a phase shift.

- **Emergence of Long-Range Correlations**: In larger systems, spins separated by large distances can become correlated near the critical point, leading to collective behavior. For a two-site system, the maximum separation is between the two sites themselves, so you cannot observe how correlations decay with distance or how an ordered phase emerges.

A two-site Ising model is therefore inherently too small to exhibit phase transitions because it lacks the extensive degrees of freedom and the ability to develop long-range order, both of which are essential for such phenomena. Phase transitions are collective effects that emerge only in systems with a large number of interacting components.

5.2 Quantum circuits for $n = 4$ sites

Increasing the number of sites allows for us to examine more interesting physics that was not captured by the $n = 2$ case, such as a phase transition. Here we consider a system with $n = 4$ sites, and therefore $n_q = 4$ qubits in the simulation.

Increasing the size of the system means we now need to start considering boundary conditions. Below we consider two options: open-boundary conditions (OBC) and periodic-boundary conditions (PBC).

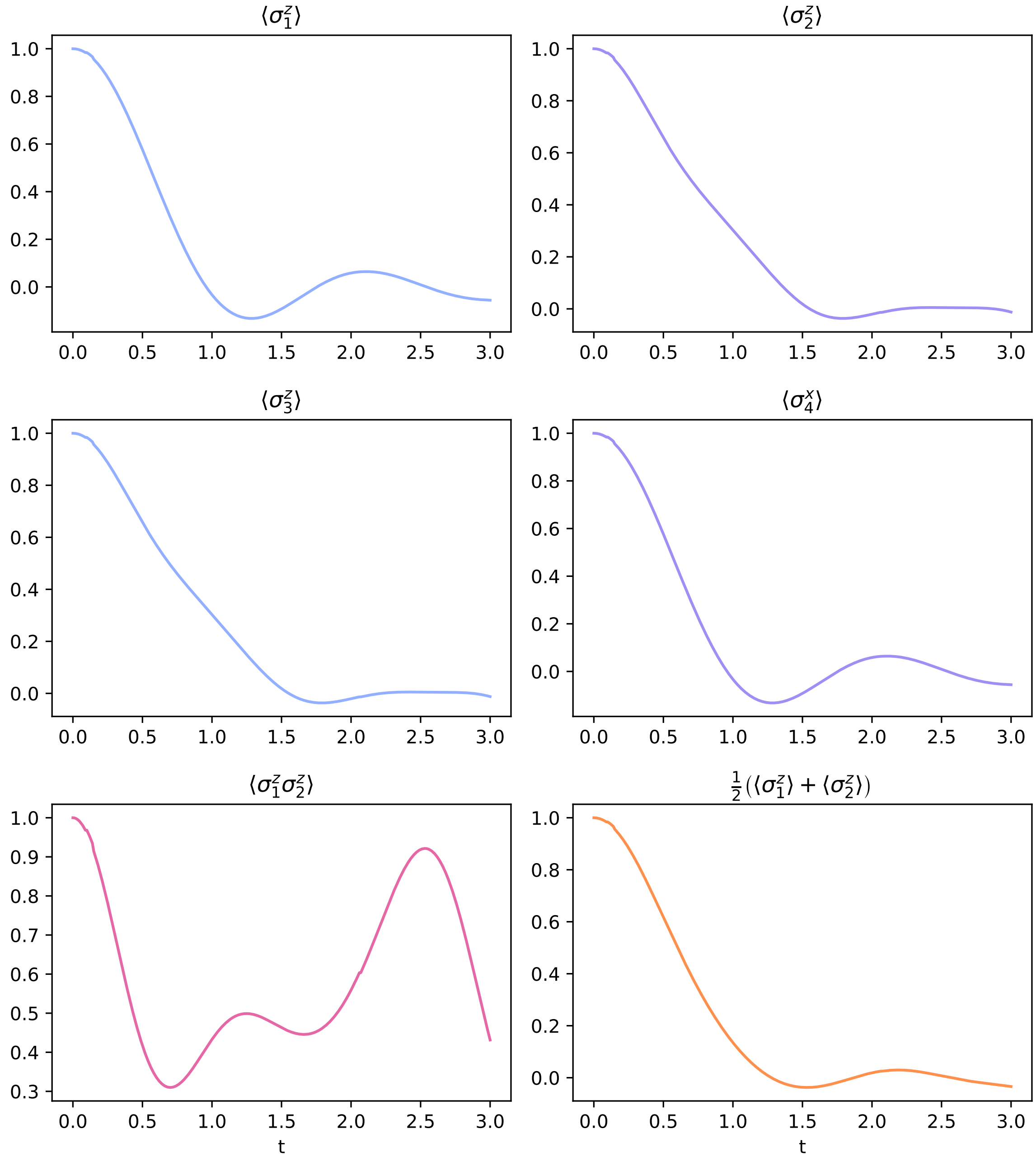


Figure 7. The time evolution of physical observables for the $n = 4$ site Ising model with OBC.

5.2.1 Open-Boundary Conditions

Let us first consider OBC. This is the easiest extension of our $n = 2$ model from above, with the Hamiltonian taking the form:

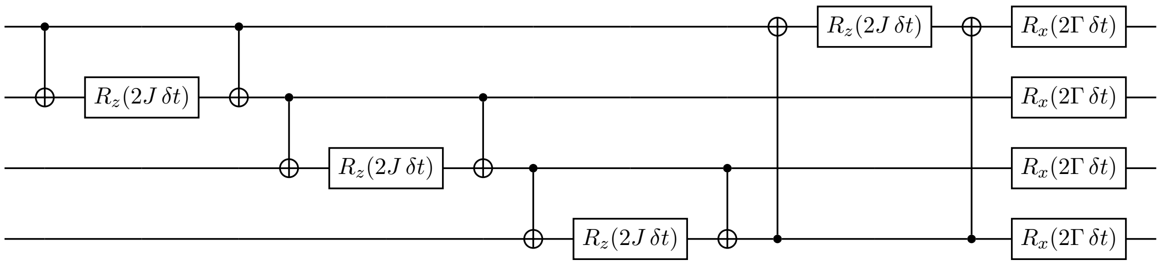


Figure 8. Circuit decomposition for the one-dimensional Ising model with $n = 4$ lattice sites and periodic boundary conditions.

$$H_{OBC} = -J \sum_{i=1}^{n-1} \sigma_i^z \sigma_{i+1}^z - \Gamma \sum_{i=1}^{n} \sigma_i^x. \tag{14}$$

Therefore, for $n = 4$ sites, we have

$$H_{OBC} = -J \left[\sigma_1^z \sigma_2^z + \sigma_2^z \sigma_3^z + \sigma_3^z \sigma_4^z\right] - \Gamma \left[\sigma_1^x + \sigma_2^x + \sigma_3^x + \sigma_4^x\right]. \tag{15}$$

The total magnetisation along the z-axis is now given by

$$M_z = \frac{1}{n} \sum_i \langle \sigma_i^z \rangle. \tag{16}$$

We can implement this Hamiltonian on the quantum computer in the same way as before, and the circuit diagram is shown in Figure 6

Here we start to see some of the spins go out of alignment, as expected from the couplings $J = \Gamma = 1$. The system size is still too small to see a phase transition, but we can see the indication that this will happen as we increase n.

5.2.2 Periodic-Boundary Conditions

We now consider PBC, i.e. a lattice on a circle. The Hamiltonian takes the form

$$H_{PBC} = -J \sum_{i=1}^{n} \sigma_i^z \sigma_{\overline{i+1}}^z - \Gamma \sum_{i=1}^{n} \sigma_i^x. \tag{17}$$

where $\overline{i+1}$ means $\overline{n+1} = 1$, and thus the system is periodic. For the $n = 4$ qubit case, the Hamiltonian takes the form

$$H_{OBC} = -J \left[\sigma_1^z \sigma_2^z + \sigma_2^z \sigma_3^z + \sigma_3^z \sigma_4^z + \sigma_4^z \sigma_1^z\right] - \Gamma \left[\sigma_1^x + \sigma_2^x + \sigma_3^x + \sigma_4^x\right]. \tag{18}$$

We once again simulate this in the same way but by altering the circuit slightly, adding another $\sigma_i^z \sigma_{i+1}^z$ term. The circuit now takes the form shown in Figure 8.

We can now run the time-evolution simulation and study the same observables as the OBC case. The results are shown in Figure 9. We see that the boundary conditions have a

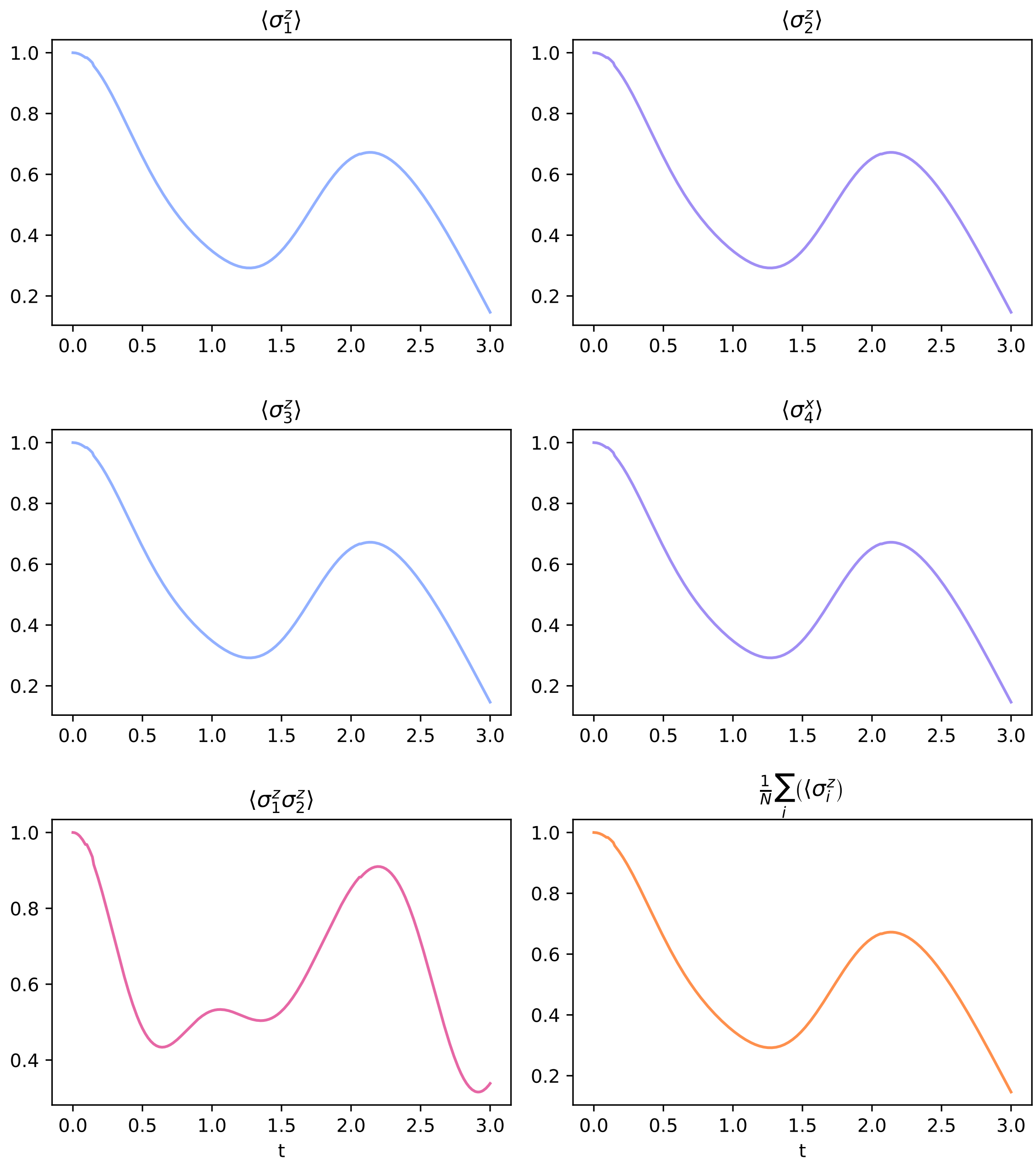


Figure 9. The time evolution of physical observables for the $n = 4$ site Ising model with PBC.

large effect on the model for small lattices. The presence of a potential phase transition is not visible in the PBC case. As we increase the lattice size, the OBC and PBC cases should start to agree.

6 Conclusions

In these notes, and the attached Python notebook, we have explored Hamiltonian Simulation on quantum devices. We have constructed the quantum circuits for the one-dimensional Ising model, and have examined the real-time evolution of different physical observables. The demonstrator's notebook will be available to you after the class, and you will be able to see some more experiments we can do with the Ising model.

A Gate Decomposition

To implement unitary operations on a quantum device, one often has to decompose the operation into a series of gates on the quantum circuit. In Section 4.2, we did exactly this to simulate the real-time evolution of the Ising model Hamiltonian. Single qubit gate operations are straightforward to implement on the quantum device as rotations, however gate decompositions of multi-qubit operations can be less obvious. Here we explicitly outline the gate decomposition of the $\sigma_z\sigma_z$ term in the time-evolution of the Ising model Hamiltonian from Equation (3.3).

A.1 Circuit decomposition of $e^{iJ\delta t\,\sigma_i^z\sigma_{i+1}^z}$

In Section 4.2 we made the observation that the $\sigma_i^z\sigma_{i+1}^z$ term in Equation (3.3) can be implemented using a controlled-Z (CZ) operation, a two-qubit operation which acts upon the computational basis in the following way

$$\begin{aligned} CZ|00\rangle &= |00\rangle, \qquad & CZ|10\rangle &= \ \ |10\rangle, \\ CZ|00\rangle &= |01\rangle, \qquad & CZ|10\rangle &= -|11\rangle. \end{aligned} \tag{A.1}$$

As a result, the CZ has the form

$$e^{-i\frac{\pi}{4}\sigma_i^z\sigma_{i+1}^z - I}. \tag{A.2}$$

For our purposes, we wish to abstract the CZ operation such that we obtain the unitary operation

$$U(\theta) = e^{i\frac{\theta}{2}\sigma_i^z\sigma_{i+1}^z}, \tag{A.3}$$

and observe the angle $\theta = 2J\delta t$.

In Section 4.2 we identified that this can be achieved by decomposing U as a series of gates:

1. CNOT controlling from the first qubit and acting on the second qubit,
2. R_z rotation on the second qubit with $\theta = 2J\delta t$,
3. CNOT controlling from the first qubit and acting on the second qubit.

Below, we provide a proof that this gate decomposition indeed achieves a two-qubit unitary operation corresponding to the $\sigma_i^z\sigma_{i+1}^z$ term in Equation (3.3). We begin by defining the initial state of the system

$$|q_1\rangle \otimes |q_2\rangle, \tag{A.4}$$

where q_1, $q_2 \in \{0, 1\}$ are defined in the computational basis. The action of the first CNOT-gate flips the state of the second qubit if the first qubit is in the $|1\rangle$ state, and does nothing if the first qubit is in the $|0\rangle$ state. We write this as

$$|q_1\rangle \otimes |q_2\rangle \xrightarrow{\text{CNOT}} |q_1\rangle \otimes |q_2 \oplus q_1\rangle. \tag{A.5}$$

We then apply an R_z operation on the second qubit, yielding the state

$$|q_1\rangle \otimes |q_2 \oplus q_1\rangle \xrightarrow{R_z(\theta)} |q_1\rangle \otimes e^{-i\frac{\theta}{2}\sigma^z_{q_2\oplus q_1}}|q_2 \oplus q_1\rangle, \tag{A.6}$$

where $\sigma^z_{q_2\oplus q_1}$ indicates that the rotation is acting on state $q2 \oplus q1$. We now apply a second CNOT-gate acting in the same way as the previous operation, yielding

$$|q_1\rangle \otimes e^{-i\frac{\theta}{2}\sigma^z_{q_2\oplus q_1}}|q_2 \oplus q_1\rangle \xrightarrow{\text{CNOT}} |q_1\rangle \otimes e^{-i\frac{\theta}{2}\sigma^z_{q_2\oplus q_1}}|q_2 \oplus q_1 \oplus q_1\rangle. \tag{A.7}$$

Since $q_2 \oplus q_1 = q_2 + q_1 \mod 2$, then $\sigma^z_{q_2\oplus q_1} = \sigma^z_{q_2}\sigma^z_{q_1}$, thus the final state is

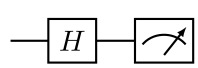
$$e^{-i\frac{\theta}{2}\sigma^z_{q1}\sigma^z_{q2}}|q_1 q_2\rangle, \tag{A.8}$$

which is exactly U from Equation (A.3). Therefore, in the circuit picture, U is implemented as in Figure 2.

B Measuring Observables

Measuring observables is crucial for extracting data from quantum devices. In this exercise, we have considered $\langle\sigma_z\rangle$ or derivations thereof only. This is realised by directly measuring the qubit, as the computational basis, 0 and 1, corresponds directly to the eigenvalues of the σ_z operator, -1 and 1. However, how do we measure other observables? As we can only measure the qubit in the computational basis, if we wish to measure a different observable from $\langle\sigma_z\rangle$, then we must carry out a basis change to the computational basis. For example, below we consider the circuits for measuring $\langle\sigma_x\rangle$ and $\langle\sigma_y\rangle$:

- **Measuring** $\langle\sigma_x\rangle$: To measure the expectation value with respect to σ_x, we must change basis to the computational basis by first applying a Hadamard gate and then measuring in the computational basis:



- **Measuring** $\langle\sigma_y\rangle$: To measure the expectation value with respect to σ_y, we must apply a rotation to the qubit by first applying an $S^\dagger$ gate followed by a Hadamard gate and then measuring in the computational basis: