Transverse-Field Ising Model

We will perform quantum dynamics (QD) simulation (*cf.* lecture 1) on a quantum computer for the transverse-field Ising model (TFIM) Hamiltonian (*cf.* lecture 2) for two spins,

$$H = -J\sigma_0^z\sigma_1^z - B\sum_{j=0}^{1}\sigma_j^x, \tag{1}$$

where σ_j^z and σ_j^x are Pauli Z and X matrices acting on the j-th spin, J is the exchange coupling, and B is the magnetic field along the x axis.

Time evolution of a two-spin wave function, $|\Psi(t)\rangle = |\psi_0(t)\rangle|\psi_1(t)\rangle$ ($|\psi_j(t)\rangle$ is the wave function of the j-th spin at time t), for small time step Δt is governed by (*cf.* https://aiichironakano.github.io/phys516/03QD.pdf)

$$|\Psi(t+\Delta t)\rangle = \exp(-iH\Delta t)|\Psi(t)\rangle \tag{2}$$

in the atomic unit. Using Trotter expansion, the time-propagation operator is approximated as

$$\exp(-iH\Delta t) = \exp(i\Delta tJ\sigma_0^z\sigma_1^z)\exp(i\Delta tB\sigma_0^x)\exp(i\Delta tB\sigma_1^x) + O(\Delta t^2). \tag{3}$$

Let us first consider the transverse-field propagator $\exp\left(i\Delta tB\sigma_j^x\right)$ acting on the j-th spin independent of the other spin. We use the eigendecomposition (see Appendix) of Pauli X matrix,

$$\sigma^x = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4}$$

Note that

$$\sigma^x H = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = H\sigma^z, \tag{5}$$

where H is the Hadamard gate (which is column-aligned eigenvectors $(1/\sqrt{2}, \pm 1/\sqrt{2})^T$ of σ^x with respective eigenvalues ± 1), or equivalently

$$\sigma^x = H\sigma^z H, \tag{6}$$

where we have used the fact H is a symmetric orthogonal matrix, *i.e.*, $H^{-1} = H^T = H$ and thus

$$H^2 = I \tag{7}$$

(I is the identity matrix).

Using Taylor expansion of the time propagator and Eqs. (6) and (7) (the procedure is called telescoping),

$$\exp\left(i\Delta tB\sigma^x\right) = \sum_{n=0}^{\infty}\frac{(i\Delta tB)^n}{n!}\sigma^{x\,n} = \sum_{n=0}^{\infty}\frac{(i\Delta tB)^n}{n!}(H\sigma^z H)^n =$$

$$\sum_{n=0}^{\infty}\frac{(i\Delta tB)^n}{n!}\overbrace{H\sigma^z HH\sigma^z H\cdots H\sigma^z H}^{n\text{ times}}\ (\text{every internal HH product becomes } I) =$$

$$H\sum_{n=0}^{\infty}\frac{(i\Delta tB)^n}{n!}\sigma^{z\,n}H = H\sum_{n=0}^{\infty}\frac{(i\Delta tB)^n}{n!}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}^n H = H\begin{pmatrix} \sum_{n=0}^{\infty}\frac{(i\Delta tB)^n}{n!} & 0 \\ 0 & \sum_{n=0}^{\infty}\frac{(-i\Delta tB)^n}{n!} \end{pmatrix}H =$$

$$H\begin{pmatrix} e^{i\Delta tB} & 0 \\ 0 & e^{-i\Delta tB} \end{pmatrix}H = HR_z(-2\Delta tB)H = \frac{1}{2}\begin{pmatrix} e^{i\Delta tB} + e^{-i\Delta tB} & e^{i\Delta tB} - e^{-i\Delta tB} \\ e^{i\Delta tB} - e^{-i\Delta tB} & e^{i\Delta tB} + e^{-i\Delta tB} \end{pmatrix} =$$

$$\begin{pmatrix} \cos(\Delta tB) & i\sin(\Delta tB) \\ i\sin(\Delta tB) & \cos(\Delta tB) \end{pmatrix} = R_x(-2\Delta tB). \tag{8}$$

In terms of the native gates on IBM Q computers, Eq. (8) can be implemented using either rotation around the *z* axis, $R_z(\theta)$, along with Hadamard gate H, or solely using rotation around the *x* axis, $R_x(\theta)$. Here, R_z and R_x gates are defined as

$$R_z(\theta) = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}, \tag{9}$$

$$R_x(\theta) = \begin{pmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{pmatrix}. \tag{10}$$

(see https://github.com/Qiskit/qiskit-tutorials/blob/master/tutorials/circuits/3_summary_of_quantum_operations.ipynb).

Next, we consider the exchange-coupling propagator $\exp(i\Delta t J\sigma_0^z\sigma_1^z)$. We first consider a tensor product of operators multiplied by a scalar constant,

$$i\Delta t J\sigma_0^z \otimes \sigma_1^z = i\Delta t J \begin{pmatrix} 1\cdot\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & 0\cdot\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ 0\cdot\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & -1\cdot\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} i\Delta t J & 0 & 0 & 0 \\ 0 & -i\Delta t J & 0 & 0 \\ 0 & 0 & -i\Delta t J & 0 \\ 0 & 0 & 0 & i\Delta t J \end{pmatrix}. \tag{11}$$

Since this is a diagonal matrix, it can be exponentiated element by element as

$$\exp(i\Delta t J\sigma_0^z\sigma_1^z) = \begin{pmatrix} \exp(i\Delta t J) & 0 & 0 & 0 \\ 0 & \exp(-i\Delta t J) & 0 & 0 \\ 0 & 0 & \exp(-i\Delta t J) & 0 \\ 0 & 0 & 0 & \exp(i\Delta t J) \end{pmatrix} = \begin{pmatrix} R_z(-2\Delta t J) & 0 \\ 0 & R_z(2\Delta t J) \end{pmatrix}. \tag{12}$$

Now consider the following sequence of quantum gates operating on two qubits, q_0 and q_1,

$$G = CX(q_0, q_1) \cdot R_1^z(-2\Delta t J) \cdot CX(q_0, q_1), \tag{13}$$

where

$$CX(q_0, q_1) = \begin{pmatrix} I & 0 \\ 0 & X \end{pmatrix} \tag{14}$$

is the controlled *X* (CNOT) gate, with q_0 and q_1 being the control and target bits, and R_1^z is the R^z gate acting on q_1. When operating on two qubits, R_1^z signifies a tensor product,

$$I \otimes R^z(-2\Delta t J) = \begin{pmatrix} 1\cdot R^z(-2\Delta t J) & 0\cdot R^z(-2\Delta t J) \\ 0\cdot R^z(-2\Delta t J) & 1\cdot R^z(-2\Delta t J) \end{pmatrix} = \begin{pmatrix} R^z(-2\Delta t J) & 0 \\ 0 & R^z(-2\Delta t J) \end{pmatrix}. \tag{15}$$

Substituting Eqs. (14) and (15) in Eq. (13), we obtain

$$G = \begin{pmatrix} I & 0 \\ 0 & X \end{pmatrix}\begin{pmatrix} R^z(-2\Delta t J) & 0 \\ 0 & R^z(-2\Delta t J) \end{pmatrix}\begin{pmatrix} I & 0 \\ 0 & X \end{pmatrix} = \begin{pmatrix} R^z(-2\Delta t J) & 0 \\ 0 & XR^z(-2\Delta t J)X \end{pmatrix}. \tag{16}$$

Here,

$$XR^z(-2\Delta t J)X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \exp(i\Delta t J) & 0 \\ 0 & \exp(-i\Delta t J) \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \exp(-i\Delta t J) \\ \exp(i\Delta t J) & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} \exp(-i\Delta t J) & 0 \\ 0 & \exp(i\Delta t J) \end{pmatrix} = R^z(2\Delta t J). \tag{17}$$

Substituting Eq. (17) in Eq. (16) and compare the result with Eq. (12), we arrive at the identity,

$$G = CX(q_0, q_1)R_1^z(-2\Delta tJ)CX(q_0, q_1) = \begin{pmatrix} R^z(-2\Delta tJ) & 0 \\ 0 & R^z(2\Delta tJ) \end{pmatrix} = \exp(i\Delta tJ\sigma_0^z\sigma_1^z). \quad (18)$$

where the last equality results from Eq. (12). Namely, $G = CX(q_0, q_1) \cdot R_1^z(-2\Delta tJ) \cdot CX(q_0, q_1)$ is a quantum-gate implementation of the exchange-coupling propagator $\exp(i\Delta tJ\sigma_0^z\sigma_1^z)$.

Combining Eqs. (8) and (18) for the transverse-field and exchange-coupling time propagators, respectively, quantum-circuit implementation for a single time step of time evolution for the TFIM model, Eq. (1), is given by

$$\exp(-iH\Delta t) = \exp(i\Delta tJ\sigma_0^z\sigma_1^z)\exp(i\Delta tB\sigma_0^x)\exp(i\Delta tB\sigma_1^x) = \\ CX(q_0, q_1)R_1^z(-2\Delta tJ)CX(q_0, q_1)R_0^x(-2\Delta tB)R_1^x(-2\Delta tB). \quad (18)$$

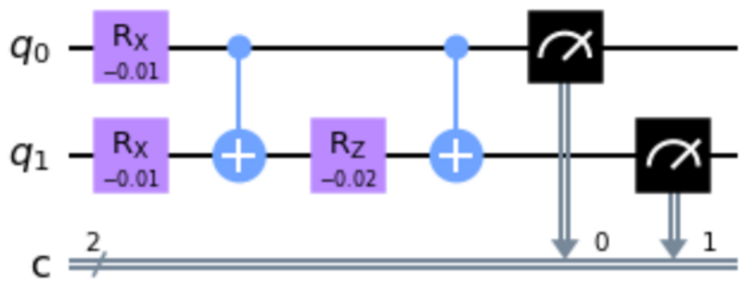


Fig. 1: Quantum circuit for time evolution of TFIM in IBM Quantum Lab.

Hands-on Exercise (try it at https://quantum-computing.ibm.com using IBM Quantum Lab)

Execute the following Qiskit program to perform a single time step of QD simulation. Here, we have used model parameters, $J = 1$, $B = 0.5$ and $\Delta t = 0.01$, in atomic units.

```
##### Single step of Trotter propagation in transverse-field Ising model #####
import numpy as np
# Import standard Qiskit libraries
from qiskit import QuantumCircuit, transpile, Aer, IBMQ
from qiskit.tools.jupyter import *
from qiskit.visualization import *
from ibm_quantum_widgets import *
from qiskit.providers.aer import QasmSimulator
# Load your IBM Quantum account
provider = IBMQ.load_account()
### Physical parameters (atomic units) ###
J = 1.0     # Exchange coupling
B = 0.5     # Transverse magnetic field
dt = 0.01   # Time-discretization unit
### Build a circuit ###
circ = QuantumCircuit(2, 2)  # 2 quantum & 2 classical registers
circ.rx(-2*dt*B, 0)  # Transverse-field propagation of spin 0
circ.rx(-2*dt*B, 1)  # Transverse-field propagation of spin 1
circ.cx(0, 1)        # Exchange-coupling time propagation (1)
circ.rz(-2*dt*J, 1)  #                                   (2)
circ.cx(0, 1)        #                                   (3)
circ.measure(range(2), range(2))  # Measure both spins
circ.draw('mpl')
```

This will build a circuit and draw it, which should then be transpiled and run on a simulator as follows.

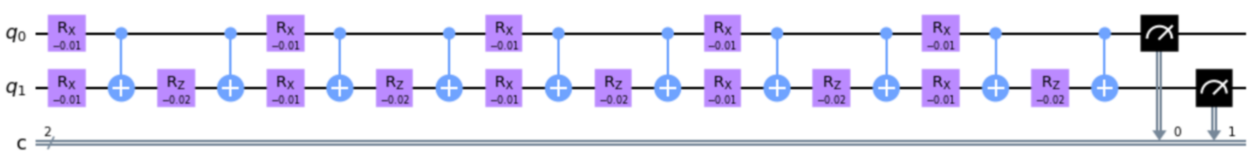
```
### Simulate on OpenQASM backend ###

# Use Aer's Qasm simulator
from qiskit.providers.aer import QasmSimulator
backend = QasmSimulator()
# Transpile the quantum circuit to low-level QASM instructions
from qiskit import transpile
circ_compiled = transpile(circ, backend)
# Execute the circuit on the Qasm simulator, repeating 1024 times
job_sim = backend.run(circ_compiled, shots=1024)
# Grab the results from the job
result_sim = job_sim.result()
# Get the result
counts = result_sim.get_counts(circ_compiled)
# Plot histogram
from qiskit.visualization import plot_histogram
plot_histogram(counts)
```

Table I: Qiskit program for single-time-step QD simulation of TFIM: tfim-1step.qiskit.

After opening a Qiskit (ipykenel) notebook, you can copy and paste the above code into a cell in the Python notebook. Here, we have used QASM simulator as a backend. Try increasing the value of *dt* and re-running the program to see how the result changes (though the Trotter expansion, Eq. (3), will no longer be valid and hence an incorrect result). For Python programming underlying Qiskit, see A. Scopatz and K. D. Huff, *Effective Computation in Physics* at Safari Online (https://libraries.usc.edu/databases/safari-books).

Extension (try it at https://quantum-computing.ibm.com using IBM Quantum Lab)

You can perform quantum dynamics simulation in a correct way by time stepping. Extend the Qiskit program for single-time-step QD simulation of TFIM model (tfim-1step.qiskit) to simulate the same model for $t_{\text{tot}} = 5\Delta t$ ($\Delta t = 0.01$).



Appendix: Eigendecomposition

For a 2×2 Hermitian matrix,

$$\mathbf{A} = \begin{bmatrix} a & b \\ b^* & a \end{bmatrix}, \tag{A1}$$

where a and b are real and complex numbers, respectively, consider an eigenvalue problem,

$$\begin{bmatrix} a & b \\ b^* & a \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \varepsilon \begin{bmatrix} u \\ v \end{bmatrix}. \tag{A2}$$

or equivalently

$$\begin{bmatrix} \varepsilon - a & -b \\ -b^* & \varepsilon - a \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{A3}$$

For nontrivial solutions (*i.e.*, other than $u = v = 0$), the determinant of the matrix in Eq. (A3) should be zero. (Otherwise, one can invert Eq. (A3) to get $u = v = 0$.) Hence,

$$\begin{vmatrix} \varepsilon - a & -b \\ -b^* & \varepsilon - a \end{vmatrix} = (\varepsilon - a)^2 - |b|^2 = 0, \text{ Secular (characteristic) equation} \tag{A4}$$

which has two solutions,

$$\varepsilon_\pm = a \pm |b|. \text{ Eigenvalues} \tag{A5}$$

The corresponding eigenvectors can be obtained by solving Eq. (A3) for these eigenvalues

$$\begin{bmatrix} |b| & -b \\ -b^* & |b| \end{bmatrix} \begin{bmatrix} u_+ \\ v_+ \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}; \begin{bmatrix} -|b| & -b \\ -b^* & -|b| \end{bmatrix} \begin{bmatrix} u_+ \\ v_+ \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{A6}$$

with the answers (note the degeneracy of the two linear equations for each eigenvalue, *e.g.*, $|b|u_+ - bv_+ = 0 \Longrightarrow \left(\times \frac{-b^*}{|b|}\right) -b^*u_+ + |b|v_+ = 0$)

$$\mathbf{w}_\pm = \begin{bmatrix} u_\pm \\ v_\pm \end{bmatrix} = \frac{1}{\sqrt{2}|b|} \begin{bmatrix} b \\ \pm|b| \end{bmatrix}. \text{ Eigenvectors} \tag{A7}$$

In Eq. (A7), we have normalized each eigenvector so that

$$\mathbf{w}_\pm^\dagger \mathbf{w}_\pm = [u_\pm^* \quad v_\pm^*] \begin{bmatrix} u_\pm \\ v_\pm \end{bmatrix} = \frac{\overbrace{b^*b}^{|b|^2} + |b|^2}{2|b|^2} = 1, \tag{A8}$$

where $\mathbf{w}_\pm^\dagger$ denotes the Hermitian conjugate (or conjugate transpose) of $\mathbf{w}_\pm$. Also, the two eigenvectors are orthogonal:

$$\mathbf{w}_\mp^\dagger \mathbf{w}_\pm = [u_\mp^* \quad v_\mp^*] \begin{bmatrix} u_\pm \\ v_\pm \end{bmatrix} = \frac{\overbrace{b^*b}^{|b|^2} - |b|^2}{2|b|^2} = 0. \tag{A9}$$

Now, define a 2×2 matrix composed of column aligned eivenvectors,

$$\mathbf{U} = [\mathbf{w}_+ \quad \mathbf{w}_-] = \begin{bmatrix} u_+ & u_- \\ v_+ & v_- \end{bmatrix} = \frac{1}{\sqrt{2}|b|} \begin{bmatrix} b & b \\ |b| & -|b| \end{bmatrix}, \tag{A10}$$

then

$$\mathbf{U}^\dagger \mathbf{U} = \begin{bmatrix} \mathbf{w}_+^\dagger \\ \mathbf{w}_-^\dagger \end{bmatrix} [\mathbf{w}_+ \quad \mathbf{w}_-] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \mathbf{I}, \tag{A11}$$

where $\mathbf{I}$ is the 2×2 identity matrix and we have used the orthonormalization relations, Eqs. (A8) and (A9). Using the explicit formula for $\mathbf{U}$ in Eq. (A10), we can also verify that $\mathbf{U}\mathbf{U}^\dagger = \mathbf{I}$ and hence $\mathbf{U}$ is a unitary matrix:

$$\mathbf{U}^\dagger\mathbf{U} = \mathbf{U}\mathbf{U}^\dagger = \mathbf{I}. \text{ Unitary} \tag{A12}$$

The two solutions of Eq. (A2) can now be combined into a matrix form as

$$\begin{cases} \begin{bmatrix} a & b \\ b^* & a \end{bmatrix} \begin{bmatrix} u_+ \\ v_+ \end{bmatrix} = \varepsilon_+ \begin{bmatrix} u_+ \\ v_+ \end{bmatrix} \\ \begin{bmatrix} a & b \\ b^* & a \end{bmatrix} \begin{bmatrix} u_- \\ v_- \end{bmatrix} = \varepsilon_- \begin{bmatrix} u_- \\ v_- \end{bmatrix} \end{cases} \Leftrightarrow \underbrace{\begin{bmatrix} a & b \\ b^* & a \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} u_+ & u_- \\ v_+ & v_- \end{bmatrix}}_{\mathbf{U}} = \underbrace{\begin{bmatrix} u_+ & u_- \\ v_+ & v_- \end{bmatrix}}_{\mathbf{U}} \underbrace{\begin{bmatrix} \varepsilon_+ & 0 \\ 0 & \varepsilon_- \end{bmatrix}}_{\mathbf{D}}, \tag{A13}$$

i.e.,

$$\mathbf{AU} = \mathbf{UD}, \tag{A14}$$

where we have defined a diagonal matrix,

$$\mathbf{D} = \begin{bmatrix} \varepsilon_+ & 0 \\ 0 & \varepsilon_- \end{bmatrix}. \tag{A15}$$

$\because \begin{bmatrix} u_+ & u_- \\ v_+ & v_- \end{bmatrix} \begin{bmatrix} \lambda_+ \\ 0 \end{bmatrix} = \lambda_+ \begin{bmatrix} u_+ \\ v_+ \end{bmatrix}$ and $\begin{bmatrix} u_+ & u_- \\ v_+ & v_- \end{bmatrix} \begin{bmatrix} 0 \\ \lambda_- \end{bmatrix} = \lambda_- \begin{bmatrix} u_- \\ v_- \end{bmatrix}$ 1st & 2nd-column pickers

Multiplying both sides of Eq. (A14) by $\mathbf{U}^\dagger$ from the right hand and using the unitary, Eq. (A12), we obtain

$$\mathbf{A} = \mathbf{UDU}^\dagger. \text{ Eigendecomposition} \tag{A16}$$

or more explicitly

$$\begin{bmatrix} a & b \\ b^* & a \end{bmatrix} = \frac{1}{\sqrt{2}|b|} \begin{bmatrix} b & b \\ |b| & -|b| \end{bmatrix} \begin{bmatrix} a + |b| & 0 \\ 0 & a - |b| \end{bmatrix} \frac{1}{\sqrt{2}|b|} \begin{bmatrix} b & b \\ |b| & -|b| \end{bmatrix}. \tag{A17}$$

(Example) Pauli X matrix, *i.e.*, $a = 0$ and $b = 1$

$$\mathbf{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \mathbf{HZH}. \tag{A18}$$

where $\mathbf{H}$ and $\mathbf{Z}$ are matrix representations of Hadamard and Pauli Z gates.