

1 The Hamiltonian

We consider a Hamiltonian acting on n qubits:

$$H = \alpha(s_1 \otimes s_2 \otimes \cdots \otimes s_n) \quad (1)$$

where s_i are Pauli matrices (X, Y, Z), and α is a scalar. Our goal is to implement the time evolution operator efficiently:

$$e^{-itH} = e^{-it\alpha(s_1 \otimes s_2 \otimes \cdots \otimes s_n)}. \quad (2)$$

2 The Challenge

- H is a $2^n \times 2^n$ matrix, making direct exponentiation impractical.
- Quantum circuits use polynomially many gates ($O(\text{poly}(n))$), so we need an efficient approach.

3 Unitary Transformation Trick

We use the key identity:

$$Ue^{-i\alpha H}U^\dagger = e^{-i\alpha UHU^\dagger}. \quad (3)$$

This follows from the definition of the matrix exponential.

Proof. Expanding the power series:

$$e^{-i\alpha H} = \sum_{k=0}^{\infty} \frac{(-i\alpha H)^k}{k!}, \quad (4)$$

and applying conjugation by U :

$$Ue^{-i\alpha H}U^\dagger = U \left(\sum_{k=0}^{\infty} \frac{(-i\alpha H)^k}{k!} \right) U^\dagger. \quad (5)$$

Using $UHU^\dagger = H'$, we get:

$$Ue^{-i\alpha H}U^\dagger = \sum_{k=0}^{\infty} \frac{(-i\alpha UHU^\dagger)^k}{k!} = e^{-i\alpha H'}. \quad (6)$$

□

4 Diagonalizing H

Each Pauli matrix s_i can be diagonalized by a single-qubit unitary U_i :

5 Diagonalization of Pauli Terms

6 Single-Qubit Pauli Matrix Diagonalization

7 Pauli Matrices

The Pauli matrices are fundamental operators in quantum mechanics:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (7)$$

- **Pauli-X diagonalization:**

$$HXH = Z \quad (8)$$

The Hadamard gate H transforms X to diagonal Z form.

- **Pauli-Y diagonalization:**

$$U_Y Y U_Y^\dagger = Z \quad \text{where} \quad U_Y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \quad (9)$$

The unitary U_Y transforms Y to diagonal Z form.

Applying these transformations to all qubits, we rewrite the evolution operator as:

$$e^{-itH} = (U_1 \otimes \dots \otimes U_n) e^{-i\alpha t(z_1 \otimes \dots \otimes z_n)} (U_1^\dagger \otimes \dots \otimes U_n^\dagger), \quad (10)$$

where z_i are now either I or Z , making the Hamiltonian diagonal.

8 Why This Helps

By diagonalizing H , we reduce the problem to implementing:

$$e^{-i\alpha t Z \otimes Z \otimes \dots \otimes Z}, \quad (11)$$

which is simple because:

- Pauli Z matrices are diagonal, making exponentiation trivial, example of diagonalization.
- The circuit needs only controlled phase gates, requiring $O(n)$ quantum gates.

9 Conclusion

Using unitary transformations, we efficiently simulate the time evolution of a tensor-product Pauli Hamiltonian in polynomial time, making it feasible for quantum computation.