Lecture notes: quantum circuit architecture for Pauli strings exponentials

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Abstract
The purpose of these notes is to explain how to build the quantum circuit that will encode a Pauli string exponential. These operations play a key role in quantum computation for quantum chemistry as they appear in various quantum algorithms. We can find them in the quantum circuit encoding of the Unitary Coupled Cluster ansatz for the VQE algorithm (Variational Quantum Eigensolver), or in the encoding of the time evolution operator for the QPE algorithm (Quantum Phase Estimation). To help the reader, I will first present all the basic ingredients, then I will explain step by step the architectures of the circuits.

Contents

1. Basics one- and two-qubit gates and Pauli-strings

1.1 Pauli operators X, Y, Z

First, let us introduce important single-qubit quantum transformations : the Pauli operators X_q, Y_q and Z_q. Their gate representation is given in figure 1.

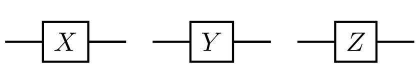

Figure 1: Representation of the Pauli gates.

The three different Pauli operators present the following matrix shape in the local basis (associated to the qubit "q")

$$X_q = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y_q = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z_q = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (1)$$

Here we have introduced the index "q" to refer to the particular qubit these operators are attached to. Based on these matrix forms, a pletora of useful properties can be derived. We are going to enumerate the most important ones for our future work.

- Pauli operators are hermitian :

$$X_q = X_q^\dagger, \quad Y_q = Y_q^\dagger, \quad Z_q = Z_q^\dagger \quad (2)$$

- Pauli operators are involutory (self-inverse) :

$$X_q^2 = Y_q^2 = Z_q^2 = \mathbf{1}_q \quad (3)$$

- Complete matrix product of three Pauli operators resolve the identity of the qubit q Hilbert space :

$$\mathbf{1}_q = -iX_qY_qZ_q \quad (4)$$

- A useful trick is that a Z_q operator sandwiched by two X_q or Y_q produces a minus sign :

$$X_qZ_qX_q = Y_qZ_qY_q = -Z_q \quad (5)$$

  This can be demonstrated using the previous definition (resolution of the identity).

1.1.1 Rotation gates $R_{X,Y,Z}(\theta)$

Now let us focus on the qubit rotations. For any Pauli operator (X_q, Y_q, Z_q), a rotation of the qubit q can be generated via a unitary operator. Such an unitary operator takes the shape of complex exponential of the associated Pauli matrix. For example, the following operation

$$e^{-i\theta Z_q} = \cos(\theta)\mathbf{1}_q - i\sin(\theta)Z_q \quad (6)$$

produces a rotation for the qubit q of angle θ around the Z_q axis. Note that the cosine/sine representation of this operator holds thanks to the algebraic properties of the Pauli operator.

Even if this transformation is very general, in the literature (and in practice) rotations are introduced with the concept of "rotation gates" which present a slightly different angular parametrization. For example, to do a rotation around the Z_q axis we have the following gate

$$\begin{aligned} R_{Z_q}(\theta') &= e^{-i\frac{\theta'}{2}Z_q} \\ &= \cos(\theta'/2)\mathbf{1} - i\sin(\theta/2)Z_q \end{aligned} \tag{7}$$

We see here the presence of a factor 2 which simply represents a difference of angular parametrization. This difference is not a problem, but we want here to stress that in order to implement an angular rotation of θ on a qubit, we should use in a circuit a rotation gate $R_{Z_q}(2\theta)$. Figure 2 illustrates the diagram that is usually employed to represent a rotation gate.

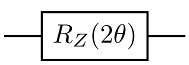

Figure 2: Diagram of a Z_q rotation gate.

1.2 Control-X gate $C^X_{qq'}$ (CNOT)

Another important gate is the two-qubit $C^X_{qq'}$ gate whose matrix shape is

$$C^X_{qq'} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{8}$$

This operator, also called "CNOT", depends on two ingredients : a first control qubit q which, when active, generates a flip of the state of a second target qubit q'. In tensorial representation, this operator is described as

$$C^X_{qq'} = |0_q\rangle\langle 0_q| \otimes \mathbf{1}_{q'} + |1_q\rangle\langle 1_q| \otimes X_{q'} \tag{9}$$

Based on this, we clearly see that the $C^X_{qq'}$ operator is hermitian

$$C^X_{qq'} = {C^X_{qq'}}^\dagger \tag{10}$$

and involutory

$$C^X_{qq'} {C^X_{qq'}}^\dagger = {C^X_{qq'}}^\dagger C^X_{qq'} = \mathbf{1}_q \otimes \mathbf{1}_{q'} \tag{11}$$

In a quantum circuit, we will denote the action of this two-qubit gate via a diagram as illustrated in figure 3.

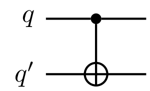

Figure 3: $C^X_{qq'}$ gate with a control qubit q and a target qubit q'.

1.3 Pauli strings $\mathcal{P}$

Let us now introduce a central object : the Pauli string. A Pauli string $\mathcal{P}$ refers to a chain (*i.e.* a tensor product) of different Pauli operators, each one acting on one qubit. As an example, we can imagine a Pauli string for 4 different qubits such that

$$\mathcal{P} = Z_0 \otimes X_1 \otimes \mathbf{1}_2 \otimes Y_3 \tag{12}$$

with Z_0 acting on the qubit $q = 0$, X_1 on the qubit $q = 1$, and so on. Note that in the following if an identity is present for any qubit we will intentionally disregard its notation. Therefore, we can introduce a shorthand notation for the precedent Pauli string like

$$\mathcal{P} = Z_0 \otimes X_1 \otimes \mathbf{1}_2 \otimes Y_3 \longrightarrow Z_0X_1Y_3 \tag{13}$$

In practice, Pauli strings usually appear when building the quantum circuit for a Unitary Coupled Cluster ansatz or for a time evolution propagator (see the lectures realized during the workshop). Due to the nice properties of the Pauli operators, we can show that exponential of Pauli strings actually follows

$$e^{-i\theta\mathcal{P}} = \cos(\theta)\mathbf{1} - i\sin(\theta)\mathcal{P} \tag{14}$$

with θ a phase parameter and $\mathbf{1}$ the resolution of the identity over the total set of qubits considered.

2. Quantum circuit to implement exponentials of Pauli strings

2.1 Generating extended Z Pauli string exponentials

Our first tool, will be to use C^X gates to sandwich a Z-rotation gate. We can that this process extend the effect of this rotation to a second qubit. More precisely, considering a control qubit q and a target qubit (with the condition $q < q'$), we can show that the following property holds

$$e^{-i\theta Z_q Z_{q'}} = C^X_{qq'}\ e^{-i\theta Z_{q'}}\ C^X_{qq'} \tag{15}$$

To demonstrate this property, let us use the trigonometric decomposition of the complex exponential (introduced in previous section)

$$C^X_{qq'}\ e^{-i\theta Z_{q'}}\ C^X_{qq'} = \cos(\theta)\mathbf{1} - i\sin(\theta) C^X_{qq'}\ Z_{q'}\ C^X_{qq'} \tag{16}$$

Here we also used the fact that $C^X_{qq'}$ gates are involutory. Then, using the tensorial representation of the $C^X_{qq'}$ gate and the trick $XZX = -Z$, we can demonstrate the following useful property

$$C^X_{qq'}\ Z_{q'}\ C^X_{qq'} = Z_q Z_{q'} \tag{17}$$

Putting this result back into (16) allows to conclude the proof of (15) with

$$e^{-i\theta Z_q Z_{q'}} = \cos(\theta)\mathbf{1} - i\sin(\theta) Z_q Z_{q'} \tag{18}$$

Based on this, we can then define a quantum circuit architecture to implement any exponential of Z-Pauli strings. Figures (4-7) illustrate all the possible quantum circuits realizing such a transformation on a register of three qubits.

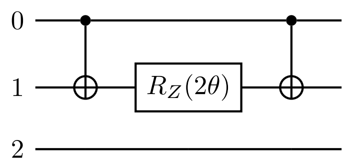

Figure 4: Circuit generating $\exp(-i\theta Z_0 Z_1)$

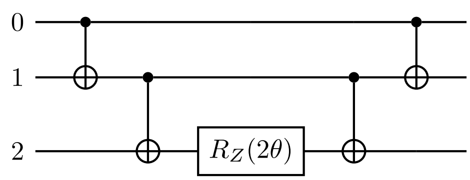

Figure 5: Circuit generating $\exp(-i\theta Z_0 Z_1 Z_2)$

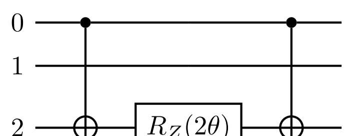

Figure 6: Circuit generating $\exp(-i\theta Z_0 Z_2)$

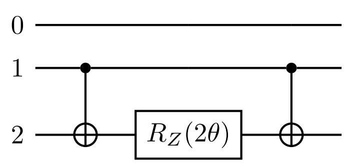

Figure 7: Circuit generating $\exp(-i\theta Z_1 Z_2)$

2.2 From Z to X, Y operators in exponential

We know how to generate any kind of Z-Pauli string in an exponential. Starting from this, we will now learn how to change Z_q operator in an exponential with a X_q or Y_q operator. To introduce this trick, we sandwich the Z-Pauli string exponential by two rotation gates implementing rotations of $\pi/4$ of the qubit q around the Y_q-axis (*i.e.* $R_{Y_q}(\pi/2)$). Using the trigonometric decomposition (see previous section), we can indeed show

$$\begin{aligned} R_{Y_q}(\pi/2)\ e^{-i\theta Z_0 \dots Z_q \dots Z_N}\ R^\dagger_{Y_q}(\pi/2) = \\ e^{-i\theta Z_0 \dots R_{Y_q}(\pi/2) Z_q R^\dagger_{Y_q}(\pi/2) \dots Z_N} \end{aligned} \tag{19}$$

Then, using the trigonometric decomposition on the rotation operator we can show

$$R_{Y_q}(\pi/2) Z_q R^\dagger_{Y_q}(\pi/2) = X_q \tag{20}$$

Thus, we see here the trick

$$R_{Y_q}(\pi/2)\ e^{-i\theta Z_0 \dots Z_q \dots Z_N}\ R^\dagger_{Y_q}(\pi/2) = e^{-i\theta Z_0 \dots X_q \dots Z_N} \tag{21}$$

We can then replace any Z_q operator by a X_q using the rotation $R_{Y_q}(\pi/2)$. Note that the same type of trick holds if we want to obtain Y_q instead of X_q. However in this case the transformation we should use is $R_{X_q}(-\pi/2)$: a rotation of $-\pi/4$ of the qubit q around the X_q-axis. Using this rotation, we can show the following property

$$R_{X_q}(-\pi/2) Z_q R^\dagger_{X_q}(-\pi/2) = Y_q \tag{22}$$

which allows us to change a Z_q operator by a Y_q in the exponential.

3. Example of quantum circuit

Finally, if we combine the two tricks we have introduced before, we can then decompose any exponential of Pauli-string into a succession of elementary transformations. To give an example, let us decompose the following unitary :

$$e^{-i\theta Z_A X_B} = \cos(\theta)\mathbf{1} - i\sin(\theta) Z_A X_B \tag{23}$$

We have then the following circuit decomposition:

$$\begin{aligned} e^{-i\theta Z_A X_B} &= R_{Y_B}(\pi/2)\ e^{-i\theta Z_A Z_B}\ R_{Y_B}(-\pi/2) \\ &= R_{Y_B}(\pi/2)\ C^X_{AB}\ e^{-i\theta Z_B}\ C^X_{AB}\ R_{Y_B}(-\pi/2). \end{aligned} \tag{24}$$

Figure 8 illustrates the circuit architecture that implements the precedent unitary (with a parameter 2θ).

Remark : my apologies, but in my slides the circuits introducing the Pauli exponentials should be reversed around the central Z-rotation gate. Indeed, when translating a series of operators into a circuit, the operator on the very right is implemented first in the circuit, namely on the left. In other terms, the rotations $R_Y(-\pi/2)$ and $R_X(\pi/2)$ should be on the left and not on the right in the quantum circuits (here, the figure 8 includes this correction).

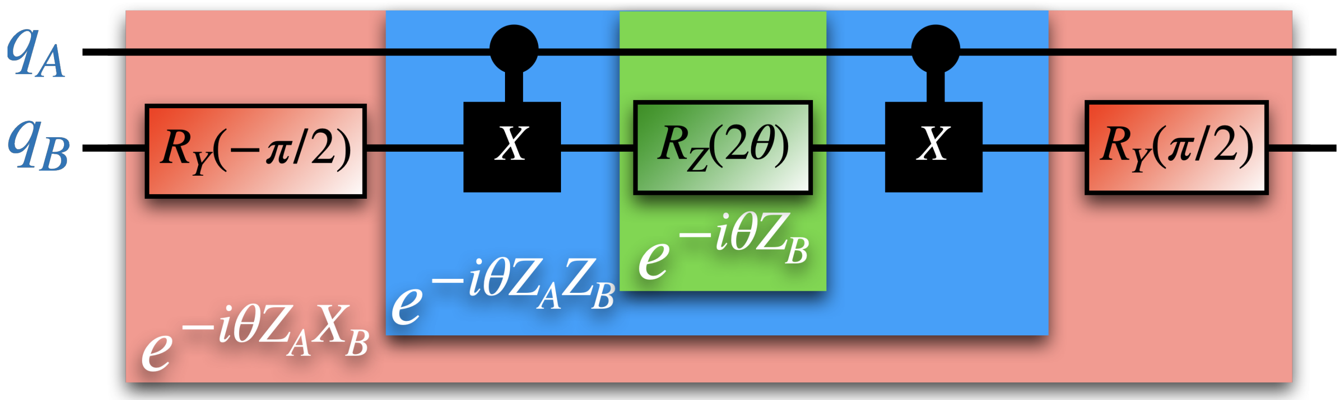

Figure 8: Illustration of the quantum circuit implementing the operator $e^{-i\theta Z_A X_B}$.