

# decomposition

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## 1 Decomposition

1.1 In this notebook we are going to explain step-by-step our optimal decomposition

## 2 1) Trotterization

We decide to split the XXX Hamiltonian into two pieces  $H = H_1 + H_2$  (instead of 6):

$$H_1 = I^{(0)} \otimes \sigma_x^{(1)} \otimes \sigma_x^{(2)} + I^{(0)} \otimes \sigma_y^{(1)} \otimes \sigma_y^{(2)} + I^{(0)} \otimes \sigma_z^{(0)} \otimes \sigma_z^{(1)}$$
$$H_2 = \sigma_x^{(0)} \otimes \sigma_x^{(1)} \otimes I^{(2)} + \sigma_y^{(0)} \otimes \sigma_y^{(1)} \otimes I^{(2)} + \sigma_z^{(0)} \otimes \sigma_z^{(1)} \otimes I^{(2)}$$

so using Trotter's formula:

$$e^{-iHt} = e^{-i(H_1+H_2)t} \simeq \left( e^{-iH_1 \frac{t}{N}} e^{-iH_2 \frac{t}{N}} \right)^N$$

Now we need to compute a sigle Trotter Step in function of  $\frac{t}{N}$

```
[ ]: import numpy as np
from sympy import *
from sympy.physics.quantum import TensorProduct as Tp
import warnings
warnings.filterwarnings('ignore')

X = Matrix([[0,1],[1,0]]) #defining the pauli matrices
Y = Matrix([[0,-I],[I,0]])
Z = Matrix([[1,0],[0,-1]])
Id = eye(2)

H1 = Tp(X,X,Id) + Tp(Y,Y,Id) + Tp(Z,Z,Id)
H1
```

```
[ ]: 
$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

```

```
[ ]: a = symbols("a")

m = Matrix([
    [exp(-I*a),0,0,0],
    [0,cos(a)*exp(I*a),-I*sin(a)*exp(I*a),0],
    [0,-I*sin(a)*exp(I*a),cos(a)*exp(I*a),0],
    [0,0,0,exp(-I*a)]
])
m
```

```
[ ]:
```

$$\begin{bmatrix} e^{-ia} & 0 & 0 & 0 \\ 0 & e^{ia} \cos(a) & -ie^{ia} \sin(a) & 0 \\ 0 & -ie^{ia} \sin(a) & e^{ia} \cos(a) & 0 \\ 0 & 0 & 0 & e^{-ia} \end{bmatrix}$$

```
[ ]: exp_H1p = Tp(m, Id)
exp_H1p
```

```
[ ]:
```

$$\begin{bmatrix} e^{-ia} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & e^{-ia} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & e^{ia} \cos(a) & 0 & -ie^{ia} \sin(a) & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{ia} \cos(a) & 0 & -ie^{ia} \sin(a) & 0 & 0 \\ 0 & 0 & -ie^{ia} \sin(a) & 0 & e^{ia} \cos(a) & 0 & 0 & 0 \\ 0 & 0 & 0 & -ie^{ia} \sin(a) & 0 & e^{ia} \cos(a) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & e^{-ia} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & e^{-ia} \end{bmatrix}$$

where  $a = \frac{2t}{N}$

We can also compute  $H_2$

```
[ ]: exp_H2p = Tp(Id,m)
exp_H2p
```

```
[ ]:
```

$$\begin{bmatrix} e^{-ia} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & e^{ia} \cos(a) & -ie^{ia} \sin(a) & 0 & 0 & 0 & 0 & 0 \\ 0 & -ie^{ia} \sin(a) & e^{ia} \cos(a) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{-ia} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{-ia} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & e^{ia} \cos(a) & -ie^{ia} \sin(a) & 0 \\ 0 & 0 & 0 & 0 & 0 & -ie^{ia} \sin(a) & e^{ia} \cos(a) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & e^{-ia} \end{bmatrix}$$

So, the final form of a Trotter step is :

$$e^{-iHt} = e^{-i(H_1+H_2)t} \simeq \left( e^{-iH_1 \frac{t}{N}} e^{-iH_2 \frac{t}{N}} \right)^N$$

$$T_{step} = e^{-iH_1 \frac{t}{N}} e^{-iH_2 \frac{t}{N}} =$$

```
[ ]: Trotter_Step = exp_H1p * exp_H2p
Trotter_Step
```

```
[ ]: 
$$\begin{bmatrix} e^{-2ia} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \cos(a) & -i \sin(a) & 0 & 0 & 0 & 0 \\ 0 & -ie^{2ia} \sin(a) \cos(a) & e^{2ia} \cos^2(a) & 0 & -i \sin(a) & 0 & 0 \\ 0 & 0 & 0 & \cos(a) & 0 & -ie^{2ia} \sin(a) \cos(a) & -e^{2ia} \sin^2(a) \\ 0 & -e^{2ia} \sin^2(a) & -ie^{2ia} \sin(a) \cos(a) & 0 & \cos(a) & 0 & 0 \\ 0 & 0 & 0 & -i \sin(a) & 0 & e^{2ia} \cos^2(a) & -ie^{2ia} \sin(a) \cos(a) \\ 0 & 0 & 0 & 0 & 0 & -i \sin(a) & \cos(a) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

```

## 3 2) Single Column Decomposition

This Decomposition works only in a symmetry preserving subspace of the Hamiltonian. In this case we are in the magnetization  $m=2$  subspace.

We need to find a  $U_{best}$  gate for which  $T_{step}^n |110\rangle = U_{best} |110\rangle$  and reduces the depth of the circuit. If the initial state is a vector of the computational basis this decomposition coincides with the preparation of a specific column of the matrix, in this case the 7th column.

The idea is to find a generic circuit that preserves the symmetry and depends on 2d real parameters, where d is the dimension of the subspace.

Instead of repeating the Trotter Step we numerically calculate  $T_{step}^n$  and find the parameters of the optimized circuit. In this case we need at least a six parameters circuit.

### 3.1 2.1) Parametric Circuit

To find the most generic magnetization preserving circuit we start by defining a general 2-qubit operator that do this and depends on 3 parameters:

```
[ ]: a1, r1, f1 = symbols("a1 r1 f1")

H = Matrix([
    [1/sqrt(2), 1/sqrt(2)],
    [1/sqrt(2), -1/sqrt(2)]
])

cx_01= Matrix([
    [1,0,0,0],
    [0,0,0,1],
    [0,0,1,0],
    [0,1,0,0]
])

def ry(alpha):    # generic ry gate
    return Matrix([
        [cos(alpha/2), -sin(alpha/2)],
        [sin(alpha/2), cos(alpha/2)]
    ])
```

```

    ])

def rz(alpha):    # generic rz gate
    return Matrix([
        [exp(-1j*(alpha/2)),0],
        [0,exp(1j*(alpha/2))]
    ])

M1 =  $\square$ 
 $\rightarrow$ Matrix(simplify(Tp(rz(2*f1),Id)*Tp(Id,H)*cx_01*Tp(ry(a1),ry(a1))*cx_01*Tp(Id,H)*Tp(rz(2*r1)
M1

```

$$[ ]: \begin{bmatrix} e^{1.0i(-f_1-r_1)} & 0 & 0 & 0 \\ 0 & e^{-1.0i(f_1+r_1)} \cos(a_1) & -e^{-1.0i(f_1-r_1)} \sin(a_1) & 0 \\ 0 & e^{1.0i(f_1-r_1)} \sin(a_1) & e^{1.0i(f_1+r_1)} \cos(a_1) & 0 \\ 0 & 0 & 0 & e^{1.0i(f_1+r_1)} \end{bmatrix}$$

We need at least six parameters so we decide to apply  $M_1$  to qubits  $[0, 1]$  and  $M_2$  to  $[1, 2]$ .

$$U_{best} = (I \otimes M_2(f_2, r_2, a_2))(M_1(f_1, r_1, a_1) \otimes I)$$

```

[ ]: a2, r2, f2 = symbols("a2 r2 f2")
M2 =  $\square$ 
 $\rightarrow$ Matrix(simplify(Tp(rz(2*f2),Id)*Tp(Id,H)*cx_01*Tp(ry(a2),ry(a2))*cx_01*Tp(Id,H)*Tp(rz(2*r2)

Ubest = Tp(M2, Id) * Tp(Id, M1)
Ubest

```

$$[ ]: \begin{bmatrix} e^{1.0i(-f_1-r_1)} e^{1.0i(-f_2-r_2)} & 0 & 0 & 0 \\ 0 & e^{-1.0i(f_1+r_1)} e^{1.0i(-f_2-r_2)} \cos(a_1) & -e^{-1.0i(f_1-r_1)} e^{1.0i(-f_2-r_2)} \sin(a_1) & 0 \\ 0 & e^{1.0i(f_1-r_1)} e^{-1.0i(f_2+r_2)} \sin(a_1) \cos(a_2) & e^{1.0i(f_1+r_1)} e^{-1.0i(f_2+r_2)} \cos(a_1) \cos(a_2) & 0 \\ 0 & 0 & 0 & 0 \\ 0 & e^{1.0i(f_1-r_1)} e^{1.0i(f_2-r_2)} \sin(a_1) \sin(a_2) & e^{1.0i(f_1+r_1)} e^{1.0i(f_2-r_2)} \sin(a_2) \cos(a_1) & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Perfect, now imposing the equality between the elements of the 7<sup>th</sup> column (relative to  $|110\rangle$ ) of the parametric matrix  $U_{best}$  and of the numerical evaluation  $(T_{step})^n$  matrix we can define our Gate.

So, the  $(T_{step})^n$  matrix is easily computed here:

```

[ ]: steps = 42
time = np.pi
U = eye(8)

for _ in range(steps):
    U=U*Trotter_Step
    U=U.subs(a,2*time/steps)

```

U=U.evalf(40)

U.evalf(4)

[ ]:

$$\begin{bmatrix} 1.0 - 2.873 \cdot 10^{-16}i & 0 & 0 & 0 & 0 \\ 0 & 0.4367 + 0.3027i & 0.07228 + 0.526i & 0 & -0.5554 + 0.3569i \\ 0 & -0.05856 + 0.6128i & -0.1395 - 0.5654i & 0 & 0.07228 + 0.526i \\ 0 & 0 & 0 & 0.4367 + 0.3027i & 0 \\ 0 & -0.5507 + 0.1882i & -0.05856 + 0.6128i & 0 & 0.4367 + 0.3027i \\ 0 & 0 & 0 & 0.07228 + 0.526i & 0 \\ 0 & 0 & 0 & -0.5554 + 0.3569i & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

We impose the following equation in order to have the same values on the 7<sup>th</sup> column of both the matrices:

$$\begin{cases} b_0 = \text{im}(U_{4,7}) \\ b_1 = \text{im}(U_{6,7}) \\ b_2 = \text{im}(U_{7,7}) \\ \alpha_0 = \text{re}(U_{4,7}) \\ \alpha_1 = \text{re}(U_{6,7}) \\ \alpha_2 = \text{re}(U_{7,7}) \end{cases}$$

$$\begin{cases} -f_1 + r_1 - f_2 + r_2 = \text{atan}(\frac{b_0}{\alpha_0}) = x_0 \\ -\pi - f_1 + r_1 + f_2 + r_2 = \text{atan}(\frac{b_1}{\alpha_1}) = x_1 \\ f_1 + r_1 + f_2 + r_2 = \text{atan}(\frac{b_2}{\alpha_2}) = x_2 \\ \sin(a_1)\sin(a_2) = |U_{4,7}| = \sqrt{\alpha_0^2 + b_0^2} \\ \sin(a_1)\cos(a_2) = |U_{6,7}| = \sqrt{\alpha_1^2 + b_1^2} \\ \cos(a_1) = |U_{7,7}| = \sqrt{\alpha_2^2 + b_2^2} \end{cases}$$

solving them one can find:

$$\begin{cases} r_1 = \frac{x_0 + x_2}{2} \\ r_2 = 0 \\ f_2 = \frac{x_2 - x_1 - \pi}{2} \\ f_1 = \frac{x_0 - x_1 - \pi}{2} \\ a_1 = \arccos(\sqrt{\alpha_2^2 + b_2^2}) \\ a_2 = \arccos(\frac{\sqrt{\alpha_1^2 + b_1^2}}{\sin(a_1)}) \end{cases}$$

### 3.2 3) Decomposition of $M_1$ and $M_2$ operators

We need to find the minimal decomposition of the M gate. The M gate acts as generic 1 qubit gate on the subspace  $|10\rangle, |01\rangle$  and as a phase for  $|00\rangle$  and  $|11\rangle$ . So we used the Givens Rotation gate as defined in: “<https://arxiv.org/pdf/2104.05695.pdf>” that perform a RY in the subspace  $|10\rangle, |01\rangle$  with just 2 cnots. We can think to do a ZYZ decomposition to finally obtain :

$$M = (I \otimes RZ(f))G(r)(I \otimes RZ(a))$$

```
[ ]: from qiskit import Aer, QuantumCircuit, QuantumRegister, execute

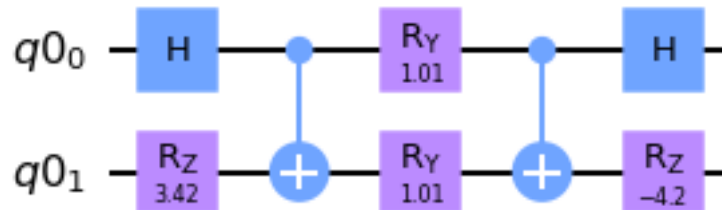
r1=float(atan2(im(U[3*8+6]),re(U[3*8+6]))+atan2(im(U[6*8+6]),re(U[6*8+6])))/2
r2=0
f1=float(atan2(im(U[6*8+6]),re(U[6*8+6]))-atan2(im(U[5*8+6]),re(U[5*8+6]))-np.
    ↪pi)/2
f2=float((atan2(im(U[6*8+6]),re(U[6*8+6]))-atan2(im(U[3*8+6]),re(U[3*8+6])))/
    ↪2-f1)
a1=float(acos(abs(U[6*8+6])))
a2=float(acos(abs(U[5*8+6])/sin(a1)))

qr1=QuantumRegister(2)
M1_qc=QuantumCircuit(qr1, name="M1")

M1_qc.rz(2*r1,qr1[1])
M1_qc.h(qr1[0])
M1_qc.cx(qr1[0],qr1[1])
M1_qc.ry(a1,qr1)
M1_qc.cx(qr1[0],qr1[1])
M1_qc.h(qr1[0])
M1_qc.rz(2*f1,qr1[1])

M1_qc.draw(output="mpl")
```

[ ]:

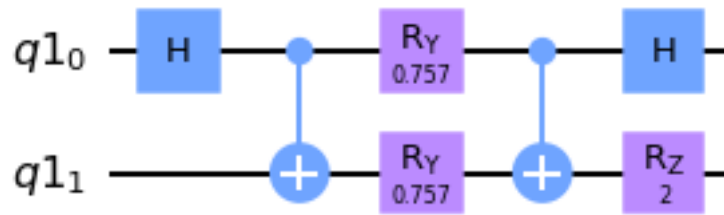


```
[ ]: qr2=QuantumRegister(2)
M2_qc=QuantumCircuit(qr2, name="M2")

#M2_qc.rz(2*r2,qr2[1])
M2_qc.h(qr2[0])
M2_qc.cx(qr2[0],qr2[1])
M2_qc.ry(a2,qr2)
M2_qc.cx(qr2[0],qr2[1])
M2_qc.h(qr2[0])
M2_qc.rz(2*f2,qr2[1])
```

```
M2_qc.draw(output="mpl")
```

```
[ ]:
```



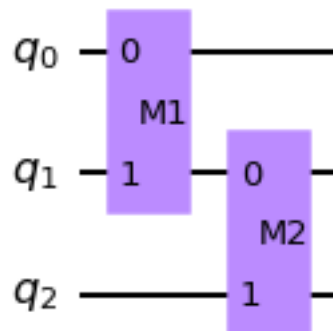
### 3.3 Buiding the final evolution circuit

```
[ ]: qr = QuantumRegister(3 ,name="q")
      qc = QuantumCircuit(qr, name="U")

      qc.append(M1_qc, [qr[0],qr[1]])
      qc.append(M2_qc, [qr[1],qr[2]])

      qc.draw(output="mpl")
```

```
[ ]:
```



```
[ ]: def matrix_from_circuit(qc, phase=0):
      backend = Aer.get_backend('unitary_simulator')
      job = execute(qc, backend, shots=32000)
      result = job.result()
      A=result.get_unitary(qc, decimals=10)*np.exp(1j*phase)
      return Matrix(A)
```

You can see that the 7<sup>th</sup> columns are equivalent.

```
[ ]: ## 7th column of the matrix representation of the quantumcircuit.
Matrix([matrix_from_circuit(qc)[j*8+6] for j in range(8)])
```

```
[ ]: 
$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ -0.5506938802 + 0.1881775479i \\ 0 \\ -0.0585630369 + 0.6128121094i \\ 0.4367423281 + 0.3026768721i \\ 0 \end{bmatrix}$$

```

```
[ ]: ## 7th column of the matrix obtained multiplying n times trotter_steps_matrix  
↪with itself.  
Matrix([U.evalf(10)[j*8+6] for j in range(8)])
```

```
[ ]: 
$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ -0.5506938803 + 0.1881775479i \\ 0 \\ -0.0585630369 + 0.6128121094i \\ 0.4367423281 + 0.3026768721i \\ 0 \end{bmatrix}$$

```

In conclusion we have a circuit with a fixed depth (4 cnots and 11 single qubit gates) for every choices of time and number of Trotter Steps