

# Quantum Computing Assignment 7 - Group 18

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## Exercise 7.1

### (Schmidt Decomposition & Schrödinger Equation)

(a) Part 1

$$|\psi\rangle = \frac{1}{\sqrt{2}} * (|00\rangle + |11\rangle)$$

$$|\psi\rangle = \sum A_{ij} |ij\rangle$$

$$A = \frac{1}{\sqrt{2}} * \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$svd(A) = \frac{1}{\sqrt{2}} * \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} * \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} * \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$$

Schmidt decomposition is

$$|\psi\rangle = \sum \lambda_{\alpha} * |\psi_{A,\alpha}\rangle * |\psi_{B,\alpha}\rangle$$

$$= [|\psi_{A,0}\rangle |\psi_{A,1}\rangle] * \begin{bmatrix} \lambda_0 & 0 \\ 0 & \lambda_1 \end{bmatrix} * [|\psi_{A,0}\rangle |\psi_{A,1}\rangle]$$

$$= \frac{1}{\sqrt{2}} [-|0\rangle \quad -|1\rangle] * \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} * \begin{bmatrix} -|0\rangle \\ -|1\rangle \end{bmatrix}$$

Part 2

$$|\psi\rangle = \frac{1}{2} * (|00\rangle + |01\rangle + |10\rangle + |11\rangle)$$

$$A = \frac{1}{2} * \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

$$svd(A) = \frac{1}{\sqrt{2}} * \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} * \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} * \frac{1}{\sqrt{2}} * \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Schmidt decomposition is

$$\begin{aligned} |\psi\rangle &= \sum \lambda_\alpha * |\psi_{A,\alpha}\rangle * |\psi_{B,\alpha}\rangle \\ &= [|\psi_{A,0}\rangle |\psi_{A,1}\rangle] * \begin{bmatrix} \lambda_0 & 0 \\ 0 & \lambda_1 \end{bmatrix} * [|\psi_{A,0}\rangle |\psi_{A,1}\rangle] \\ &= \frac{1}{2} [|0\rangle + |1\rangle \quad |0\rangle - |1\rangle] * \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} * \begin{bmatrix} |0\rangle + |1\rangle \\ |0\rangle - |1\rangle \end{bmatrix} \end{aligned}$$

(b)

Given  $U_t = e^{-iHt}$ , as  $\hbar = 1$  &  $H = \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix}$

Since  $H$  is Hermitian, i.e;  $H^2 = I$

We can use Eq. 2.20, i.e;  $e^{iAx} = \cos(x)I + i \sin(x)A$  to represent  $U_t$  as follows:

$$\begin{aligned} U_t = e^{-iHt} &\implies U_t = \cos(t) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - i \sin(t) \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix} \\ &\implies \begin{pmatrix} \cos(t) & 0 \\ 0 & \cos(t) \end{pmatrix} - \begin{pmatrix} i \sin(t)\omega_1 & 0 \\ 0 & i \sin(t)\omega_2 \end{pmatrix} \\ &\implies U_t = \begin{pmatrix} \cos(t) - i \sin(t)\omega_1 & 0 \\ 0 & \cos(t) - i \sin(t)\omega_2 \end{pmatrix} \quad (\mathbf{A}) \end{aligned}$$

Using **(A)** we can solve for  $|\psi(t)\rangle$  given  $|\psi(0)\rangle$ .

$$(i) \quad |\psi(0)\rangle = |0\rangle$$

$$\begin{aligned} \implies |\psi(t)\rangle &= \begin{pmatrix} \cos(t) - i \sin(t)\omega_1 & 0 \\ 0 & \cos(t) - i \sin(t)\omega_2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ \implies |\psi(t)\rangle &= \begin{pmatrix} \cos(t) - i \sin(t)\omega_1 \end{pmatrix} |0\rangle \end{aligned}$$

$$(ii) |\psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$\implies |\psi(t)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \cos(t) - i \sin(t)\omega_1 & 0 \\ 0 & \cos(t) - i \sin(t)\omega_2 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\implies |\psi(t)\rangle = \frac{1}{\sqrt{2}} \left( \begin{pmatrix} \cos(t) - i \sin(t)\omega_1 \\ 0 \end{pmatrix} |0\rangle + \begin{pmatrix} 0 \\ \cos(t) - i \sin(t)\omega_2 \end{pmatrix} |1\rangle \right)$$

(c) Given  $H = \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix} + \epsilon \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

This can be re-written as:

$$H = \bar{\omega} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \Delta \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \epsilon \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \equiv \bar{\omega} I + \sqrt{\Delta \omega^2 + \epsilon^2} (\vec{v} \cdot \vec{\sigma})$$

Where  $\bar{\omega}$  is assumed to be  $\frac{\omega_1 + \omega_2}{2}$  &  $\Delta \omega = \frac{\omega_1 - \omega_2}{2}$

$$\implies Ht = \bar{\omega}tI + \Delta \omega tZ + \epsilon tX \implies e^{-iHt} = e^{-i\bar{\omega}tI - i\Delta \omega tZ - i\epsilon tX} \approx \underbrace{e^{-i(\bar{\omega}t)I}}_{(A)} \cdot \underbrace{e^{-i(\Delta \omega t)Z}}_{(B)} \cdot \underbrace{e^{-i(\epsilon t)X}}_{(C)}$$

Using Eq. 2.20 in (A):  $\begin{pmatrix} \cos(\bar{\omega}t) & 0 \\ 0 & \cos(\bar{\omega}t) \end{pmatrix} - \begin{pmatrix} i \sin(\bar{\omega}t) & 0 \\ 0 & i \sin(\bar{\omega}t) \end{pmatrix} = \begin{pmatrix} e^{-i(\bar{\omega}t)} & 0 \\ 0 & e^{-i(\bar{\omega}t)} \end{pmatrix}$

Using Eq. 2.20 in (B):  $\begin{pmatrix} \cos(\Delta \omega t) - i \sin(\Delta \omega t) & 0 \\ 0 & \cos(\Delta \omega t) + i \sin(\Delta \omega t) \end{pmatrix} = \begin{pmatrix} e^{-i(\Delta \omega t)} & 0 \\ 0 & e^{i(\Delta \omega t)} \end{pmatrix}$

Using Eq. 2.20 in (C):  $\begin{pmatrix} \cos(\epsilon t) & -i \sin(\epsilon t) \\ -i \sin(\epsilon t) & \cos(\epsilon t) \end{pmatrix}$

$$\implies U_t = e^{-iHt} \approx (A)(B)(C)$$

$$(A)(B) : \begin{pmatrix} e^{-i(\bar{\omega}t)} & 0 \\ 0 & e^{-i(\bar{\omega}t)} \end{pmatrix} \times \begin{pmatrix} e^{-i(\Delta \omega t)} & 0 \\ 0 & e^{i(\Delta \omega t)} \end{pmatrix} = \begin{pmatrix} e^{-i(\bar{\omega} + \Delta \omega)t} & 0 \\ 0 & e^{i(\Delta \omega - \bar{\omega})t} \end{pmatrix} = \begin{pmatrix} e^{-i(\omega_1)t} & 0 \\ 0 & e^{-i(\omega_2)t} \end{pmatrix}$$

$$U_t = \begin{pmatrix} e^{-i(\omega_1)t} & 0 \\ 0 & e^{-i(\omega_2)t} \end{pmatrix} \times \begin{pmatrix} \cos(\epsilon t) & -i \sin(\epsilon t) \\ -i \sin(\epsilon t) & \cos(\epsilon t) \end{pmatrix} = \begin{pmatrix} e^{-i(\omega_1)t} \cos(\epsilon t) & -i e^{-i(\omega_1)t} \sin(\epsilon t) \\ -i e^{-i(\omega_2)t} \sin(\epsilon t) & e^{-i(\omega_2)t} \cos(\epsilon t) \end{pmatrix}$$

$$|\psi(t)\rangle = U_t |0\rangle \implies |\psi(t)\rangle = \begin{pmatrix} e^{-i(\omega_1)t} \cos(\epsilon t) \\ -i e^{-i(\omega_2)t} \sin(\epsilon t) \end{pmatrix}$$

$$\therefore \langle 1 | \psi(t) \rangle = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} e^{-i(\omega_1)t} \cos(\epsilon t) \\ -i e^{-i(\omega_2)t} \sin(\epsilon t) \end{pmatrix} = -i e^{-i(\omega_2)t} \sin(\epsilon t)$$

(d)

$$|\psi(t)\rangle = U_t|\psi(0)\rangle$$

$$\rho = \sum_j p_j |\psi_j(t)\rangle \langle \psi_j(t)| = \sum_j p_j U_t |\psi(0)\rangle \langle \psi(0)| U_t^\dagger = U_t A U_t^\dagger$$

$$U_t = e^{\frac{-iHt}{\hbar}}$$

$$\frac{dU_t}{dt} = \frac{-iH}{\hbar} U_t$$

$$\frac{d\rho}{dt} = \left(\frac{-iH U_t}{\hbar}\right) * A U_t^\dagger + U_t^\dagger A \left(\frac{iH U_t^\dagger}{\hbar}\right)$$

$$= \frac{-i}{\hbar} [H\rho - \rho H]$$

$$i\hbar \frac{d\rho(t)}{dt} = [H\rho - \rho H] = [H, \rho(t)]$$

Thus the derivation of Von Neumann equation is proved.

## (Python/Numpy implementation of the partial trace)

(a)

```
In [39]: # ANSWER 7.2
# a)

import numpy as np
def partial_trace(rho,dimA,dimB):
    reshaped_dm = rho.reshape([dimA,dimB,dimA,dimB])
    # compute the partial trace
    rho_A= np.einsum('ijik->jk', reshaped_dm)
    rho_B = np.einsum('jiki->jk', reshaped_dm)
    a = (rho_A,rho_B)
    return a

In [40]: dimA=4
dimB=8
rho = np.random.randn(dimA*dimB,dimA*dimB)
partial_trace(rho,dimA,dimB)

Out[40]: (array([[ 1.4201677 ,  2.39504506, -2.2483172 ,  2.10753928,  2.22660272,
 -0.23774537,  3.38391736, -0.12099788],
 [ -0.07790885,  3.0741709 , -2.12218315, -0.96384127,  3.82175562,
 -4.2751483 ,  4.63409173,  1.07739852],
 [-0.43215101,  1.88827875,  1.51959742,  0.70667535,  1.10531461,
  1.57533666,  0.67035551,  4.23955212],
 [ 3.02463034,  2.97591351,  1.12200783,  0.33641079,  0.58748035,
  0.69172361, -2.75042606, -0.84158349],
 [ 1.51968918,  1.12140566,  4.87596295,  0.11029747,  1.18433153,
  3.03211712,  1.33704395,  0.84814695],
 [-1.88134385, -0.49163687, -6.78719296, -3.6769222 , -0.5633687 ,
  0.65842035, -4.53086354,  0.97387264],
 [-0.82960378, -2.51742567, -0.21867956, -3.36792719,  1.11556678,
  3.45606045, -0.68361483,  3.60800759],
 [-0.78327494,  2.02959473,  2.21159498, -0.4650718 , -0.95604822,
  0.17083995,  2.68733761,  1.86004572]]),
 array([[ 2.55597097,  5.6823249 , -1.77814963, -4.2631279 ],
 [-5.22056583,  4.04964453,  1.63559599, -3.48303142],
 [ 2.57096543,  2.19484942,  2.94299248,  3.3851535 ],
 [-5.73840189, -0.36136427, -1.98193132, -0.17907841]]))
```

(b)

```
In [41]: # Answer b)
psi = np.array([1,0,0,1])/np.sqrt(2)
rho1=np.outer(psi,psi.conj())
print(rho1)
partial_trace(rho1,2,2)

[[0.5 0.  0.  0.5]
 [0.  0.  0.  0. ]
 [0.  0.  0.  0. ]
 [0.5 0.  0.  0.5]]

Out[41]: (array([[0.5, 0. ],
 [0. , 0.5]]), array([[0.5, 0. ],
 [0. , 0.5]]))
```

(c)

```
In [48]: # Answer c)
def construct_random_density_matrix(d):
    """
    Construct a complex random density matrix of dimension d x d.
    """
    # ensure that rho is positive semidefinite
    A = (np.random.randn(d, d) + 1j*np.random.randn(d, d))/np.sqrt(2)
    rho = A @ A.conj().T
    # normalization
    rho /= np.trace(rho)
    return rho

def construct_random_operator(d):
    """
    Construct a complex random Hermitian matrix of dimension d x d.
    """
    # ensure that M is Hermitian
    A = (np.random.randn(d, d) + 1j*np.random.randn(d, d))/np.sqrt(2)
    M = 0.5*(A + A.conj().T)
    return M
```

```
In [84]: rho3 = construct_random_density_matrix(4)
M= construct_random_operator(2)
rho_A, rho_B=partial_trace(rho3, 2, 2)
LHS=np.trace(rho_B*M)
RHS=np.trace(np.kron(M, np.identity(2))*rho3)
print(LHS, RHS)
#ma=np.mean((np.square(np.subtract(LHS, RHS))))
print(RHS-LHS)

np.isclose(LHS, RHS, rtol=1e-05, atol=1e-06)

(-0.2859130294523684+6.635801494981807e-20j) (-0.2859130294523684+6.635801494981807e-20j)
0j
```

Out[84]: True