exercise 3

working with (important) matrices

solutions due

until **November 26, 2024** at **23:30** via **ecampus**

Note: Carefully read and follow the solution submission instructions which are detailed in task 3.9.

If your submission does not adhere to the guidelines in task 3.9, your solutions will not be accepted / graded.

general remarks

These exercises expose you to various objects and their properties where some of those are of utmost importance in quantum computing.

We therefore encourage you to make an effort to really understand what you are doing when you solve the following tasks.

Ideally, all of the following problems would be solved with pen and paper only (getting used to this may come in handy in the near future when may find yourself in a situation where you have to solve similar problems but no computer access). If you do not want or cannot do this, then we suggest working with `sympy`.

mathematical preliminaries

These exercises are the first in which we are working with the ket vectors

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Their inner products are

$$\langle 0 | 0 \rangle = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 1$$

$$\langle 0 | 1 \rangle = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0$$

$$\langle 1 | 0 \rangle = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 0$$

$$\langle 1 | 1 \rangle = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 1$$

Their outer products are

$$|0\rangle\langle 0| = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$|0\rangle\langle 1| = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

$$|1\rangle\langle 0| = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

$$|1\rangle\langle 1| = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

task 3.1 [10 points]

getting to know the Pauli matrices

The four Pauli matrices are 2×2 Hermitian matrices over $\mathbb{C}$ and given by

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad Y = \begin{bmatrix} 0 & -i \\ +i & 0 \end{bmatrix} \qquad Z = \begin{bmatrix} +1 & 0 \\ 0 & -1 \end{bmatrix}$$

In this course, its exercises, and exam, we refer to the objects on the left of the equal signs as operators and to the objects on the right of the equal signs as the matrix representations of said operators.

Here are your tasks:

a) **[2 points]** Compute the matrix representations of the operators $I^\dagger I$, $X^\dagger X$, $Y^\dagger Y$, and $Z^\dagger Z$ and write them down. Discuss what you observe. What other general property of Pauli matrices besides from being Hermitian does your observation imply.

b) **[2 points]** Compute the matrix representations of the operators I^2, X^2, Y^2, and Z^2 and write them down. Discuss what you observe. What other general property of Pauli matrices besides from being Hermitian does your observation imply.

c) **[2 points]** Write I, X, Y, and Z in terms of linear combinations of outer products of $|0\rangle$ and $|1\rangle$.

d) **[2 points]** Use your results from subtask c) to quickly determine the eigenvectors of I, X, Y, and Z. Write them down in terms of linear combinations of $|0\rangle$ and $|1\rangle$.

e) **[2 points]** Determine the eigenvalues of I, X, Y, and Z and write them down.

task 3.2 [5 points]

important friends of the Pauli matrices

Let M be an $m \times m$ matrix over $\mathbb{C}$ and recall the definition of its matrix exponential

$$e^{M} = \sum_{k=0}^{\infty} \frac{1}{k!} M^{k} \tag{1}$$

Here are your tasks:

a) **[1 point]** Use (1) to compute the matrix representation of operator

$$R_X(\theta) \equiv e^{-i\,\frac{\theta}{2}\,X} = \ldots$$

b) **[3 points]** Use (1) to compute the matrix representation of operator

$$R_Y(\theta) \equiv e^{-i\,\frac{\theta}{2}\,Y} = \ldots$$

c) **[1 point]** Use (1) to compute the matrix representation of operator

$$R_Z(\theta) \equiv e^{-i\,\frac{\theta}{2}\,Z} = \ldots$$

task 3.3 [5 points]

an important identity

Let A be an involutory matrix over $\mathbb{C}$ and $\vartheta \in [0, 2\,\pi)$.

Here is your task:

Prove the equality

$$e^{i\,\vartheta\,A} = \cos(\vartheta)\,I + i\,\sin(\vartheta)\,A$$

task 3.4 [5 points]

another interesting matrix

Here is yet another interesting matrix

$$V = \frac{1}{\sqrt{2}} \begin{bmatrix} +i & -i \\ +1 & +1 \end{bmatrix}$$

Here are your tasks:

a) **[2 points]** Would you say that V is unitary? How would you decide this? Discuss this in your own words.

b) **[3 points]** Here is another bold claim: Every matrix $M \in \mathbb{C}^{2\times 2}$ can be written as a linear combination of the Pauli matrices. If this is true, then we should be able to compute V as follows

$$V = c_I I + c_X X + c_Y Y + c_Z Z$$

Determine the appropriate coefficients and write them down.

task 3.5 [5 points]

the beam splitter matrix

Here is yet another matrix which we will meet it later on during the lectures

$$B = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix}$$

Here is your task:

Compute the following matrix powers $B^0, B^1, B^2, \ldots, B^8$. For the fun of it, also compute B^{16} and B^{32}. Do you observe anything noteworthy when looking at all your resulting matrices? Discuss your observations in your own words.

task 3.6 [5 points]

Boolean functions as matrices

Let $x, y \in \{0, 1\}$ be two bits and represent them in terms of 2-dimensional vectors, namely

$$\boldsymbol{x} = \begin{bmatrix} 1 \\ x \end{bmatrix} \qquad \text{and} \qquad \boldsymbol{y} = \begin{bmatrix} 1 \\ y \end{bmatrix}$$

Here are your tasks:

a) **[1 point]** Consider this 2×2 matrix

$$\boldsymbol{M} = \begin{bmatrix} 0 & +1 \\ +1 & -1 \end{bmatrix}$$

and fill in the following truth table

x	y	$\boldsymbol{x}^\intercal \boldsymbol{M} \boldsymbol{y}$
0	0	$\dots$
0	1	$\dots$
1	0	$\dots$
1	1	$\dots$

Which Boolean function did you just compute?

b) **[1 point]** Consider this 2×2 matrix

$$\boldsymbol{M} = \begin{bmatrix} +1 & 0 \\ 0 & -1 \end{bmatrix}$$

and fill in the following truth table

x	y	$\boldsymbol{x}^\intercal \boldsymbol{M} \boldsymbol{y}$
0	0	$\dots$
0	1	$\dots$
1	0	$\dots$
1	1	$\dots$

Which Boolean function did you just compute?

c) **[3 points]** Can every bivariate Boolean function $f : \{0, 1\}^2 \to \{0, 1\}$ be represented in terms of a 2×2 matrix? Answer this correctly and carefully discuss your mathematical reasoning (proof or disproof).

task 3.7 [5 points]

3D vectors as matrices

Every vector $\boldsymbol{x} \in \mathbb{R}^3$ can be represented by a traceless Hermitian matrix $\boldsymbol{X} \in \mathbb{C}^{2\times 2}$ using the following mapping

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \mapsto \boldsymbol{X} = \begin{bmatrix} +x_3 & x_1 - i\,x_2 \\ x_1 + i\,x_2 & -x_3 \end{bmatrix}$$

Here are your tasks:

a) **[1 point]** Consider the three standard basis vectors

$$\boldsymbol{e}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \qquad \boldsymbol{e}_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \qquad \boldsymbol{e}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

in $\mathbb{R}^3$ and compute the corresponding matrices $\boldsymbol{X}_1$, $\boldsymbol{X}_2$, and $\boldsymbol{X}_3$. What do you observe? Discuss your results.

b) **[2 points]** Consider any two $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$, represent them as $\boldsymbol{X}, \boldsymbol{Y} \in \mathbb{C}^{2\times 2}$, and prove the following identity

$$\boldsymbol{x}^\intercal \boldsymbol{y} = \frac{1}{2}\,\mathrm{tr}\big[\boldsymbol{X}\boldsymbol{Y}\big]$$

c) **[2 points]** Note that $\boldsymbol{X}$ and $\boldsymbol{Y}$ are square matrices of the same size. Show that, for matrices like these, we have the identity

$$\mathrm{tr}\big[\boldsymbol{X}\boldsymbol{Y}\big] = \mathrm{tr}\big[\boldsymbol{Y}\boldsymbol{X}\big]$$

Remark: Given your results for this task, it is clear that the above method of computing inner products of real valued 3D vectors complies with the symmetry axiom for inner products of *real valued* vectors. That is, we have

$$\boldsymbol{x}^\intercal \boldsymbol{y} = \frac{1}{2}\,\mathrm{tr}\big[\boldsymbol{X}\boldsymbol{Y}\big] = \frac{1}{2}\,\mathrm{tr}\big[\boldsymbol{Y}\boldsymbol{X}\big] = \boldsymbol{y}^\intercal \boldsymbol{x}$$

task 3.8 [10 points]

an important identity

In lecture 05, we considered the most general possible wave function for a 1D particle trapped in a well

$$\Psi(x,t) = \sum_{j=1}^{\infty} a_j \, \Psi_j(x,t) = \sum_{j=1}^{\infty} a_j \, \psi_j(x) \, \phi_j(t)$$

where the Born rule tells us that

$$\begin{aligned} 1 = \int \Psi^*\big(x,t\big) \, \Psi\big(x,t\big) \, dx &= \int \Big(\sum_j a_j^* \, \Psi_j^*(x,t) \Big) \Big(\sum_k a_k \, \Psi_k(x,t) \Big) \, dx \\ &= \int \bigg(a_1^* \, \psi_1^*(x) \, e^{+\frac{i\,E_1\,t}{\hbar}} + a_2^* \, \psi_2^*(x) \, e^{+\frac{i\,E_2\,t}{\hbar}} + \ldots \bigg) \\ &\quad \cdot \bigg(a_1 \, \psi_1(x) \, e^{-\frac{i\,E_1\,t}{\hbar}} + a_2 \, \psi_2(x) \, e^{-\frac{i\,E_2\,t}{\hbar}} + \ldots \bigg) \, dx \\ &= \sum_j \sum_k a_j^* a_k \, e^{\frac{i\,(E_j - E_k)\,t}{\hbar}} \int \psi_j^*(x) \, \psi_k(x) \, dx \end{aligned}$$

We then claimed that

$$\int \psi_j^*(x) \, \psi_k(x) \, dx = \delta_{jk} = \begin{cases} 1 & \text{if} \;\; j = k \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

and therefore obtained

$$1 = \int \Psi^*\big(x,t\big) \, \Psi\big(x,t\big) \, dx = \sum_j |a_j|^2$$

Here is your task:

Prove that (2) is true. You may work with the fact that $\psi_j(x)$ and $\psi_k(x)$ are eigenfunctions of some Hermitian Hamiltonian $\hat{H} = \hat{H}^\dagger$ with distinct real eigenvalues E_j and E_k such that

$$\begin{aligned} \hat{H} \psi_j(x) &= E_j \, \psi_j(x) \\ \hat{H} \psi_k(x) &= E_k \, \psi_k(x) \end{aligned}$$

task 3.9

submission of presentation and code

Prepare a presentation / set of slides about your solutions and results. **Submissions of only jupyter notebooks will not be accepted.**

Your slides should help you to give a scientific presentation of your work (i.e. to give a short talk in front of your fellow students and instructors and answer any questions they may have).

W.r.t. to formalities, please make sure that

- your presentation contains a title slide which lists the **names and matriculation numbers** of everybody in your team who contributed to the solutions.

W.r.t. content, please make sure that

- your presentation contains about 12 to 15 content slides but not more
- your presentation is concise and clearly structured
- your presentation answers questions such as
  - "what was the task / problem we considered?"
  - "what difficulties (if any) did we encounter?"
  - "how did we solve them?"
  - "what were our results?"
  - "what did we learn?"

Save / export your slides as a PDF file and upload it to eCampus.

Furthermore, please name all your code files in a manner that indicates which task they solve (e.g. `task-1-5.py`) and put them in an archive or a ZIP file.

Upload this archive / ZIP file with your code snippets to eCampus.