Homework sheet 1 – Due 01/31/2025

With solutions: Solutions are in blue throughout.

Problem 1: Basics of linear algebra [1 + 1 + (1+1+2) + (1+1+2) = 10 points]

Consider a finite dimensional linear vector space V (its dual is denoted V^*) with inner product $\langle \cdot | \cdot \rangle : V^* \times V \to \mathbb{C}$. A simple example to be kept in mind throughout the exercise is $V = \mathbb{C}^N$ with scalar products defined as $\langle a|b\rangle = \sum_{\sigma=1}^N a_\sigma^* b_\sigma$. For our quantum mechanics applications, such a vector space is the prototype for Hilbert spaces.

a) Prove that, for a Hermitian operator $\hat{A}$ with (right) eigenstate $|a\rangle$ (i.e. $\hat{A}|a\rangle = a|a\rangle$) the dual state $\langle a|$ is a (left) eigenstate with the same eigenvalue a and that $a \in \mathbb{R}$.

First, we see that

$$\langle a| \hat{A} = [\hat{A}^\dagger |a\rangle]^* = [\hat{A}|a\rangle]^* = [a|a\rangle]^* = \langle a| a^*. \tag{1}$$

Second use that

$$a = \frac{\langle a|\hat{A}|a\rangle}{\langle a|a\rangle} = \frac{\langle a|\hat{A}^\dagger|a\rangle^*}{\langle a|a\rangle^*} = \frac{\langle a|\hat{A}|a\rangle^*}{\langle a|a\rangle^*} = a^*. \tag{2}$$

b) Prove the <u>Schwarz-inequality</u>

$$\langle \phi|\phi\rangle \langle \psi|\psi\rangle \geq |\langle \phi|\psi\rangle|^2. \tag{3}$$

The proof is trivial when one vector is zero and the inequality is saturated. Consider now the case of non-zero $|\psi\rangle$.

$$|\chi\rangle = |\phi\rangle - \frac{|\psi\rangle \langle \psi|\phi\rangle}{\langle \psi|\psi\rangle}. \tag{4}$$

The overlap with $|\psi\rangle$ vanishes by construction

$$\langle \psi|\chi\rangle = \langle \psi|\phi\rangle - \frac{\langle \psi|\psi\rangle \langle \psi|\phi\rangle}{\langle \psi|\psi\rangle} = 0. \tag{5}$$

We reverse the equation

$$|\phi\rangle = |\chi\rangle + \frac{|\psi\rangle \langle \psi|\phi\rangle}{\langle \psi|\psi\rangle} \tag{6}$$

to express the norm of $|\phi\rangle$ as

$$\| \, |\phi\rangle \, \|^2 = \| \, |\chi\rangle \, \|^2 + \frac{|\, \langle\psi|\phi\rangle \,|^2}{\| \, |\psi\rangle \, \|^2} \geq \frac{|\, \langle\psi|\phi\rangle \,|^2}{\| \, |\psi\rangle \, \|^2} . (Q.E.D.) \tag{7}$$

c) Consider the <u>direct sum</u> $V = U \oplus W$, where U, V, W are all finite dimensional linear vector spaces. *This means the following: Let $U \subseteq V, W \subseteq V$ and the space spanned by $U \cup W$ (as obtained by summing elements of U, W using the addition defined for V) is a linear subvectorspace of V. If additionally $U \cap W = \{0\}$ the sum of U and W is called direct.*

i) Show that each $|v\rangle \in V$ can be uniquely decomposed in $|v\rangle = |u\rangle + |w\rangle$ with $|u\rangle \in U, |w\rangle \in W$.

Let's denote the dimension of the Hilbert spaces as $d_{U,V,W}$ respectively.

- All vectors of the ONB of U, $\{|u_i\rangle\}_{i=1}^{d_U}$, and W, $\{|w_i\rangle\}_{i=1}^{d_W}$, are orthonormal by the assumption $U \cap W = \{0\}$. Hence $\{|u_i\rangle\}_{i=1}^{d_U} \cup \{|w_i\rangle\}_{i=1}^{d_W}$ form an ONB for V.
- Thus any $|v\rangle$ can be uniquely decomposed as

$$|v\rangle = \underbrace{\sum_{i=1}^{d_U} |u_i\rangle \langle u_i|v\rangle}_{\in U} + \underbrace{\sum_{i=1}^{d_W} |w_i\rangle \langle w_i|v\rangle}_{\in W} \quad (Q.E.D.). \tag{8}$$

ii) Consider the map $P : V \to V$ defined by

$$P : |v\rangle = |u\rangle + |w\rangle \mapsto P\,|v\rangle := |w\rangle \,. \tag{9}$$

Show that P is a projection (i.e. it's a linear operation with $P^2 = P$). Determine the eigenspace of P.

We effectively define the projection operator as the operation of dropping all coefficents in front of $|u_i\rangle$ in the expansion

$$|v\rangle = \sum_{i=1}^{d_U} \underbrace{c_{u_i}}_{\text{drop these}} |u_i\rangle + \sum_{i=1}^{d_W} c_{w_i} \,|w_i\rangle \,. \tag{10}$$

Clearly, repeating the operation twice is the same as doing it once, hence $P^2 = P$. Moreover the operation is linear, i.e.

$$P[\lambda \,|v\rangle] = P[\sum_{i=1}^{d_U} \lambda c_{u_i} \,|u_i\rangle + \sum_{i=1}^{d_W} \lambda c_{w_i} \,|w_i\rangle = \lambda[P\,|v\rangle]. \tag{11}$$

The eigenspace of P is W.

iii) Construct an explicit eigenbasis for state vectors $|v\rangle, |u\rangle, |w\rangle$ in their respective spaces. Express the dimension of the vector space V in terms of the dimension of vector spaces U, W. Construct a matrix representation for P from subexercise ii).

Part of this was done in i). It's obvious that $d_V = d_U + d_W$. The matrix of P is then represented as

$$P = \begin{pmatrix} \mathbf{0}_{d_U \times d_U} & \mathbf{0}_{d_U \times d_W} \\ \mathbf{0}_{d_W \times d_U} & \mathbf{I}_{d_W \times d_W} \end{pmatrix} \tag{12}$$

where we chose an ONB on V

$$\left\{ \begin{pmatrix} |u_1\rangle \\ 0_{d_W} \end{pmatrix}, \begin{pmatrix} |u_2\rangle \\ 0_{d_W} \end{pmatrix}, \ldots, \begin{pmatrix} |u_{d_U}\rangle \\ 0_{d_W} \end{pmatrix}, \begin{pmatrix} 0_{d_u} \\ |w_1\rangle \end{pmatrix}, \begin{pmatrix} 0_{d_u} \\ |w_2\rangle \end{pmatrix}, \ldots, \begin{pmatrix} 0_{d_u} \\ |w_{d_W}\rangle \end{pmatrix} \right\} \tag{13}$$

d) Consider the direct product $V = U \otimes W$, where U, V, W are all finite dimensional linear vector spaces. *This means the following: Let* $|u\rangle \in U, |w\rangle \in W$. *The direct (outer) product is a bilinear operation* $\otimes : U \times W \to V$, *such that* $\otimes : (|u\rangle, |w\rangle) \mapsto |u\rangle \otimes |w\rangle \equiv |u, w\rangle$.

i) Show that the Schwarz-inequality in U, W implies the Schwarz inequality in V, i.e. that for any $|u_1, w_1\rangle, |u_2, w_2\rangle \in V$

$$\langle u_1, w_1 | u_1, w_1\rangle \langle u_2, w_2 | u_2, w_2\rangle \geq |\langle u_1, w_1 | u_2, w_2\rangle|^2 \tag{14}$$

We remind ourselves that, since U, W have an inner product $\langle . | . \rangle$, one may uniquely define an inner prodouct on V by

$$\langle u_1, w_1 | u_2, w_2\rangle_V = \langle u_1 | u_2\rangle_U \langle w_1 | w_2\rangle_W . \tag{15}$$

(The subscript here highlights that $u_{1,2}$ have their inner product w.r.t the definition within U, and $w_{1,2}$ w.r.t W.)
Having reviewed these basics we find the Schwarz inequality trivially

$$\begin{aligned} \| \, |u_1, w_1\rangle \, \|^2 \| \, |u_2, w_2\rangle \, \|^2 &= \| \, |u_1\rangle \, \|^2 \| \, |u_2\rangle \, \|^2 \| \, |w_1\rangle \, \|^2 \| \, |w_2\rangle \, \|^2 \\ &\geq |\langle u_1 | u_2\rangle|^2 \, |\langle w_1 | w_2\rangle|^2 \equiv |\langle u_1, w_1 | u_2, w_2\rangle|^2 . \end{aligned} \tag{16}$$

ii) Consider a linear operator O on U, i.e. $O : |u\rangle \mapsto O|u\rangle$. Explain why the properties of the outer product imply that this operator is represented as $O \otimes \mathbf{I}$ on elements of V, where $\mathbf{I}$ is the identity operation.

Let's denote $O|u\rangle = |Ou\rangle$. The definition $|u, w\rangle \equiv |u\rangle \otimes |w\rangle \in V$ implies $|Ou, w\rangle = |Ou\rangle \otimes |w\rangle$. This motivates the representation

$$O \otimes \mathbf{I} : |u\rangle \otimes |w\rangle \mapsto |Ou\rangle \otimes |w\rangle = (O|u\rangle) \otimes |w\rangle , \tag{17}$$

as it leaves $|w\rangle$ invariant. Of course, the operation $O \otimes \mathbf{I}$ inherits properties of linearity from O, e.g.

$$O \otimes \mathbf{I} : (\lambda |u\rangle) \otimes |w\rangle \mapsto (O\lambda |u\rangle) \otimes |w\rangle = \lambda[(O|u\rangle) \otimes |w\rangle], \tag{18}$$

in view of the bilinearity of $\otimes$.

iii) Construct an explicit eigenbasis for state vectors $|v\rangle, |u\rangle, |w\rangle$ in their respective spaces. Express the dimension of the vector space V in terms of the dimension of vector spaces U, W. Construct a matrix representation for O from subexercise ii).

We use the same notations as in part c). The outer product implies that for vectors

$$|u\rangle = \sum_{i=1}^{d_U} c_{u_i} |u_i\rangle \tag{19}$$

$$|w\rangle = \sum_{i=1}^{d_W} c_{w_i} |w_i\rangle \tag{20}$$

$$\Rightarrow |u\rangle \otimes |w\rangle = \sum_{i=1}^{d_U} \sum_{j=1}^{d_W} c_{u_i} c_{w_j} |u_i\rangle \otimes |w_j\rangle \,. \tag{21}$$

Using the inner product reviewed in i) we see that $\{|v_{(ij)}\rangle\}_{(ij)}$ is an ONB, where $|v_{(ij)}\rangle := |u_i\rangle \otimes |w_j\rangle$ and $i = 1, \ldots, d_U$, $j = 1, \ldots, d_W$. Hence the dimension of V is $d_V = d_U d_W$.

Exercise 2: Pauli matrices [2 + 1+ 2 + 1+ 2+ 1 + 1 = 10 points]

The Pauli matrices are

$$\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{22}$$

Prove the following:

a) $\{\sigma_i, \sigma_j\} = 2\delta_{ij}$, where $\{A, B\} = AB + BA$ is the anticommutator and δ_{ij} the Kronecker delta. (This implies that the Pauli matrices form a *Clifford algebra*.)

It is obvious that $\sigma_i^2 = 1$. Let's now consider the multiplication of two non-equal Pauli matrices

$$\sigma_1\sigma_2 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i\sigma_z, \quad \sigma_2\sigma_3 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = i\sigma_x, \quad \sigma_3\sigma_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\sigma_y \tag{23a}$$

$$\sigma_2\sigma_1 = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = -i\sigma_z, \quad \sigma_3\sigma_2 = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} = -i\sigma_x, \quad \sigma_1\sigma_3 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -i\sigma_y \tag{23b}$$

The sum of first and second line yields zero, QED.

b) $\sigma_i = \sigma_i^\dagger = -\sigma_y \sigma_i^T \sigma_y$

It is manifest that all σ_i are Hermitian. Next we see that

$$\sigma_{x,z}^T = \sigma_{x,z}, \text{ but } \sigma_y^T = -\sigma_y \tag{24}$$

As well as (from part a)

$$\sigma_y \sigma_{x,z} \sigma_y = -\sigma_{x,z}, \text{ but } \sigma_y \sigma_y \sigma_y = \sigma_y. \tag{25}$$

Combining the two implies the property summarized above.

c) $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$, where $[A, B] = AB - BA$ is the commutator and ϵ_{ijk} the Levi-Civita-tensor. (The Pauli matrices fulfill the *angular momentum algebra* (up to a constant).)

The solution follows from the solution of a) by subtraction of the two lines in Eq. (23)

d) $\mathrm{tr}\,[\sigma_i \sigma_j] = 2\delta_{ij}$

For $i \neq j$ the product of Pauli matrices is a third Pauli matrix, see Eq. (23), which in turn is manifestly traceless. For $i = j$ we have the trace of the unit matrix. QED.

e) Any complex 2×2 matrix M can be expanded uniquely as $M = m_0 \mathbf{1} + \sum_{i=1}^3 m_i \sigma_i$, where $\mathbf{1}$ is the 2×2 identity. Determine m_0, m_i.

Complex $2x2$ matrices contain 4 complex variables, hence they form a 4-dimensional vector space with inner product $\mathrm{tr}\,[AB]$. The Pauli matrices and $\mathbf{1}$ form an ONB on this vector space. Multiplying the equation on both sides by $\mathbf{1}$ or a Pauli matrix and taking the trace yields

$$m_0 = \frac{1}{2}\mathrm{tr}\,[M], \tag{26}$$

$$m_1 = \frac{1}{2}\mathrm{tr}\,[\sigma_x M], \tag{27}$$

$$m_2 = \frac{1}{2}\mathrm{tr}\,[\sigma_y M], \tag{28}$$

$$m_3 = \frac{1}{2}\mathrm{tr}\,[\sigma_z M]. \tag{29}$$

f) Any traceless, Hermitian 2×2 matrix H can be uniquely expanded as $H = \sum_{i=1}^3 h_i \sigma_i$, where $h_i = \mathrm{tr}\,[H\sigma_i]/2 \in \mathbb{R}$.

To prove this, we use part d) and see that hermiticity implies that all coeffients be real. If H is tracles, m_0 vanishes.

g) Any unitary 2×2 matrix U with unit determinant, $\det[U] = 1$, can be expanded as $U = a_0 \mathbf{1} + i \sum_i a_i \sigma_i$, where $a_{0,1,2,3}$ are all real numbers and $\sum_{i=0}^{3} a_i^2 = 1$.

To prove this, we again use part d). The determinant of U fixes

$$1 = m_0^2 - \sum_{i=1}^{3} m_i^2. \tag{30}$$

Since this expression ought to be true for any U, also for traceless U we conclude $m_i \in i\mathbb{R}$. Analogously we conclude $m_0 \in \mathbb{R}$. Next unitarity implies

$$\mathbf{1} = (m_0^* + \sum_{i=1}^{3} m_i^* \sigma_i)(m_0 + \sum_{j=1}^{3} m_j \sigma_j) \tag{31}$$

$$= \sum_{i=0}^{4} |m_i|^2 + \sum_{i=1}^{3} (m_0^* m_i + c.c) \sigma_i + \sum_{i=1}^{3} \sum_{j=1}^{3} m_i^* m_j i \epsilon_{ijk} \sigma_k. \tag{32}$$

Multiplying by $\mathbf{1}$ or σ_i leads to four equations

$$1 = \sum_{i=0}^{4} |m_i|^2 \tag{33}$$

$$0 = (m_0^* \vec{m} + c.c) + i \vec{m}^* \times \vec{m}. \tag{34}$$

Since $\vec{m} = (m_1, m_2, m_3) \in i\mathbb{R}$, $m_0 \in \mathbb{R}$ the assertion follows.

Exercise 3: States, Operators, Expectation values [1+2 +2 + 2+1 + 2 = 10 points]

Consider a 3-dimensional Hilbert space and the four states

$$|\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |\psi_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{35}$$

and

$$|\tilde{\psi}\rangle = C[|\psi_2\rangle + |\psi_3\rangle]. \tag{36}$$

Let the states $|\psi_i\rangle, i = 1, 2, 3$ be the eigenstates of an operator $\hat{A}$ with eigenvalues a_i, i.e. $\hat{A} |\psi_i\rangle = a_i |\psi_i\rangle$.

Further consider an operator $\hat{B}$, which in the basis of $|\psi_i\rangle$ is given by

$$\hat{B} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & i \\ 0 & -i & 3 \end{pmatrix}. \tag{37}$$

a) Determine the constant C such that $|\tilde{\psi}\rangle$ is normalized.

Clearly, $C = 1/\sqrt{2}$.

b) Determine $\hat{A}\,|\tilde{\psi}\rangle$ and the expectation value $\langle\tilde{\psi}|\hat{A}|\tilde{\psi}\rangle$.

$$\hat{A}\,|\tilde{\psi}\rangle = \frac{1}{\sqrt{2}}\left[a_2\,|\psi_2\rangle + a_3\,|\psi_3\rangle\right] \tag{38}$$

$$\langle\tilde{\psi}|A|\tilde{\psi}\rangle = \frac{1}{2}\left[a_2 + a_3\right] \tag{39}$$

c) Determine $\hat{B}\,|\tilde{\psi}\rangle$ and the expectation value $\langle\tilde{\psi}|\hat{B}|\tilde{\psi}\rangle$.

$$\hat{B}\,|\tilde{\psi}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & i \\ 0 & -i & 3 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 2+i \\ -i+3 \end{pmatrix} \tag{40}$$

$$\langle\tilde{\psi}|B|\tilde{\psi}\rangle = 5/2 \tag{41}$$

d) Is it possible to diagonalize $\hat{A}$ and $\hat{B}$ simultaneously? Calculate the commutator $[\hat{A},\hat{B}]$.

Only if $a_{1,2,3}$ are all equal.

$$[A,B] = \begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & i \\ 0 & -i & 3 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & i \\ 0 & -i & 3 \end{pmatrix}\begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix} \tag{42}$$

$$= \begin{pmatrix} a_1 & 0 & a_1 \\ 0 & a_2 & a_2 i \\ 0 & -ia_3 & a_3 \end{pmatrix} - \begin{pmatrix} a_1 & 0 & a_3 \\ 0 & a_2 & ia_3 \\ 0 & -ia_2 & a_3 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0 & a_1 - a_3 \\ 0 & 0 & (a_2 - a_3)i \\ 0 & -i(a_3 - a_2) & 0 \end{pmatrix} \tag{43}$$

e) Consider the operator $\hat{\rho}$ defined by

$$\hat{\rho} = \frac{1}{3}\,|\psi_1\rangle\,\langle\psi_1| + \frac{1}{3}\,|\tilde{\psi}\rangle\,\langle\tilde{\psi}| \tag{44}$$

and express it explicitly as a matrix in the basis of $|\psi_i\rangle\,, i = 1,2,3$.

Comment: $\hat{\rho}$ is called a density matrix. A state whose density matrix is not given by a single "ket-bra" $|.\rangle\langle.|$ is called *pure*, if instead the density matrix is a sum over $|.\rangle\langle.|$ with non-zero coefficients, the states is called *mixed*.

$$\hat{\rho} = \frac{1}{3}|\psi_1\rangle\langle\psi_1| + \frac{1}{6}[|\psi_2\rangle\langle\psi_2| + |\psi_2\rangle\langle\psi_3| + |\psi_3\rangle\langle\psi_2| + |\psi_3\rangle\langle\psi_3|] \tag{45}$$

$$= \frac{1}{3}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 1/2 \\ 0 & 1/2 & 1/2 \end{pmatrix} \tag{46}$$

f) Calculate the expectation values of $\hat{A}, \hat{B}$ with respect to the mixed state $\hat{\rho}$.

Comment: For mixed states, the expectation value of an operator is $\langle\hat{O}\rangle = \mathrm{tr}\,[\hat{\rho}\hat{O}]$, where tr is the trace and $\hat{O}$ and arbitrary operator. Convince yourself that for pure states, this expectation value is the same as the expectation value $\langle\hat{O}\rangle = \langle\psi|\hat{O}|\psi\rangle$ discussed in the lecture.

$$\langle\hat{A}\rangle = [a_1 + a_2/2 + a_3/2]/3 \tag{47}$$

$$\langle\hat{B}\rangle = \frac{1}{3}\mathrm{tr}\,[\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & i \\ 0 & -i & 3 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 1/2 \\ 0 & 1/2 & 1/2 \end{pmatrix}] = \frac{1}{3}[1 + (1 + i/2) + (-i/2 + 3/2)] = \frac{7}{6}. \tag{48}$$