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Tutorial 7 (Schmidt decomposition and purifications[1])

(a) Prove the following theorem:

Theorem (**Schmidt decomposition**) Suppose $|\psi\rangle$ is a pure state of a composite system, AB. Then there exist orthonormal states $|i_\mathsf{A}\rangle$ for system A, and orthonormal states $|i_\mathsf{B}\rangle$ for system B such that

$$|\psi\rangle = \sum_i \lambda_i \, |i_\mathsf{A}\rangle |i_\mathsf{B}\rangle,$$

where λ_i are non-negative real numbers satisfying $\sum_i \lambda_i^2 = 1$ known as *Schmidt coefficients*.

(b) Show that, as consequence of the Schmidt decomposition, the deduced density matrices for subsystems A and B have the same eigenvalues if the composite system is in a pure state $|\psi\rangle$.

(c) Given a density operator ρ^A on a quantum system A, construct a pure state $|\psi\rangle$ on an extended quantum system AR such that $\rho^\mathsf{A} = \mathrm{tr}_\mathsf{R}[|\psi\rangle\langle\psi|]$. This procedure is known as *purification*.

Exercise 7.1 (Schmidt decomposition and Schrödinger equation)

(a) Consider a composite system consisting of two qubits. Find the Schmidt decompositions of the states

$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \quad \text{and} \qquad \frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle).$$

Hint: For the second state, the required singular value decomposition agrees with the spectral decomposition of a matrix. It might be instructive to compare your result with exercise 4.2(a).

The Schrödinger equation

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle$$

describes how a quantum state $|\psi(t)\rangle$ governed by a Hamiltonian operator H evolves in time (cf. Tutorial 7). In case H itself is time independent, it is solved by

$$|\psi(t)\rangle = U_t|\psi(0)\rangle \quad \text{with} \quad U_t = \mathrm{e}^{-iHt/\hbar}.$$

U_t is the unitary *time evolution operator*. In parts (b) and (c), we absorb $\hbar$ into H, effectively setting $\hbar = 1$.

(b) Consider the Hamiltonian operator

$$H = \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix}$$

acting on a single qubit, with the "frequency" parameters $\omega_1, \omega_2 \in \mathbb{R}$. Find U_t and $|\psi(t)\rangle$ for the initial state (i) $|\psi(0)\rangle = |0\rangle$ and (ii) $|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$.

(c) We now add a small perturbation of strength ϵ to the Hamiltonian:

$$H = \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix} + \epsilon \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Compute U_t and the "overlap" $\langle 1|\psi(t)\rangle$ between $|1\rangle$ and $|\psi(t)\rangle$ for the initial state $|\psi(0)\rangle = |0\rangle$.

Hint: Represent H in terms of the identity and Pauli-X and Z matrices: $H = \bar{\omega} I + \sqrt{\Delta\omega^2 + \epsilon^2}\,(\vec{v} \cdot \vec{\sigma})$ with $\Delta\omega = (\omega_1 - \omega_2)/2$ and suitable $\bar{\omega} \in \mathbb{R}$, $\vec{v} \in \mathbb{R}^3$, and then use Eq. (2.25) from the script.

(d) Based on the Schrödinger equation, derive the following *von Neumann equation* for a density matrix $\rho(t) = \sum_j p_j \, |\psi_j(t)\rangle\langle\psi_j(t)|$:

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

Here $[\cdot, \cdot]$ is the matrix commutator.

Hint: Use the product rule for computing the time derivative of each term $|\psi_j(t)\rangle\langle\psi_j(t)|$.

[1] M. A. Nielsen, I. L. Chuang: *Quantum Computation and Quantum Information*. Cambridge University Press (2010), Section 2.5

Exercise 7.2 (Python/NumPy implementation of the partial trace)

(a) Implement the partial trace operation for arbitrary dimensions using Python/NumPy. Specifically, you should write a function with signature `partial_trace(rho, dimA, dimB)`, where `rho` is the density matrix of the composite quantum system, and `dimA`, `dimB` specify the dimensions of subsystems A and B, respectively. (Thus `rho` is a $\texttt{dimA} \cdot \texttt{dimB} \times \texttt{dimA} \cdot \texttt{dimB}$ matrix.) The function should return a tuple $(\rho^{\mathsf{A}}, \rho^{\mathsf{B}})$ containing the reduced density matrices $\rho^{\mathsf{A}} = \mathrm{tr}_{\mathsf{B}}[\texttt{rho}]$ and $\rho^{\mathsf{B}} = \mathrm{tr}_{\mathsf{A}}[\texttt{rho}]$.

Hint: First reshape `rho` into a $\texttt{dimA} \times \texttt{dimB} \times \texttt{dimA} \times \texttt{dimB}$ tensor using `numpy.reshape`. Then apply `numpy.trace` to trace out certain dimensions.

(b) Apply your function to $\rho = |\psi\rangle\langle\psi|$ with the Bell state $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. The reduced density matrices should both be equal to $\frac{I}{2}$.

Hint: Represent $|\psi\rangle$ as vector (NumPy array) of length 4. `numpy.outer(psi, psi.conj())` computes the outer product $|\psi\rangle\langle\psi|$.

(c) Test your implementation by constructing a random density matrix ρ on the composite system and a random observable M on subsystem A, and then numerically verifying that $\mathrm{tr}[M\rho^{\mathsf{A}}] = \mathrm{tr}[(M \otimes I)\rho]$ (up to numerical rounding errors).

You can use the following functions to obtain ρ and M:

```
import numpy as np


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
```

Hint: In Python $\geq$ 3.5, the `@` operator performs the matrix product.