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Quantum Information Science I

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Problem Set #2 Solution

1. **Density matrices**. A density matrix (also sometimes known as a *density operator*) is a representation of statistical mixtures of quantum states. This exercise introduces some examples of density matrices, and explores some of their properties.

   (a) Let $|\psi\rangle = a|0\rangle + b|1\rangle$ be a qubit state. Give the matrix $\rho = |\psi\rangle\langle\psi|$, which you may compute using linear algebra using the vector representations of $|\psi\rangle$ and $\langle\psi|$. What are the eigenvectors and eigenvalues of ρ?
   Answer:

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} a \\ b \end{pmatrix} \begin{pmatrix} a^* & b^* \end{pmatrix} = \begin{pmatrix} |a|^2 & ab^* \\ ba^* & |b|^2 \end{pmatrix}$$

   The eigenvalues of ρ are 1 and 0 and the corresponding eigenvectors are

$$\begin{pmatrix} a \\ b \end{pmatrix}, \begin{pmatrix} b^* \\ -a^* \end{pmatrix}$$

   (b) Let $\rho_0 = |0\rangle\langle 0|$ and $\rho_1 = |1\rangle\langle 1|$. Give the matrix $\sigma = \frac{\rho_0+\rho_1}{2}$. What are the eigenvectors and eigenvalues of σ?
   Answer:

$$\sigma = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

   The eigenvalues of σ are both $\frac{1}{2}$ and the eigenvectors are

$$|0\rangle, |1\rangle$$

   or any two orthogonal vectors in this Hilbert space.

   (c) Compute $\mathrm{tr}(\rho^2)$ and $\mathrm{tr}(\sigma^2)$. In general, $\mathrm{tr}(M^2) \leq 1$, with equality if and only if M is a pure state.
   Answer:

$$\mathrm{tr}\rho^2 = \mathrm{tr}(|\psi\rangle\langle\psi|)^2 = \mathrm{tr}(|\psi\rangle\langle\psi|) = 1,$$
$$\mathrm{tr}(\sigma^2) = \frac{1}{4}\mathrm{tr}(|0\rangle\langle 0| + |1\rangle\langle 1|)^2 = \frac{1}{4}\mathrm{tr}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{1}{2}$$

2. **Exponential of the Pauli matrices**. Let $\vec{v}$ be any real, three-dimensional unit vector and θ a real number. Prove that

$$\exp(i\theta\vec{v}\cdot\vec{\sigma}) = \cos(\theta)I + i\sin(\theta)\vec{v}\cdot\vec{\sigma}, \tag{1}$$

   where $\vec{v}\cdot\vec{\sigma} \equiv \sum_{i=1}^{3} v_i\sigma_i$, and σ_i are the Pauli matrices, $\sigma_1 = X$, $\sigma_2 = Y$, $\sigma_3 = Z$.

Answer:

$$\exp(i\theta\vec{v}\cdot\vec{\sigma}) = \sum_{k=0}^{\infty}\frac{1}{k!}(i\theta\vec{v}\cdot\vec{\sigma})^k = \sum_{k'=0}^{\infty}\frac{(-1)^{k'}}{(2k')!}(\theta\vec{v}\cdot\vec{\sigma})^{2k'} + \sum_{k'=0}^{\infty}\frac{i(-1)^{k'}}{(2k'+1)!}(\theta\vec{v}\cdot\vec{\sigma})^{2k'+1}$$

The powers of Pauli matrices have a simple form. Note that,

$$(\vec{v}\cdot\vec{\sigma})^2 = (\sum_{i=1}^{3} v_i\sigma_i)^2 = \sum_{i,j=1}^{3} v_i v_j \sigma_i\sigma_j$$

The commutation relation between Pauli matrices satisfies that

$$\sigma_i\sigma_j + \sigma_j\sigma_i = 0 \text{ and } \sigma_i^2 = I$$

Hence,

$$(\vec{v}\cdot\vec{\sigma})^2 = \sum_{i=1}^{3} v_i^2 I = I$$

Therefore,

$$(\theta\vec{v}\cdot\vec{\sigma})^{2k'} = \theta^{2k'}I \quad (\theta\vec{v}\cdot\vec{\sigma})^{2k'+1} = \theta^{2k'+1}\vec{v}\cdot\vec{\sigma}$$

and

$$\exp(i\theta\vec{v}\cdot\vec{\sigma}) = \sum_{k'=0}^{\infty}\frac{(-1)^{k'}}{(2k')!}\theta^{2k'}I + i\sum_{k'=0}^{\infty}\frac{(-1)^{k'}}{(2k'+1)!}\theta^{2k'+1}\vec{v}\cdot\vec{\sigma} = \cos\theta I + i\sin\theta\vec{v}\cdot\vec{\sigma}$$

3. **Hadamard operator on n qubits**. The Hadamard operator on one qubit may be written as

$$H = \frac{1}{\sqrt{2}}\Big[(|0\rangle + |1\rangle)\langle 0| + (|0\rangle - |1\rangle)\langle 1|\Big]. \tag{2}$$

Show explicitly that the Hadamard transform on n qubits, $H^{\otimes n}$, may be written as

$$H^{\otimes n} = \frac{1}{\sqrt{2^n}}\sum_{x,y}(-1)^{x\cdot y}|x\rangle\langle y|. \tag{3}$$

Write out an explicit matrix representation for $H^{\otimes 2}$.
Answer:
Hadamard transform on 1 qubit can be written as

$$H = \frac{1}{\sqrt{2}}\Big[(|0\rangle + |1\rangle)\langle 0| + (|0\rangle - |1\rangle)\langle 1|\Big] = \sum_{x_1,y_1}(-1)^{x_1\cdot y_1}|x_1\rangle\langle y_1|$$

Here $x_1 \cdot y_1$ is multiplication mod 2.

Hadamard transform on n qubits can be written as

$$H^{\otimes n} = \otimes_{i=1}^{n} (\sum_{x_i, y_i} (-1)^{x_i \cdot y_i} |x_i\rangle\langle y_i|)$$

Define $|x\rangle = \otimes |x_i\rangle$, $|y\rangle = \otimes |y_i\rangle$, $x \cdot y = \sum_{i=1}^{n} x_i \cdot y_i$

Therefore,

$$H^{\otimes n} = \otimes_{i=1}^{n} (\sum_{x_i, y_i} (-1)^{x_i \cdot y_i} |x_i\rangle\langle y_i|) = \sum_{x,y} (\otimes_{i=1}^{n} (-1)^{x_i \cdot y_i} |x_i\rangle\langle y_i|) = \sum_{x,y} (-1)^{x \cdot y} |x\rangle\langle y|$$

In particular,

$$H^{\otimes 2} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

4. **Single qubit rotations**. Define the rotation operator

$$R_{\hat{n}}(\theta) \equiv \exp(-i\theta\, \hat{n} \cdot \vec{\sigma}/2) = \cos\left(\frac{\theta}{2}\right) I - i \sin\left(\frac{\theta}{2}\right) (n_x X + n_y Y + n_z Z)\,, \tag{4}$$

where $\hat{n}$ is a real three-dimensional unit vector.

1. Prove that an arbitrary single qubit unitary operator can be written in the form $U = \exp(i\alpha) R_{\hat{n}}(\theta)$, for some real numbers α and θ.

   Answer:

   A single qubit operator $U = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ can be expanded in terms of $\{I, X, Y, Z\}$ as $U = a_0 I + a_1 X + a_2 Y + a_3 Z$, where

$$a_0 = \frac{a+d}{2} \quad a_1 = \frac{b+c}{2} \quad a_2 = \frac{c-b}{2i} \quad a_3 = \frac{a-d}{2}$$

   U is unitary if $U^\dagger U = I$.

$$\begin{aligned} U^\dagger U &= (a_0^* I + a_1^* X + a_2^* Y + a_3^* Z)(a_0 I + a_1 X + a_2 Y + a_3 Z) \\ &= (|a_0|^2 + |a_1|^2 + |a_2|^2 + |a_3|^2) I + (a_0^* a_1 + a_1^* a_0 + i a_2^* a_3 - i a_3^* a_2) X + \\ &\quad (a_0^* a_2 - i a_1^* a_3 + a_2^* a_0 + i a_3^* a_1) Y + (a_0^* a_3 + i a_1^* a_2 - i a_2^* a_1 + a_3^* a_0) Z \end{aligned}$$

   This requires that

$$\begin{aligned} |a_0|^2 + |a_1|^2 + |a_2|^2 + |a_3|^2 &= 1 \\ a_0^* a_1 + a_1^* a_0 + i a_2^* a_3 - i a_3^* a_2 &= 0 \\ a_0^* a_2 - i a_1^* a_3 + a_2^* a_0 + i a_3^* a_1 &= 0 \\ a_0^* a_3 + i a_1^* a_2 - i a_2^* a_1 + a_3^* a_0 &= 0 \end{aligned}$$

Define $\cos\left(\frac{\theta}{2}\right) = |a_0|$, then $|a_1|^2 + |a_2|^2 + |a_3|^2 = |\sin\left(\frac{\theta}{2}\right)|$.
Define

$$n_x = |a_1|/|\sin\left(\frac{\theta}{2}\right)|$$
$$n_y = |a_2|/|\sin\left(\frac{\theta}{2}\right)|$$
$$n_z = |a_3|/|\sin\left(\frac{\theta}{2}\right)|$$

Obviously, $n_x^2 + n_y^2 + n_z^2 = 1$ and $\hat{n}$ is a three dimensional unit vector.
Define $\exp(i\alpha) = a_0/\cos\left(\frac{\theta}{2}\right)$. Denote the phase of a_1, a_2, a_3 as α_1, α_2, α_3 respectively.
As

$$\begin{aligned} 0 &= a_0^* a_1 + a_1^* a_0 + i a_2^* a_3 - i a_3^* a_2 \\ &= \exp(i(\alpha_1 - \alpha))\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)n_x + \exp(i(\alpha - \alpha_1))\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)n_x + \\ &\quad i\exp(i(\alpha_3 - \alpha_2))\sin^2\left(\frac{\theta}{2}\right)n_y n_z - i\exp(i(\alpha_2 - \alpha_3))\sin^2\left(\frac{\theta}{2}\right)n_y n_z \\ &= 2\cos(\alpha - \alpha_1)\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)n_x + 2i\sin(\alpha_3 - \alpha_2)\sin^2\left(\frac{\theta}{2}\right)n_y n_z \end{aligned}$$

Therefore, $\cos(\alpha - \alpha_1) = 0$, $\sin(\alpha_2 - \alpha_3) = 0$. Hence $\alpha_1 = \alpha - \pi/2$, $\alpha_2 = \alpha_3$.
Similarly, we find, $\alpha_2 = \alpha_3 = \alpha - \pi/2$, $\alpha_1 = \alpha_2 = \alpha_3$.
Therefore,

$$\begin{aligned} a_0 &= \exp(i\alpha)\cos\left(\frac{\theta}{2}\right) \\ a_1 &= -i\exp(i\alpha)\sin\left(\frac{\theta}{2}\right)n_x \\ a_2 &= -i\exp(i\alpha)\sin\left(\frac{\theta}{2}\right)n_y \\ a_3 &= -i\exp(i\alpha)\sin\left(\frac{\theta}{2}\right)n_z \end{aligned}$$

That is,

$$U = \exp(i\alpha)\left(\cos\left(\frac{\theta}{2}\right)I - i\sin\left(\frac{\theta}{2}\right)(n_x X + n_y Y + n_z Z)\right) = \exp(i\alpha)R_{\hat{n}}(\theta)$$

2. Find values for α, θ, and $\hat{n}$ giving the Hadamard gate H.
Answer:

$$H = \frac{1}{\sqrt{2}}(X + Z)$$

$$\alpha = \pi/2, \theta = \pi, n_x = \frac{1}{\sqrt{2}}, n_y = 0, n_z = \frac{1}{\sqrt{2}}$$

3. Find values for α, θ, and $\hat{n}$ giving the phase gate

$$S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}. \tag{5}$$

Answer:

$$S = \frac{1+i}{2} I + \frac{1-i}{2} Z$$

$$\alpha = \pi/4, \theta = \pi/2, n_x = 0, n_y = 0, n_z = 1$$