Solutions:
Homework Set 6 — Density matrix

Due June 20, 2021

1. The trace of an operator is defined as $\mathrm{Tr}\{A\} = \sum_m \langle m|A|m\rangle$, where $\{|m\rangle\}$ is an arbitrary orthonormal basis set. Introduce a second basis set, and use it to prove that the trace is independent of the choice of basis.

Let $\{|\alpha\rangle\}$ be an arbitrary second basis. In the basis $\{|m\rangle\}$, the trace is

$$\mathrm{Tr}\{A\} = \sum_m \langle m|A|m\rangle. \tag{1}$$

In basis $\{|\alpha\rangle\}$, it is

$$\mathrm{Tr}\{A\} = \sum_\alpha \langle \alpha|A|\alpha\rangle. \tag{2}$$

We can insert a complete set of m states

$$\mathrm{Tr}\{A\} = \sum_{\alpha,m} \langle \alpha|m\rangle\langle m|A|\alpha\rangle. \tag{3}$$

re-ordering gives

$$\mathrm{Tr}\{A\} = \sum_{\alpha,m} \langle m|A|\alpha\rangle\langle \alpha|m\rangle \tag{4}$$

We recognize the identity operator $I = \sum_\alpha |\alpha\rangle\langle\alpha|$, which leads to the original expression

$$\mathrm{Tr}\{A\} = \sum_m \langle m|A|m\rangle. \tag{5}$$

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2. Prove the linearity of the trace operation by proving

$$\text{Tr}\{aA + bB\} = a\text{Tr}\{A\} + b\text{Tr}\{B\} \tag{6}$$

$$\begin{aligned}
\text{Tr}\{aA + bB\} &= \sum_m \langle m|(aA + bB)|m\rangle && (7)\\
&= a\sum_m \langle m|A|m\rangle + b\sum_m \langle m|B|m\rangle && (8)\\
&= a\text{Tr}\{A\} + b\text{Tr}\{B\} && (9)
\end{aligned}$$

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3. Prove the cyclic property of the trace by proving

$$\text{Tr}\{ABC\} = \text{Tr}\{BCA\} = \text{Tr}\{CAB\} \tag{10}$$

$$\begin{aligned}
\text{Tr}\{ABC\} &= \sum_{m_1} \langle m_1|ABC|m_1\rangle && (11)\\
&= \sum_{m_1,m_2,m_3} \langle m_1|A|m_2\rangle\langle m_2|B|m_3\rangle\langle m_3|C|m_1\rangle && (12)\\
&= \sum_{m_1,m_2,m_3} \langle m_3|C|m_1\rangle\langle m_1|A|m_2\rangle\langle m_2|B|m_3\rangle = \text{Tr}\{CAB\} && (13)\\
&= \sum_{m_1,m_2,m_3} \langle m_2|B|m_3\rangle\langle m_3|C|m_1\rangle\langle m_1|A|m_2\rangle = \text{Tr}\{BCA\} && (14)
\end{aligned}$$

Note that this is not equivalent to non-cyclic permutations , $\text{Tr}\{ABC\} \neq \text{Tr}\{BAC\}$

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4. Which of the following density matrices correspond to a pure state?

$$\rho_1 = \begin{pmatrix} \frac{2}{7} & 0 \\ 0 & \frac{5}{7} \end{pmatrix} \tag{15}$$

$$\rho_2 = \begin{pmatrix} \frac{1}{4} & i\frac{\sqrt{3}}{4} \\ -i\frac{\sqrt{3}}{4} & \frac{3}{4} \end{pmatrix} \tag{16}$$

$$\rho_3 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{17}$$

$$\rho_4 = \begin{pmatrix} \frac{1}{5} & \frac{\sqrt{2}}{5} \\ \frac{\sqrt{2}}{5} & \frac{4}{5} \end{pmatrix} \tag{18}$$

A pure state must satisfy $\rho^2 = \rho$, or equivalently $\mathrm{Tr}\rho^2 = \mathrm{Tr}\rho = 1$. Checking this, we have

ρ_1: Mixed

ρ_2: Pure

ρ_3: Pure

ρ_4: Mixed

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5. The density matrix evolves with time. Derive the equation of motion

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H, \rho(t)] \tag{19}$$

using the Schrodinger equation and the most general form of the density operator

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \tag{20}$$

$$\frac{d}{dt}\rho(t) = \frac{d}{dt}\sum_i p_i|\psi_i\rangle\langle\psi_i| \tag{21}$$

$$= \sum_i p_i \left[\left(\frac{d}{dt}|\psi_i\rangle\right)\langle\psi_i| + |\psi_j\rangle\left(\frac{d}{dt}\langle\psi_i|\right)\right] \tag{22}$$

$$= \sum_i p_i \left[-\frac{i}{\hbar}H|\psi_i\rangle\langle\psi_i| + \frac{i}{\hbar}|\psi_i\rangle\langle\psi_i|H\right] \tag{23}$$

$$= -\frac{i}{\hbar}H\sum_i p_i|\psi_i\rangle\langle\psi_i| + \frac{i}{\hbar}\left(\sum_i p_i|\psi_i\rangle\langle\psi_i|\right)H \tag{24}$$

$$- -\frac{i}{\hbar}[H,\rho] \tag{25}$$

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6. A spin-$\frac{1}{2}$ particle is in a statistical ensemble with a 50% probability to be in the $|+_z\rangle$ state (the eigenstate of S_z with eigenvalue $\hbar/2$) a 50% chance to be in $|+_x\rangle$ (the eigenstate of S_x with eigenvalue $\hbar/2$). [Note that these states are not orthogonal. Don't worry about that yet.] Use the standard procedure,

$$\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i| \tag{26}$$

to write this density operator in terms of states in the $|\pm_z\rangle$ basis, and then as a matrix using this basis. Use the density matrix to compute the probability that a measurement of the z-component of spin will return value $+\hbar/2$.

Now solve the eigenvalue/eigenvector problem for the density matrix. The eigenstates you find are eigenstates of spin along a definite axis — that is, eigenstates of $S \cdot \hat{n}$ for some unit vector $\hat{n}$. Find $\hat{n}$. What is the entropy of the density matrix, and is it the same as you would guess at the beginning, knowing that there is a 50% chance to be in each of two states? What would be a more proper description of the density matrix, in terms of probabilities to be in orthogonal states?

We have a mixed state of $|\psi_1\rangle = |+_z\rangle$ with probability 1/2, and $|\psi_2\rangle = |+_x\rangle = 1/\sqrt{2}(|+_z\rangle + |-_z\rangle)$ with probability 1/2. The density operator is then

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \tag{27}$$

$$= \frac{1}{2}|+_z\rangle\langle +_z| + \frac{1}{2}|+_x\rangle\langle +_x| \tag{28}$$

$$= \frac{1}{2}|+_z\rangle\langle +_z| + \frac{1}{2}\frac{1}{\sqrt{2}}\left(|+_z\rangle + |-_z\rangle\right)\frac{1}{\sqrt{2}}\left(\langle +_z| + \langle -_z|\right) \tag{29}$$

$$= \frac{3}{4}|+_z\rangle\langle +_z| + \frac{1}{4}|+_z\rangle\langle -_z| + \frac{1}{4}|-_z\rangle\langle +_z| + \frac{1}{4}|-_z\rangle\langle -_z| \tag{30}$$

$$= \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{pmatrix} \tag{31}$$

The expectation value for S_z is

$$\mathrm{Tr}(\rho S_z) = \mathrm{Tr}\left[\begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{pmatrix}\begin{pmatrix} \frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix}\right] \tag{32}$$

$$= \frac{\hbar}{8}\mathrm{Tr}\left[\begin{pmatrix} 3 & -1 \\ 1 & -1 \end{pmatrix}\right] \tag{33}$$

$$= \frac{\hbar}{2}\left(\frac{3}{4} - \frac{1}{4}\right) \tag{34}$$

$$= \frac{\hbar}{4} \tag{35}$$

with probability of measuring $+\hbar/2$

$$p(+_z) = \langle +_z|\rho|+_z\rangle \tag{36}$$

$$= \frac{3}{4} \tag{37}$$

and probability of measuring $-\hbar/2$

$$p(-_z) = \langle -_z|\rho|-_z\rangle \tag{38}$$

$$= \frac{1}{4} \tag{39}$$

The eigenvectors are

$$\psi_1 = \frac{1}{2(2+\sqrt{2})}\begin{pmatrix}1+\sqrt{2}\\ 1\end{pmatrix} \tag{40}$$

$$\psi_2 = \frac{1}{2(2-\sqrt{2})}\begin{pmatrix}1-\sqrt{2}\\ 1\end{pmatrix} \tag{41}$$

and eigenvalues $\lambda_1 = \frac{1}{4}(2+\sqrt{2})$ and $\lambda_2 = \frac{1}{4}(2-\sqrt{2})$

For the angle of $\hat{n}$, we note that the vector is in the $x-z$ plane, so the azimuthal angle is $\phi = 0$ and we only need to know the angle θ with respect to the z axis, $\hat{n} = (\sin\theta, \cos\theta)$. The eigenvalues of $S \cdot \hat{n}$ have the form

$$\psi = \begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}\end{pmatrix} \tag{42}$$

$$\implies \theta_1 = 2\tan^{-1}\frac{1}{1+\sqrt{2}} \tag{43}$$

$$= \frac{\pi}{4} \tag{44}$$

$$\theta_2 = 2\tan^{-1}\frac{1}{1-\sqrt{2}} \tag{45}$$

$$= -\frac{3\pi}{4} \tag{46}$$

And finally we have

$$\hat{n} = (\sin\theta, 0, \cos\theta) \tag{47}$$

$$\implies \hat{n}_1 = \frac{1}{\sqrt{2}}(1,0,1) \tag{48}$$

$$\hat{n}_2 = -\frac{1}{\sqrt{2}}(1,0,1) \tag{49}$$

The entropy is

$$S(\rho) \equiv -\mathrm{Tr}\left[\rho \log \rho\right] \tag{50}$$

$$= -\sum_i \lambda_i \log \lambda_i \tag{51}$$

$$= -\frac{1}{4}(2+\sqrt{2})\log\left[\frac{1}{4}(2+\sqrt{2})\right] - \frac{1}{4}(2-\sqrt{2})\log\left[\frac{1}{4}(2-\sqrt{2})\right] \tag{52}$$

$$\simeq 0.6 \tag{53}$$

(using base 2 logarithm to measure in bits).

This is different then the case where the system has equal probability to be in every state of an orthogonal basis (e.g., 1/2 probability $|+_z\rangle$ and 1/2 probability $|-_z\rangle$). In that case the entropy is maximual $S = 1$.

The simpler way to describe the system is being in state ψ_1 with probability λ_1 and state ψ_2 with probability λ_2, the orthogonal basis where the density matrix is diagonal:

$$\rho = \lambda_1|\psi_1\rangle\langle\psi_2| + \lambda_2|\psi_2\rangle\langle\psi_2| \tag{54}$$