Prof. Dr. Viatcheslav Mukhanov Winter term 2019/2020

Exercises on Quantum Mechanics II (TM1/TV)

Problem set 4, discussed November 11 - November 15, 2019

Exercise 25 (central tutorial)

(i) Consider a system Σ described by a state $|\,\psi_\Sigma\rangle$ and its corresponding density matrix $\hat\rho_\Sigma$, composed of subsystems I and II; prove that the two definitions of density matrix for the subsystem I, $\hat\rho_I$, are equivalent:

a) For every operator that acts only on the subsystem I, $\hat A = \hat A_I \otimes \mathbb{1}$, the density matrix $\hat\rho_I$ is defined such that

$$\bar A = \mathrm{tr}\left(\hat\rho_I \hat A_I\right) = \bar A_I \tag{1}$$

b)

$$\hat\rho_I = \mathrm{tr}_{II}\left(\hat\rho_\Sigma\right) = \sum_n \left\langle {}^{II}\delta^n \,|\, \hat\rho_\Sigma | {}^{II}\delta_n \right\rangle \tag{2}$$

where $\{\left|\, {}^{II}\delta_n\right\rangle\}_{n\in\mathbb{N}}$ is an orthonormal basis for II.

(ii) Prove that in general (i.e. also for mixed states) for density matrices the following relations hold:

a) $\mathrm{tr}\,\hat\rho = 1$;

b) $\hat\rho$ is an hermitian operator;

c) $\hat\rho$ is a positive operator, i.e. $\langle\psi\,|\,\hat\rho|\psi\rangle \geq 0 \quad \forall\,|\,\psi\rangle$;

d) All the eigenvalues of $\hat\rho$ are between 0 and 1;

e) $\left\langle\psi\,|\,\hat\rho - \hat\rho^2|\psi\right\rangle \geq 0 \quad \forall\,|\,\psi\rangle$;

f) If $\hat\rho^2 = \hat\rho$ then there exists a vector $|\,\phi\rangle$ for which $\hat\rho = |\,\phi\rangle\langle\phi\,|$ (pure state).

Solution

(i) Let's first recall the definition for a general density matrix that describes a subsystem I of a general system Σ. Suppose to have an operator that acts only on the subsystem I, $\hat A = \hat A_I \otimes \mathbb{1}$. The density matrix $\hat\rho_I$ is defined such that

$$\bar A = \mathrm{tr}\left(\hat\rho_I \hat A_I\right) = \bar A_I \tag{3}$$

Therefore, given a generic **normalized** state for the whole system $|\,\psi_\Sigma\rangle = \sum_{ij} = c^{ij}\left|\,{}^I\delta_i\right\rangle\left|\,{}^{II}\delta_j\right\rangle$ we have:

$$\begin{aligned}
\bar A = \left\langle\psi_\Sigma\,|\,\hat A|\psi_\Sigma\right\rangle &= \sum_{ijkl}\left(c_{ij}\left\langle{}^I\delta^i\,|\left\langle{}^{II}\delta^j\,|\right.\right.\right)\left(\hat A_I\otimes\mathbb{1}\right)\left(c^{kl}\left|\,{}^I\delta_k\right\rangle\left|\,{}^{II}\delta_l\right\rangle\right) = \\
&= \sum_{ijkl} c_{ij}c^{kl}\left\langle{}^{II}\delta^j\,|\,{}^{II}\delta_l\right\rangle\left\langle{}^I\delta^i\,|\,\hat A_I|{}^I\delta_k\right\rangle = \sum_{ijk} c_{ij}c^{kj}\left\langle{}^I\delta^i\,|\,\hat A_I|{}^I\delta_k\right\rangle = \\
&= \sum_{ik}\left(\rho_I\right)_i^k\left(\hat A_I\right)_k^i = \mathrm{tr}\left(\hat\rho_I\hat A_I\right)
\end{aligned} \tag{4}$$

where we defined $\left(\rho_I\right)_i^k = \sum_j c_{ij}c^{kj}$.

Therefore we have

$$\hat\rho_I = \sum_{ik}\left(\rho_I\right)_i^k\left|\,{}^I\delta_k\right\rangle\left\langle{}^I\delta^i\,\right| \tag{5}$$

Let's now calculate $\mathrm{tr}_{II}\left(\hat{\rho}_\Sigma\right)$:

$$\begin{aligned}\mathrm{tr}_{II}\left(\hat{\rho}_\Sigma\right) &= \sum_n \left\langle {}^{II}\delta^n \,|\, \hat{\rho}_\Sigma | {}^{II}\delta_n \right\rangle = \sum_n \left\langle {}^{II}\delta^n \,|\, \psi_\Sigma \right\rangle \left\langle \psi_\Sigma \,|\, {}^{II}\delta_n \right\rangle = \sum_{ijk} c_{ij} c^{kj} \left| {}^{I}\delta_k \right\rangle \left\langle {}^{I}\delta^i \right| = \\ &= \sum_{ik} \left(\rho_I\right)^k_i \left| {}^{I}\delta_k \right\rangle \left\langle {}^{I}\delta^i \right| = \hat{\rho}_I\end{aligned} \tag{6}$$

(ii) From now on we omit the superscript I in the basis elements, since we are dealing only with subsystem I.

a) The property of the trace follows straightforwardly

$$\mathrm{tr}\left(\hat{\rho}_I\right) = \sum_i \left(\rho_I\right)^i_i = \sum_{ij} c_{ij} c^{ij} = \sum_{ij} |c_{ij}|^2 \overset{|\,\psi_\Sigma\rangle\text{norm.}}{=} 1 \tag{7}$$

b)

$$\hat{\rho}_I^\dagger = \sum_{ik} \left(\rho_I^*\right)^i_k |\,\delta_i\rangle \left\langle \delta^k \right| = \sum_{ijk} c^{ij} c_{kj} |\,\delta_i\rangle \left\langle \delta^k \right| = \hat{\rho}_I \tag{8}$$

c) We shall call $\hat{\rho}_I$ just $\hat{\rho}$ from now on, with the properties defined above.
Since we have just proven $\hat{\rho}$ to be hermitian, it means that it can be diagonalized in some orthonormal basis $\{|\,\rho_k\rangle\}_{k\in\mathbb{N}}$ through some unitary matrix $(U)^i_j = u^i_j$, i.e. $\hat{\rho}_{\text{diag.}} = \hat{U}\hat{\rho}\hat{U}^\dagger$. Therefore we have:

$$\hat{\rho} = \sum_k \rho_k \,|\,\rho_k\rangle \left\langle \rho^k \right| \quad \text{where} \quad |\,\rho_k\rangle = u^i_k \,|\,\delta_i\rangle \quad \text{and} \quad \{\rho_k\}_{k\in\mathbb{N}} \quad \text{are the eigenvalues of} \quad \hat{\rho} \tag{9}$$

The relation between the eigenvalues and the coefficients of $\hat{\rho}$ is given by the transformation that diagonalizes $\hat{\rho}$. It follows that

$$\begin{aligned}\rho_k &= \sum_{nm} u^k_n (\rho)^n_m (u^*)^m_k = \sum_{nmj} u^k_n c^{nj} c_{mj} (u^*)^m_k = \sum_j \left(\sum_n c^{nj} u^k_n\right) \left(\sum_m c^{mj} u^k_m\right)^* = \\ &= \sum_j \left|\sum_n c^{nj} u^k_n\right|^2 \geq 0 \quad \forall k\end{aligned} \tag{10}$$

Therefore

$$\langle \psi \,|\, \hat{\rho} | \psi \rangle = \sum_k \rho_k |\, \langle \psi \,|\, \rho_k \rangle \,|^2 \geq 0 \tag{11}$$

since we have proved $\rho_k \geq 0 \quad \forall k$.

d) This is immediate since all the eigenvalues are positive and the their sum (the trace of $\hat{\rho}$) is 1.

e)

$$\left\langle \psi \,|\, \hat{\rho} - \hat{\rho}^2 | \psi \right\rangle = \sum_k (\rho_k - \rho_k^2) |\, \langle \psi \,|\, \rho_k \rangle \,|^2 \geq 0 \tag{12}$$

since $\rho_k \geq \rho_k^2$ (ρ_k is between 0 and 1).

f) It means that

$$\sum_k (\rho_k - \rho_k^2) |\, \langle \psi \,|\, \rho_k \rangle \,|^2 = 0 \quad \forall \,|\, \psi\rangle \quad \Rightarrow \quad \rho_k = \rho_k^2 \quad \Rightarrow \quad \rho_k \in \{0, 1\} \tag{13}$$

Therefore, $\hat{\rho}$ must be of the form

$$\hat{\rho} = |\,\rho_k\rangle \left\langle \rho^k \right| \tag{14}$$

with a particular k; that is the definition of a pure state.

Exercise 26 (central tutorial)

(i) A harmonic oscillator has an equal classical probability 1/3 to be found in each of the states $|0\rangle$, $|1\rangle$ and $4|0\rangle + 3|1\rangle$. Write down the corresponding density matrix $\hat{\rho}$ explicitly.

(ii) Consider a system Σ consisting of two subsystems I and II. Σ is in a pure state $|\psi_\Sigma\rangle$, where $|\psi_\Sigma\rangle$ is a vector in the product space. The density matrices $\hat{\rho}_{I,II}$ and $\hat{\rho}_\Sigma$ are defined as in the lecture. Remembering that

$$\hat{\rho}_I = \mathrm{tr}_{II}\,\hat{\rho}_\Sigma \equiv \left\langle {}^{II}\delta^i \,|\, \hat{\rho}_\Sigma | {}^{II}\delta_i \right\rangle \quad \text{and} \quad \hat{\rho}_{II} = \mathrm{tr}_I\,\hat{\rho}_\Sigma \equiv \left\langle {}^{I}\delta^i \,|\, \hat{\rho}_\Sigma | {}^{I}\delta_i \right\rangle \tag{15}$$

and given that $\{|n\rangle\}_{n\in\mathbb{N}}$ is a set of orthonormal vectors, calculate the density matrix for subsystems I and II, for

$$|\psi_\Sigma\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle \otimes |1\rangle + |1\rangle \otimes |2\rangle\right) \tag{16}$$

(iii) Consider $\hat{\rho}_I$ of the previous point. Does it correspond to a pure or to a mixed state?

(iv) Given a density matrix, the entropy of the described state is given by $S = -\,\mathrm{tr}(\hat{\rho}\log(\hat{\rho}))$. Express the entropy as a function of the eigenvalues of $\hat{\rho}$.
It can be shown that the maximum entropy is reached when all eigenvalues are equal, i.e. when every state is possible with the same probability; what is the maximum entropy for a Hilbert space of dimension d? What is the entropy of a pure state? Calculate the entropy of $\hat{\rho}_I$ and $\hat{\rho}_{II}$ of the previous part.

Solution

(i) First of all, we need all states to be normalized. In particular, we have to normalize the third state

$$4|0\rangle + 3|1\rangle \quad \rightarrow \quad \frac{4}{5}|0\rangle + \frac{3}{5}|1\rangle \tag{17}$$

Now we can build the density matrix of the harmonic oscillator as follows

$$\begin{aligned}\hat{\rho} &= \sum_i p_i\,|\psi_i\rangle\langle\psi_i| \overset{p_i=1/3}{=} \frac{1}{3}\sum_i |\psi_i\rangle\langle\psi_i| = \\ &= \frac{1}{3}\left[|0\rangle\langle 0| + |1\rangle\langle 1| + \left(\frac{4}{5}|0\rangle + \frac{3}{5}|1\rangle\right)\left(\frac{4}{5}\langle 0| + \frac{3}{5}\langle 1|\right)\right] \\ &= \frac{41}{75}|0\rangle\langle 0| + \frac{34}{75}|1\rangle\langle 1| + \frac{12}{75}\left(|0\rangle\langle 1| + |1\rangle\langle 0|\right)\end{aligned} \tag{18}$$

(ii) For the sake of legibility we adopt the following notation:

$$|n\rangle \otimes |m\rangle \equiv |nm\rangle \quad , \quad \langle n| \otimes \langle m| \equiv \langle nm| \tag{19}$$

In this notation the state is

$$|\psi_\Sigma\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |12\rangle) \tag{20}$$

Therefore

$$\hat{\rho}_\Sigma = |\psi_\Sigma\rangle\langle\psi_\Sigma| = \frac{1}{2}(|01\rangle + |12\rangle)(\langle 01| + \langle 12|) = \frac{1}{2}(|01\rangle\langle 01| + |12\rangle\langle 12| + |01\rangle\langle 12| + |12\rangle\langle 01|) \tag{21}$$

Tracing out the subsystem II and I we find

$$\hat{\rho}_I = \mathrm{tr}_{II}\,\hat{\rho}_\Sigma = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) \tag{22}$$

$$\hat{\rho}_{II} = \mathrm{tr}_I\,\hat{\rho}_\Sigma = \frac{1}{2}(|1\rangle\langle 1| + |2\rangle\langle 2|) \tag{23}$$

(iii) We have from the previous point $\hat{\rho}_I = \mathrm{tr}_{II}\,\hat{\rho}_\Sigma = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$. It corresponds to a mixed state, and we have two ways of proving it.

a) Suppose $\hat{\rho}_I$ is a pure state; then it must be possible to write it as $\hat{\rho}_I = |\,\phi_I\rangle\langle\phi_I\,|$, with $|\,\phi_I\rangle = \sum_n a_n\,|\,n\rangle$. In this assumption:

$$|\,\phi_I\rangle\langle\phi_I\,| = \sum_{nm} a_n a_m^*\,|\,n\rangle\langle m\,| \tag{24}$$

We can immediately set to 0 the coefficients a_i with $i > 1$ since the corresponding states do not appears in $\hat{\rho}_I$. We have therefore:

$$|\,\phi_I\rangle\langle\phi_I\,| = |a_0|^2\,|\,0\rangle\langle 0\,| + |a_1|^2\,|\,1\rangle\langle 1\,| + a_0 a_1^*\,|\,0\rangle\langle 1\,| + a_1 a_0^*\,|\,1\rangle\langle 0\,| \tag{25}$$

We can see that there exists no choice of a_0, a_1 such that $|\,\phi_I\rangle\langle\phi_I\,| = \hat{\rho}_I$.

b) The second way relies on the fact that for pure states $\hat{\rho}^2 = \hat{\rho}$.

$$\hat{\rho}_I^2 = \frac{1}{2}\hat{\rho}_I \neq \hat{\rho}_I \tag{26}$$

and therefore it is not a pure state.

(iv) Since the density matrix is an hermitian operator it can be diagonalized in a certain orthonormal basis $\{|\,\rho_k\rangle\}_{k\in\mathbb{N}}$; each element of the basis is related to an eigenvalue p_k. Applying the cyclicity of the trace and the definition of logarithm of an operator, the result holds:

$$S = -\sum_k p_k \log(p_k) \tag{27}$$

The maximum entropy in a Hilbert space of dimension d is reached when $p_k = p = \frac{1}{d} \quad \forall k$. The entropy is then:

$$S = -\sum_{k=0}^{d-1} p_k \log(p_k) = -\sum_{k=0}^{d-1} p\log(p) = -d\frac{1}{d}\log\left(\frac{1}{d}\right) = \log(d) \tag{28}$$

For a pure state $\hat{\rho} = |\,\psi\rangle\langle\psi\,|$; it is a diagonal operator with one eigenvalue 1, its eigenvector $|\,\psi\rangle$ and all the others eigenvalues are 0. It follows that the entropy for a pure state is always $S_{\text{pure}} = 0$.

Given the density matrices of the subsystem I and II of the previous point we immediately see that they are both diagonal, with $p_0, p_1 = \frac{1}{2}$ and $p_1, p_2 = \frac{1}{2}$, respectively; the entropy is therefore

$$S_I = S_{II} = \log(2) \tag{29}$$

Exercise 27

Let us now consider a continuous system of two particles Σ, which consists of two subsystems I and II. As before, Σ is in a pure state, which in this case can be expanded as

$$|\,\psi_\Sigma\rangle = \int \psi(x,y)\,|\,x\rangle\,|\,y\rangle\,dxdy \tag{30}$$

Show that:

$$\bar{x} = \operatorname{tr}\hat{\rho}_I\hat{x}_I = \int x\rho_I(x,x)dx \tag{31}$$

$$\bar{p} = \operatorname{tr}\hat{\rho}_I\hat{p}_I = -i\hbar\int dx'\left[\frac{\partial\rho_I(x',x)}{\partial x'}\right]_{x=x'} \tag{32}$$

Solution Let us first show that given an operator $\hat{A}$ which acts only on the subsystem I, i.e. $\hat{A} = \hat{A}_I \otimes \mathbb{1}$, we have

$$\bar{A} = \operatorname{tr}\hat{\rho}_I\hat{A}_I \tag{33}$$

Proof:

$$\begin{aligned}\bar{A} = \langle\psi_\Sigma\,|\,\hat{A}\,|\,\psi_\Sigma\rangle &= \left(\int dx'dy'\psi^*(x',y')\,\langle x'\,|\,\langle y'\,|\right)\hat{A}\left(\int dxdy\psi(x,y)\,|\,x\rangle\,|\,y\rangle\right) = \\ &= \int dxdx'dydy'\,\langle y'\,|\,y\rangle\,\psi^*(x',y')\psi(x,y)\,\langle x'\,|\,\hat{A}_I\,|\,x\rangle = \int dxdx'\rho_I(x,x')\,\langle x'\,|\,\hat{A}_I\,|\,x\rangle = \\ &= \rho_{Ix'}^{x}A_{Ix}^{x'} = \operatorname{tr}\hat{\rho}_I\hat{A}_I\end{aligned} \tag{34}$$

where

$$\rho_I(x,x') = \int dy \psi^*(x',y)\psi(x,y) \tag{35}$$

Now we have

$$\begin{aligned} \bar{x} = \mathrm{tr}(\hat{\rho}_I \hat{x}) = \rho^x_{I x'} x^{x'}_x = \int dx dx' \rho_I(x,x') \langle x' \,|\, \hat{x}_I \,|\, x\rangle = \\ = \int dx dx' x \rho_I(x,x') \delta(x-x') = \int dx x \rho_I(x,x) \end{aligned} \tag{36}$$

and

$$\begin{aligned} \bar{p} = \mathrm{tr}(\hat{\rho}_I \hat{p}) = \rho^x_{I x'} p^{x'}_x = \int dx dx' \rho_I(x,x') \langle x' \,|\, \hat{p}_I \,|\, x\rangle = \\ = i\hbar \int dx dx' \rho_I(x,x') \frac{\partial}{\partial x}\delta(x-x') = -i\hbar \int dx' \left[\frac{\partial \rho_I(x,x')}{\partial x}\right]_{x=x'} \end{aligned} \tag{37}$$

Exercise 28

Calculate the energy, pressure and entropy of a thermal radiation of temperature T in a volume V.

Hint: You may use the relation for the free energy $F(T,V)$ which is known from the lecture:

$$F(T,V) = 2k_B T V \int \frac{d^3k}{(2\pi)^3} \ln\left[1 - e^{-\beta\hbar\omega}\right] \tag{38}$$

with

$$\beta = \frac{1}{k_B T} \tag{39}$$

You may also need the following result:

$$\int_0^\infty dx x^2 \ln\left[1 - e^{-x}\right] = -\frac{\pi^4}{45} \tag{40}$$

Solution Following the hint, we will start with the expression for the free energy obtained in the lecture, and make it nicer:

$$\begin{aligned} F(T,V) = 2k_B T V \int \frac{d^3k}{(2\pi)^3} \ln\left[1 - e^{-\beta\hbar\omega}\right] = \frac{k_B T V}{\pi^2} \int_0^\infty dk k^2 \ln\left[1 - e^{-\beta\hbar\omega}\right] = \\ = \frac{c\hbar V}{\pi^2}\left(\frac{k_B T}{c\hbar}\right)^4 \int_0^\infty dx x^2 \ln\left[1 - e^{-x}\right] \\ \Longrightarrow F(T,V) = -\frac{4\sigma}{3c} V T^4 \qquad , \qquad \sigma = \frac{\pi^2 k_B^4}{60 c^2 \hbar^3} \end{aligned} \tag{41}$$

where in the first line we used the isotropy of the momentum space and $\omega = ck$, and in the second line used the substitution $x = \beta\hbar c k$.
Now we have

$$\begin{aligned} S = -\frac{\partial F}{\partial T} = \frac{16\sigma}{3c} V T^3 \\ E = F + TS = \frac{4\sigma}{c} V T^4 \\ P = -\frac{\partial F}{\partial V} = \frac{4\sigma}{3c} T^4 \end{aligned} \tag{42}$$

Exercise 29

The matrix elements (in coordinate representation) of the density matrix $\hat{\rho}_u = e^{-\beta\hat{H}}$ for a free particle in a three dimensional volume V, satisfy the diffusion equation

$$\frac{\partial \rho_u(\vec{x},\vec{x}';\beta)}{\partial\beta} = \frac{\hbar^2}{2m}\Delta_{\vec{x}} \rho_u(\vec{x},\vec{x}';\beta) \tag{43}$$

with the initial condition $\rho_u(\vec{x}, \vec{x}'; 0) \equiv \delta(\vec{x} - \vec{x}')$.
Show that this equation has the following solution:

$$\rho_u(\vec{x}, \vec{x}'; \beta) = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}} \exp\left[-\frac{m}{2\hbar^2\beta}(\vec{x} - \vec{x}')^2\right] \tag{44}$$

Solution Calculating both sides gives:

$$\frac{\partial\rho_u(\vec{x}, \vec{x}'; \beta)}{\partial\beta} = \left(\frac{m}{2\pi\hbar^2}\right)^{\frac{3}{2}} \left[-\frac{3}{2}\beta^{-\frac{5}{2}} + \frac{m}{2\hbar^2}(\vec{x} - \vec{x}')^2\beta^{-\frac{7}{2}}\right] \exp\left[-\frac{m}{2\hbar^2\beta}(\vec{x} - \vec{x}')^2\right] \tag{45}$$

On the other hand

$$\frac{\hbar^2}{2m}\Delta_{\vec{x}}\rho_u(\vec{x}, \vec{x}'; \beta) = \frac{\hbar^2}{2m}\left(\frac{m}{2\pi\hbar^2}\right)^{\frac{3}{2}} \left[-6\frac{m}{2\hbar^2}\beta^{-\frac{5}{2}} + 4\left(\frac{m}{2\hbar^2}\right)^2(\vec{x} - \vec{x}')^2\beta^{-\frac{7}{2}}\right] \exp\left[-\frac{m}{2\hbar^2\beta}(\vec{x} - \vec{x}')^2\right] \tag{46}$$

The initial condition is satisfied by this solution too, as for $\beta = 0$ the exponential term suppresses everything unless $\vec{x} - \vec{x}' = 0$. The correct normalisation can be seen by a change of variables and performing the gaussian integral:

$$\int_{\mathbb{R}^3} d^3x\ \rho_u(\vec{x}, \vec{x}'; \beta) = \int_{\mathbb{R}^3} d^3x \left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}} \exp\left[-\frac{m}{2\hbar^2\beta}(\vec{x} - \vec{x}')^2\right] \overset{\vec{v}=\vec{x}-\vec{x}'}{=} \left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}} \int_{\mathbb{R}^3} d^3v \exp\left[-\frac{m}{2\hbar^2\beta}(\vec{v})^2\right] =$$

$$\overset{|\vec{v}|^2=v_x^2+v_y^2+v_z^2}{=} \left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}} \left(\int_{-\infty}^{\infty} dv\ \exp\left[-\frac{m}{2\hbar^2\beta}v^2\right]\right)^3 \overset{\frac{m}{2\hbar^2\beta}v^2=w^2}{=} \left(\frac{1}{\pi}\right)^{\frac{3}{2}} \left(\int_{-\infty}^{\infty} dw\ \exp\left[-w^2\right]\right)^3 =$$

$$= \left(\frac{1}{\pi}\right)^{\frac{3}{2}} \left(\sqrt{\pi}\right)^3 = 1 \tag{47}$$

Exercise 30

Consider the three dimensional Hilbert spaces $\mathcal{H}_i$, $i = 1, 2, 3$. Take the tensor product $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$. Let $|\,0\rangle$, $|\,1\rangle$, $|\,2\rangle$ be an orthonormal basis in a single three dimensional Hilbert space. Then a basis of the tensor product is given by $|\,xyz\rangle$, where $x, y, z \in \{0, 1, 2\}$. Pick the following two states in $\mathcal{H}$:

$$|\,\psi\rangle = |\,000\rangle \qquad |\,\phi\rangle = \frac{1}{\sqrt{3}}(|\,000\rangle + |\,111\rangle + |\,222\rangle) \tag{48}$$

(i) Compute the reduced density matrix for the system with Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ for each case.

(ii) Compute the entanglement entropy in each case using your result.

Solution

(i) Firstly note that both density matrix are given by:

$$\rho_\psi = |\,000\rangle\langle 000\,| \qquad \rho_\phi = |\,\phi\rangle\langle\phi\,| = \frac{1}{3}(|\,000\rangle + |\,111\rangle + |\,222\rangle)(\langle 000\,| + \langle 111\,| + \langle 222\,|) \tag{49}$$

Therefore, tracing over $\mathcal{H}_3$ we obtain the required density matrices:

$$\rho_{\psi_{12}} = \mathrm{tr}_{\mathcal{H}_3}\rho_\psi = |\,00\rangle\langle 00\,| \tag{50}$$

$$\rho_{\phi_{12}} = \mathrm{tr}_{\mathcal{H}_3}\rho_\phi = \frac{1}{3}(|\,00\rangle\langle 00\,| + |\,11\rangle\langle 11\,| + |\,22\rangle\langle 22\,|) \tag{51}$$

(ii) In order to compute the entanglement entropy is useful to visualize (50) and (51) as matrices in the basis $|\,00\rangle, |\,11\rangle, |\,22\rangle, |\,01\rangle, |\,10\rangle$ .... In such a basis both are diagonal and so the logarithm of the matrix becomes the matrix of the logarithm of the components. Then trivially one obtains, after matrix multiplication, the entanglement entropy for both systems:

$$S_{\psi_{12}} = -\mathrm{tr}_{\mathcal{H}_1\otimes\mathcal{H}_2}\rho_{\psi_{12}}\log\rho_{\psi_{12}} = 0 \tag{52}$$

$$S_{\phi_{12}} = -\mathrm{tr}_{\mathcal{H}_1\otimes\mathcal{H}_2}\rho_{\phi_{12}}\log\rho_{\phi_{12}} = -\log\frac{1}{3} = \log 3 \tag{53}$$

General information

The *lecture* takes place on:
Monday at 10:00 - 12:00 c.t. in B 052 (Theresienstraße 37)
Friday at 10:00 - 12:00 c.t. in B 052 (Theresienstraße 37)
The *central tutorial* takes place on Monday at 12:00 - 14:00 c.t. in B 139 (Theresienstraße 37)
The *webpage* for the lecture and exercises can be found at

`https://www.physik.uni-muenchen.de/lehre/vorlesungen/wise_19_20/T_M1_TV_-Quantum-Mechanics-II`