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

$$\bar{A} = \operatorname{tr}\left(\hat{\rho}_I \hat{A}_I\right) = \bar{A}_I \tag{1}$$

b)

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

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) $\operatorname{tr}\hat{\rho} = 1$;

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).

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

$$\hat{\rho}_I = \operatorname{tr}_{II}\hat{\rho}_\Sigma \equiv \left\langle {}^{II}\delta^i \,|\, \hat{\rho}_\Sigma | {}^{II}\delta_i \right\rangle \quad \text{and} \quad \hat{\rho}_{II} = \operatorname{tr}_{I}\hat{\rho}_\Sigma \equiv \left\langle {}^{I}\delta^i \,|\, \hat{\rho}_\Sigma | {}^{I}\delta_i \right\rangle \tag{3}$$

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

$$|\,\psi_\Sigma\rangle = \frac{1}{\sqrt{2}}\left(|\,0\rangle \otimes |\,1\rangle + |\,1\rangle \otimes |\,2\rangle\right) \tag{4}$$

(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 $S = -\operatorname{tr}(\hat{\rho}\log(\hat{\rho}))$. 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.

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

$$|\,\psi_\Sigma\rangle = \int \psi(x,y)\,|\,x\rangle\,|\,y\rangle\,dxdy \tag{5}$$

Show that:

$$\bar{x} = \text{tr}\,\hat{\rho}_I \hat{x}_I = \int x\rho_I(x,x)dx \tag{6}$$

$$\bar{p} = \text{tr}\,\hat{\rho}_I \hat{p}_I = -i\hbar \int dx' \left[\frac{\partial \rho_I(x',x)}{\partial x'}\right]_{x=x'} \tag{7}$$

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:

$$F(T,V) = 2k_BTV \int \frac{d^3k}{(2\pi)^3} \ln\left[1 - e^{-\beta\hbar\omega}\right] \tag{8}$$

with

$$\beta = \frac{1}{k_BT} \tag{9}$$

You may also need the following result:

$$\int_0^\infty dx x^2 \ln\left[1 - e^{-x}\right] = -\frac{\pi^4}{45} \tag{10}$$

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

$$\frac{\partial \rho_u(\vec{x},\vec{x}';\beta)}{\partial\beta} = \frac{\hbar^2}{2m}\Delta_{\vec{x}}\rho_u(\vec{x},\vec{x}';\beta) \tag{11}$$

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:

$$\rho_u(\vec{x},\vec{x}';\beta) = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}} \exp\left[-\frac{m}{2\hbar^2\beta}(\vec{x}-\vec{x}')^2\right] \tag{12}$$

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 $\mathcal{H}$:

$$|\,\psi\rangle = |\,000\rangle \qquad\qquad |\,\phi\rangle = \frac{1}{\sqrt{3}}(|\,000\rangle + |\,111\rangle + |\,222\rangle) \tag{13}$$

(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.

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`