Problem set for “Density matrix”
Due April 20, 2020

Problem I: Density matrix for a two-level system

Consider the two-level system whose Hilbert space is spanned by the two basis vectors
\[ |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \]

(a) Show that the most general time-independent Hermitian Hamiltonian for the two level system can be written in the form
\[ H = \sigma_0 h^0 + \sum_{a=1}^{3} \sigma_a h^a \equiv \sigma_0 h^0 + \sigma_a h^a \equiv h^0 + \vec{h} \cdot \vec{\sigma}, \]

where \( h^0 \) and \( \vec{h} = (h^1, h^2, h^3) \) are four real constants, \( \sigma_a (a = 1, 2, 3) \) are the conventional Pauli matrices,
\[ \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \]

and
\[ \sigma_0 = 1 \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \]

(b) Show that the most general density matrix for the two-level system can be written in the form
\[ \rho = \frac{1}{2} \sigma^0 + \sigma_a s^a \equiv \frac{1}{2} + \vec{s} \cdot \vec{\sigma}, \]

where \( \vec{s} = (s^1, s^2, s^3) \) are three real numbers satisfying the condition
\[ (s^1)^2 + (s^2)^2 + (s^3)^2 \leq \frac{1}{4}. \]

(c) Show that the \( s^a \) in (2) coincide with the expectation values of the “spin operators” \( \frac{1}{2} \sigma_a \), i.e.,
\[ \vec{s} = \frac{1}{2} \langle \vec{\sigma} \rangle. \]

(d) Re-write the Liouville-von Neumann equation
\[ i\hbar \frac{\partial \rho}{\partial t} = [H, \rho] \]
for the general time-independent Hamiltonian \( \vec{s} = (s^1, s^2, s^3) \) parameterizing the general density matrix \( \rho \). Give a simple physical interpretation of the obtained system of differential equations and then write the solution of the Liouville-von Neumann equation where the initial value of \( \vec{s} \) at \( t = 0 \) is given: \( \vec{s}(0) = \vec{s}_0 \).

**Hint:** It is useful to know the following properties of the Pauli matrices:

\[
\begin{align*}
\text{Tr}(\sigma_a) &= 0 , \\
\{\sigma_a, \sigma_b\} &\equiv \sigma_a \sigma_b + \sigma_b \sigma_a = 2 \delta_{ab} , \\
[\sigma_a, \sigma_b] &= 2i \varepsilon_{abc} \sigma_c ,
\end{align*}
\]

where \( \varepsilon_{abc} \) is the totally antisymmetric Levi-Civita symbol.

(e) Construct the Lagrangian governes the two level system.

### Problem II: Quantum mechanical entropy

A quantum mechanical system, defined by the Hamiltonian \( H \), is described by a density matrix \( \rho \), which has an associated von Neumann entropy

\[
S_{\text{vN}}[\rho] \equiv -\text{Tr}(\rho \log \rho) .
\]

(a) Using the method of Lagrange multipliers, find the density operator \( \rho_{\text{ext}} \) which extremizes the functional \( S_{\text{vN}}[\rho] \), subject to the constraint of fixed average energy:

\[
\langle H \rangle = \text{Tr}(\rho H) = E \quad \text{given and fixed} .
\]

Show that \( \rho_{\text{ext}} \) is given by

\[
\rho_{\text{ext}} = \rho(\beta) \equiv Z^{-1} e^{-\beta H} ,
\]

where

\[
Z = Z(\beta) = \text{Tr}(e^{-\beta H})
\]

and the parameter \( \beta \) is defined by the equation:

\[
E = -\partial_\beta \log (Z(\beta))
\]

(here we assume that trace \( \text{Tr}(e^{-\beta H}) \) does exist and eq.4 has a solution w.r.t. \( \beta \)).

(b) Show that

\[
S_{\text{vN}}[\rho(\beta)] = -\beta^2 \partial_\beta (\beta^{-1} \log Z(\beta)) .
\]

(c) Show that the solution to part (a) is stationary, i.e.,

\[
\frac{\partial \rho_{\text{ext}}}{\partial t} = 0 .
\]

(d) Show that among all stationary density matrices the solution \( \rho_{\text{ext}} \) (if it exists) of the extremization problem corresponds to the maximum of the von Neumann entropy.

\[\text{Note: This simple problem is of fundamental importance in theoretical physics. However, since it lies beyond the scope of this course, it is optional and will not be graded.}\]
Problem III: Density matrix $\rho(\beta) = Z^{-1} e^{-\beta H}$ for the oscillator

(a) Evaluate the matrix elements $\langle q' \mid \rho(\beta) \mid q'' \rangle$ of the density matrix

$$\rho(\beta) \equiv Z^{-1} e^{-\beta H} , \quad H = \frac{p^2}{2m} + \frac{m \omega^2}{2} q^2$$

for a one-dimensional harmonic oscillator in the $q$-representation, where $p = \hbar \frac{\partial}{\partial q}$.

Hint: Recall that the eigenfunction $\langle q \mid n \rangle \equiv \psi_n(q)$ ($n = 0, 1, 2, \ldots$) with the eigenvalue $E_n = \frac{(n + \frac{1}{2}) \hbar \omega}{2}$ is given by

$$\psi_n(q) = \left( \frac{m \omega}{\pi \hbar} \right)^{\frac{1}{4}} \frac{H_n(\xi)}{\sqrt{2^n n!}} e^{-\xi^2} , \quad \xi = \sqrt{\frac{m \omega}{\hbar}} q .$$

The Hermite polynomials $H_n(\xi)$ are defined as

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2} = e^{\xi^2} \sqrt{\pi} \int_{-\infty}^{\infty} du (-2iu)^n e^{-u^2+2i\xi u} . \quad (5)$$

Use the last expression in the integral form.

(b) Using the result from (a) show that the random variable $q$ is normally distributed, i.e.,

the PDF $w(q) = \langle q \mid \rho(q) \rangle$ is given by

$$w(q) = \frac{1}{Z} \sum_{n=0}^{\infty} e^{-\beta E_n} |\psi_n(q)|^2 = \frac{1}{\sqrt{2\pi \sigma^2}} e^{-\frac{q^2}{2\sigma^2}} . \quad (6)$$

Show that the variance

$$\sigma^2 = \langle q^2 \rangle_\beta \equiv Z^{-1} \text{Tr}(e^{-\beta H} q^2) ,$$

is simply related to the mean energy, $E \equiv \text{Tr}(\rho(\beta) H)$:

$$\sigma^2 = \frac{E}{m \omega^2} . \quad (7)$$

Compare the PDF (6), (7) with the PDF for the ensemble of classical non-interacting harmonic pendulums from Problem V(c), HW2.

(c) Evaluate

$$\langle p^2 \rangle_\beta \equiv Z^{-1} \text{Tr}(e^{-\beta H} p^2)$$

from the density matrix in the $q$-representation and check that

$$\langle \frac{m \omega^2 q^2}{2} \rangle_\beta = \langle \frac{p^2}{2m} \rangle_\beta = \frac{E}{2} .$$

(d) Discuss the classical limit $\hbar \to 0$ for $\langle q' \mid e^{-\beta H} \mid q'' \rangle$ and the normalization factor $Z$. In particular show that in the classical limit $Z$ turns out to be the classical statistical integral

$$Z_{\hbar \to 0} \to \int_{-\infty}^{+\infty} \frac{dq dp}{h} e^{-\beta H(q,p)} .$$
Problem IV: Density matrix $\rho(\beta)$ in the $q$-representation

(a) Show that the $q$-representation of a density matrix $\rho(\beta) \equiv Z^{-1} e^{-\beta H}$ for a Hamiltonian $H(q, p)$ is given by

$$\langle q' | \rho(\beta) | q'' \rangle = Z^{-1} \exp \left[ -\beta H \left( q', \frac{\hbar}{i} \frac{\partial}{\partial q'} \right) \right] \delta(q' - q'').$$

(8)

Here $H \left( q', \frac{\hbar}{i} \frac{\partial}{\partial q'} \right)$ is the $q$-representation of the Hamiltonian and $\delta(q' - q'')$ is the Dirac delta function.

(b) Apply the result to a free particle $H(\vec{p}) = \vec{p}^2 / 2m$ and evaluate the density matrix in the $q$-representation. Show that, in this case, the normalization factor $Z$ exactly coincides with the classical statistical integral:

$$Z = \int \int \frac{d^3\vec{r}}{\hbar^3} \frac{d^3\vec{p}}{\hbar^3} e^{-\beta H(\vec{p})}.$$ 

Problem V: Quantum rotator in two dimensions

Consider a rotator in two dimensions with the Hamiltonian

$$H = \frac{p_\phi^2}{2I}, \quad \text{where} \quad 0 \leq \phi < 2\pi, \quad p_\phi = \frac{\hbar}{i} \frac{d}{d\phi}.$$ 

(a) Using the result of Problem IV, find the density matrix $\rho(\beta) \equiv Z^{-1} e^{-\beta H}$ in the $\phi$-representation. Express the result in terms of the Jacobi theta function (see [http://mathworld.wolfram.com/JacobiThetaFunctions.html](http://mathworld.wolfram.com/JacobiThetaFunctions.html))

$$\vartheta_3(z, q) = \sum_{m=-\infty}^{\infty} q^{m^2} e^{2\pi i m z} = \text{EllipticTheta}[3, z, q].$$

(9)

(b) Show that the normalization factor $Z = Z(\beta)$ satisfies the “duality” relation

$$Z(\beta) = \sqrt{\frac{2\pi I}{\beta \hbar^2}} Z \left( \frac{4\pi^2 I^2}{\hbar^4 \beta} \right).$$

Using this relation show that $Z$ becomes the classical statistical integral in the classical limit $\hbar \to 0$:

$$Z(\beta)|_{\hbar \to 0} \to \frac{1}{\hbar} \int_0^{2\pi} d\phi \int_{-\infty}^{+\infty} dp_\phi e^{-\beta p_\phi^2 / 2\hbar}.$$ 

Hint: Use the Poisson summation formula:
\[
\sum_{n=-\infty}^{\infty} f(n) = \sum_{n=-\infty}^{\infty} \hat{f}(2\pi n),
\]

(10)

where \( \hat{f}(k) \) is the Fourier transform of \( f \):

\[
\hat{f}(k) = \int_{-\infty}^{+\infty} dx \ f(x) \ e^{-ikx}.
\]