Problem 8.1: Density matrix

ID: ex_density_matrix_2:aqt2223

Learning objective

The purpose of this problem is to get familiar with the concept of the density matrix (operator) and calculate some important properties.

In general, the density matrix is given by

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|$$

(1)

where $p_i$ is the probability to be in the state $|\psi_i\rangle$.

a) Show that $\rho^\dagger = \rho$ and $\text{tr}(\rho) = 1$. 

b) Show that $\text{tr}(\rho^2) \leq 1$ and equality holds for a pure state. Show also that for a pure state $\rho^2 = \rho$.

c) Show that the expectation value of an operator $O$ is given by $\langle O \rangle = \text{tr}(\rho O)$.

d) Show that the equation of motion of the density matrix $\rho(t)$ of a system with Hamiltonian $H$ is given by the von Neumann equation

$$i\hbar \partial_t \rho(t) = [H, \rho(t)].$$

(2)

e) Consider a canonical ensemble at temperature $T$. Show that for a system with Hamiltonian $H$, the thermal density matrix is given by

$$\rho = \frac{1}{Z} \sum_n e^{-\beta E_n} |n\rangle \langle n| = \frac{1}{Z} e^{-\beta H},$$

(3)

where $\beta = \frac{1}{k_B T}$, $Z = \text{tr}(e^{-\beta H})$ is the partition function, and $H |n\rangle = E_n |n\rangle$.

Problem 8.2: Planck’s radiation law

ID: ex_plancks_radiation_law:aqt2223

Learning objective

In this problem, you derive Planck’s radiation law of a black body which was a pioneering result in modern physics and quantum theory in particular.

First, consider a single mode of the electromagnetic field (without polarization) with Hamiltonian

$$H = \hbar \omega_k a_k^\dagger a_k.$$
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a) Calculate the partition sum \( Z \) and write down the thermal state \( \rho \) at temperature \( T \).
b) Calculate the mean particle number \( \bar{n} = \langle n \rangle \) and the mean energy \( \bar{E} = \langle H \rangle \) for the thermal state \( \rho \).

In order to derive Planck’s radiation law, consider a three-dimensional box of volume \( V = L^3 \) with periodic boundary conditions. The Hamiltonian of the system is now given by

\[
H = \sum_{k,\lambda} \hbar \omega_k a_k^\dagger a_k, \tag{5}
\]

where \( \omega_k = c|k| \) and \( \lambda \) is the polarization of the mode \( k \).

c) Based on your results in subtask b), calculate the spectral energy density \( u_\omega(T)d\omega \) and the total energy density \( u(T) \).

Hints:
- The system now consists of independent harmonic oscillators.
- The spectral energy density \( u_\omega d\omega \) is given by the product of the energy and the density of states in the frequency interval \([\omega, \omega + d\omega]\).
- In order to calculate the density of states, first calculate the mode spacing and then take the limit \( L \rightarrow \infty \).
- \[
\int_0^\infty dx \frac{x^3}{e^x - 1} = \frac{\pi^4}{15}.
\]

Problem 8.3: Commutator of the electric field

[Written | 3 pt(s)]

ID: ex_commutator_electric_field:aqt2223

Learning objective

This problem deals with the quantized electric field. You calculate its commutator and show that it preserves causality.

In this problem, you calculate the commutator of the electric field, \([E_i(r, t), E_j(r', t')]\).

a) In a first step, calculate the commutator \([A_i(r, t), A_j(r', t')]\) of the vector potential.

Start by decomposing the vector potential \( A(r, t) \) into its normal modes

\[
A(r, t) = \sum_{k,\lambda} \left( \frac{2\pi \hbar c^2}{V \omega_k} \right)^{1/2} \left( a_{k,\lambda} \epsilon(k, \lambda) e^{i(k \cdot r - \omega_k t)} + \text{h.c.} \right), \tag{6}
\]

where \( r \) is the spatial coordinate, \( t \) the time, \( k \) the wave vector, \( V \) the quantization volume, \( h \) Planck’s constant, \( c \) the speed of light, and \( \omega_k = c|k| \). \( a_{k,\lambda} \) denotes the annihilation operator for wave number \( k \) and polarization \( \lambda \), \( \epsilon \) is the vector of polarization.

In addition, use the completeness relation of the polarization vectors,

\[
\sum_{\lambda} \epsilon_i(k, \lambda) \epsilon^*_j(k, \lambda) = \delta_{ij} - \frac{k_i k_j}{k^2}, \tag{7}
\]
in order to bring the commutator into the following form:

\[ [A_i(r, t), A_j(r', t')] = \partial_{ij} K(\xi, \tau), \]  

with \( \xi \equiv r - r' \) and \( \tau \equiv t - t' \), where \( K(\xi, \tau) \) has to be determined.

The differential operator \( \partial_{ij} \) is defined as

\[ \partial_{ij} \equiv \frac{\partial^2}{c^2} \delta_{ij} - \partial_{\xi_i} \partial_{\xi_j}. \]  

b) Next, write the commutator for the electric field \( E \) in the following form

\[ [E_i(r, t), E_j(r', t')] = -\frac{1}{c^2} \frac{\partial^2}{\partial \tau^2} [A_i(r, t), A_j(r', t')] . \]  

c) Finally, transform the commutator into a form which is proportional to \( \delta (\xi^2 - c^2 \tau^2) \).

\[ \text{Hint: It is not required to evaluate the derivatives } \partial_{ij}, \text{ it is sufficient to perform the integration over } k. \text{ This can be done by replacing the summation } \frac{1}{V} \sum_k \rightarrow \int \frac{d^3k}{(2\pi)^3} \text{ by an integral.} \]