Quantum statistics and interactions

Exercise session I - C. Winkelmann - UGA/Phelma

Density Matrix

Until now, we have usually assumed that the quantum states at play were initially perfectly well prepared, and therefore also following perfectly determined dynamics. This of course does not mean that the measurement outcome for a given observable $\hat{A}$ in that state is certain - unless it is an eigenstate of $\hat{A}$. The density matrix formalism allows connecting the quantum mechanical formalism to systems in which the information about the initial quantum state is incomplete, and only statistically known. This very important tool - theorised by J. von Neumann around 1930 - formally connects quantum mechanics to statistical physics.

Consider a quantum system described by state vectors living in a hermitian space $\mathcal{E}$, which for convenience we will take to be of finite dimension (although the results can be extended to infinite dimension). All *kets* defined hereafter are vectors of $\mathcal{E}$.

Log of an operator. Let $\hat{A}$ be an observable of $\mathcal{E}$, $\hat{I}$ is identity and $\hat{H}$ the hamiltonian operator. If f is a sufficiently smooth function of x, then $f(\hat{A})$ is also an operator acting on $\mathcal{E}$. If an operator $\hat{B}$ can be found such that $\hat{A} = e^{\hat{B}}$ then we will write $\hat{B} = \ln(\hat{A})$.

Trace. We define the trace of an operator acting in $\mathcal{E}$ defined as follows: let $\{|n\rangle\}_n$ be an orthonormal basis of $\mathcal{E}$ and $\hat{A}$ an operator. Then

$$\mathrm{Tr}(\hat{A}) = \sum_n \langle n|\hat{A}|n\rangle.$$

Properties of the trace:

- $\mathrm{Tr}(\hat{A})$ does not depend on the orthonormal basis chosen.
- $\mathrm{Tr}(\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{A})$.
- $\mathrm{Tr}(\hat{A}+\hat{B}) = \mathrm{Tr}(\hat{A}) + \mathrm{Tr}(\hat{B})$.

Entropy. We define the Shannon entropy as $S = -k_B \sum_i p_i \ln(p_i)$, where k_B is the Boltzmann constant and p_i is the occupation probability of microstate i, with $\sum_i p_i = 1$.

1 Pure states

Suppose a quantum system is prepared in a pure (normalized) state $|\psi\rangle \in \mathcal{E}$,

1.1

Discuss the physical meaning of $\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle$.

1.2

We define the density matrix (also called density operator) associated to this state as $\hat{\rho} = |\psi\rangle\langle\psi|$. Show that $\langle A\rangle = \mathrm{Tr}(\hat{\rho}\hat{A})$.

1.3

Show that $\mathrm{Tr}(\hat{\rho}) = 1$, $\hat{\rho}^2 = \hat{\rho}$, and $\hat{\rho}^\dagger = \hat{\rho}$.

1.4

Write the density matrix for a spin 1/2 in its $\frac{1}{\sqrt{2}}\left(|+\rangle - |-\rangle\right)$ state.

1.5

The most general expression of the pure quantum state of a spin 1/2 system (or any other two-level system) is

$$|\psi\rangle = \cos(\theta/2)\,|+\rangle + \sin(\theta/2)e^{i\phi}\,|-\rangle,$$

with θ and ϕ the usual polar and longitudinal angles. We define $\mathbf{a}$ as the unitary vector in the (θ, ϕ) direction. Show that the associated density matrix is

$$\hat{\rho} = \frac{\hat{I} + \mathbf{a}\cdot\boldsymbol{\sigma}}{2},$$

where $\boldsymbol{\sigma} = 2\mathbf{S}/\hbar$ is the 3D vector of Pauli matrices.

2 Mixed states

Suppose now that we don't know exactly in which state the system was initially prepared. All we know is that it has a statistical probability p_i to be in state $|\psi_i\rangle$, with $\sum_i p_i = 1$ et $0 \leq p_i \leq 1$. We take the $\{|\psi_i\rangle\}$ to form a base. These vectors are normalized but not necessarily orthogonal.

2.1

Justify that the average measurement outcome of $\hat{A}$, which we still write $\langle\hat{A}\rangle$, is given by $\langle\hat{A}\rangle = \sum_i p_i\langle\psi_i|\hat{A}|\psi_i\rangle$.

2.2

We now define the density matrix of the system as $\hat{\rho} = \sum_i p_i|\psi_i\rangle\langle\psi_i|$. Give a matrix representation of $\hat{\rho}$. Show that $\langle\hat{A}\rangle = \mathrm{Tr}(\hat{\rho}\hat{A})$ is still true.

2.3

Show that $\mathrm{Tr}(\hat{\rho}) = 1$, $\hat{\rho}^\dagger = \hat{\rho}$. Using an example, show that in general $\hat{\rho}^2 \neq \hat{\rho}$.

2.4

Starting from the Schrödinger equation, derive the *von Neumann* equation:

$$\frac{d\hat{\rho}}{dt} = \frac{1}{i\hbar}[\hat{H}, \hat{\rho}].$$

Compare this result to a known formula from earlier lectures.

2.5

The expression $\ln\hat{\rho}$ can be problematic because it is ill defined when one of the p_i goes to 0. Show that $\hat{\rho}\ln\hat{\rho}$ is nevertheless still well defined in this limit. Show that $S = -k_B\mathrm{Tr}(\hat{\rho}\ln\hat{\rho})$.

2.6

For a non-polarized spin 1/2, that is, having the same statistical probability to be in either state $|+\rangle$ or $|-\rangle$, show that $\hat{\rho} = \hat{I}/2$. What would be the corresponding $\mathbf{a}$ vector to use to recover the expression in question 1.5?

2.7

Consider a spin 1/2, which has a statistical probability $0 \leq \alpha \leq 1$ to be in the $|+\rangle$ state. Calculate its Shannon entropy as a function of α. Draw qualitatively $S(\alpha)$ et discuss its extremae.

2.8

The spin doublet degeneracy is lifted by applying a magnetic field along z. At $t = 0$, the spin is excited to the $|+\rangle$ state. Then it gradually relaxes its energy $\propto \exp(-t/T_1)$, ending in the ground state $|-\rangle$. Describe the path of the $\mathbf{a}$ vector.

2.9

Take a spin ensemble initially in the pure state from question 1.4. Assuming a Zeeman Hamiltonian, calculate the dynamics of $\hat{\rho}$. Let us now assume that the off-diagonal elements (coherences) have an additional decay $\propto \exp(-\gamma t)$, with $\hbar\gamma$ much smaller than the Zeeman energy. Find the expectation value of the x-component of the spin and plot it as a function of time.

3 Density matrix of a particle with angular momentum 1

(after a problem by F. Porter / Caltech)

The general rule for a matrix (operator) to be permissible as a density matrix is that it has to be (i) hermitian, (ii) of trace 1, and (iii) non-negative definite (in other words, for any state $|\Psi\rangle$, we have $\langle\Psi|\hat{\rho}|\Psi\rangle \geq 0$).

Suppose we have a system with total angular momentum 1. In the basis of the three eigenvectors of the z-component of angular momentum, J_z, with eigenvalues +1, 0,-1, respectively, we assume an ensemble described by the density matrix

$$\hat{\rho} = \frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

3.1

Check that $\hat{\rho}$ is permissible as a density matrix. Does it describe a pure or a mixed state?

3.2

Given the ensemble described by $\hat{\rho}$, what is the average value of J_z?

3.3

What is the spread (standard deviation) in measured values of J_z?

4 Thermodynamical equilibrium

4.1

We now consider a system of N *distinguishable* and non-interacting (paramagnetic) spin 1/2 particles. Such a system is well described by the canonical ensemble. At thermal equilibrium, the population of state i, with energy ϵ_i is given by $p_i = \frac{1}{Z}\exp(-\beta\epsilon_\mathrm{i})$, with $\beta = 1/k_B T$ et Z the partition function. Show that

$$\hat{\rho} = \frac{1}{Z}\exp(-\beta\hat{H}),$$

and thus

$$Z = \mathrm{Tr}\left(\exp(-\beta\hat{H})\right).$$

4.2

Applying a constant and uniform magnetic field along z (with amplitude B), we can write $\hat{H} = -\gamma\, B\,\hat{\sigma}_z$, with γ a positive constant and $\hat{\sigma}_z$ the Pauli matrix in the z direction. Show that the magnetisation can be written

$$M_z = \frac{\gamma N}{Z}\mathrm{Tr}\left(\exp(-\beta\hat{H})\,\hat{\sigma}_z\right),$$

where Z shall be written explicitly.

4.3

Make a Taylor expansion of Z in the high-temperature limit and calculate the magnetic susceptibility to lowest order in β.

5 Entanglement and decoherence

Let us consider two entangled qubits, one called Alice, the other Bob.

5.1

Write the most general pure quantum state of the two-qubit system. Write the associated density operator $\hat{\rho}_{AB}$ in matrix form.

5.2

We call $\hat{\rho}_A$ the *reduced* density operator, obtained after tracing $\hat{\rho}_{AB}$ over Bob's subspace of states. Write $\hat{\rho}_A$ in matrix form.

5.3

Show using a well-chosen example that the reduced density operator of an entangled pure state can be a mixed state.

5.4

A qubit interacts with its environment, reaching the entangled state $|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle|E_0\rangle + |1\rangle|E_1\rangle\right)$, with $\langle 0|1\rangle = \langle E_0|E_1\rangle = 0$. Explain qualitatively how the qubit's reduced density matrix evolves when the environment evolves towards thermal equilibrium.