Department für Physik
Arnold-Sommerfeld-Zentrum
für Theoretische Physik
Ludwig-Maximillians-Universität

SoSe 05

Set 5
5/18/05

T IV: Thermodynamik und Statistik
(Prof. E. Frey)

Problem set 5

Problem 5.1 *density matrix*

For many quantum problems it is sufficient to consider only two states, by analogy to a spin 1/2 referred to as 'spin up' and 'spin down'. The corresponding Hilbert space $\mathcal{E}$ is then two-dimensional and operators acting on $\mathcal{E}$ can be represented by 2×2 matrices. Show that any operator is represented by a linear combination of the identity matrix $\mathbb{I}$ and the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Construct the normed eigenstates $|\sigma k\rangle$, $k = 1, 2, 3$ of the Pauli matrices and demonstrate that the eigenvalues σ are given by ± 1. Construct the projectors $\Lambda_{k+} = |+k\rangle\langle +k|$ and consider density matrices $\rho = \sum_{k=1}^{3} q_k \Lambda_{k+}$ with $\sum_k q_k = 1$.

1. Express the projectors Λ_{k+} in terms of the identity and the Pauli matrices. Show that the density matrix can be written as
$$\rho = \frac{1}{2}\left(\mathbb{I} + \mathbf{P} \cdot \boldsymbol{\sigma}\right), \qquad \mathbf{P} = \langle \boldsymbol{\sigma} \rangle = \mathsf{Tr}\left(\boldsymbol{\sigma}\rho\right)$$

2. For the density matrix ρ a measurement of the observable σ_1 is performed. Calculate the probability W_{1+} that the system is found in eigenstate $|+1\rangle$ after the measurement. Interpret the result in terms of the probabilities q_k.

3. Determine the expectation and variance for measuring $\mathbf{n} \cdot \boldsymbol{\sigma}$, i.e. $\langle \mathbf{n} \cdot \boldsymbol{\sigma} \rangle$ and $\langle (\mathbf{n} \cdot \boldsymbol{\sigma})^2 \rangle - \langle \mathbf{n} \cdot \boldsymbol{\sigma} \rangle^2$ for arbitrary unit vectors $\mathbf{n}$.

4. Evaluate the probabilities $W_{\mathbf{n}\pm}$ to find eigenvalues ± 1 when measuring the observable $\mathbf{n} \cdot \boldsymbol{\sigma}$ for the density matrix ρ.

5. Determine the density matrix that maximizes the functional $S[\rho] = -\mathsf{Tr}(\rho \ln \rho)$ with the constraint that probability is preserved $\mathsf{Tr}\rho = 1$ and the average $\mathbf{P} = \langle \boldsymbol{\sigma} \rangle$ is known. In general $\mathbf{P}$ can have a norm smaller than unity. Use appropriate Lagrange multipliers to enforce the constraints.

Problem 5.2 *spin precession*

A single spin described by density matrix ρ is exposed to a constant magnetic field. The Hamiltonian for the problem is given by $\mathcal{H} = -(\gamma\hbar/2)\mathbf{B}\cdot\boldsymbol{\sigma}$, where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices. Use the von Neumann equations to show that the magnetization $\mathbf{P}(t) = (\gamma\hbar/2)\mathsf{Tr}\rho(t)\boldsymbol{\sigma}$ obeys the classical equation of motion

$$\dot{\mathbf{P}}(t) = -\mathbf{B}\times\mathbf{P}(t)$$

* Assume a collection of spins in an external magnetic field $\mathbf{B}_0$. Additionally there may be small random local fields, such that the Larmor frequency $\omega = \gamma B$ is statistically distributed. Assuming a Gaussian or Lorentzian distribution for ω characterized by mean $\omega_0 = \gamma B_0$ and variance $1/T^2$ derive the time dependence of the average magnetization $\overline{\mathbf{P}(t)}$ by averaging the solution of the classical equation of motion for a single spin and show that it quickly looses phase coherence.

Problem 5.3 *entangled states*

The density matrix of a subsystem is usually in a mixed state even if the entire system is in a pure state. Assuming that the wave function of the entire system is merely a product of wave functions for the subsystem and the reservoir, show that the density matrix of the subsystem corresponds to a pure state.

If the total system is described by a pure state and the density matrix of the subsystem describes a pure state, show that the wave function of the total system necessarily factorizes.

Can you construct a mixed state for the density matrix such that the subsystem is in a pure state?

Problem 5.4 *Pressure ensemble*

Use the NPT (constant pressure) ensemble with the phase space density

$$\rho_P = Z_P^{-1}\exp\left(-\beta\mathcal{H} - \beta PV\right), \qquad Z_P(T,P,N) = \int_0^\infty dV \int \frac{d^{3N}r\,d^{3N}p}{N!h^{3N}}\exp\left(-\beta\mathcal{H} - \beta PV\right)$$

and the definition of averages to show that

$$Z_P(T,P,N) = Z_P(T,P_0,N)\langle e^{\beta(P_0-P)V}\rangle_0\,.$$

Here $\langle\cdot\rangle_0$ denotes averaging with respect to ρ_P at pressure P_0. Derive the corresponding expansion of the free enthalpy $G(T,P,N) = -k_BT\ln Z_P(T,P,N)$ in terms of the cumulants of the volume.

In the thermodynamic limit, i.e. $N\to\infty$, P and T fixed, derive the thermodynamic relations

$$G(T,P,N) = F(T,\langle V\rangle,N) + P\langle V\rangle\,, \qquad dG = -SdT + \langle V\rangle dP + \mu dN$$