
Seventh Problem Set for Physics 847 (Statistical Physics II)

Winter quarter 2004

Important date: Mar 16 9:30am-11:18am final exam

Due date: Tuesday, Feb 24

18. Spin 1 atom

12 points

An atom with spin 1 has a Hamiltonian $\hat{H} = A\hat{S}_z^2 + B(\hat{S}_x^2 - \hat{S}_y^2)$, where \hat{S}_x , \hat{S}_y , and \hat{S}_z are the x , y , and z component of the spin angular momentum operator. In the basis of eigenstates of the operator \hat{S}_z these three operators have the matrix representations

$$\hat{S}_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \hat{S}_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \text{and} \quad \hat{S}_y = \frac{\hbar}{i\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}.$$

At time $t = 0$ the atom is initially in an eigenstate of \hat{S}_z with eigenvalue $+\hbar$.

- Write the density matrix (in the basis of eigenstates of \hat{S}_z) at $t = 0$.
- Compute the density matrix at time t in the basis of eigenstates of \hat{S}_z .
- Compute the average z component of the spin at time t .

19. Extremality of density operators I

12 points

We want to look in more detail in which sense the density operators of the canonical and grand canonical ensemble maximize the entropy. To this end we want to prove the identity

$$\text{Tr} \hat{\rho}_1 (\ln \hat{\rho}_2 - \ln \hat{\rho}_1) \leq 0 \tag{1}$$

for *any* pair of density operators ρ_1 and ρ_2 . In the next problem we apply this identity to the canonical and the grand canonical density operators.

- Use the Cauchy-Schwarz inequality applied to the scalar product $\langle \hat{A}, \hat{B} \rangle \equiv \text{Tr} \hat{A} \hat{B}^\dagger$ in order to prove $\text{Tr} \hat{\rho}_1^{1/2} \hat{\rho}_2^{1/2} \leq 1$. A fractional power of an operator is defined by $\hat{A}^x \equiv \exp(x \ln \hat{A})$ where \exp and \ln are defined by their power series.
- Use induction on n in order to prove

$$\text{Tr}(\hat{\rho}_1^{1-2^{-n}} \hat{\rho}_2^{2^{-n}}) \leq 1$$

for any integer $n \geq 1$. (Hint: Rewrite $\hat{\rho}_1^{1-2^{-n}} \hat{\rho}_2^{2^{-n}} = \hat{\rho}_1^{1/2} (\hat{\rho}_1^{1/2-2^{-n}} \hat{\rho}_2^{2^{-n}})$ and use the Cauchy-Schwarz inequality again.)

- c) Take the limit $n \rightarrow \infty$ in order to prove the identity (1).

20. Extremality of density operators II

8 points

Now, we want to use Eq. (1) in order to see in which sense the density operators of the canonical and grand canonical ensemble maximize the entropy.

- a) Let $\hat{\rho}_2$ be the density operator of the canonical ensemble and $\hat{\rho}_1$ be an arbitrary density operator. Define $E \equiv \text{Tr}\hat{\rho}_2\hat{H}$, $E' \equiv \text{Tr}\hat{\rho}_1\hat{H}$, $S \equiv -k_B\text{Tr}\hat{\rho}_2\ln\hat{\rho}_2$, and $S' \equiv -k_B\text{Tr}\hat{\rho}_1\ln\hat{\rho}_1$. Show that

$$S \geq S' + \frac{1}{T}(E - E').$$

- b) Let $\hat{\rho}_2$ be the density operator of the grand canonical ensemble and $\hat{\rho}_1$ be an arbitrary density operator. Define $E \equiv \text{Tr}\hat{\rho}_2\hat{H}$, $E' \equiv \text{Tr}\hat{\rho}_1\hat{H}$, $N \equiv \text{Tr}\hat{\rho}_2\hat{N}$, $N' \equiv \text{Tr}\hat{\rho}_1\hat{N}$, $S \equiv -k_B\text{Tr}\hat{\rho}_2\ln\hat{\rho}_2$, and $S' \equiv -k_B\text{Tr}\hat{\rho}_1\ln\hat{\rho}_1$. Show that

$$S \geq S' + \frac{1}{T}[E - E' - \mu'(N - N')].$$