33-765 — Statistical Physics

Department of Physics, Carnegie Mellon University, Spring Term 2020, Deserno

Problem sheet #10

35. Equivalent characterizations of pure quantum states *(3 points)*

If we have a normalized state vector $|\psi\rangle \in \mathscr{H}$, then the quantum state $W = |\psi\rangle\langle\psi|$ is pure: it obviously satisfies $W = W^2$. Prove that *the converse is also true*: If a quantum state satisfies $W = W^2$, then there exists a vector $|\psi\rangle$ such that $W = |\psi\rangle\langle\psi|$.
Hint: Start with the spectral expansion of W. What extra condition does $W = W^2$ impose on the expansion coefficients?

36. Equivalent characterizations of eigenstates *(4 points)*

If a quantum state W is an eigenstate of an observable A, then measurements of A in that state are sharp: $\sigma_A^2 = \langle A^2\rangle - \langle A\rangle^2 = 0$. But the converse also holds: $\sigma_A^2 = 0 \Rightarrow AW = \alpha W$ for some $\alpha \in \mathbb{R}$. Prove this in the special case where W is a pure state!
Hint: The probably quickest way to see this involves applying the Cauchy-Schwarz inequality to the vectors $|\psi\rangle$ and $A|\psi\rangle$.

37. Quantum fluctuations can only increase the free energy *(4 points)*

Consider the quantum mechanical one-particle Hamiltonian $H(P,Q) = \frac{1}{2m}P^2 + V(Q)$ and its classical analogue. In this problem we want to prove the following inequality between the quantum and the classical free energy for this system:

$$F_{\text{classical}} \;\leq\; F_{\text{quantum}} \,. \tag{1}$$

You will need to use (*but not prove!*) the so-called *Golden-Thompson inequality*, which states that for two selfadjoint operators A and B, which don't necessarily commute, we have $\text{Tr}[\text{e}^{A+B}] \leq \text{Tr}[\text{e}^{A}\text{e}^{B}]$ (provided these traces also exist).
Hint: Express the trace in position space: $\text{Tr}(\,\cdot\,) = \int dq\, \langle q| \cdot |q\rangle$. It will also be useful to recall that $\langle q|p\rangle = \frac{1}{\sqrt{h}}\text{e}^{ipq/\hbar}$.

38. A system of spin-1 particles on a lattice *(4 points)*

Consider a macroscopic crystal with a spin-1 quantum mechanical moment located on each of N atoms. Assume further that we can represent the energy eigenvalues of the system with a Hamiltonian of the following form:

$$H \;=\; B\sum_{n=1}^{N}\sigma_n + D\sum_{n=1}^{N}\sigma_n^2 \,, \tag{2}$$

where the σ_n can independently take on the values -1, 0, and $+1$, and B and D are constants representing an external magnetic field and an internal "crystal field", respectively. The entire system is in contact with a heat bath at temperature T.

1. Calculate the canonical partition function and the free energy of this system.
2. Calculate the magnetization per spin, $m = \frac{1}{N}\big\langle \sum_{n=1}^{N}\sigma_n\big\rangle$, and plot $m(B)$ for selected values of βD.

39. Polylogarithms *(5 points)*

The quantum grand potential of ideal Bose and Fermi gases can be expressed analytically via special functions called "polylogarithms." Before we do that in class, let's first learn a bit more about them. The polylogarithm is defined as follows:

$$\text{L}_\nu(z) = \frac{1}{\Gamma(\nu)}\int_0^\infty \text{d}t\;\frac{t^{\nu-1}}{z^{-1}\text{e}^{t}-1} \qquad z<1\,,\quad \nu>0\,. \tag{3}$$

Prove that the polylogarithm has the following properties:

1. For $\nu > 1$, we can rewrite it as $\text{L}_\nu(z) = -\dfrac{1}{\Gamma(\nu-1)}\displaystyle\int_0^\infty \text{d}t\; t^{\nu-2}\,\log\Big(1 - z\,\text{e}^{-t}\Big)$.
2. $z\,\dfrac{\text{d}}{\text{d}z}\,\text{L}_{\nu+1}(z) = \text{L}_\nu(z)$.
3. For $|z| \leq 1$ we also have $\text{L}_\nu(z) = \displaystyle\sum_{n=1}^{\infty}\frac{z^n}{n^\nu}$. *(Hint: Rewrite parts of the definition (3) using a geometric series.)*
4. $\dfrac{\text{d}}{\text{d}z}\,\text{L}_\nu(z) > 0$ and $\dfrac{\text{d}}{\text{d}\nu}\,\text{L}_\nu(z) < 0$. (The latter is true for all z, but it suffices if you prove it for positive z!)
5. $\text{L}_\nu(0) = 0$; $\quad \text{L}_\nu(1) = \zeta(\nu)$ (= Riemann zeta function); $\quad \text{L}_0(x) = \dfrac{x}{1-x}$; $\quad \text{L}_1(x) = -\log(1-x)$.