33-765 Homework 10

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35. Equivalent Characterizations of Pure Quantum States

If we have a normalized state vector $|\psi\rangle \in \mathcal{H}$, then the quantum state $W = |\psi\rangle\langle\psi|$ is pure, and it is obvious that $W = W^2$. Prove that the converse is also true: If a quantum state satisfies $W = W^2$, then there exists a vector $|\psi\rangle$ such that $W = |\psi\rangle\langle\psi|$.

If W is a quantum state, we can surely expand it in eigenstates:

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

Since $W = W^2$,

$$W^2 = \sum_{ij} p_i p_j |\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j| = \sum_{ij} p_i p_j |\psi_i\rangle\langle\psi_j|\delta_{ij} = \sum_i p_i^2 |\psi_i\rangle\langle\psi_i|$$

so

$$p_i = p_i^2$$

or $p_i = 1 \quad \text{or} \quad 0$. We require $\sum_i p_i = 1$ for normalization, so at most one of the p_i can be 1 while the others must be zero, so the state can be represented by a single eigenvector.

36. Equivalent Characterizations of Eigenstates

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: $\sigma_A^2 = 0 \implies AW = \alpha W$ for some $\alpha \in \mathbb{R}$. Prove this in the special case where W is a pure state!

The Cauchy-Schwarz inequality states that

$$|\langle u|v\rangle|^2 \leq \langle u|u\rangle\langle v|v\rangle$$

The equality condition means that the vectors are linearly dependent, or $u = \lambda v$. For our vectors, we have

$$|\langle\psi| A |\psi\rangle|^2 \leq \langle\psi|\psi\rangle\langle\psi| A^\dagger A |\psi\rangle$$
$$\langle A\rangle^2 \leq \langle A^2\rangle$$

From our assumption that $\sigma_A^2 = 0$, we know that this must be an equality, but that also implies that the vectors are linearly dependent:

$$A|\psi\rangle = \lambda|\psi\rangle$$

or equivalently

$$A|\psi\rangle\langle\psi| = \lambda|\psi\rangle\langle\psi|$$

37. Quantum Fluctuations Can Only Increase the Free Energy

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

$$F_{\text{classical}} \leq F_{\text{quantum}}.$$

You will need to use the Golden-Thompson inequality, which states that for two self-adjoint operators A and B which might not commute, $\operatorname{Tr} e^{A+B} \leq \operatorname{Tr}\left(e^{Ae^B}\right)$.

$$\begin{aligned}
Z_{\text{QM}} = \operatorname{Tr}\left[e^{-\beta\left(\frac{P^2}{2m}+V(Q)\right)}\right] &\leq \operatorname{Tr}\left[e^{-\beta\frac{P^2}{2m}}e^{-\beta V(Q)}\right] \\
&\leq \int \mathrm{d}q\, \langle q| e^{-\beta\frac{P^2}{2m}}e^{-\beta V(Q)}|q\rangle \\
&\leq \int \mathrm{d}q \int \mathrm{d}p\, \langle q| e^{-\beta\frac{P^2}{2m}}|p\rangle\langle p| e^{-\beta V(Q)}\langle q| \\
&\leq \int \mathrm{d}q \int \mathrm{d}p\, e^{-\beta\frac{p^2}{2m}}e^{-\beta V(q)}\frac{1}{\sqrt{h}}e^{\imath pq/\hbar}e^{-\imath pq/\hbar} \\
&\leq \frac{1}{h}\int \mathrm{d}q \int \mathrm{d}p\, e^{-\beta\frac{p^2}{2m}}e^{-\beta V(q)} \\
Z_{\text{QM}} &\leq Z_{\text{CM}}
\end{aligned}$$

Therefore, $\ln(Z_{\text{QM}}) \leq \ln(Z_{\text{CM}})$ so $-F_{\text{QM}} \leq -F_{\text{CM}}$ or $F_{\text{QM}} \geq F_{\text{CM}}$.

38. A System of Spin-1 Particles on a Lattice

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:

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

where the σ_n can independently take values in $\{-1, 0, +1\}$ 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.

We can factorize over each particle, so $Z = Ne^{-\beta H}$. I'll then divide this up into exponentials where σ_n is equal to each of its respective values:

$$\begin{aligned}
Z &= Ne^{-\beta\left(B\sum_n \sigma_n + D\sum_n \sigma_n^2\right)} \\
&= N\prod_{n=1}^{N} e^{-\beta(B\sigma_n + D\sigma_n^2)} \\
&= \left(e^{-\beta\underbrace{(-B+D)}_{\sigma_n=-1}} + e^{-\beta\underbrace{(0)}_{\sigma_n=0}} + e^{-\beta\underbrace{(B+D)}_{\sigma_n=1}}\right)^N \\
&= \left(\left(e^{\beta B} + e^{\beta B}\right)e^{-\beta D} + 1\right)^N \\
Z &= \left(2\cosh(\beta B)e^{-\beta D} + 1\right)^N
\end{aligned}$$

so

$$F = -k_B T \ln\Bigl(\left[2\cosh(\beta B)e^{-\beta D} + 1\right]^N\Bigr)$$

2. Calculate the magnetization per spin, $m = \frac{1}{N}\left\langle \sum_{n=1}^{N}\sigma_n\right\rangle$, and plot $m(B)$ for selected values of βD.

I don't understand what I'm supposed to do here.

39. Polylogarithms

The quantum grand potential of ideal Bose and Fermi gases can be expressed analytically via special functions called polylogarithms. The polylogarithm is defined as follows:

$$L_\nu(z) = \frac{1}{\Gamma(\nu)}\int_0^\infty \mathrm{d}t\,\frac{t^{\nu-1}}{z^{-1}e^t - 1} \qquad z < 1, \quad \nu > 0.$$

Prove that the polylogarithm has the following properties:

1. For $\nu > 1$, we can rewrite it as $L_\nu(z) = -\frac{1}{\Gamma(\nu-1)}\int_0^\infty \mathrm{d}t\, t^{\nu-2}\ln(1 - ze^{-t})$.

$$L_\nu(z) = \frac{1}{\Gamma(\nu)}\int_0^\infty \underbrace{t^{\nu-1}}_{u}\underbrace{(z^{-1}e^t - 1)\,\mathrm{d}t}_{\mathrm{d}v}$$

$$v = \ln\bigl(1 - ze^{-t}\bigr)$$

$$\mathrm{d}u = (\nu - 1)t^{\nu-2}\,\mathrm{d}t$$

so

$$\begin{aligned}
L_\nu(z) &= \frac{1}{\Gamma(\nu)}\left[\cancel{t^{\nu-1}\ln\bigl(1 - ze^{-t}\bigr)\Big|_0^\infty}^{\,0} - \int(\nu-1)t^{\nu-2}\ln\bigl(1 - ze^{-t}\bigr)\,\mathrm{d}t\right] \\
&= -\underbrace{\frac{(\nu-1)}{\Gamma(\nu)}}_{\frac{1}{\Gamma(\nu-1)}}\int_0^\infty \mathrm{d}t\, t^{\nu-2}\ln\bigl(1 - ze^{-t}\bigr)
\end{aligned}$$

2. $z\frac{\mathrm{d}}{\mathrm{d}z}L_{\nu+1}(z) = L_\nu(z)$.

$$
\begin{aligned}
z\,\mathrm{d}z\,L_{\nu+1}(z) &= -\frac{z}{\Gamma(\nu)}\int_0^\infty \mathrm{d}t\,\frac{\mathrm{d}}{\mathrm{d}z}t^{\nu-1}\ln\bigl(1-ze^{-t}\bigr)\\
&= -\frac{z}{\Gamma(\nu)}\int_0^\infty \mathrm{d}t\,t^{\nu-1}\frac{1}{1-ze^{-t}}e^{-t}\\
&= \frac{z}{\Gamma(\nu)}\int_0^\infty \mathrm{d}t\,t^{\nu-1}\frac{1}{e^t-z}\\
&= \frac{1}{\Gamma(\nu)}\int_0^\infty \mathrm{d}t\,t^{\nu-1}\frac{1}{z^{-1}e^t-1}
\end{aligned}
$$

3. For $|z| \leq 1$ we also have $L_\nu(z) = \sum_{n=1}^\infty \frac{z^n}{n^\nu}$.

$$
\begin{aligned}
L_\nu(z) &= \frac{1}{\Gamma(\nu)}\int_0^\infty \mathrm{d}t\,t^{\nu-1}\left(\frac{1}{\frac{e^t}{z}\left(1-\frac{z}{e^t}\right)}\right)\\
&= \frac{1}{\Gamma(\nu)}\int_0^\infty \mathrm{d}t\,t^{\nu-1}\frac{z}{e^t}\left(\frac{1}{1-\frac{z}{e^t}}\right)\\
&= \frac{1}{\Gamma(\nu)}\int_0^\infty \mathrm{d}t\,t^{\nu-1}\sum_{n=1}^\infty\left(\frac{z}{e^t}\right)^n\\
&= \frac{1}{\Gamma(\nu)}\sum_{n=1}^\infty z^n\int_0^\infty e^{-nt}t^{\nu-1}\,\mathrm{d}t\\
&= \frac{1}{\Gamma(\nu)}\sum_{n=1}^\infty z^n\frac{\Gamma(\nu)}{n^\nu}\\
&= \sum_{n=1}^\infty \frac{z^n}{n^\nu}
\end{aligned}
$$

4. $\frac{\mathrm{d}}{\mathrm{d}z}L_\nu(z) > 0$ and $\frac{\mathrm{d}}{\mathrm{d}\nu}L_\nu(z) < 0$.

$$
\frac{\mathrm{d}}{\mathrm{d}z}L_\nu(z) = \frac{\mathrm{d}}{\mathrm{d}z}\sum_n \frac{z^n}{n^\nu} = \sum_n \frac{z^{n-1}}{n^{\nu-1}}
$$

Both the numerator and denominator are positive as long as $z > 0$.

$$
\frac{\mathrm{d}}{\mathrm{d}\nu}L_\nu(z) = \sum_n\left(-\frac{z^n}{n^\nu}\ln(n)\right)
$$

Again, every term is positive (aside from the explicit negative sign), which makes the entire thing negative.

5. $L_\nu(0) = 0$, $L_\nu(1) = \zeta(\nu)$, $L_0(x) = \frac{x}{1-x}$, and $L_1(x) = -\ln(1-x)$.

$$
L_\nu(0) = \sum_n \frac{0^n}{n^\nu} = \sum_n 0 = 0
$$

$$
L_\nu(1) = \sum_n \frac{1}{n^\nu} = \zeta(\nu)
$$

This is just how the Riemann zeta function is defined.

$$
L_0(x) = \sum_n \frac{x^n}{n^0} = \sum_n x^n = \frac{x}{1-x}
$$

This is by the properties of a geometric series.

$$L_1(x) = \sum_n \frac{x^n}{n}$$

The Taylor series for $\ln(z)$ is

$$\ln(z) = \sum_n \frac{(-1)^{n-1}}{n} z^n$$

so

$$-\ln(1-x) = -\sum_n \frac{(-1)^{n-1}}{n}(1-x)^n = -\sum_n \frac{(-1)^{n-1}}{n}\left(\sum_{k=0}^{n}\binom{n}{k}1^{n-k}(-x)^k\right) = \sum_n \frac{x^n}{n}$$

since the binomial coefficient with $(-1)^k$ will cancel out $(-1)^{n-1}$ in the outside summation.