M12T.3 FERROMAGNET

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1. Problem

Consider a classical one-dimensional magnet with Hamiltonian:

$$H = -J \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1},$$

where each $\vec{S}_i$ is a classical (3-component) vector spin of fixed length S.

1.1. **(a.)** Calculate $\langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle$ at equilibrium at temperature T.

We first desire the partition function $\mathcal{Z}$. Recognize that $\vec{S}_i \cdot \vec{S}_{i+1} = S^2 \cos(\theta_i)$, where θ_i is the angle betwixt the vectors. The partition function must account for every state of the chain, for which it is easiest to integrate over every possible θ. However, we must recognize that in 3D there is another degree of freedom betwixt the vectors, the angle ϕ. Regardless of the ϕ orientation, the dot product is unnaffected for a given θ, and thus we expect the ϕ dependence to appear as a degeneracy factor.

Now, integrating the Boltzmann factor for our Hamiltonian over every possible θ, we get:

$$\mathcal{Z} = \int e^{\beta H} \, d\Omega = \int e^{\beta J S^2 \sum_{i=1}^{N} \cos(\theta_i)} \, d\Omega$$

$$= \prod_{i=1}^{N} \int_0^{2\pi} \int_0^{\pi} \sin(\theta_i) e^{\beta J S^2 \cos(\theta_i)} \, d\theta \, d\phi$$

Where $\beta \equiv \frac{1}{k_B T}$. By letting the substitution $u = \cos(\theta_i)$, the integral is quickly solved to yield:

$$\mathcal{Z} = \prod_{i=1}^{N} \frac{2\pi}{S^2 \beta J} (e^{\beta J S^2} - e^{-\beta J S^2})$$

And since the dependence on i vanished, from the product we simply get the result:

$$\mathcal{Z} = \left(\frac{4\pi}{S^2 \beta J} \sinh(\beta J S^2) \right)^N$$

Now, we find $\langle H \rangle$ from $\mathcal{Z}$ trivially:

$$\langle H \rangle = -\frac{\partial}{\partial \beta} ln(\mathcal{Z}) = -N \frac{\partial}{\partial \beta} \big(ln(\sinh(\beta J S^2)) - ln(\beta) + const \big)$$

$$= -NJS^2 \coth(\beta J S^2) + \frac{N}{\beta}$$

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But from our Hamiltonian, we can also see the relation:

$$\langle H \rangle = -J \left\langle \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1} \right\rangle = -JN \left\langle \vec{S}_i \cdot \vec{S}_{i+1} \right\rangle ,$$

which together implies:

$$\langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle = \coth\left(\frac{JS^2}{k_B T}\right) S^2 - \frac{k_B T}{J}$$

1.2. **(b.)** Calculate the specific heat per spin $c(T)$ of the system in the limit $N \to \infty$.

$$c(T) \equiv \frac{1}{N}\frac{\partial \langle H \rangle}{\partial T} = \frac{1}{N}\frac{\partial \beta}{\partial T}\frac{\partial \langle H \rangle}{\partial \beta}$$

$$= -\frac{1}{Nk_B T^2}\left((-NJS^2(1 - \coth^2(\beta J S^2)) JS^2 - \frac{N}{\beta^2}\right)$$

$$c(T) = \frac{J^2 S^4}{k_B T^2}\left(1 - \coth^2\left(\frac{JS^2}{k_B T}\right)\right) + k_B$$

1.3. **(c.)** Consider the $T \to 0$ limit of part b). Is this consistent with the behavior of $c(T)$ for a **quantum** ferromagnet ($J > 0$) of spin S with this same Hamiltonian? If not, estimate (roughly) and state the correct quantum behavior of $c(T)$ for small T, explaining your reasoning.

Off hand, we can recall that in a classical system there is no "freezing out" of degrees of freedom, so there will remain finite $c(T)$ for even the $T \to 0$ limit. However, in the quantum system we expect the specific heat to go to zero for low enough T because the quantized energy levels will make certain degrees of freedom unavailable. But this is very hand-wavy, let us try to back it up with the math.

First, we notice that $\coth(x) \equiv \left(\frac{e^x + e^{-x}}{e^x - e^{-x}}\right)$. In our classical $c(T)$ from part b), our coth argument goes as $1/T$, so as we take the limit $T \to 0$, $x \to \infty$. We see then that the coth term goes to unity in our low T limit, which actually eliminates the entire first term[1]. Thus, $\lim_{T\to 0} c(T) = k_B$ in the classical case.

Our only change in the quantum model is that $\vec{S}_i \cdot \vec{S}_{i+1} = \pm S^2$ instead of relying on relative angle θ. Thus, our partition function is not an integral, but a simple sum of two terms:

$$\mathcal{Z} = \prod_{i=1}^{N} \left(e^{\beta J S^2} + e^{-\beta J S^2}\right) = (2\cosh(\beta J S^2))^N.$$

This yields a new value of $\langle H \rangle$:

$$\langle H \rangle = -NJS^2 \tanh(\beta J S^2),$$

giving the new $c_Q(T)$:

$$c_Q(T) = \frac{JS^2}{k_B T^2}\left(1 - \tanh^2\left(\frac{JS^2}{k_B T}\right)\right).$$

[1] Actually, there is that $1/T^2$ in the first term of $c(T)$ that causes a problem, but in the limit we obtain $0/0$, and we apply L'Hospital's rule (twice in fact) to find out that the coth term goes to one faster than $T \to 0$, in which case the entire term vanishes. The two application of L'Hospital's rule are omitted here for clarity.

Now, tanh is the inverse of coth, so it also goes to unity in the $T \to 0$ limit, so again the first term vanishes[2], but this time there is no second, constant term. We conclude $\lim_{T\to 0} c_Q(T) = 0$. Thus, the classical model is not consistent with the low-T behavior of the quantum model.

[2]Except again we have the T^2 term in the denominator, but L'Hospital again saves us in the exact same way. See footnote 1.