Specific heat of classical-spin chains

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Sepcific heat of the chain of harmonic oscillators

Assume the Hamiltonian of the chain of N coupled harmonic oscillators to be

$$\mathcal{H} = \sum_{k=1}^{N} \frac{m}{2}\dot{u}_k^2 + \frac{1}{2}\sum_{k=1}^{N} K_e (u_{k+1} - u_k)^2$$

The specific heat is obtained from the thermal average of the energy $E = \langle \mathcal{H} \rangle$ through the relation

$$C_N = \frac{\partial E}{\partial T} \qquad (1)$$

Q1 Using the equipartition theorem **compute the specific heat** of the whole chain C_N.

We have seen in the lecture that, after having performed a Fourier transformation

$$u_k = \frac{1}{\sqrt{N}} \sum_q \tilde{u}_q e^{iqk} ,$$

the Hamiltonian takes the following form in the reciprocal space:

$$\mathcal{H} = \sum_q \left[K_e\,(1 - \cos q)\,|\tilde{u}_q|^2 + \frac{1}{2} m\,|\dot{\tilde{u}}_q|^2 \right] .$$

Applying the equipartition theorem to each independent d.o.f. yields

$$\begin{cases} K_e\,(1 - \cos q)\,\langle |\tilde{u}_q|^2 \rangle = \frac{1}{2} k_B T \\ \frac{1}{2} m \langle |\dot{\tilde{u}}_q|^2 \rangle = \frac{1}{2} k_B T \end{cases}$$

so that the thermal average of the energy reads

$$\langle \mathcal{H} \rangle = N \left(\frac{1}{2} k_{\mathrm{B}} T + \frac{1}{2} k_{\mathrm{B}} T \right) = N k_{\mathrm{B}} T$$

from which the famous Dulong–Petit law follows: $C_N = N k_{\mathrm{B}}$.

Sepcific heat of the 1D Ising model

In the absence of external filed ($B = 0$), the Hamiltonian of the 1D Ising model reads

$$\mathcal{H} = -J \sum_i S_i^z S_{i+1}^z .$$

The computation of the partition function $\mathcal{Z}$ encompasses a sum over 2^N values of the spin variables $S_i^z = \pm 1$

$$\mathcal{Z} = \mathcal{T}r \left\{ \mathrm{e}^{-\beta \mathcal{H}} \right\} = \sum_{S_i^z = \pm 1} \mathrm{e}^{-\beta \mathcal{H}\left(\{S_i^z\}\right)} .$$

This calculation is facilitated defining the *transfer matrix*

$$T_{i,i+1} = \mathrm{e}^{\kappa S_i^z S_{i+1}^z} = \begin{pmatrix} \mathrm{e}^{\kappa} & \mathrm{e}^{-\kappa} \\ \mathrm{e}^{-\kappa} & \mathrm{e}^{\kappa} \end{pmatrix} ,$$

with $\kappa = \beta J$, which allows rewriting

$$\mathcal{Z} = \sum_{S_i^z = \pm 1} T_{1,2} T_{2,3} \ldots T_{N-1,N} T_{N,1} = \mathcal{T}r \left\{ T^N \right\}$$

where periodic boundary conditions have been assumed. Since the trace of a matrix is independent of the basis on which the matrix is expressed, it is convenient to express T on its eigenstates so that $\mathcal{Z}$ becomes

$$\mathcal{Z} = \lambda_+^N + \lambda_-^N ,$$

with $\lambda_\pm$ being the two eigenvalues of T. In the thermodynamic limit $N \to \infty$ only the contribution of the largest eigenvalue survives

$$\mathcal{Z} = \lambda_+^N .$$

1. Using the fact that the thermal average of the energy is

$$E = \langle \mathcal{H} \rangle = \frac{1}{\mathcal{Z}} \mathcal{T}r \left\{ \mathcal{H} e^{-\beta \mathcal{H}} \right\} = -\frac{1}{\mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial \beta}$$

compute the eigenvalues of the transfer matrix and use the largest one λ_+ **to compute** $E = \langle \mathcal{H} \rangle$.

The eigenvalues of the transfer matrix T *are the solution of the characteristic polynomial*

$$\left(\lambda - \mathrm{e}^{\kappa}\right)^2 - \mathrm{e}^{-2\kappa} = 0$$

namely

$$\lambda_\pm = \mathrm{e}^{\kappa} \pm \mathrm{e}^{-\kappa}.$$

Hence we find the expression of the partition function

$$\mathcal{Z} = \lambda_+^N + \lambda_-^N \overset{N \to \infty}{=} \lambda_+^N = \left[2 \cosh\left(\beta J\right)\right]^N .$$

From above we know that

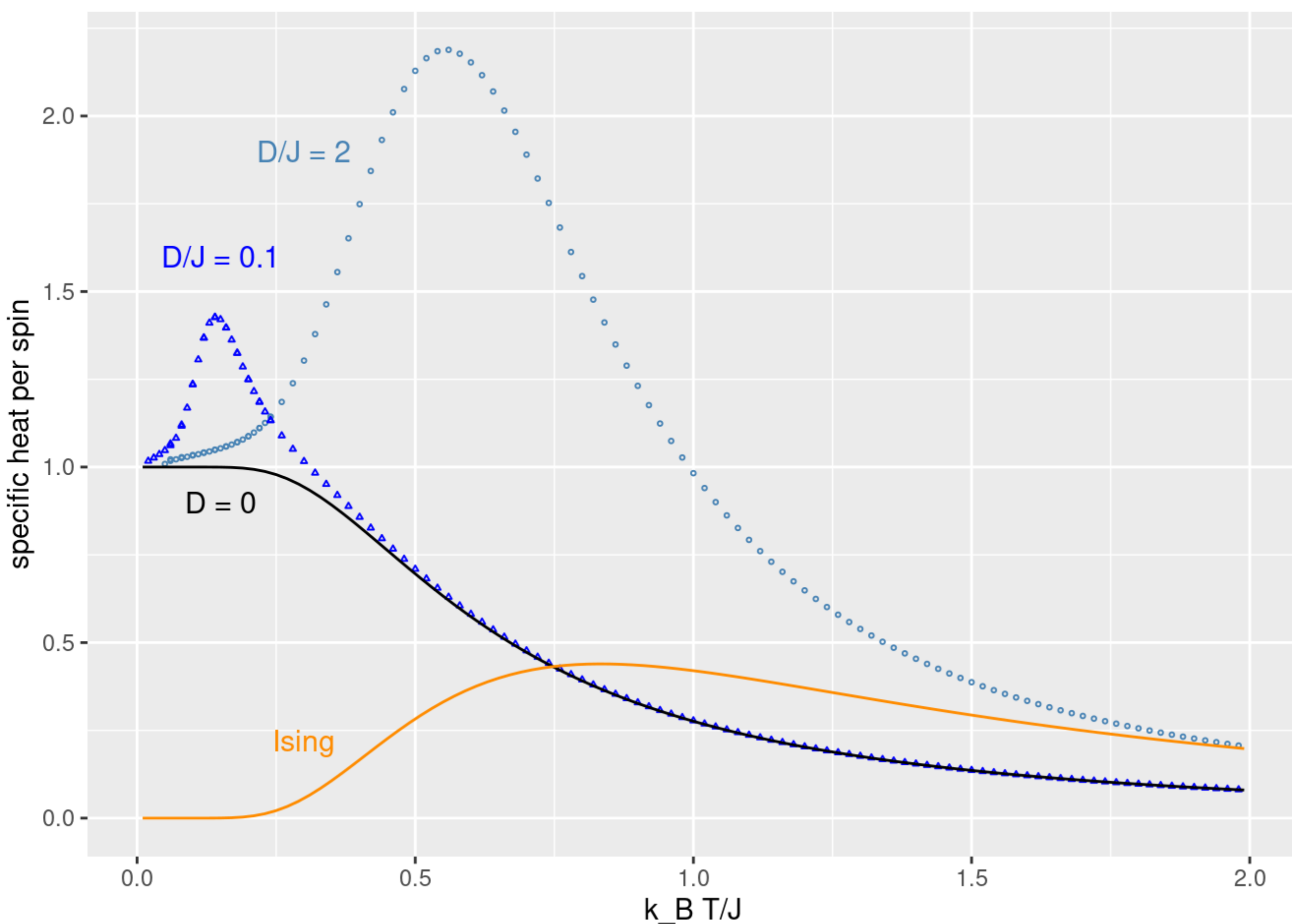
$$E = \langle \mathcal{H} \rangle = -\frac{1}{\mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial \beta} = -\frac{1}{\lambda_+^N} \frac{\partial}{\partial \beta} [2 \cosh(\beta J)]^N = -NJ \frac{\cosh^{N-1}(\beta J)}{\cosh^N(\beta J)} \sinh(\beta J) = -NJ \tanh(\beta J).$$

2. Using Eq.(1) **compute the specific heat** of the whole chain C_N.
   After deriving E, we can simply calculate the specific heat of the entire chain by

$$C_N = \frac{\partial E}{\partial T} = NJ\left(1 - \tanh^2(\beta J)\right) \frac{J}{k_B T^2} = \frac{NJ^2}{k_B T^2 \cosh^2(\beta J)}.$$

Comparison between different models

The following script plots the magnetic contribution to the specific heat computed for 1D (infinite chain) classical Heisenberg model with uniaxial anisotropy in $B = 0$. In the vertical axis the specific heat per spin is reported in units of k_B; in the horizontal axis the temperature in units of the exchange coupling $k_B T/J$. For comparison the analytic results obtained for the isotropic Heisenberg model (with $D = 0$) and for the Ising model are also plotted with solid lines.



1. Explain with your own words **why at low T the specific heat tends to the constant value** equal to k_B for all the three curves involving classical Heisenberg spins (symbols and black solid line).
   Hint: establish an analogy between the linear excitations in the 1D Heisenberg model and the chain of

harmonic oscillators discussed in the first exercise.
The classical Heisenberg model behaves at low-T as a system of coupled harmonic oscillators and, therefore, the Dulong–Petit law applies. For the 1D case, the linearized Hamiltonian has two independent d.o.f. in the Fourier space, which provide a constant contribution to the specific heat per spin equal to k_{B}.

2. Why does the specific heat of the Ising model approach zero when T tends to zero?
Because the elementary excitations of the Ising model are not spin waves but domain walls (DWs) with a finite energy gap w.r.t. to the ground state (each spin variable can only take quantized values ± 1). For this reason, the specific heat per spin vanishes as $T \to 0$ and it displays a Schottky anomaly at intermediate temperatures.
***Disambiguation**: Note that when $D \neq 0$ the spin-waves dispersion relation $\omega(q)$ is also gaped. However, as we are dealing with classical spins, the Fourier amplitude of a certain mode varies continuously and can be made indefinitely small. As a consequence, the Dulong–Petit law applies till $T \to O^+$. The situation is different when spin-waves are treated quantum-mechanically.*

3. Do you expect the classical Heisenberg model to reproduce the specific heat observed in realistic samples at low temperature?
No, because the energy spectrum of real systems is quantized at low-T, and the specific heat should vanish accordingly (think, e.g., of the Einstein or the Debey models of heat capacity).

4. Provide an argument to explain why the curve for $D/J = 0.1$ approaches the behavior of the *isotrpic* Heisenberg model at the highest computed temperatures.
The anisotropy is not relevant for $k_B T \gg D$ or better when $k_B T$ is significantly larger than the DW energy (equal to $2\sqrt{2DJ}$ in this case).

5. Provide an argument to explain why the curve for $D/J = 2$ approaches the behavior of the Ising model at the highest computed temperatures.
Hint: wait for the lecture on domain walls if you have no idea.
In this limit, domain walls are sharp and their energy is $2J$, namely the same as for the Ising model.