Microcanonical ensembles of 32x32 spins in Ising Model.

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It is well known that different thermodynamic ensembles do not coincide for finite systems. Likewise, it is well established – but hardly recognized – that these differences may distinguish certain ensembles as more appropriate than others even if one is ultimately interested in the thermodynamic limit of infinite system size. To illustrate this point we present as an example the famous second order phase transition in the two-dimensional Ising model and compare the canonical and microcanonical specific heat for a lattice of 32×32 spins.

I. GENERAL CONSIDERATIONS

A. Laplace-Transform

Assume we know the microcanonical partition function $\Omega_N(E)$ (conventionally referred to as the "density of states") of some finite system consisting of N particles. The canonical partition function is then given by

$$Z_N(T) \;=\; \sum_E \Omega_N(E)\, \mathrm{e}^{-\beta E}, \qquad (1)$$

which is essentially the Laplace-transform of $\Omega_N(E)$ with respect to $\beta \equiv 1/k_\mathrm{B}T$. Since this is well known to be a "smoothing" operation, any features which are present in $\Omega_N(E)$ will be flattened out in $Z_N(T)$, even though they are still present (Laplace-Transforms can be inverted!). However, just because they are *in principle* present in $Z_N(T)$ doesn't necessarily mean we can readily see them.

B. Legendre-Transform

Let us define the microcanonical entropy and the canonical free energy as

$$S_N(E) \;:=\; k_\mathrm{B}\,\log[\Omega_N(E)] \qquad (2)$$

$$\text{and} \qquad F_N(T) \;:=\; -k_\mathrm{B}T\,\log[Z_N(T)] \qquad (3)$$

Eqn. (1) can then be rewritten as

$$\begin{aligned} \mathrm{e}^{-\beta N f_N(T)} \;&=\; \sum_E \mathrm{e}^{-\beta[E - T S_N(E)]} \\ &=\; \sum_e \mathrm{e}^{-\beta N[e - T s_N(e)]}, \end{aligned} \qquad (4)$$

where we defined the specific energy $e = E/N$, entropy $s_N = S_N/N$ and free energy $f_N = F_N/N$. If the thermodynamic limit exists, f_N and s_N should approach limiting functions f_∞ and s_∞, respectively. Moreover, in this case the sum can be treated by a Laplace-evaluation [6], leading to

$$f_\infty(T) \;=\; \mathrm{min}_e\{e - T s_\infty(e)\}, \qquad (5)$$

showing that the connection of the partition functions via a Laplace transform becomes – in the thermodynamic limit! – a connection of the corresponding potentials via a Legendre transform.

C. Specific Heat

Let us define the microcanonical temperature by

$$\frac{1}{T_N^\mathrm{mic}} \;=\; \frac{\partial S_N(E)}{\partial E}. \qquad (6)$$

This equation can (in principle) be solved for E and yields the microcanonical equation of state $E_N^\mathrm{mic}(T_N^\mathrm{mic})$. Differentiating this with respect to T_N^mic gives the microcanonical specific heat

$$c_N^\mathrm{mic}(T_N^\mathrm{mic}) = \frac{\partial e_N^\mathrm{mic}}{\partial T_N^\mathrm{mic}} = -\left(\frac{\partial s_N}{\partial e}\right)^2 \left(\frac{\partial^2 s_N}{\partial e^2}\right)^{-1}. \qquad (7)$$

Alternatively, we may also start from the free energy, but then we get the canonical specific heat

$$c_N^\mathrm{can}(T^\mathrm{can}) = -T\,\frac{\partial^2 f_N}{\partial T^2} = N k_\mathrm{B}\,\frac{\langle e^2\rangle_N - \langle e\rangle_N^2}{(k_\mathrm{B}T^\mathrm{can})^2}, \qquad (8)$$

where the angular brackets denote *canonical* averages over the finite system.

Below we will illustrate the difference between these two functions with the help of the two-dimensional Ising model.

II. THE TWO-DIMENSIONAL ISING MODEL

A. Hamiltonian

Imagine a square lattice of $N = L \times L$ "spins" s_i, each of which can take the value ± 1 and has an interaction energy with any of its nearest neighbors s_j of $-J s_i s_j$. The Hamiltonian (in zero external field) is thus given by

$$H \;=\; -J \sum_{\langle i,j\rangle} s_i s_j, \qquad (9)$$

where the sum is over all pairs of nearest neighbors, denoted by $\langle i,j\rangle$. We will assume $J > 0$.