Microcanonical and canonical two-dimensional Ising model: An example

Markus Deserno
Department of Chemistry and Biochemistry, UCLA, USA
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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 $\beta \equiv 1/k_{\rm B}T$. 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

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

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

Eqn. (1) can then be rewritten as

$$\mathrm{e}^{-\beta N f_N(T)} \;=\; \sum_E \mathrm{e}^{-\beta[E - TS_N(E)]} \;=\; \sum_e \mathrm{e}^{-\beta N[e - Ts_N(e)]}, \qquad (4)$$

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

$$f_\infty(T) \;=\; \min_e\{e - Ts_\infty(e)\}, \qquad (5)$$

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

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

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

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

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

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

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 $-Js_is_j$. 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 $J > 0$.

B. Free energy and entropy

The two-dimensional Ising model in zero external field can be solved exactly [1], in the sense that the free energy

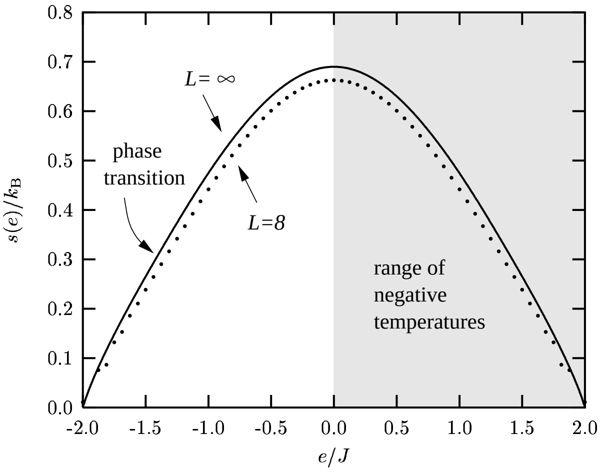

FIG. 1: Entropy of the two-dimensional Ising model for an 8×8 lattice (dots) as well as for the infinite lattice (solid line).

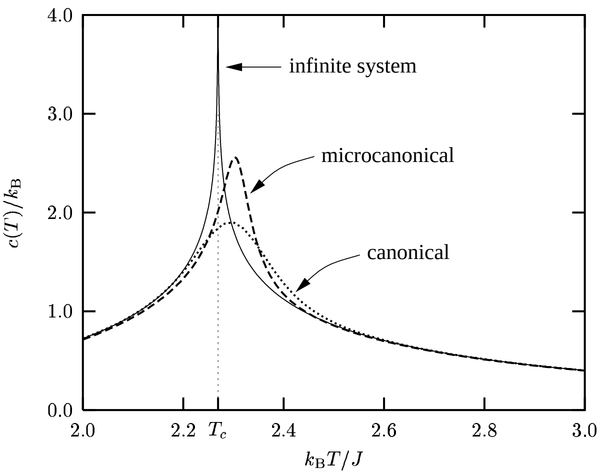

FIG. 2: Specific heat of the two-dimensional Ising model. The solid line is the result for the infinite system [4], the long-dashed and dotted lines correspond to the microcanonical and canonical result for a finite 32×32 lattice, respectively.

can be written down analytically—even for finite systems of $L_x \times L_y$ spins [2]. The *entropy* of *finite* systems can be obtained from the free energy of finite systems via an inverse Laplace transform, as described in Ref. [3]. We thus know the functions f_N and s_N. Fig. 1 shows the entropy $s_N(e)$ for an 8×8 Ising lattice as well as for the infinite lattice. The symmetry of the Ising model implies that $s_N(e) = s_N(-e)$, but positive values of the energy correspond to negative temperatures and are hence inaccessible when coupled to a heat bath. The non-analytic point in $s_\infty(e)$ where the phase-transition occurs is indicated.

C. Specific heat

Since we know the thermodynamic potentials we can compute the heat capacities from Eqn. (7) and (8). Fig. 2 shows the result for a finite lattice of 32×32 spins. Several things may be noted:

1. Canonical and microcanonical specific heat do not coincide with each other or with the result of the thermodynamic limit.

2. The deviations are pronounced at the critical point but become small away from it.

3. The features visible in c^{mic} are “sharper” developed than the features in c^{can}.

Comment 1 just demonstrates the fact that different ensembles do not coincide for finite systems. Comment 2 says that “how finite” a system appears does not only depend on its size alone. It also depends on the size of fluctuations. At the critical point fluctuations on all length scales occur, hence any finite system will appear small in the sense that it cannot accommodate sufficiently long-ranged fluctuations. Away from the critical point fluctuations are weaker and correlations quickly decay with distance, hence systems that are sufficiently large compared to the correlation length are essentially infinite for all practical means and purposes. Comment 3 finally demonstrates that typical features of phase transitions – here: a peak in the specific heat – may be better “developed” when looked at microcanonically.

The fact that the microcanonical ensemble often proves advantageous when analyzing phase transitions is little known and even less appreciated. The reader will find some exemplary material in Refs. [5].

[1] L. Onsager, Phys. Rev. **65**, 117 (1944).
[2] B. Kaufman, Phys. Rev. **76**, 1232 (1949).
[3] P. D. Beale, Phys. Rev. Lett. **76**, 78 (1996).
[4] M. Plischke and B. Bergersen, *Equilibrium Statistical Physics*, 2nd ed., World Scientific, Singapore (1994).
[5] A. Hüller, Z. f. Phys. **95**, 63 (1994); M. Promberger and A. Hüller, Z. f. Phys. **97**, 341 (1995); D. H. E. Gross, A. Ecker, and X. Z. Zhang, Ann. Phys. **5**, 446 (1996); M. Deserno, Phys. Rev. E **56**, 5204 (1997); M. Kastner M, M. Promberger M, and A. Hüller, J. Stat. Phys. **99**, 1251 (2000).

[6] Given the integral $I_N := \int \mathrm{d}x \; \mathrm{e}^{Nf(x)}$; if f is continuous, then $\lim_{N\to\infty} \log(I_N)/N = \max_x f(x)$. Assuming that the first correction stems from the immediate neighborhood of the point $\bar{x}$ where f is maximal, a quadratic expansion of the exponent yields $\log(I_N)/N \sim f(\bar{x}) - \log(-Nf''(\bar{x})/2\pi)/2N$.