Thermodynamic constraints on equilibrium fluctuations of an order parameter

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Supplementary Material

Here, we discuss in appendix A applications of the Crooks like fluctuation relation, namely Eq. (2) of the main text, as a way to infer free energy of the full system from a study of the fluctuations in the sub-part; and in appendix B, details on the proof of the bound for the order parameter fluctuations and applications to the Curie-Weiss model.

Appendix A: Free energy determination from Crooks like fluctuation relation

We now discuss the possibility to apply the Crooks like fluctuation theorem, namely Eq. (2) to determine the free energy of the full system. Now, the relevant asymmetry function is

$$\tilde{Y}_m = \frac{1}{\beta B n} \ln \frac{P_{\mathbf{B}}(m)}{P_0(m)}. \tag{A1}$$

For the full system, a plot of this quantity as a function of the magnetic energy density MB is shown in fig. 1. As expected, for any conditions (temperature, system size..) this plot is a straight line of slope 1, which intersects the x-axis at the value $MB = \Delta F$, corresponding to the free energy of the full system. In the conditions of this figure, we find $\Delta F \simeq 2$ in units of $k_B T$.

Let us then analyze *local* fluctuations in a finite box above the critical point where the decomposition of Eq. (7) of the main text can be used. The correction factor Ω_B introduced in Eq. (6) then takes the following form: $\Omega_B(\mathbf{M}_n) = \alpha_n \mathbf{M}_n \cdot \mathbf{B} + \beta \mathbf{B}^2 \sigma^2/2$, where σ^2 is the variance of ξ_n. Therefore, the asymmetry function $\tilde{Y}_m$ for the box fluctuations should be a straight line of slope $1+\alpha_n$, which is indeed the case as shown in fig. 1. The difference in the intersection points of the asymmetry functions with the x-axis for *local* and *global* fluctuations is the bias in the free energy due to the coarse-graining. This bias is proportional to the variance of ξ, namely $\beta \mathbf{B}^2 \sigma^2/2$. In the conditions of the figure, a direct evaluation of the bias using Eq. (7) confirms that it is of the order of 1.17, which accounts exactly for the difference of the two intersection points.

This example shows that the determination of the free energy from *local* fluctuations is in general difficult due to the bias on the free energy. Unlike the situation considered in Ref. [1], a simple shift in the fluctuation relation is not enough to remove this bias, and additional information on the fluctuations in the rest of the system is needed.

Appendix B: Bound on the fluctuations of the global and local order parameter

In this section, we provide more details on the derivation of the bounds on the fluctuations of the *global* and *local* order parameter given in the main text and we apply them to the case of the Curie-Weiss model. We first start with the case of fluctuations of the *global* order parameter.

1. Bound on the fluctuations of the global order parameter

Let us illustrate the bound on the fluctuations of the global order parameter

$$\frac{\mathrm{Var}(M_N)}{\langle M_N \rangle} \leq \frac{k_B T}{B}, \tag{B1}$$

derived in the main text in the specific case of the Curie-Weiss model.

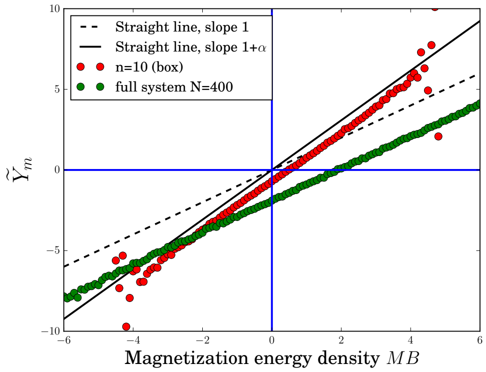

FIG. 1. Asymmetry function $\tilde{Y}_m$ for the Ising-model versus the magnetization density m for temperature $T = 3$, a magnetic field $h = 0.05$, a box of $n = 10 \times 10$ spins and a full system of 400 spins.

In the large system limit, the probability distribution of the magnetization is expected to behave exponentially as a function of the number of spins N. As a result, the fluctuations of the *global* magnetization are well described by the large deviation function defined in Eq. (13) of the main text. As shown in [2], this large deviation function takes the following simple form for the Curie-Weiss model with Ising spins :

$$\Phi_{\mathbf{B}}(m) = \frac{1+m}{2}\ln\frac{1+m}{2} + \frac{1-m}{2}\ln\frac{1-m}{2} - \frac{1}{2}\beta J m^2 - \beta B m - \beta f(B). \tag{B2}$$

where $f(B)$ is the Helmholtz free energy per spin. The following derivatives will be needed in the following:

$$\Phi'_{\mathbf{B}}(m) = \frac{1}{2}\ln\frac{1+m}{1-m} - \beta J m - \beta B = \tanh^{-1}(m) - \beta J m - \beta B, \tag{B3}$$

$$\Phi''_{\mathbf{B}}(m) = \frac{1}{1-m^2} - \beta J, \tag{B4}$$

and

$$\Phi'''_{\mathbf{B}}(m) = \Phi'''_{\mathbf{0}}(m) = \frac{2m}{(1-m^2)^2}. \tag{B5}$$

The most probable value of the magnetization, $m^*(B)$ given the magnetic field B, satisfies the relation $\Phi'_{\mathbf{B}}(m^*) = 0$, which leads to the well-known self-consistent equation

$$m = \tanh(\beta J m + \beta B). \tag{B6}$$

Above the critical temperature $k_B T_c = J$, this equation has one solution, whereas below this temperature, there are three solutions. Furthermore, since $-1 \le m \le 1$, $\Phi''_B(m) \ge \Phi''_B(0) = 1 - \beta J$ for all m.

As explained in the main text, the bound on the fluctuations of the order parameter, namely Eq. (B1) follows from the following lower bound of the second derivative of the large deviation function, namely

$$\Phi''_{\mathbf{B}}(m^*) \ge \frac{\beta B}{m^*}. \tag{B7}$$

Since Eq. (B6) defines $m^* = m^*(B)$ or equivalently $B = B(m^*)$, one can report the expression $\beta B(m^*) = \tanh^{-1}(m^*) - \beta J m^*$ for B into the right hand side of Eq. (B7), with the result that the inequality is equivalent to following function $h(m)$ been positive, with

$$h(m) = \frac{1}{1-m^2} - \frac{\tanh^{-1}(m)}{m}, \tag{B8}$$

on the interval $[-1, 1]$. Incidentally, this also shows that the inequality of Eq. (B7) must hold irrespective of the temperature. Since $h(m)$ is of the form $f'(m) - f(m)/m$, and f is convex for $m \ge 0$ and concave for $m \le 0$, the positivity of $h(m)$ follows from such properties of $f(m)$. Here this can be checked explicitly using the second derivative of f, which equals $\Phi_{\mathbf{0}}''(m)$ given above, but in fact the argument is general, and the precise expression of f should be unimportant as long as f is convex.

As a numerical confirmation of the generality of Eq. (B1), fig. (6) of the main text shows $\mathrm{Var}(M_N)/\langle M_N \rangle$ obtained from simulations of the 2D-Ising model against $k_B T/B$. This figure confirms that the bound is indeed satisfied at this temperature which is near the critical temperature and in such conditions, the bound is very tight, specially in the region of low magnetic field as expected. At temperatures below T_c, the bound is also satisfied but it is much less tight due to the magnetization taking non-zero values, which reduces the ratio $\mathrm{Var}(M_N)/\langle M_N \rangle$ significantly.

Finally, let us check directly that the inequality of Eq. (B7) is saturated when $B \to 0$, irrespective of the value of the temperature. The right hand side has the following limit

$$\lim_{B\to 0} \frac{B}{m^*} = \left(\left.\frac{dm^*}{dB}\right|_{B\to 0} \right)^{-1}, \tag{B9}$$

if we assume the function $m^*(B)$ differentiable. By differentiating Eq. (B7), one obtains the following limit,

$$\left.\frac{dm^*}{dB}\right|_{B\to 0} = \frac{\beta(1-m^*(0)^2)}{1-\beta J(1-m^*(0)^2)}. \tag{B10}$$

Using the explicit expression of the second derivative of $\Phi_{\mathbf{B}}(m)$ from Eq. (B4), it is straightforward to check that the inequality of Eq. (B7) becomes an equality when $B \to 0$ irrespective of the temperature.

2. Bound on the fluctuations of the local order parameter

We now turn to fluctuations of the *local* order parameter, obtained from the observation of a sub-part of the full system. We emphasize that the large deviation function is now defined with respect to that sub-part, and that the magnetization density is $m = M_n/n$. Let us first discuss the general case first and then the applications to the Curie-Weiss model.

The *local* fluctuation relation, when formulated in terms of large deviation functions, takes the following form:

$$\phi_{\mathbf{B}}(\mathbf{m}) - \phi_{\mathbf{B}}(-\mathbf{m}) = -2\beta \mathbf{B}\cdot\mathbf{m} - \frac{\beta\Gamma(n\mathbf{m})}{n}, \tag{B11}$$

$$= -2\beta B m - \beta\frac{\Gamma(n\mathbf{m})}{n}, \tag{B12}$$

where in the first step, we have introduced the function Γ defined in the main text. In terms of the asymmetry function Y_m given in Eq. (9), this is equivalent to

$$Y_m = m + \frac{\Gamma(n\mathbf{m})}{2Bn}. \tag{B13}$$

In the main text, we have proposed the following bound for the large deviation function $\phi_B(\mathbf{m})$:

$$\phi_{LR}(\mathbf{m}) = \beta B Y_{m^*} \frac{(\mathbf{m}-\mathbf{m}^*)^2}{2(\mathbf{m}^*)^2}, \tag{B14}$$

which is such that $\phi_{LR}(\pm\mathbf{m}^*) = \phi_{\mathbf{B}}(\pm\mathbf{m}^*) = 0$ and in addition $\phi_{LR}'(\mathbf{m}^*) = \phi_{\mathbf{B}}'(\mathbf{m}^*) = 0$. In contrast, the derivatives of the two functions are not equal in general at $-\mathbf{m}^*$ unlike the previous case for the fluctuations of the *global* order parameter. Indeed, from the *local* fluctuation relation and the property $\phi_{\mathbf{B}}(\mathbf{m}^*) = 0$, one deduces that

$$\phi_B'(-\mathbf{m}^*) = -2\beta B - \beta\Gamma'(n\mathbf{m}^*), \tag{B15}$$

while from Eq. (B14), one obtains

$$\phi_{LR}'(-\mathbf{m}^*) = -2\beta B - \beta\frac{\Gamma(n\mathbf{m}^*)}{n\mathbf{m}^*}. \tag{B16}$$

Therefore, we see that these derivatives are equal at $-\mathbf{m}^*$, *i.e.* $\phi_{\mathbf{B}}'(-\mathbf{m}^*) = \phi_{LR}(-\mathbf{m}^*)$ only if

$$\Gamma'(n\mathbf{m}^*) = \frac{\Gamma(n\mathbf{m}^*)}{n\mathbf{m}^*}. \tag{B17}$$

From this and given that $\Gamma(0) = 0$, this condition is satisfied whenever one of these conditions is met:

- when $\mathbf{m}^* \to 0$, which is for instance the case when $\mathbf{B} \to \mathbf{0}$ and $T > T_c$.
- when the size of the sub-part goes to zero $n \to 0$.
- when the asymmetry function Y_m is a linear function of m of the form $Y_m = (1+\alpha_n)m$.

When one of these conditions hold, the function ϕ_{LR} approximates $\phi_{\mathbf{B}}$ for all values of the magnetization. When $Y_m = (1+\alpha_n)m$, we have $\Gamma(n\mathbf{m}) = 2Bm\alpha_n$ and an equivalent expression of ϕ_{LR} is:

$$\phi_{LR}(\mathbf{m}) = \beta B_{eff} \frac{(\mathbf{m}-\mathbf{m}^*)^2}{2m^*}, \tag{B18}$$

in terms of the effective field $B_{eff} = (1+\alpha_n)B$.

From such an approximation, one obtains the bound on the fluctuations of the *local* order parameter, given in Eq. (20) of the main text, by the same arguments used above for the full system.

3. Applications to the mean-field case

Following [3]-[4], we have

$$\phi_{\mathbf{B}}(\mathbf{m}) = I(\mathbf{m}) - \beta \mathbf{B}\cdot\mathbf{m} - \frac{\beta J}{2}\mathbf{m}^2 \frac{n}{N} - \frac{N\beta f(\mathbf{B})}{n} + \beta f(\mathbf{B} + Jn\mathbf{m}/N)\left(\frac{N}{n} - 1\right), \tag{B19}$$

where $I(\mathbf{m})$ is the rate function for the fluctuations of the *local* order parameter with zero magnetic field.

The correction factor Γ introduced in the main text is

$$\Gamma(n\mathbf{m}) = \left(1 - \frac{N}{n}\right)\left(f(B + \frac{Jnm}{N}) - f(B - \frac{Jnm}{N})\right), \tag{B20}$$

which agrees with Eq. (12) of the main text.

In fig. 3, we show the large deviation function $\phi_{\mathbf{B}}(\mathbf{m})$ and its linear-response approximation $\phi_{LR}(\mathbf{m})$ for a size ratio of the sub-part to the full system of 1/9. In these conditions, we see that ϕ_{LR} is not tangent at the point $m = -m^*$ although both functions $\phi_{LR}(m)$ and $\phi(m)$ take the same value there.

Now, if we move to a smaller size ratio of the sub-part to the full system, as in fig. 3, where it is about 1/100, we observe that ϕ_{LR} appears tangent at $m = -m^*$ which makes ϕ_{LR} a more acceptable lower bound of $\phi_{\mathbf{B}}$. It is in such conditions, where the bound on the fluctuations of the *local* fluctuations, Eq. (20) should hold.

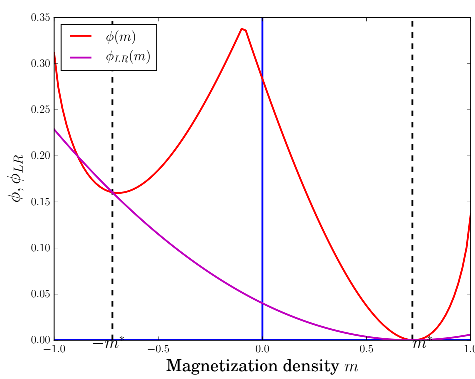

FIG. 2. Large deviation function $\phi_{\mathbf{B}}(\mathbf{m})$ and its linear-response approximation $\phi_{LR}(\mathbf{m})$ for the *local* fluctuations of the magnetization density $\mathbf{m}$ in the Curie-Weiss model for a temperature $T = 0.8$ (in the ferromagnetic phase) and a magnetic field $B = 0.01$. The size ratio of the sub-part to the full system is 1/9.

[1] R. García-García, S. Lahiri, and D. Lacoste, Phys. Rev. E **93**, 032103 (2016).
[2] P. Gaspard, J. Stat. Mech. **2012**, P08021 (2012).

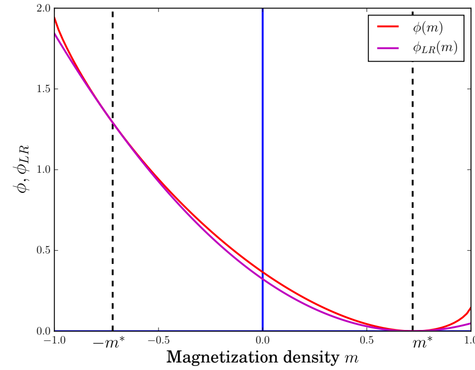

FIG. 3. Large deviation function $\phi_{\mathbf{B}}(\mathbf{m})$ and its linear-response approximation $\phi_{LR}(\mathbf{m})$ for the *local* fluctuations of the magnetization density $\mathbf{m}$ in the Curie-Weiss model for a temperature $T = 0.8$ (in the ferromagnetic phase) and a magnetic field $h = 0.01$. The size ratio of the sub-part to the full system is $1/100$.

[3] D. Lacoste and P. Gaspard, Phys. Rev. Lett. **113**, 240602 (2014).

[4] D. Lacoste and P. Gaspard, J. Stat. Mech. (2015).