LDT for magnetic order

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1 1D Ising model

1.1 Description of the model

The simplest magnetic toy model that we can try are large deviation equations on, is the one-dimensional Ising model. We have a chain of N up/down spins,

$$\mu_j = \pm 1, \quad j = 1, .., N$$

The interaction energy function of N spins is written as,

$$H = -J \sum_{j=1}^{N} \mu_j \mu_{j+1}$$

with $J > 0$. Only nearest neighbohrs interact and periodic boundaries apply as usual,

$$\mu_{N+1} = \mu_1$$

The order parameter of the problem is the total magnetization,

$$\mu = \frac{1}{N} \sum_{j=1}^{N} \mu_j, \quad -1 \leq \mu \leq 1$$

There is no thermodynamic phase transition but for a finite simulation the order parameter follows a probability distribution that we wish to describe.

1.2 Monte Carlo simulation

Standard Metropolis algorithm was employed. Periodic Boundaries were applied as well. I had to choose the thermodynamic conditions (βJ and N) as well as the relaxation time (τ) in a way that enough high μ configurations were sampled. After a lot of experimentation I ended up using,

$$N = 100$$

$$\beta J = 0.9$$

$$20 * 10^6 \quad MC \quad \text{relaxation}$$

$$80 * 10^6 \quad MC \quad \text{sampling}$$

1.3 Large deviations theory

With the transfer matrix method we calculate the scaled cumulant generating function as a function of an intensive, external field variable, γ that is conjugate to the random variable μ. After that we can use the fact that,

$$\mu(\gamma) = \frac{d\lambda(\gamma)}{d\gamma}$$

in order to express the SCGF as a function of the extensive variable,

$$\lambda(\mu) = \ln \left(\frac{\sqrt{(1-\mu^2)e^{2\beta J} + \mu^2 e^{-2\beta J}} + e^{-\beta J}}{2\sqrt{1-\mu^2}\cosh \beta J} \right)$$

The equation of state then reads,

$$\gamma(\mu) = \ln\left(\frac{\mu e^{-2\beta J} + \sqrt{1-\mu^2(1-e^{4\beta J})}}{\sqrt{1-\mu^2}}\right)$$

From the Gaertner-Ellis theorem we can calculate the rate function,

$$I(\mu) = \mu\gamma(\mu) - \lambda(\mu) = \int_0^{\mu} \gamma(\mu')d\mu'$$

Notice how the Legendre transform nicely reduces to the reversible work theorem from classical thermodynamics. The corresponding probability distribution is,

$$P(\mu) = \frac{e^{-NI(\mu)}}{\int_{-1}^{1} d\mu' e^{-NI(\mu')}}$$

1.4 Small fluctuation approach

In the small field limit, $\gamma \to 0$, we have the following expression for the SCGF,

$$\lambda(\gamma) = \frac{1}{2}e^{2\beta J}\gamma^2$$

The equation of state is now linear,

$$\mu(\gamma) = e^{2\beta J}\gamma$$

or equivalently we can say,

$$\gamma(\mu) = e^{-2\beta J}\mu$$

The SCGF as a function of the extensive parameter now is,

$$\lambda(\mu) = \frac{1}{2}e^{-2\beta J}\mu^2$$

The rate function is,

$$I(\mu) = \mu\gamma(\mu) - \lambda(\mu) = \int_0^{\mu} \gamma(\mu')d\mu' = \frac{1}{2}e^{-2\beta J}\mu^2$$

Notice how the SCGF and the rate function are exactly the same. This is to be expected at the central limit theorem level of approximation. Finally, the probability distribution follows from the rate function as before. We can calculate,

$$\langle\mu\rangle|_{\gamma=0} = \frac{d\lambda(\gamma)}{d\gamma}|_{\gamma=0} = e^{2\beta J}\gamma = 0$$

which makes sense since the distribution's mean is zero. We can also calculate this directly from the distribution,

$$\langle\mu\rangle = \frac{\int_{-1}^{1} \mu' e^{-NI(\mu')}d\mu'}{\int_{-1}^{1} e^{-NI(\mu')}d\mu'} = 0$$

From symmetry it is easy to evaluate the integral directly. The equations pass the test here so let us try the second cumulant. From the SCGF we have the following answer,

$$\langle\mu^2\rangle|_{\gamma=0} = \frac{1}{N}\frac{d^2\lambda(\gamma)}{d\gamma^2}|_{\gamma=0} = \frac{1}{N}e^{2\beta J}$$

but if we calculate this straight from the distribution we get,

$$\langle\mu^2\rangle = \frac{\int_{-1}^{1} \mu'^2 e^{-NI(\mu')}d\mu'}{\int_{-1}^{1} e^{-NI(\mu')}d\mu'} = \frac{1}{2a} - \frac{\sqrt{a}}{a}\frac{1}{\sqrt{\pi}}\frac{e^{-a}}{\mathrm{erf}\,(\sqrt{a})}, \quad a = \frac{1}{2}Ne^{-2\beta J}$$

and in the limit $N \to \infty$ the second cumulant goes to,

$$\langle\mu^2\rangle \to \frac{1}{2a} = \frac{1}{N}e^{2\beta J}$$

Which is the same as the answer we got from the SCGF.

1.5 Comparison and discussion

I compared the effective rate functions for all three methods.

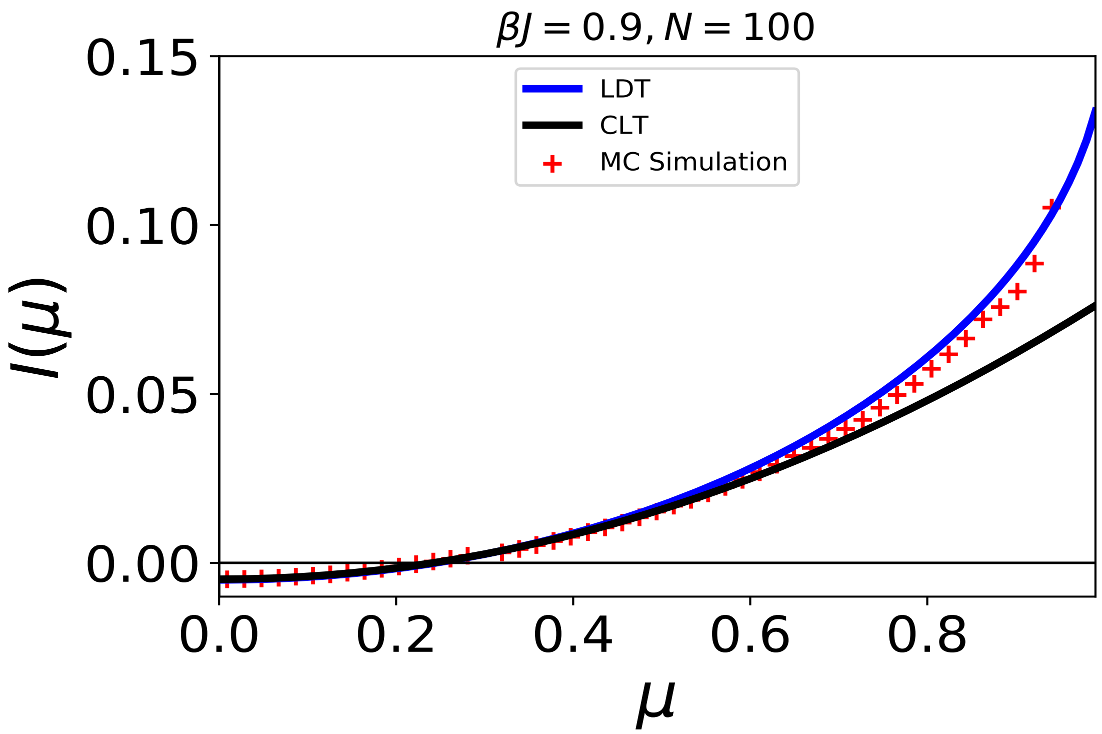

Figure 1: The effective rate functions for the three approaches. I only show the right branch, $\mu \in [0, 1]$, because it was sampled more efficiently during the Monte Carlo simulation.

2 2D XY model

2.1 Description of the model

Let us imagine a two-dimensional rectangular lattice with a spin placed on each lattice site. Only neighboring spins interact and this time the spins are able to rotate around and not just take up/down values. The random variables are now vectors,

$$\vec{\mu}_j = (\cos\theta_j, \sin\theta_j)$$

The interaction energy is,

$$H = -J\sum_{j=1}^{N}\cos\left(\theta_{j+1} - \theta_j\right)$$

The scalar magnetic order parameter,

$$\mu = \frac{1}{N}\sqrt{\left(\sum_{j=1}^{N}\cos\theta_j\right)^2 + \left(\sum_{j=1}^{N}\sin\theta_j\right)^2} = \frac{1}{N}\sqrt{\sum_{j,k=1}^{N}\cos\left(\theta_j - \theta_k\right)}$$

goes from $\mu = 0$ (disorder) to $\mu = 1$ (order). Similarly to liquid crystals but this time the directions $\hat{x}$ and $-\hat{x}$ are not the same so we measure one-fold and not two-fold orientational order. There is no thermodynamic transition because of the Mermin-Wagner theorem and the system behaves according to the Kosterlitz-Thouless theory. I think we can leave all the details aside and focus on the fact that in high temperatures the system is in a orientationally isotropic phase. As we decrease the temperature correlations between the orientations of spins start to grow and fluctuations in the order parameter distribution are more and more important. For that reason, our equations should be applicable as they are written but for one-fold order.

2.2 Monte Carlo simulation

Again I chose thermodynamic conditions (βJ and N) as well as the relaxation time (τ) in a way that enough high μ configurations were sampled. For the deep isotropic phase I chose,

$$N = 784$$

$$\beta J = 0.01, \quad \text{Deep} \quad \text{Isotropic}$$

$$20 * 10^6 \quad MC \quad \text{relaxation}$$

$$80 * 10^6 \quad MC \quad \text{sampling}$$

and for the "pre-transitional" phase I chose,

$$N = 784$$

$$\beta J = 0.9, \quad \text{Pre-transitional} \quad \text{Isotropic}$$

$$20 * 10^6 \quad MC \quad \text{relaxation}$$

$$80 * 10^6 \quad MC \quad \text{sampling}$$

2.3 Large deviations theory

Same as the Liquid Crystal equations. Look at the report with title "The 2D solution - Rate functions and equations of state (28th of July update)" - page 9.

2.4 Small fluctuation approach

Same as the Liquid Crystal equations. Look at the report with title "The 2D solution - Rate functions and equations of state (28th of July update)"

2.5 Comparison and discussion

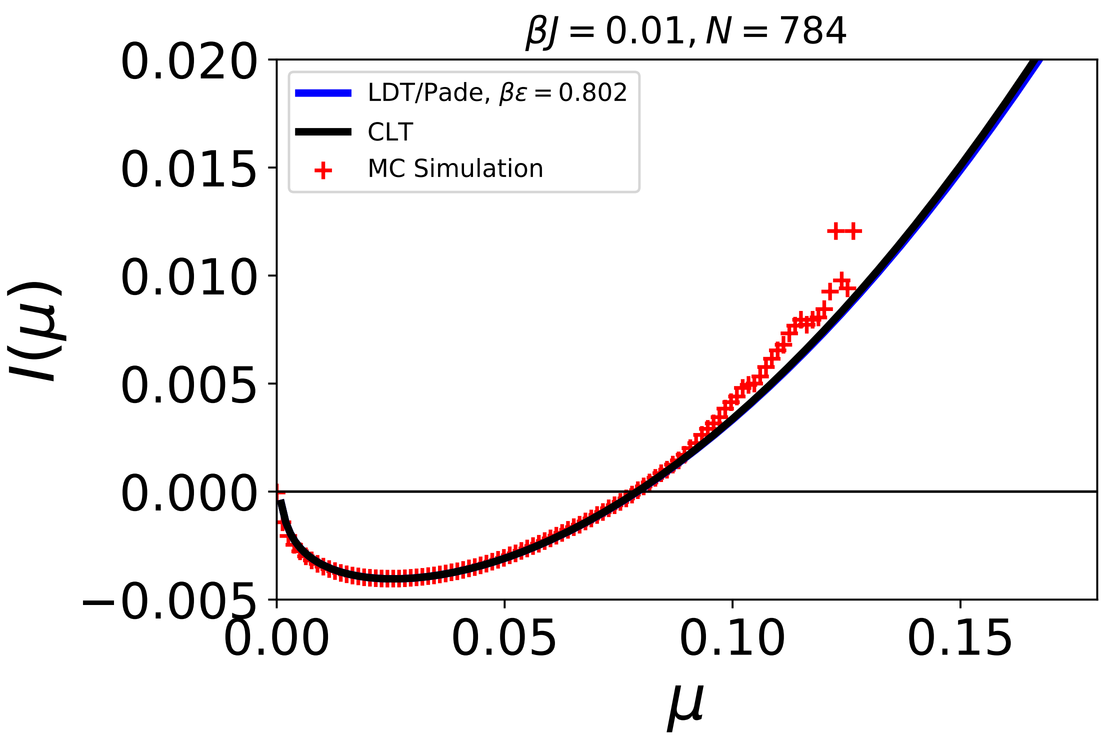

Figure 2: The high temperature isotropic phase of the 2DXY model. Sampling stops before we can see differencies between LDT and CLT. Just like the isotropic phase of 2DLC.

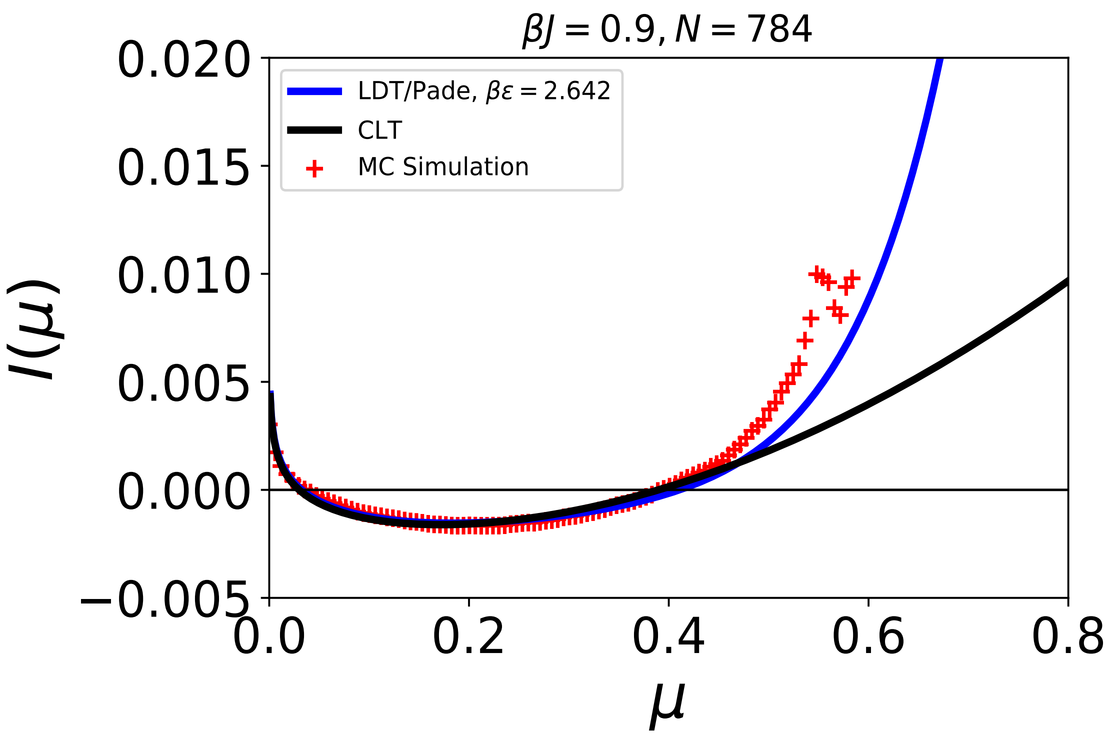

Figure 3: The low temperature isotropic phase of the 2DXY model. Fluctuations at these thermodynamic conditions are perhaps too strong and I should go to bigger N. I just wanted to illustrate the idea that perhaps our equations could be relevant to studies of the XY model.