Microcanonical solution of lattice models with long range interactions

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Abstract

We present a general method to obtain the microcanonical solution of lattice models with long range interactions. As an example, we apply it to the long range Ising chain, focusing on the role of boundary conditions.

Key words: Long range interactions, Ising chain, optimization under constraint.
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1 Introduction

Throughout the paper, systems in $d$ dimensions with a pairwise interaction potential which decays at large distances as $V(r) \sim 1/r^{d+\sigma}$ with $-d \leq \sigma \leq 0$, will be referred to as systems with long range interactions. Recently, such systems have attracted much attention, since they are believed to be in some cases candidates for the application of Non Extensive Thermostatistics, introduced by Tsallis. Actually, even the standard statistical mechanics of these systems are still not well studied.

Last year, Campa et al. [1], and, in a more general fashion, Vollmayr-Lee and Luijten [2], gave the solution within the standard canonical ensemble; however, it is known, from the study of self-gravitating systems and other models, that long range interactions may produce inequivalences between the results of the canonical and microcanonical ensembles [3–6]. A complete understanding of these models requires thus a microcanonical solution. We present in this letter a simple procedure to obtain the microcanonical solution of long-range interacting lattice systems, and illustrate it on the Ising case, focusing on the

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1 E-mail: Julien.Barr@ens-lyon.fr
2 Such interactions are sometimes called in the literature nonintegrable

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influence of boundary conditions.

2 The $\alpha$-Ising model

To study the influence of the long range interactions, we introduce a generalization of the one dimensional Ising model, with an additional parameter $\alpha$ controlling the decay of the interaction between two sites. The Hamiltonian reads:

$$H = -\frac{1}{2\tilde{N}} \sum_{ij} \frac{S_i S_j}{d_{ij}^\alpha}$$  \hspace{1cm} (1)

In this expression, the sum extends over all pairs of sites; $d_{ij}$ is the distance between the sites $i$ and $j$, and it depends on the boundary conditions: if we use periodic boundary conditions, the system must be seen as a closed ring, and $d_{ij} = \min(|i - j|, N - |i - j|)$; if we use free boundary conditions, then $d_{ij} = |i - j|$. Finally $\tilde{N} \propto N^{1-\alpha}$ is a rescaling factor chosen in order to obtain an extensive energy [1]; $\alpha = 0$ (non decreasing interactions) leads to $\tilde{N} = N$, which is the usual rescaling factor for mean-field Hamiltonians.

3 The coarse graining procedure

To describe the system, we use a coarse grained magnetization function $m(x)$, and we rescale the total length of the lattice to one, so that $0 \leq x \leq 1$. For a finite chain, with a grain size $n$, $m$ would be defined as follows

$$m(jn/N) = \frac{1}{n} \sum_{i=nj+1}^{n(j+1)} S_i$$ \hspace{1cm} (2)

To justify this approach, let us consider the interaction matrix $K_{ij} = \frac{1}{2\tilde{N}} \frac{1}{d_{ij}^\alpha}$. If the boundary conditions are periodic, $K$ appears to be cyclic, and is explicitly diagonalizable. One obtains for the spectrum and the eigenvectors (each eigenvalue corresponds to a two dimensional eigenspace except the $k = 0$ one):

$$\lambda_k = 2 \tilde{N}^{-1} \sum_{i=1}^{N/2-1} \frac{\cos(2\pi ki/N)}{i^\alpha}$$ \hspace{1cm} (3)
\[ u_j^{(k)} = \cos(2\pi kj/N) \]
\[ v_j^{(k)} = \sin(2\pi kj/N) \]

This spectrum has a very interesting property. On the one hand, if one fixes the wavenumber \( k \), the corresponding eigenvalue goes to some finite value when \( N \) goes to infinity, thanks to the choice of \( \tilde{N} \). On the other hand, if one fixes \( k/N = x \), which amounts to fix the wavelength of the eigenmode considered in units of the lattice spacing, the corresponding eigenvalue \( \lambda(x) \) goes to zero when \( N \) goes to infinity, whatever \( x \) is, provided it is non zero Fig. 1. This means that all these modes involving a possibly large but finite number of spins in one wavelength are irrelevant in the \( N \to \infty \) limit. Consequently, the coarse graining procedure, which drops precisely these short wavelengths modes is adequate to describe the system. It is important to notice that under more general boundary conditions, the spectrum is not explicitly computable, but heuristic arguments and numerical checks show that the qualitative properties described above are unchanged.

Using the coarse grained magnetization, we may now write the energy as

\[
H = -\frac{N}{2} \int_0^1 \int_0^1 m(x)m(y)K_\alpha(x,y) \, dx \, dy
\]  

(4)

with \( K_\alpha(x,y) = \text{cste}/d(x,y)^\alpha \), where the constant is chosen through \( \tilde{N} \) so that the maximal eigenvalue of \( K_\alpha \) is 1 (this facilitates the comparison between

Fig. 1. Spectrum of the interaction matrix with periodic boundary conditions. The curves correspond to \( \alpha = 1.5 \), for \( N = 50 \) (dotted), \( N = 200 \) (dashed), \( N = 800 \) (full line). The symbols correspond to \( \alpha = 0.5 \), for \( N = 50 \) (stars), \( N = 200 \) (circles), \( N = 800 \) (crosses). In the short range case (\( \alpha = 1.5 \)) the spectrum tends to a smooth curve, whereas in the long range case (\( \alpha = 0.5 \)), it shrinks on the \( y \)-axis as \( N \) increases, indicating that all modes with \( k/N \neq 0 \) are irrelevant in the thermodynamic limit.
different values of $\alpha$). The energy may also be written as $H = -N \sum_k \lambda_k \tilde{m}_k^2$ where $\tilde{m}_k$ is the amplitude of the eigenmode $k$ in the function $m(x)$.

4 Expression of the entropy

Given a magnetization profile $m(x)$, it is possible to determine approximately the corresponding number of microscopic configurations, using again the fact that $m$ varies slowly, on scales involving an infinite number of spins. After some easy combinatorial algebra and the use of Stirling formula, the logarithm of the number of configuration reads

$$S(m(x)) = -\frac{N}{2} \int_0^1 \left[ (1 + m) \ln \left( \frac{1+m}{2} \right) + (1 - m) \ln \left( \frac{1-m}{2} \right) \right] dx \quad (5)$$

The above expression of the entropy is valid for the Ising model; in general, the appropriate form of the entropy has to be derived, through some usually easy combinatorial calculus. To obtain the most probable magnetization profile in the microcanonical ensemble, we now have to maximize $S$ with respect to $m$, keeping $H$ constant\footnote{Let us note that the canonical solution is also available, through the minimization of $\beta H - S$ at fixed $\beta$}.

5 Application to the Ising model

Let’s now calculate the most probable magnetization profile for the $\alpha$-Ising model using the procedure described above, first for periodic boundary conditions, then for free boundary conditions.

Using a Lagrange multiplier $\beta$, we can write a necessary and sufficient condition to get a stationary point of equation (5) with the constraint given by equation (4); after a few algebra, we are left with

$$m(x) = \tanh \left( \beta \int_0^1 K_\alpha(x, y)m(y) \, dy \right) \quad (6)$$

with $\beta$ given by the energy constraint. If we use periodic boundary conditions, it is easy to see that $\int K_\alpha(x, y) \, dy$ is independent of $x$, so that equation (6)
together with the energy constraint admits a uniform solution for \( m(x) \). Furthermore, a second order calculation would show that this uniform solution is always a local entropy maximum (in other words, the eigenvalues associated to non-uniform modes are too weak to destabilize the uniform solution). On the contrary, if the boundary conditions are free, the constants are not eigenvectors of the kernel \( K_\alpha(x, y) \) anymore, and the solutions will be non-uniform.

To verify these predictions, we use a numerical optimization algorithm. Starting from a variety of initial magnetization profiles, we always get the same equilibrium solution, suggesting that for both type of boundary conditions, there is only one entropy maximum.

As expected, the profile is uniform and independent of \( \alpha \) for periodic boundary conditions; this is the microcanonical counterpart of the universality found in [1]. Figure 2 shows the results of the numerical computations for free boundary conditions: the profile depends on \( \alpha \), and becomes more and more uniform as \( \alpha \) goes to zero, as should be expected. The \( \alpha \)-Ising model does not display any phase transition in the microcanonical ensemble, just as the mean-field one. To study the phase transitions with long range interactions, one should introduce a slightly more complex model, for instance the Blume-Emery-Griffiths one, [6]; work along this line is in progress.

6 Conclusion

We have described a general method to obtain the microcanonical solution of lattice models with long range interaction, taking advantage of the quasi mean-field structure induced by the long range interactions. Although the

![Fig. 2. Magnetization profile at energy \(-0.1\), for free boundary conditions and \( \alpha = 0.2 \) (full line), \( \alpha = 0.5 \) (dotted line), \( \alpha = 0.8 \) (dashed line): the system is inhomogeneous. For periodic boundary conditions, the magnetization profile is homogeneous and invariant under a change of \( \alpha \).](image-url)
procedure has been illustrated with the Ising chain, it is straightforward to
generalize it to various lattice models (Potts models, X-Y type models, Blume-
Emery-Griffiths model...) in any dimension, by modifying the expression of
the entropy; it will be applied in subsequent work to systems displaying phase
transitions.
The problem reduces to an optimization problem under constraint, which is
very similar to that obtained after a statistical analysis of the two dimensional
Euler equation in fluid mechanics [7], and where the boundary conditions play
a central role. Despite the huge gain in complexity with respect to the initial
states counting problem, it is not easy to solve and requires in some cases a
numerical treatment.

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References

[1] A. Campa, A. Giansanti and D. Moroni , to appear in Chaos, Solitons and
Fractals.

[2] B. P. Vollmayr-Lee and E. Luijten , Phys. Rev. E 63, 031108 (2001).

[3] T. Padmanabhan, Phys. Rep. 188, 285 (1990).

[4] D. Lynden-Bell and R. Wood, Mon. Not. R. Astron. Soc. 138, 495 (1968).

[5] D. Lynden-Bell, Physica A 263, 293 (1999).

[6] J. Barré, D. Mukamel and S. Ruffo, in Phys. Rev. Lett., 87, 030601 (2001).

[7] R. Robert and J. Sommeria, J. Fluid. Mech 229, 291 (1991).