Statistical mechanics of long range interactions

Introduction

In presence of long range interactions, some of our usual intuition for statistical mechanics and thermodynamics is not valid anymore. For instance, it has been known for a long time to astrophysicists that self-gravitating systems may exhibit a negative specific heat. Inequivalence between statistical mechanics at fixed energy or fixed temperature, that is inequivalence between statistical ensembles, may also occur. The underlying reason for these unusual behaviors is lack of energy additivity: a long range interacting system with internal energy E cannot be divided into two macroscopic parts with internal energy E_1 and E_2 such that $E = E_1 + E_2$.

This in turn allows us to be more precise on the definition of long range interactions: an interaction is long range in this sense when it renders the internal energy not additive, which is often equivalent to say that the range of the interaction is comparable to the size of the system.

Systems with long range interactions, according to the above definition, are rather common in physics: self gravitating systems, that we already mentioned; point vortices, and more generally vortex-vortex interactions in 2D turbulence and related geophysical flows; wave-particles interactions, where the wave conveys the interaction over long distance... These long range interacting systems also share some phenomenology with small systems: in a system of a few dozens of particles (an atomic cluster for instance), the range of the interaction is comparable to the size of the system [1].

Many of the usual statistical mechanics analytical methods focus on partition function calculations, in the canonical or grand canonical ensembles. In presence of long range interactions however, ensembles may be inequivalent, and it can be argued in many cases that the microcanonical one, at fixed energy, is the most relevant: a galaxy, an atomic cluster, or an unforced 2D fluid for instance can be considered as isolated on reasonable time scales. This calls for the development of analytical methods for microcanonical calculations.

Large deviation, a tool for microcanonical calculations

In the presence of long range interactions, a given particle, or spin, interacts with many others. As a consequence, it feels a local field averaged over many particles, which fluctuations are thus much smaller than in the case of a nearest neighbor interaction. This is the basic observation that allows for the use of large deviation techniques to exactly solve a large number of problems with long range interactions, in the canonical as well as in the microcanonical ensembles. This general method was described in a mathematically rigorous setting by R. S. Ellis [2]; we applied it to several models of different types in [3]. Fig. 1 shows an exemple of ensemble inequivalence and negative specific heat in a mean field (that is the interaction is of infinite range) spin system. The Hamiltonian is given by

$$H = \Delta \sum_{i=1}^{N} S_i^2 - \frac{J}{2N} (\sum_{i=1}^{N} S_i)^2 \ , \qquad (1)$$

where the spins S_i can take the values $0, 1, -1$.

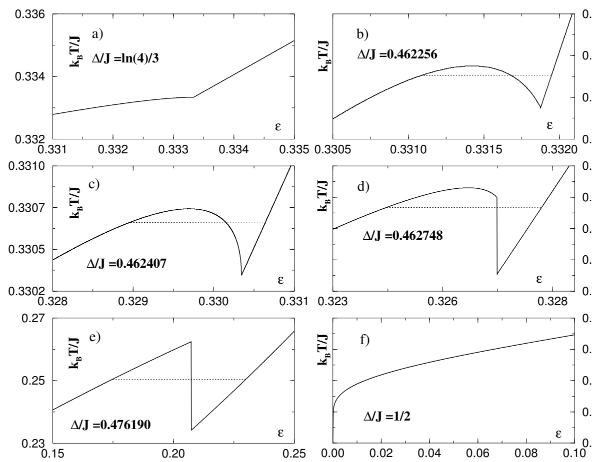

Figure 1: Temperature vs energy relation in the microcanonical ensembles for different values of Δ/J. A negative specific heat region is visible on panels b, c and d. The dotted line indicates the canonical solution when different from the microcanonical one. There is ensemble inequivalence on panels b to e.

Application to a model of free electron laser

Wave-particles systems, where the interaction between particles is mediated by a wave, may sometimes be considered as long range interacting systems. Indeed, the wave is a macroscopic degree of freedom, propagating in the whole system, inducing effective long range interactions. One example is a free electron laser (FEL). In such a device, a beam of relativistic electrons travels in a region of variable magnetic field (an undulator), and interacts with the light it emits. In some conditions, this light is amplified through an energetic transfer from the kinetic energy of the electrons. A very simplified model of this phenomenon is given by the following Hamiltonian:

$$H_N = \sum_{j=1}^{N} \frac{p_j^2}{2} - N\delta A^2 + 2A \sum_{j=1}^{N} \sin(\theta_j - \varphi) \quad . \quad (2)$$

The p_i's represent the velocities relative to the center of mass of the N electrons and the conjugated variables θ_i characterize their positions with respe to the co-propagating wave. The complex electr magnetic field variable, $\mathbf{A} = A\,e^{i\varphi}$, defines the ar plitude and the phase of the dominating mode (and $\mathbf{A}^\star$ are conjugate variables). δ is a paramet which measures the average deviation from the re onance condition. Starting from an initially sma value, A is amplified and saturates to an asymptot value. Analytic calculations of this asymptotic valu by definition deep in the non linear regime, are n very common in the field. Fig. 2 compares nume ical results and large deviation calculations for th asymptotic value [4].

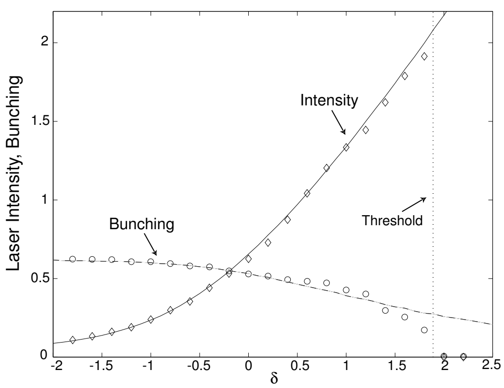

Figure 2: Laser intensity and a parameter characterizing the bunching of the electron beam as a function of the detuning parameter δ. Symbols are numerical results, solid lines are the analytical curves. Above the threshold, there is no amplification.

Application to a model of micromagnetism

When considering a small numbers of particles (say for instance a few tens), the range of the interaction is necessarily comparable to the size of the whole system. Some effects similar to those induced by long range interactions may thus be expected in that case [1], and the same analytical techniques might be useful. An example of such small samples is molecular magnetism: the spins of atoms in a single molecule interact with one another, and one is interested in the total magnetization of the molecule, and how it may change sign. We studied a toy model for this magnetization reversal, aiming at demonstrating the potential use of large deviation techniques in this setting [5]. The toy model is an assembly of Heisenberg spins, with Hamiltonian

$$H = B\sum_{i=1}^{N} S_i^z + \frac{J}{2}\sum_{i=1}^{N}\sum_{j\neq i}(S_i^x S_j^x - S_i^y S_j^y), \qquad (3)$$

As a first step, we study the classical dynamics of the model; some results are presented on Fig. 3. Future work implies turning to more realistic models of real molecules like Mn-12-acetate.

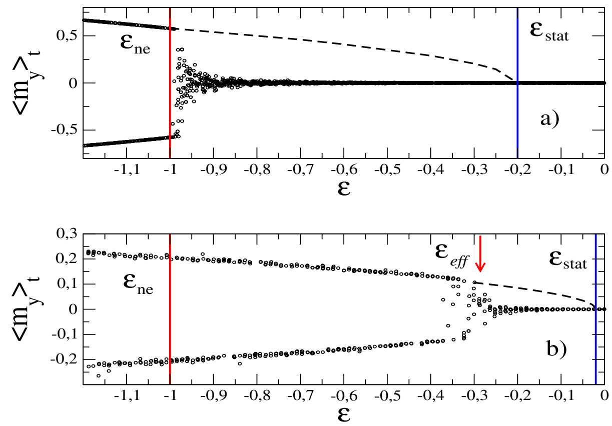

Figure 3: The top panel is for $N = 5$, the bottom one for $N = 50$. Numerically computed temporal average of the total magnetization m_y, as a function of the energy per spin ε. The agreement with the large deviation calculation (dashed line) is excellent when $m_y \neq 0$. In addition, this calculation estimates the ε for which m_y falls to 0: $\varepsilon = -1$ for the top panel, $\varepsilon = -.28$ for the bottom one.

References

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