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Abnormal kinetic energy fluctuations and critical behaviors in the microcanonical Lattice Gas model

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In this paper we present a microcanonical lattice gas model with a fluctuating volume. In the first order liquid - gas phase transition region thermodynamical anomalies such as a back-bending in the caloric curve and a negative heat capacity are observed. This phenomenon induces abnormal kinetic energy fluctuations and is associated with a critical fragment size distribution. The relevance of these findings for the experimental detection of a liquid - gas phase transition in finite systems is discussed.

Phase transitions are universal properties of interacting matter which have been widely studied in the thermodynamical limit of infinite systems. However, in many physical situations this limit cannot be accessed and phase transitions should be reconsidered from a more general point of view. This is for example the case of matter under long range forces like gravitation [1]: even if self - gravitating systems are very large they cannot be considered as infinite because of the non saturating nature of the force. Other cases are provided by microscopic or mesoscopic systems. Metallic clusters can melt before being vaporized [2]. Quantum fluids may undergo Bose condensation or super-fluid phase transition [3]. Dense hadronic matter is predicted to merge in a quark and gluon plasma phase [4] while nuclei are expected to exhibit a liquid - gas phase transition [5]. For all these systems the experimental issue is how to sign a possible phase transition in a finite system.

Specifically in microcanonical finite systems where the state is defined only through its total energy, the entropy is known to present a convex intruder in first order phase transitions [6]. As a consequence the heat capacity C is expected to exhibit two divergences separated by a negative branch. To identify the phase transition we need a direct tool to explicitly extract thermodynamical state variables from experimental data. It has recently been proposed [7] that, for a given total energy, the average partial energy stored in a part of the system may provide a microcanonical thermometer while the associated fluctuations can be used to construct the heat capacity.

In this article we would like to test these ideas on an exactly solvable model for second and first order phase transitions, the Lattice Gas Model of Lee and Yang [8]. This is a simplified model which can be interpreted as a schematic representation of a classical fluid with a Van der Waals type of equation of state. In our numerical implementation the N sites of a lattice are characterized by an occupation number $\tau = 0$ or 1 . Particles occupying nearest neighboring sites interact with an energy ϵ . A kinetic energy term is also included so that the Hamiltonian is given by

$$\hat{H} = \sum_{i=1}^N \frac{p_i^2}{2m} \tau_i + \sum_{i,j}^N \frac{\epsilon}{2} \tau_i \tau_j \quad (1)$$

where the second sum runs only over neighboring sites.

In the liquid-gas phase transition, since the order parameter is the density difference between the two phases, the volume is essential in determining thermodynamical properties. Many studies have been performed considering periodic boundary conditions in order to avoid the effects of the surface [9]. Systems in a fixed cubic volume have also been investigated [10]. However, in most practical cases the volume is not defined through boundary conditions but is an experimental observable known at best in average. For example the (average) radius of a hot source can be defined through interferometry or through comparisons with statistical models. From a theoretical point of view this implies that at equilibrium the entropy of the system should be maximized under the constraint of a specific value for the average volume. In the absence of a preferred direction, an average volume can be defined through the one-body observable

$$\hat{V} = \frac{4\pi}{3} \sum_{i=1}^N r_i^3 \tau_i \quad (2)$$

where r_i is the distance to the center of the lattice.

Introducing first a canonical description in which the energy observable $\hat{H}$ as well as the volume $\hat{V}$ are known in average we have to introduce the associated Lagrange multipliers β, λ so that the partition function reads

$$Z_{\beta,\lambda} = \sum_{(n)} \exp \left(-\beta U^{(n)} - \lambda V^{(n)} \right) \quad (3)$$

Here, $U^{(n)}$ and $V^{(n)}$ are the expectation values of the operators $\hat{H}$ and $\hat{V}$ in the n^{th} event, β is the inverse of the canonical temperature $\beta = 1/T_{can}$, and the quantity $P = -\lambda/\beta$ has the dimension of a pressure. Therefore, a statistical ensemble of events associated with an average volume can easily be generated through a canonical sampling using a constrained Hamiltonian $\hat{E} = \hat{H} - P$

$\hat{V}$ where $P \hat{V}$ can be considered as a constraining one-body external field. The averaged constrained energy $E = U - PV$ can be interpreted as an enthalpy. The actual value of the pressure parameter must be defined to get the desired average volume. In the calculations shown below a number $A = 216$ of particles is fixed; to illustrate a first order phase transition the pressure P is chosen in such a way that the isobar crosses the canonical coexistence line at about the half of the critical temperature. The numerical realization of the model is a three dimensional cubic lattice characterized by a size large enough ($N = 8000$) so that the boundary conditions do not affect the calculations with a constraining pressure. Canonical statistical averages are taken over events obtained with a standard Metropolis sampling of the lattice occupations according to the partition function (3) [11].

For finite systems the various ensembles are not equivalent because fluctuations cannot be neglected. Since energy is a directly accessible observable in each event, the correct statistical framework is the microcanonical ensemble. An easy way to access microcanonical quantities is to sort the canonical partitions according to their total energy. When both energy and volume are considered as thermodynamical observables one should in principle sort the canonical events sampled for a given temperature and pressure as a function of the energy and the volume. However, if the pressure is fixed it is sufficient to sort the events as a function of the constrained energy E so that at a given temperature β the canonical distribution reads

$$P_\beta(E) = \frac{W(E)}{Z_\beta} \exp(-\beta E) \quad (4)$$

where W is the degeneracy of the state. In a sampling of N_0 events the probability P_β can be estimated from the number N_β of events falling in the enthalpy bin of size ΔE around E , $P_\beta(E) \Delta E \approx N_\beta(E)/N_0$. Equation (4) can be inverted leading to the entropy $S(E) \equiv \log(W(E))$. This allows a direct estimation of the microcanonical caloric curve

$$T^{-1}(E) \equiv \frac{\partial S(E)}{\partial E} = \beta + \frac{\partial \log N_\beta(E)}{\partial E} \quad (5)$$

which is valid for every β . Therefore using many canonical sampling at different β one can directly compute the microcanonical caloric curve (5).

Figure 1a presents the energy distributions at different β . According to equation (4) the logarithm of these probabilities directly gives the entropy apart from a linear correction. Far from the coexistence region the distribution presents the expected Gaussian behavior. When we get close to the coexistence region the observed double bump is a direct evidence of the convex intruder expected in the entropy in the case of a finite microcanonical system undergoing a first order phase transition. This

can be better seen on the associated microcanonical caloric curve presented in Figure 1b. For each canonical ensemble the total energy exhibits large fluctuations allowing the calculation of the microcanonical temperature over a wide range of energies using equation (5). The fact that the microcanonical temperatures defined from various canonical ensembles at different β all agree within the statistical error bars is a demonstration of the accuracy of the Metropolis sampling. The reconstructed microcanonical caloric curve presents the expected back-bending in the coexistence region due to the anomalous convexity of the entropy. This induces a negative branch in the microcanonical heat capacity $C = (\partial_E T)^{-1}$ as shown in Figure 1c. The anomalous curvature of the thermodynamical potential is a clear signature of a first order phase transition, the distance between the two poles being a direct measure of the latent heat. Increasing the pressure, the two poles get closer up to the critical point where they merge before they disappear.

FIG. 1. a) Total constrained energy (enthalpy) distributions associated with various canonical β . b) Microcanonical temperature as a function of the enthalpy per particle from various canonical samplings at the different β shown above (symbols) and the corresponding average (line). c) Microcanonical heat capacity.

It is interesting to compare the microcanonical and canonical caloric curves as shown in Figure 2. In finite systems two canonical caloric curves can be defined, corresponding to the average and most probable energy associated to a given β . In infinite systems these two energies are equal because fluctuations can be neglected. Far from the phase transition the canonical and microcanonical curves agree. Indeed as seen in Fig. 1a the canonical energy distribution is Gaussian showing that the two ensembles only differ through minor fluctuation corrections.

Moreover, from equation (5) we can see that the most probable canonical energy is characterized by the equality of the microcanonical and canonical temperatures. In the coexistence region however the predictions of the two ensembles differ in a noticeable manner. The canonical caloric curves are by definition monovaluated while this restriction does not apply to the microcanonical case: in the back-bending region the canonical caloric curve associated with the most probable energy presents a discontinuity equivalent to the Maxwell construction. The observed energy jump is directly related to the latent heat of the first order phase transition. Because of fluctuations the average energy presents a smoother behavior with however a clear slope change in the transition region. It should be noticed that the partitions which fall in the energy region corresponding to the canonical temperature jump are hardly sampled by the canonical ensemble, but are accessible in the microcanonical ensemble. Therefore, in a finite system the microcanonical sorting of events allows to study regions of the phase diagram which are forbidden in the canonical formalism. These regions are characterized by specific properties such as negative heat capacities which we will now study in more detail. In particular it is important to identify experimental observables which can directly inform us about these peculiar properties.

FIG. 2. Microcanonical caloric curve (full line) compared with the most probable (dots) and average (line) canonical energy for each β .

It has been recently proposed that the microcanonical latent heat can be measured using partial energy fluctuations [7]. The total energy E (here including the external constraining potential field) of the considered system can be decomposed into two independent components, its kinetic and potential energy: $E = E_k + E_p$. In a microcanonical ensemble with a total energy E the total degeneracy factor $W(E) = \exp(S(E))$ is thus simply given by the folding product of the individual degeneracy factors $W_i(E_i) = \exp(S_i(E_i))$ of the two subsystems

$i = k, p$. One can then define for the total system as well as for the two subsystems the microcanonical temperatures T_i and the associated heat capacities C_i . Since we are dealing with a classical gas the kinetic equation of state is simply given by $E_k = 3AT_k/2$ and the kinetic heat capacity is a constant, $C_k = 3A/2$. If we now look at the kinetic energy distribution when the total energy is E we get

$$P_k^E(E_k) = \exp(S_k(E_k) + S_p(E - E_k) - S(E)) \quad (6)$$

FIG. 3. As a function of the total energy per particle are shown: a): the average kinetic energy (dots) multiplied by 2/3 compared with the microcanonical temperature (line); b): the kinetic energy fluctuations (dots) compared with the canonical expectation (line); c) The heat capacity extracted from the fluctuations (dots) compared with the exact one (line).

Using Eq.(6) we directly get that the most probable partitioning of the total energy E between the potential and kinetic components is characterized by a unique microcanonical temperature $\bar{T} \equiv T_k(\bar{E}_k^E) = T_p(E - \bar{E}_k^E)$. Therefore the most probable kinetic energy $\bar{E}_k^E$ can be used as a thermometer as shown in Figure 3a. Using a Gaussian approximation for $P_k^E(E_k)$ the kinetic energy variance can be calculated as

$$\sigma_k^2 = \bar{T}^2 \frac{C_k C_p}{C_k + C_p} \quad (7)$$

where C_k and C_p are the microcanonical heat capacities calculated for the most probable energy partition. As shown in Figures 3b and 3c when C_p diverges and then becomes negative, σ_k^2 remains positive but overcomes the canonical expectation $\sigma_k^2 = \bar{T}^2 C_k$. This anomalously large kinetic energy fluctuation is a signature of the first

order phase transition. Equation (7) can be inverted to extract from the observed fluctuations the heat capacity

$$C \simeq C_k + C_p = \frac{\bar{T}^2 C_k^2}{\bar{T}^2 C_k - \sigma_k^2} \quad (8)$$

Figure 3c shows that the heat capacity extracted from the kinetic energy fluctuations is in very good agreement with the exact one. This means that kinetic energy fluctuations are an experimentally accessible measure of the heat capacity which allows to sign divergences and negative branches characteristic of the phase transition.

FIG. 4. Microcanonical fragment size distribution (symbols) and distribution of the heaviest fragment in each event (dashed lines) at three different total energies. Full line: power law with a critical exponent $\tau = 2.3$

In order to better characterize the back-bending region it is interesting to examine the properties of the associated microcanonical partitions. In our calculation microcanonical events at a total energy E are obtained by first performing a canonical metropolis sampling with a β parameter such that the resulting average energy is E . Then microcanonical events with the exact energy E are simply picked out of the generated canonical ensemble. It should be noticed that in the back-bending region the average energy is constructed out of a double bumped energy distribution meaning that it may correspond to a minimum of the canonical probability. Therefore the microcanonical sampling can be different from the typical partitions of the corresponding canonical distribution. Figure 4 presents microcanonical fragment mass distributions in the back-bending region. At the lowest energy, in the first uprising branch of the caloric curve, the fragment distribution shows an exponential fall off of light fragments associated with the gas phase and a big liquid drop, characteristic of a subcritical system. At the highest energy corresponding to the gas branch of the caloric curve, the distribution resembles to a typical supercritical vaporized system. In the middle of the back-bending region the size of the 'liquid' fraction is

comparable to the one of the other fragments and a critical distribution is observed. For comparison a power law with a critical exponent $\tau = 2.3$, expected from the liquid-gas universality class, is also shown in Fig 4. The observation of a critical behavior of the fragment size distribution in the coexistence region has already been reported in the canonical lattice-gas context [9]. The present study additionally suggests that anomalous fluctuations, coming from the negative heat capacity characteristic of a microcanonical first order phase transition, are to be expected in the region where the fragment size distribution becomes critical. The conjunction of these two observations signs a first order phase transition.

In this paper we have investigated the properties of a microcanonical lattice gas model with a finite volume known only in average. We have shown that a negative heat capacity should be associated with the fragmentation of systems undergoing a liquid-gas phase transition. This phenomenon, which is a specific feature of first order phase transitions in finite systems in the microcanonical ensemble, can be signed through the observation of abnormally large kinetic energy fluctuations when events are sorted out in total energy bins. We have shown that in the transition energy region the fragment size distribution exhibits a critical behavior in agreement with the theoretical expectation for a liquid gas phase transition. These two pieces of informations can thus be used together to experimentally detect a thermodynamical first order phase transition.

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