Distribution of the largest fragment in the lattice gas model

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The distribution of the largest fragment is studied in different regions of the lattice gas model phase diagram. We show that first- and second-order transitions can be clearly distinguished in the grancanonical ensemble, while signals typical of a continuous transition are seen inside the coexistence region if a mass conservation constraint is applied. Some possible implications of these findings for heavy-ion multifragmentation experiments are discussed.

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I. INTRODUCTION

Since the first heavy-ion experiments were conducted, the size of the largest cluster A_M detected in multifragmentation events has been tentatively associated with an order parameter for the fragmentation phase transition [1]; if this is true, we should expect for this observable a double-humped distribution if the transition is first order [2], while its fluctuations should obey the first scaling law if the transition is continuous [3]. Experimental multifragmentation data show in this respect somewhat contradictory evidences. An analysis of 80*A* MeV Au+Au peripheral collisions from the Indra-Aladin collaboration [4] reports a bimodal distribution of a variable closely correlated to A_M. On the other hand, the functional relationship between the two first moments of A_M in central Xe+Cu collisions [5] shows a change of slope which has been interpreted as a transition from the $\Delta = 1/2$ to the $\Delta = 1$ scaling law, as expected for a generic continuous transition [3]. From the theoretical point of view, it is well known [6–10] that in finite systems many different pseudocritical behaviors can be observed inside the coexistence region of a first-order phase transition. Particularly concerning the order parameter fluctuations, simulations have been performed in the framework of the Ising model with fixed magnetization (IMFM) in Ref. [11]. That study showed the distribution of A_M to approximately obey the first scaling law even at subcritical densities, i.e., in thermodynamic conditions where no continuous transition takes place. Since the scaling is violated for very large lattices, the observed behavior was interpreted in that paper as a finite size effect that prevents the recognition of the order of a transition in a small system. An important difference subsists, though, between the theoretical study of Ref. [11] and the experimental analysis in Ref. [5]: in the first paper, the average A_M size is varied by increasing the total lattice size, meaning that the existence of a scaling law is tested in well-defined thermodynamic conditions [a single point in the $(\rho,\ T)$ state variables space]. In the experimental case, it is not possible to freely vary the source size, therefore, different regions of $\langle A_M \rangle$ are explored by varying the total energy deposited in the fragmenting system. It is not *a priori* clear how these two very different procedures might be related and whether they could be equivalent.

In this paper, we analyze the distribution of A_M within the lattice gas model [12]. This model is the simplest representation of the liquid-gas phase transition; when augmented with the cluster definition through the Coniglio-Klein algorithm [13], it can also be related to a bond and site percolation problem, making this model a paradigm of the fragmentation phase transition. This model is isomorphous to the Ising spin model, and its thermodynamic properties are very precisely known: the lattice gas phase diagram contains both first- and second-order phase transitions, and basic effects, like conservation laws, which are very relevant to the experimental situation, can be easily implemented.

In the analysis of the A_M distributions, we will show that the most important finite size effect is the inequivalence between statistical ensembles [14]: the observed ambiguities can be coherently interpreted as an effect of conservation laws, the distribution of an order parameter being drastically deformed if a constraint is applied to an observable that is closely correlated to the order parameter under study.

Specifically, we will demonstrate the following points:

- In small canonical systems, a first scaling law as a function of the system size can be observed not only at the critical point but also for subcritical densities inside the coexistence region. This is in agreement with the findings reported in Ref. [11]. The difficulty in recognizing the order of the transition is due to not only the finite size effects but also and more importantly the fact that the order parameter distribution and its scaling properties are deformed by the conservation law that in the canonical ensemble acts on the total number of particles A_t, which strongly constrains the order parameter A_M.
- If the A_M size is varied by changing the system temperature at a fixed lattice size, no scaling of the largest fragment distribution is observed even if we choose a transformation that passes across the thermodynamic critical point.
- In this case, the correlation between the average $\langle A_M \rangle$ and the variance σ^2 of the largest fragment distribution exhibits a rise and fall which is imposed by the conservation law constraint; the double logarithmic derivative $\Delta' = d \ln \sigma / d\langle A_M \rangle$ appears to be a smooth decreasing function

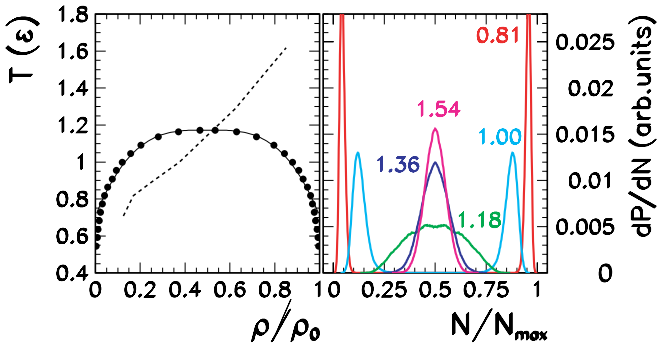

FIG. 1. (Color online) Right side: distributions of the size of the largest cluster in the grancanonical lattice gas model at different temperatures T/ϵ, with an $8 \times 8 \times 8$ lattice and at $\mu = 3\epsilon$. Left side: lattice gas phase diagram from the distributions on the right side. Dashed line: locus of the maximal A_M fluctuation in the canonical ensemble.

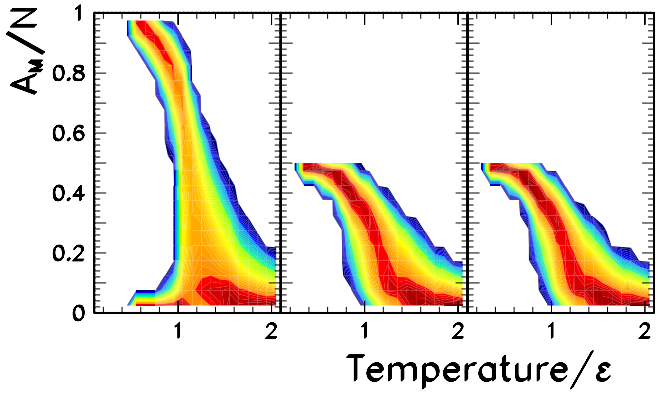

FIG. 2. (Color online) A_M distributions as a function of temperature for an $8 \times 8 \times 8$ lattice in the grancanonical (left), canonical (middle), and microcanonical (right) ensemble. In all cases the density is $\rho/\rho_0 = 1/2$.

of $\langle A_M \rangle$; even if Δ' is passing through $\Delta' = 1$ and $\Delta' = 1/2$ before becoming negative, no simple scalings $\sigma \propto \langle A_M \rangle^{\Delta}$ can actually be unambiguously isolated.

- However, we show that both the existence of a transition and a conclusion about its order can be inferred from the quantitative study of the A_M fluctuation.

II. PHASE TRANSITION IN THE LATTICE GAS MODEL

In our implementation of the lattice gas model [12], the N sites of a cubic lattice are characterized by an occupation number n_i, which is defined as $n_i = 0(1)$ for a vacancy (particle). Particles occupying nearest neighboring sites interact with a constant coupling ϵ. This model can be transformed into an Ising spin problem with a magnetic field through the mapping $s_i = n_i - 1/2$. The relative particle density ρ/ρ_0 is defined as the number of occupied sites divided by the total number of sites and is linked to the magnetization of the Ising model by $\rho/\rho_0 = m + 1/2$. In addition to this interaction, a kinetic energy is introduced. Occupied sites are characterized by a momentum vector. Observables expectation values are evaluated in the different ensembles (grancanonical, canonical, and microcanonical) sampled through standard Metropolis algorithms [8]. The chemical potential in the grancanonical implementation plays the role of the magnetic field $h = \mu - 3\epsilon$ in Ising, while the canonical lattice gas corresponds to the constant magnetization IMFM case with $m = \rho/\rho_0 - 1/2$.

The phase diagram of the model can be easily evaluated looking at the distribution of the total number of particles $A_t = \sum_{i=1}^{N} n_i$ in the grancanonical ensemble with a chemical potential $\mu = \mu_c = 3\epsilon$, which corresponds to the Ising critical field $h = 0$. The A_t distributions $P_{\beta\mu}(A_t)$ are displayed at different temperatures in the right side of Fig. 1. The presence of two different ensembles of states (bimodality) is clearly seen for all temperatures $T < T_c \approx 1.22\epsilon$. At the critical chemical potential μ_c presented in the figure, the probabilities of occurrence of the two solutions are exactly identical; if $\mu < \mu_c$ ($\mu > \mu_c$) the high (low) density peak dominates. For a fixed temperature β^{-1}, the most probable A_t as a function of μ is discontinuous at the transition point μ_c.

At the thermodynamic limit, the discontinuity in the most probable A_t as a function of μ gives rise to a discontinuity in the associated $\langle A_t \rangle(\mu)$ equation of state; this implies that the two peaks represent two coexisting phases [15,16] and that the number of particles (or equivalently the density) is the order parameter of a phase transition that is first order up to the critical point $T = T_c$. The phase diagram can be constructed by reporting the forbidden region for the most probable density, i.e., the locus of the discontinuity in the most probable. This corresponds to the two peaks in the bimodal particle number distribution observed at μ_c. The phase diagram is displayed in the left side of Fig. 1. These findings obtained in an $8 \times 8 \times 8$ lattice correspond to the phenomenology of the liquid-gas phase transition that the model is known to display at the thermodynamic limit. If we increase the lattice size, the location of the coexistence border will be modified, even if finite size corrections are especially small in this model [8]. However, it is clear from Fig. 1 that (except at the critical point which is a second-order point, where the two peaks merge to form a single distribution) the first-order character of the transition is indisputable even for a linear dimension as small as $L = 8$.

Figure 2 shows the size of the largest cluster A_M as a function of the temperature for the grancanonical, canonical, and microcanonical ensembles. The obvious correlation between A_M and A_t implies that for $T < T_c$ the A_M distribution is also double humped in the grancanonical ensemble, as explicitly shown in Ref. [17]. This means that A_M can also be taken as an order parameter of the liquid-gas phase transition; and looking at its distribution, this transition can be recognized as first order even for a system constituted of $\langle A_t \rangle = 256$ particles.

In Fig. 2 as well as in the following figures, clusters are always recognized with the so-called Coniglio-Klein algorithm [13]. It is important to note that if all cluster recognition algorithms are approximately equivalent in the low-density regime, the recognition of physical clusters in the vicinity or above the critical point demands a recognition algorithm explicitly depending on momentum space. Indeed, Ising clusters (i.e., sets of occupied nearest-neighbor sites, independent of the site momentum) do not show in three

dimensions a critical behavior at the thermodynamical critical point [18].

III. CONSERVATION LAWS AND THERMODYNAMICS

If the constraint of mass conservation is implemented (canonical lattice gas, or equivalent Ising model with fixed magnetization), the distributions of A_M drastically change [17]. In the grancanonical ensemble at $\langle \rho/\rho_0 \rangle = 1/2$, the explored microstates essentially populate the coexistence border, while the coexistence region is accessed with a negligible probability (see Fig. 1); these highly improbable grancanonical distributions are conversely the only microstates allowed by the canonical constraint at the value $\rho/\rho_0 = 1/2$; below the transition temperature, the grand canonical and canonical partitions differ drastically. Because of the mass conservation constraint, the bimodality of the A_t distribution is obviously lost in the canonical ensemble; as a consequence of the correlation between A_t and A_M, the A_M distribution also shows a unique peak (Fig. 2). If we additionally implement a total energy conservation constraint (microcanonical ensemble, right part of Fig. 2), the distributions get still narrower, but the qualitative behavior is the same as in the canonical ensemble. The normal behavior of the A_M distribution at subcritical temperatures may intuitively suggest a pure phase or a continuous transition for the canonical model. This intuition is, however, false; the characteristics and order of the transition do not depend on the statistical ensemble, and the phase diagram of Fig. 1 is still pertinent to the canonical ensemble [17]. Indeed, the relation between the two ensembles can be written as

$$\ln P_{\beta\mu}(A_t) = \ln Z_\beta(A_t) + \beta\mu A_t - \ln Z_{\beta\mu}, \tag{1}$$

where $Z_{\beta\mu}$, $Z_\beta(A_t)$ are the partition sums in the two ensembles. Equation (1) shows that in the whole region where the grancanonical distribution $P_{\beta\mu}(A_t)$ is convex, the canonical equation of state

$$\mu_{\text{can}} = -\frac{1}{\beta}\frac{\partial \ln Z_\beta}{\partial A_t} \tag{2}$$

presents a back bending, which is an unambiguous signal of a first-order phase transition [19]. At each temperature, the maxima of $P_{\beta\mu}$ correspond to the two ending points of the tangent construction for Eq. (2), i.e., to the borders of the coexistence region in the canonical ensemble.

The qualitative behavior of $A_M(T)$ in the canonical ensemble does not change with the density of the system. In particular, the A_M fluctuation passes systematically through a maximum. The locus of this maximum is displayed in the phase diagram in Fig. 1. We can see that the maximum fluctuation approximately corresponds to the transition temperature only at the critical point. At subcritical densities, this maximum lies inside the coexistence region of the first-order phase transition.

It is important to stress that this result may be somewhat model dependent. All the cluster recognition algorithms proposed in the literature show a percolation line in finite lattices, but the location of this line in the phase diagram can depend on the specific cluster definition [18]. In particular, the physical meaning of clusters in supercritical media where fragments are not separated by physical surfaces is still an object of debate [18].

In any case, the results of Fig. 2 show that the double-hump criterium for a first-order phase transition does not hold if a constraint is put on a variable closely correlated to the order parameter under study.

IV. CONSERVATION LAWS AND DELTA SCALING

We can ask the question whether a detailed study of the scaling properties of the A_M distribution may give extra information on the transition and discriminate first and second order. Following the arguments of Ref. [3], we consider the distribution

$$\Phi(z) = \Phi\left(\frac{A_M - A_M^*}{\langle A_M \rangle^\Delta}\right) = \langle A_M \rangle^\Delta P(A_M), \tag{3}$$

where A_M^* is the most probable value of A_M and $0 < \Delta \leqslant 1$ is a real number. At a continuous phase transition point, the distribution of the order parameter is expected to fulfill the first scaling law; i.e., the distribution Φ should be scale invariant with $\Delta = 1$. The scale invariance of Φ for a given value of Δ is generically referred to as Δ scaling; and the transition observed experimentally [5] from a $\Delta \approx 1/2$ to a $\Delta \approx 1$ scaling by varying the centrality of the collision and therefore the energy deposited in the system has been taken as a signal of a continuous phase transition.

A practical difficulty in testing Δ scaling is that for a given distribution the value of Δ that corresponds to scale invariance, if any, cannot be known *a priori*. This difficulty can be circumvented by using the fact that the scaling (3) imposed $\langle A_M \rangle^\Delta \propto \sigma$. Then it is immediate to verify that Eq. (3) can be equivalently written as the ensemble of the two conditions

$$\Psi\left(\frac{A_M - \widetilde{A}_M}{\sigma_{A_M}}\right) = \sigma_{A_M} P(A_M), \tag{4}$$

$$\sigma_{A_M}^2 = K \langle A_M \rangle^{2\Delta}, \tag{5}$$

where Ψ is a scale invariant distribution and K is a constant. Since in presence of a scaling, the difference between the most probable A_M^* and the average $\langle A_M \rangle$ scales like σ, $\widetilde{A}_M$ can be either one or the other. In the latter case, the occurrence of a Δ scaling study corresponds to the invariance of the centered and reduced distribution. If this distribution does not show scale invariance, we can exclude the existence of any Δ scaling law. If the function Ψ is scale invariant, this corresponds to a Δ scaling if and only if the ln-ln correlation between the average and the variance is linear; in this case, the slope of the correlation gives the value of Δ. The practical advantage of testing Eqs. (4) and (5) instead of Eq. (3) is that we can check scale invariance with no *a priori* knowledge of Δ.

The standard way of testing scale invariance is to consider a specific point of the phase diagram and consider the centered and reduced A_M distributions obtained by varying the size of the lattice and, as a consequence, the total number of particles. For the canonical case at the thermodynamical critical point,

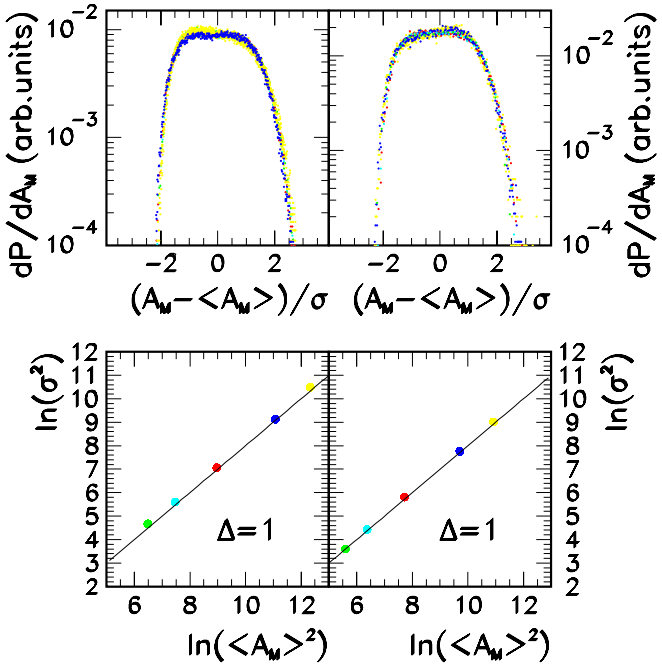

FIG. 3. (Color online) Delta scaling analysis for the canonical lattice gas model at the critical point $\rho = \rho_0/2$, $T = T_c$ (left side) and inside coexistence $\rho = \rho_0/4$ at the point of maximal A_M fluctuation (right side). Upper part: centered and reduced A_M distributions. Lower part: correlation between the first two moments and linear interpolation according to Eq. (5). The linear size of the lattice is varied as $L = 5, 6, 8, 12, 16$.

this analysis is shown on the left side of Fig. 3. Both Eqs. (4) and (5) are well verified, in agreement with the expectation of a first scaling law at a continuous transition point [3]. A comparable quality scaling is, however, observed also at subcritical densities at the temperature corresponding to the maximum A_M fluctuations (right side of Fig. 3). This finding is in agreement with Ref. [11]. Together with the analysis of the phase diagram, this means that such a scaling also approximately applies in the coexistence region of a first-order phase transition, if the order parameter is not free to fluctuate but is constrained by a conservation law.

V. DELTA SCALING AS A FUNCTION OF THE SYSTEM EXCITATION

In the experimental application to nuclear multifragmentation [5], the system size cannot be varied as freely as in the lattice gas, since the maximum size for a nuclear system is of the order of 400 particles. To explore different values of $\langle A_M \rangle$, the same system has been studied at different bombarding energies [5] and/or different impact parameters [20]. In a similar way, we kept the total number of particles constant and varied the temperature. To fix the ideas, we chose the simplest thermodynamical path from coexistence to the fluid phase passing through the critical point $\rho(T) = cte = \rho_0/2$. The resulting Ψ functions are displayed in Fig. 4. No scaling is observed: the function Ψ continuously evolves from a distribution with a tail extending toward the low mass side compared to the average at low temperature, whereas the opposite is true at high temperature.

If we look at the behavior of the variance as a function of the first moment, the ln-ln correlation is nowhere linear, showing that the large fragment fluctuation does not evolve like a power of the average fragment size. The bell-shaped behavior of this curve is due to the mass conservation constraint, which forces the fluctuation to vanish at both low and high $\langle A_M \rangle$ values. The observed maximum is in fact the maximum fluctuation point shown in Fig. 1; at the critical density, it occurs close to the critical point and for subcritical densities, it is located inside the coexistence region.

To qualitatively compare with experimental Δ-scaling analysis, we have to remember that the studied experimental distributions only cover the multifragmentation regime and do not explore the decreasing part of the $\sigma_{A_M}(\langle A_M \rangle)$ correlation which would correspond in the nuclear case to evaporation from a Compound. Focusing now on the fragmentation region, we show in Fig. 4 the best power-law interpolations of the average and variance correlation to be compared with the published experimental analysis presenting a $\Delta = 1$ to a

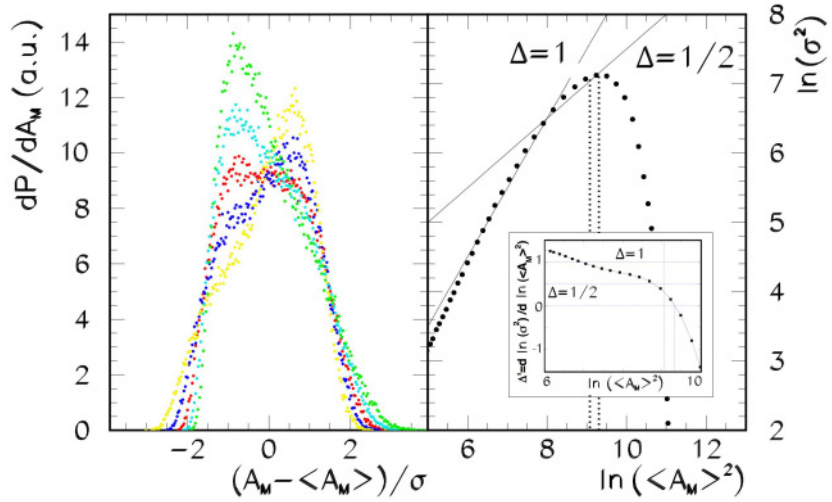

FIG. 4. (Color online) Delta scaling analysis for the canonical lattice gas model at constant density $\rho = \rho_0/2$ varying the system temperature. Left side: centered and reduced A_M distributions for temperatures varying from $T = 1.1\epsilon$ to $T = 1.25\epsilon$. Right side: correlation between the first two moments and linear interpolations according to Eq. (5). Temperatures range from $T = 0.3\epsilon$ to $T = 2.3\epsilon$. The vertical lines indicate the temperature of maximum A_M fluctuations and the critical temperature. The double logarithmic derivative Δ' is shown in the inserted figure.

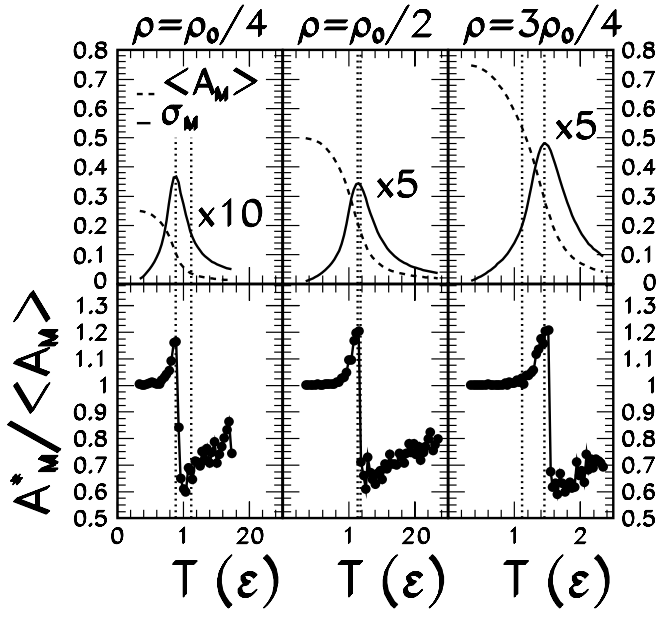

FIG. 5. First moments of the A_M/A_T distribution as a function of temperature for an $8 \times 8 \times 8$ lattice in the canonical ensemble at $\rho/\rho_0 = 1/4$ (left), $\rho/\rho_0 = 1/2$ (middle), and $\rho/\rho_0 = 3/4$ (right). Upper part: mean value (full line) and variance (dashed line). Lower part: most probable value of the A_M distribution normalized to the mean. Vertical lines indicate the temperature of maximal A_M fluctuations and the transition temperature for each density.

$\Delta = 1/2$ regime. In this interpretation, the crossing point between the two power-law fits is interpreted as a "transition" point. By construction it appears to be at a higher temperature than the maximum fluctuation, which at this critical density comes out to be close to the critical temperature.

To better study the possible occurrence of a power-law scaling of the large fragment fluctuation, we can study the double logarithmic derivative

$$\Delta' = \frac{d\sigma_{A_M}}{d\langle A_M \rangle}. \tag{6}$$

In presence of a Δ scaling, this quantity should be constant. Figure 4 shows that Δ' is a smoothly decreasing function passing through the values 1 and $1/2$ before going through 0 at the maximum fluctuation point and then becoming negative as a consequence of the mass conservation law. No plateaus of Δ' are observed, thus confirming the absence of scaling.

This violation of scaling occurs in spite of the fact that a continuous phase transition point (the thermodynamic critical point) is explored in the simulations. At this point, the distributions indeed follow the first scaling law (left side of Fig. 3), but this information is lost if the different distributions are generated by varying the temperature. This is true not only for the transition point, but also for the supercritical regime. Indeed, this regime has been shown to exhibit the second scaling law $\Delta = 1/2$ in the Potts model [3] (or something close to it, $\Delta \approx 0.6$ for the IMFM [11]), while in the representation of Fig. 4, scaling can everywhere be excluded.

The conclusion is that scale invariance can only be tested by varying the total system size. However, other information on the phase transition can be accessed through the study of the A_M distribution with a fixed total number of particles, as we will now show.

VI. SIGNALS OF PHASE TRANSITION AND OF ITS ORDER

The first two moments of the distribution in the canonical ensemble and the corresponding most probable value A_M^* are displayed in Fig. 5 for three different densities. Let us look at the $\rho < \rho_c$ case first. If the first and second moment show smooth behaviors dominated by the conservation law constraint, the transition is still apparent in the behavior of A_M^*, which rapidly changes at a temperature close to the transition point. This sudden decrease is due to a change of sign in the asymmetry of the distribution. As such, the qualitative behavior of $A_M^*(T)$ is independent of the density. A great number of continuous transition signals have been observed in different mass conserving models at densities that do not correspond to a continuous phase transition [6–11]. The same happens for the most probable value of A_M. This variable shows for all densities a sudden drop at a temperature $T_t(\rho)$ that corresponds to the maximum of the A_M fluctuations. As we already stressed, these temperatures approximately coincide with the transition temperature only at the critical density (see Fig. 1). The behavior at supercritical densities reflects a geometric phase transition that has no thermodynamic counterpart, while if fragmentation takes place at low density the A_M drop can be taken as a signal of phase coexistence.

To discriminate between the different density regimes and recognize the order of the phase transition, we have to quantify the A_M fluctuation peak. In the grancanonical ensemble, the A_t fluctuation is directly linked to the susceptibility via

$$\chi = \frac{\partial \langle A_t \rangle}{\partial \mu} = \beta \left(\sigma_{A_t}^{\mu}\right)^2. \tag{7}$$

To work out a similar expression for the canonical ensemble, let us assume that A_M and the other fragments are statistically independent, i.e., the total density of states is factorized

$$W_t(A_M, A_m, E_M, E_m) = W_M(A_M, E_M) \cdot W_m(A_m, E_m), \tag{8}$$

where we have defined the total number of particles not belonging to the largest fragment as $A_m = A_t - A_M$, and the corresponding energy $E_m = E_t - E_M$. This hypothesis is reasonably well verified in the lattice gas model, since the correlation coefficient between A_M and A_m in the grancanonical ensemble comes out to be close to zero except in the very dense regime $\rho/\rho_0 \approx 1$. The factorization of the state densities implies a convolution of the corresponding canonical partition sums

$$\begin{aligned} Z_\beta(A_t) &= \int dE_t e^{-\beta E_t} \int_0^{E_t} dE_m \int_0^{A_t} dA_m \\ &\quad \times W_m(E_m, A_m) W_M(E_t - E_m, A_t - A_m) \\ &= \int_0^{A_t} dA_m Z_\beta^M(A_M) Z_\beta^m(A_t - A_M), \end{aligned} \tag{9}$$

where Z_β^i, $i = m, M$ describe the contribution of the largest fragment and of all the others, respectively. The distribution

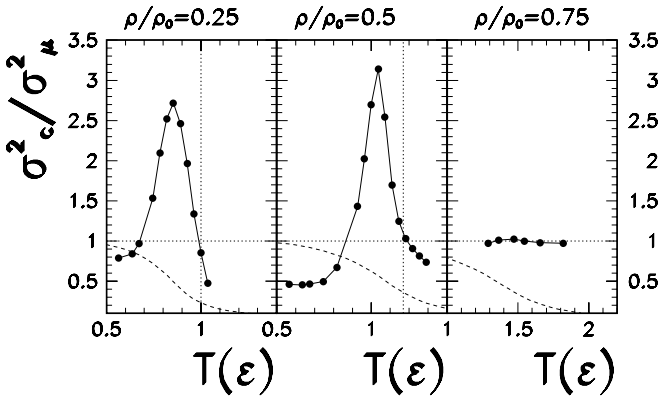

FIG. 6. Ratio between the grancanonical and canonical fluctuation of the number of particles A_m not belonging to the largest cluster, as a function of the temperature for an $8 \times 8 \times 8$ lattice at $\rho/\rho_0 = 1/4$ (left), $\rho/\rho_0 = 1/2$ (middle), and $\rho/\rho_0 = 3/4$ (right). Dashed lines: average canonical A_M values normalized to the total number of particles. Vertical lines in the two left panels: limit of the region of negative susceptibility from the canonical $\mu(A)$ equation of state Eq. (2) [8].

of the largest fragment reads

$$P_{\beta A_t}(A_M) = Z_\beta^{-1}(A_t) Z_\beta^M(A_M) Z_\beta^m(A_t - A_M). \qquad (10)$$

A Gaussian approximation of this distribution leads to [21]

$$\beta\sigma^2_{A_M} = \left[\frac{1}{\chi_m(A_t - A_M^*)} - \frac{1}{\chi_M(A_M^*)}\right]^{-1}, \qquad (11)$$

where $\sigma^2_{A_M}$ is the fluctuation of the A_M distribution, and the partial susceptibilities are defined as $\chi_i^{-1} = \frac{\partial \mu_i}{\partial A_i}(A_i^*)$.

The above derivation is valid for a system whose state density depends on the two extensive variables, number of particles A and energy E. In the case of the fragmentation transition, a third extensive variable, the volume V, has also to be considered. We show in the Appendix that in this more general case, Eq. (11) can still be derived, but a dilute limit $V_t = V_m + V_M \approx V_m$ has to be considered.

According to the general definition of phase transitions in finite systems [19,22], the generalized susceptibility associated with an order parameter is negative in a first-order phase transition in the statistical ensemble where the order parameter is subject to a conservation law. We therefore expect a negative χ_M at subcritical densities. Imposing $\chi_M < 0$ in Eq. (11) leads to

$$\sigma^2_{A_M} > \beta^{-1}\chi_m(A_t - A_M^*). \qquad (12)$$

Comparing to Eq. (7), this finally gives

$$\sigma^2_{A_M} = \sigma^2_{A_m} > \left(\sigma^\mu_{A_m}\right)^2. \qquad (13)$$

Equation (13) associates the first-order phase transition in the canonical ensemble to "abnormal" A_M fluctuations, in the same way as abnormal partial energy fluctuations sign a first-order phase transition in the microcanonical ensemble [21].

The canonical and grancanonical fluctuations are compared in Fig. 6 for three different densities. Independent of the system density our approximation Eq. (13) turns out to be incorrect at very low temperatures, when the average size of the largest cluster (dashed lines) exceeds about 80% of the available mass. In this case, the hypothesis of statistical independence between A_m and A_M cannot be justified, and the canonical mass conservation constraint trivially reduces the canonical fluctuation. However, as soon as the average A_M value drops, we can see that the region of negative susceptibility can be well reconstructed through Eq. (13), and in particular its border (vertical lines) is very precisely determined by the equality condition between the two fluctuations. At supercritical densities, the dilute gas approximation we have employed breaks down independently of the temperature, and the susceptibility cannot quantitatively be estimated from the fluctuation signal. However, in this regime, the relative fluctuation observable does not present any peak, whereas only inside the spinodal region of the first-order phase transition does the canonical fluctuation exceed the grancanonical one. Clearly this observable allows an unambiguous discrimination between the supercritical regime and phase coexistence.

VII. CONCLUSIONS

In this discussion of the role of the largest fragment in the framework of the lattice gas model, we have shown that this variable can be taken as an order parameter of the fragmentation phase transition if this latter belongs to the liquid-gas universality class. It has been already observed [11,23] that the phase transition can be tracked from the sudden drop of A_M close to the transition temperature. This drop is well fitted by a power law with a β exponent close to the expected value for the liquid-gas universality class [23], but finite size effects blur the behavior considerably for system sizes comparable to accessible nuclear sizes. However, when no constraints are affecting the fluctuations of the order parameter such as in the grand canonical ensemble, we have shown that the transition is very well defined if instead of the average we look at the most probable value of A_M. Indeed, when crossing a first-order phase transition point, this variable is discontinuous independent of the system size. The important result is that if we look at this variable, finite size effects do not constitute a major problem to identifying a phase transition or to recognizing its order.

On the other hand, important ambiguities arise from the nonequivalence of statistical ensembles inside a phase transition. Indeed, the distribution of the order parameter is strongly deformed by the presence of conservation laws in the system under study. If we look at A_M as an order parameter, the double-hump criterium for a first-order phase transition does not apply any more in the canonical or microcanonical ensemble because of the strong correlation between the conserved total number of particles and the order parameter. The mass conservation constraint induces a maximum in the fluctuation of A_M that is not necessarily correlated with the properties of the phase diagram. We observe maxima both at the critical density close to the critical point and at

subcritical densities inside the coexistence zone. Moreover, the presence of this maximum can simulate a transition from a $\Delta = 1$ to a $\Delta = 1/2$ scaling law in a region above the maximum fluctuation. It is clear that other observables have to be employed if we want to make a conclusion about the order and nature of the phase transition. One such observable is the numerical value of the fluctuation of A_M, which is by construction identical to the fluctuation of the number of particles that do not belong to the largest cluster A_m: if and only if the system crosses the phase coexistence region of a first-order phase transition, then this fluctuation overcomes the corresponding value in the grancanonical ensemble.

APPENDIX: DERIVATION OF EQ. (10)

The density of states is a function of all the relevant extensive variables of the system. For the lattice gas model, this means $W = W(E, A, V)$. If the largest fragment A_M is statistically independent from the other clusters, then

$$W_t(A_M, E_M, V_M, A_m, E_m, V_m) = W_M(A_M, E_M, V_M) \cdot W_m(A_m, E_m, V_m), \quad (14)$$

where we have defined the total number of particles not belonging to the largest fragment as $A_m = A_t - A_M$, and the corresponding energy and volume $E_m = E_t - E_M$, $V_m = V_t - V_M$. Let us first consider the case of an external temperature $T = \beta^{-1}$ and pressure $p = \beta\lambda$. Using the standard definition of the canonical isobar partition sum,

$$Z_{\beta\lambda}(A) = \int dE e^{-\beta E} \int dV e^{-pV} W(E, A, V),$$

the total partition sum can be written as

$$Z_{\beta\lambda}(A_t) = \int dE_t e^{-\beta E_t} \int dV_t e^{-pV_t} \int_0^{E_t} dE_m \int_0^{V_t} dV_m \int_0^{A_t} dA_m \times W_m(E_m, A_m, V_m) W_M(E_t - E_m, A_t - A_m, V_t - V_m),$$

or equivalently

$$Z_\beta(A_t) = \int_0^{A_t} dA_m, Z_\beta^M(A_M) Z_\beta^m(A_t - A_M), \quad (15)$$

where $Z_\beta^i, i = m, M$ describe the contribution of the largest fragment and of all the others, respectively. In the isochore case $V_m + V_M = cte$, the convolution of the partition sum is less straightforward because of the presence of the volume integral

$$Z_\beta(A_t, V_t) = \int_0^{A_t} dA_m \int_0^{V_t} dV_m Z_\beta^M \times (A_M, V_M) Z_\beta^m(A_t - A_M, V_t - V_M). \quad (16)$$

Let us introduce the partial pressures $p_i = \beta^{-1} \frac{\partial \ln Z_\beta^i}{\partial V_i}(A_i^*, V_i^*)$ and chemical potentials $\mu_i = \beta^{-1} \frac{\partial \ln Z_\beta^i}{\partial A_i}(A_i^*, V_i^*)$ at the most probable volume and mass partition A_M^*, V_M^*. Equilibrium between the two components implies $\mu_m = \mu_M$, $p_m = p_M$. A saddle-point approximation then gives

$$\begin{aligned} Z_\beta^M Z_\beta^m \approx \exp(-\beta[A_M^* f_M + A_m^* f_m]) \\ \times \exp\left\{-\beta\left[\frac{1}{2}(A_m - A_m^*)^2\left(\chi_M^{-1} + \chi_m^{-1}\right)\right.\right. \\ \left.\left. + \frac{1}{2}(V_m - V_m^*)^2\left(\kappa_M^{-1} + \kappa_m^{-1}\right)\right]\right\} \\ \times \exp\left\{-\beta\left[\frac{1}{2}(A_m - A_m^*)(V_m - V_m^*)\right.\right. \\ \left.\left. \times\left(\frac{\partial p_M}{\partial A_M} + \frac{\partial p_m}{\partial A_m}\right)\right]\right\}, \end{aligned}$$

where $f_i = -T \ln Z_\beta^i(A_i^*)/A_i^*, i = m, M$ are the most probable free energies per particle, the partial susceptibilities and compressibilities are defined as $\chi_i^{-1} = \frac{\partial \mu_i}{\partial A_i}(A_i^*, V_i^*)$, $\kappa_i^{-1} = \frac{\partial p_i}{\partial V_i}(A_i^*, V_i^*)$, and the conservation constraints make the linear terms vanish. In the dilute limit $V_t = V_m + V_M \approx V_m$ the density variation of the "gas" component m is due to its number variation $d\rho_m = dA_m/V_t$ and the volume variation can be neglected with respect to the number variation $V_m - V_m^* \ll A_m - A_m^*$ giving

$$Z_\beta(A_t, V_t) \approx \int_0^{A_t} dA_m Z_\beta^M(A_M, V_m^*) Z_\beta^{(m)}(A_t - A_M, V_t - V_m^*). \quad (17)$$

Both in the isobar (15) and in the isochore (17) case, the distribution of the largest fragment reads

$$P_{\beta A_t}(A_M) = Z_\beta^{-1} Z_\beta^M(A_M) Z_\beta^m(A_t - A_M). \quad (18)$$

Implementing the saddle-point approximation, we can identify

$$\beta\sigma_{A_M}^2 = \left[\frac{1}{\chi_m(A_t - A_M^*)} - \frac{1}{\chi_M(A_M^*)}\right]^{-1}, \quad (19)$$

where $\sigma_{A_M}^2$ is the fluctuation of the A_M distribution.

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