Phase transition in a statistical model for nuclear multifragmentation

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We use a simplified model which is based on the same physics as inherent in most statistical models for nuclear multifragmentation. The simplified model allows exact calculations for thermodynamic properties of systems of large number of particles. This enables us to study a phase transition in the model. A first order phase transition can be tracked down. There are significant differences between this phase transition and some other well-known cases. [S0556-2813(98)02803-9]

I. INTRODUCTION

Imagine that thermalization is obtained in heavy ion collisions because of two-body collisions. The compound system expands, reaches a volume larger than normal nuclear volume and finally dissociates. This dissociation will carry the signatures of a thermalized system at this expanded volume. This simple picture has been used to describe data obtained in heavy ion collisions many times, sometimes with additional inputs. In the late seventies it was first used to describe composite production in the Bevalac data [1]. At the Bevalac energy the numbers of composites were small and one was content to calculate cross sections of light mass nuclei [2]. As experimental studies of heavy-ion collisions at lower energy progressed such models could be tested in much greater details. This prompted many detailed and elaborate calculations. Today large codes exist which will calculate cross sections of composites. We mention two review articles [3,4] which provide relevant details and additional references.

Another issue that has attracted a great deal of attention is whether or not heavy ion collisions provide a window of opportunity for studying phase transitiions in nuclei. Mean field calculations [5] show that nuclear matter has Van der Waal gas type behavior and thus in the $p-\rho$ plane there would be regions of liquid-gas coexistence. It was conjectured that during disassembly the nucleus could be in the coexistence region [6]. Much of the interest in studying heavy ion collisions rests on the hope that one may discern signatures of liquid-gas phase transition in the data. The recently developed lattice gas model for nuclear disassembly addresses both the issues of fragment distributions (the major achievemnt of standard statistical model alluded above) and liquid-gas phase transition in a unified picture [7].

The purpose of the present work is to investigate the possibility of a phase transition in a simplified version of the statistical model [3]. Given that the model with its many elaborate features is able to reproduce significant details of data it is still an interesting question to ask: does this have much relevance to a phase transition which is one of the issues considered to be of primary interest in heavy ion collisions. This was briefly addressed in a recent paper [8] but we deal with this issue here with more rigor and in far greater detail. Using a technique developed in a recent paper

[9] we are able to get exact results for systems as large as 2000 particles or more. Another interesting feature is that we will be able to study ''percolative properties'' of the standard statistical model. By this we mean the ''second moment'' and the size of the largest cluster, quantities which are of relevance in a percolation model and the study of which is often very revealing [10].

II. THE MODEL AND THE CALCULATIONAL TOOLS

In the simplified model investigated here we can have monomers or composites of k nucleons. The composites have ground state energy $-W_0 k + \sigma(T)k^{2/3}$. The first term is the volume energy, with $W_0 = 16$ MeV. The second term is the surface tension term taken here as in [3] to be temperature dependent: $\sigma(T) = \sigma_0[(T_c^2 - T^2)/(T_c^2 + T^2)]^{5/4}$ with $\sigma_0 = 18$ MeV and $T_c = 18$ MeV. In most of the calculations reported in this paper σ is temperature dependent. However we also have done calculations with σ temperature independent at constant value 18 MeV and although values of specific heat, ''boiling temperature,'' etc. change, no qualitative changes are found. At a finite temperature the composite can be in the ground or one of its excited states. Excited states of composites are taken into account using the Fermi gas model. The internal energy of a composite at temperature T is $-W_0 k + \sigma(T)k^{2/3} + T^2 k/\epsilon_0$ where the last part comes from the population of excited states of the composite. The value of ϵ_0 in the above expression is taken to be 16 MeV. The intrinsic partition function of a composite of k nucleons at temperature T is $\exp(TS-E)/T$ and in the usual Fermi-gas approximation is

$$z_k = \exp[(W_0 k - \sigma k^{2/3} + T^2 k/\epsilon_0)/T]. \qquad (2.1)$$

It is assumed that the freeze-out density is small so that at disassembly different composites do not interact with each other (except through excluded volume effect).

In the grand canonical ensemble, the average number of composite of k nucleons is given by

$$\langle n_k \rangle = e^{\beta \mu k} \omega_k \qquad (2.2)$$

with

$$\omega_k = \frac{V_f}{h^3}(2\pi mT)^{3/2}k^{3/2} \times z_k \qquad (2.3)$$

where for $k > 1$, z_k is given by Eq. (2.1) and $z_1 = 1$. The chemical potential μ is fixed from the condition $\Sigma_{k=1}^{A} k n_k = A$.

Although not crucial for the work done in this paper we want to comment on the volume parameter V_f which appears in Eq. (2.3). We distinguish here between the volume V to which the compound system has expanded and the volume V_f which is the available volume for the composite of k nucleons to move around. For thermodynamics it is V_f rather than V which is to be used. The two volumes are related to each other but are not identical. We assume that composites appear with their normal volume. Thus the volume which a composite of k nucleons occupies is k/ρ_0 where $\rho_0 = 0.16$ fm^{-3}. It then follows that if the total number of nucleons fragmenting is A, the excluded volume V_{ex} is A/ρ_0 and we take the available volume for thermalization to be $V_f = V - V_{ex}$. We show most of the calculations for $\rho = A/V = 0.05$ fm^{-3}. This means calculations are done with $\tilde{\rho} = A/V_f = \rho/(1 - \rho/0.16) = 0.0727$ fm^{-3}.

We wrote down the average number of particles according to the grand canonical ensemble. We will however mostly use the canonical ensemble using a technique developed in [9]. The canonical partition function Z_A for A particles is given by [11]

$$Z_A = \sum \prod_{k \geq 1} \frac{\omega_k^{n_k}}{n_k!} \quad (2.4)$$

where n_k is the number of composites which has k nucleons and the sum above goes over all the partitions which satisfy $\Sigma k n_k = A$. The probability that a given admissible partition $P(\vec{n}) = P(n_1, n_2, n_3 \ldots)$ is obtained is given by

$$P(\vec{n}) = \frac{1}{Z_A} \prod \frac{\omega_k^{n_k}}{n_k!}. \quad (2.5)$$

The partition function Z_A can be built by recursion relation. Starting with $Z_0 = 1$ one can build all higher ones using

$$Z_p = \frac{1}{p} \sum_{k=1}^{p} k \omega_k Z_{p-k}. \quad (2.6)$$

Thus one has $Z_1 = \omega_1$, $Z_2 = \frac{1}{2}\omega_1^2 + \omega_2$, and $Z_3 = \frac{1}{6}\omega_1^3 + \omega_2\omega_1 + \omega_3$ and so on. The average value of composite number in the canonical ensemble is readily obtained [this is to be compared with Eq. (2.2) of the grand canonical ensemble]. We have $\langle n_k \rangle = \Sigma P(\vec{n}) \times n_k = (1/Z_A)\Sigma\Pi(\omega_i^{n_i}/n_i!)n_k$ which leads to $\langle n_k \rangle = \omega_k(Z_{A-k}/Z_A)$. These results apply to any choice of ω_k but in this paper we will focus only on the choice of Eq. (2.3). We like to emphasize that here the calculations in the canonical ensemble are done without any Monte-Carlo sampling to obtain various quantities of interest.

In the canonical ensemble it is straightforward to isolate the largest cluster for each "event." Calculations in which a "tag" is kept on the largest cluster proved to be of significance in percolation model analysis of data. It is possible for us to calculate $\langle k_{max} \rangle$, the average size of the largest cluster. This should be scaled by the size of the system thus we

compute $\langle k_{max} \rangle/A$. This turns out to be a very interesting quantity even in the statistical model. Campi defined reduced moments as moments in which the largest cluster is excluded. Thus the second moment is $M_2 = \Sigma_k k^2 n_k - k_{max}^2$. To compute expectation values in which the largest cluster is fixed we need to compute the partition function of such ensembles. Clearly this partition function is given by all the terms in the partition function which have $\omega_{k_{max}}$ as the highest ω_k in the term. Consider

$$\Delta Z_A(k_{max}) \equiv Z_A(\omega_1, \ldots, \omega_{k_{max}}, 0, 0, \ldots)$$
$$- Z_A(\omega_1, \ldots, \omega_{k_{max-1}}, 0, 0, \ldots). \quad (2.7)$$

We see that ΔZ_A is the partition function for ensembles with fixed maximum cluster size k_{max}, since the first term collects all terms with $\omega_{k_{max}}$ or lower, and the second term eliminates those terms which do not have an $\omega_{k_{max}}$. From this we can determine $Pr(k_{max})$, the probability of obtaining a distribution whose largest cluster is k_{max} [9],

$$Pr(k_{max}) = \frac{\Delta Z_A(k_{max})}{Z_A(\omega_1, \ldots, \omega_A)}. \quad (2.8)$$

It is now straightforward to compute $\langle k_{max} \rangle$ or the reduced moments.

Before we leave this section we would like to comment on two of the possible shortcomings of the model. One is the assumption that different composites at the time of dissociation are on the average far enough that they do not interact with each other. The only effect that can be easily taken into account is through the excluded volume effect but the simple correction that we have alluded to above is really very approximate and certainly not rigorous. Trying to take interactions between different composites would change all the equations for the partition function. We cannot correct this by simply deciding to take an arbitrarily large freeze-out volume so that interactions between different composites are indeed negligible because the major part of the physics will have been already decided and that may pertain to a smaller volume. In some sense, the lattice gas model [7] does a better job of interactions between different composites. The other approximation is in the assumption that the internal partition function is given by Eq. (2.1). That equation uses expressions for excitation energy and entropy per particle which is valid only in the infinite noninteracting nuclear matter limit. Thus there will be prefactor before the exponential in Eq. (2.1) which may completely mask the $k^{3/2}$ factor in Eq. (2.3). Other choices for the k dependence have been considered [12].

III. THE FREE ENERGY, THE LARGEST CLUSTER, AND THE SPECIFIC HEAT

The free energy of a system of A particles is given by $F = -T \ln Z_A$. The canonical partition function is directly calculated by the recurrence method of Eq. (2.6) and thus the free energy is readily available. For a system of 2800 and 1400 particles this is shown in Fig. 1 as a function of temperature. The figure suggests that there is break in the first derivative in F which occurs at about 7.3 MeV for 2800
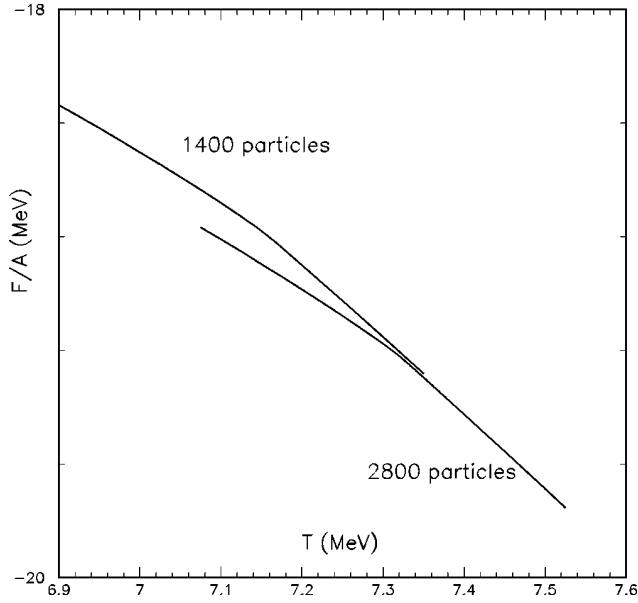
FIG. 1. The free energy per particle for (a) a system of 2800 particles and (b) a system of 1400 particles plotted as a function of temperature. The curves suggest that a break in the first derivative occurs at 7.3 MeV and at 7.15 MeV, respectively.

particles and at 7.15 MeV for 1400 particles. This means there is a first order transition here. There will be a sudden jump in entropy accompanied by an infinite specific heat at the ''boiling temperature.'' Of course although 2800 is a large number it is not the thermodynamic limit thus the specific heat would be large and proportional to A but not infinite. The behavior of the specific heat as the system size grows is shown in Fig. 2. Notice the peak becomes progres-
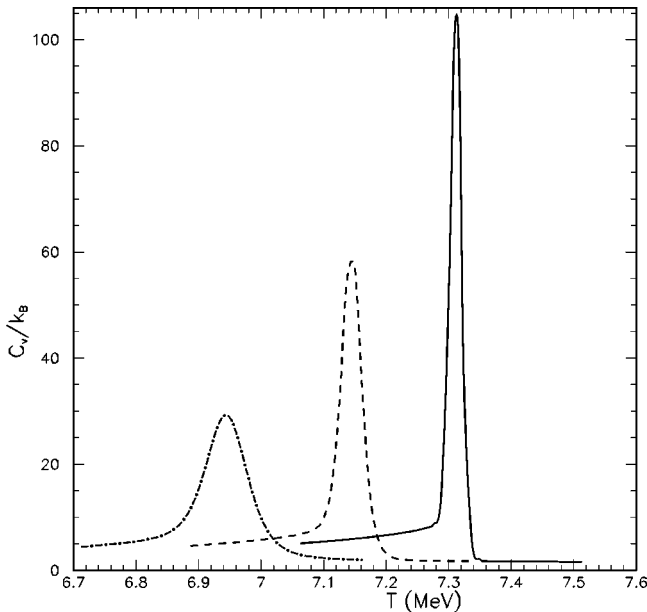

FIG. 2. Curves for C_v for 700 (dash-dot), 1400 (dash), and 2800 (solid) particles as a function of temperature. The maxima occur at 6.95 MeV, 7.15 MeV, and 7.3 MeV and coincide with what visually appear to be near breaks in the first derivatives of free energy. Notice that as the particle numbers increase, the heights of the peaks increase and the widths narrow.
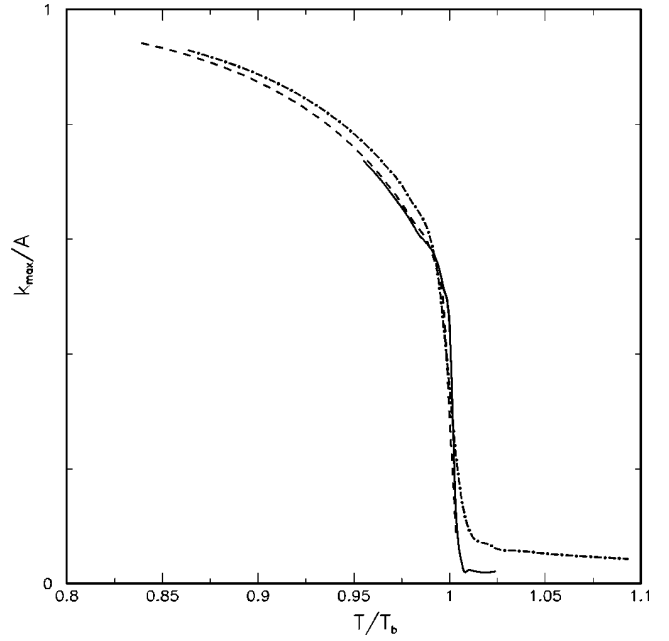

FIG. 3. Curves for $\langle k_{max} \rangle / A$ as a function of the scaled variable T/T_b where boiling temperature T_b is the temperature at which C_v is maximum. The cases shown are for 700 particles (dash-dot), 1400 particles (dash), and 2000 particles (solid line). The boiling temperatures in the respective cases are 6.97 MeV, 7.15 MeV, and 7.225 MeV. Notice that the steepness of fall increases as the particle number increases. This sudden fall begins at about 0.5 for $\langle k_{max} \rangle / A$.

sively high and narrow as the system grows larger. This huge jump in specific heat at the ''boiling point'' is readily understood if we consider the behavior of $\langle k_{max} \rangle / A$ for various size systems as function of temperature. Starting from a value higher than 0.5 it quickly drops to much lower value as the ''boiling point'' is traversed. This drop becomes progressively sharper as the system size grows. Calculations with finite systems (Fig. 3) suggest that for infinite systems $\langle k_{max} \rangle / A$ will drop from about 0.5 to at least very close to zero at the boiling point. It is the sudden disappearance of the large blob at the ''boiling point'' that is responsible for the specific heat going to infinity.

IV. ABSENCE OF A POWER LAW, EFFECTIVE τ, AND THE SECOND MOMENT

In a percolation model a power law emerges near the critical point. The yields $Y(A)$ of the composites obey $Y(A) \propto A^{-\tau}$. In the lattice gas model there is a continuous line in $\rho - T$ plane where such a power law emerges. See Ref. [8] for the prescription how the yields $Y(A)$ are calculated in the lattice gas model. The interested reader will also find in the same reference the well-known prescription of calculating $Y(A)$ in the bond percolation model. Although the power law is expected to emerge only in the neighborhood of percolation point an effective τ can always be deduced from the data using [13]

$$\frac{\Sigma_{n1}^{n2} A Y(A)}{\Sigma_{n1}^{n2} Y(A)} = \frac{\Sigma_{n1}^{n2} A A^{-\tau}}{\Sigma_{n1}^{n2} A^{-\tau}}. \tag{4.1}$$
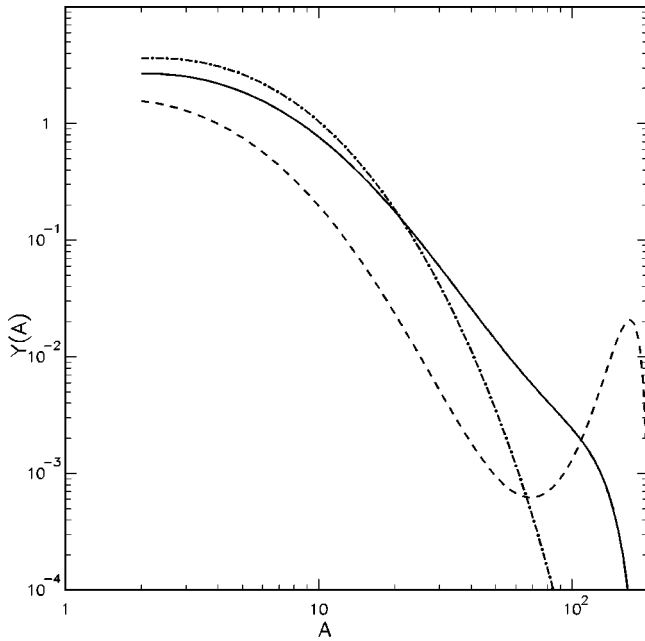
FIG. 4. Curves for yields $Y(A)$ against A at various temperatures. The disassembling system chosen has 200 particles. The temperatures chosen are 6.2 MeV (dash), 6.7 MeV (solid) (at this temperature the effective τ is lowest), and 7.2 MeV (dash-dot).

We have taken $n1 = 5$ and $n2 = 30$ which is similar to values used in other analyses. In the model pursued here we do not find the emergence of a power law. This is not just because we are using a finite number of particles. One sees a much clearer emergence of a power law in the lattice gas model even with smaller particle number than what is considered here. An example of yields $Y(A)$ in the model is demonstrated in Fig. 4. In spite of a lack of a power law below, at or above the boiling temperature deducing an effective τ using formula (4.1) is useful. As the temperature changes the value of the effective τ will go through a minimum as shown in Fig. 5. The minimum value depends upon the freeze-out density $\tilde{\rho}$ used for the calculation. For the case shown in Figs. 4 and 5 the value of the $\tau_{\min}$ was 1.84 but a lower value is found if a larger value of the freeze-out density is used; correspondingly a larger value is obtained if a lower freeze-out density is used. We also recall when a true power law emerges at a critical point the value of τ is restricted to be between 2 and 3 [14]. There is no such restriction here because there is no power law.

We now consider the second moment M_2. This will go through a maximum as the temperature changes. The maximum of M_2 and the minimum of τ_{eff} are very close to each other and they both occur close to the maximum of C_v (Fig. 5). Since experimentally a measurement of C_v is rather hard (see however [15]) it is easier to locate approximately the "boiling point" by the minimum of τ_{eff} or the maximum of M_2. The value of M_2 does not grow with particle number but saturates around 11.6.

V. BOILING POINT FOR INFINITE MATTER

We return to Figs. 1 and 2. While the figures clearly show evidence of the occurence of a first-order transition and the ever increasing values of the specific heat it is difficult from
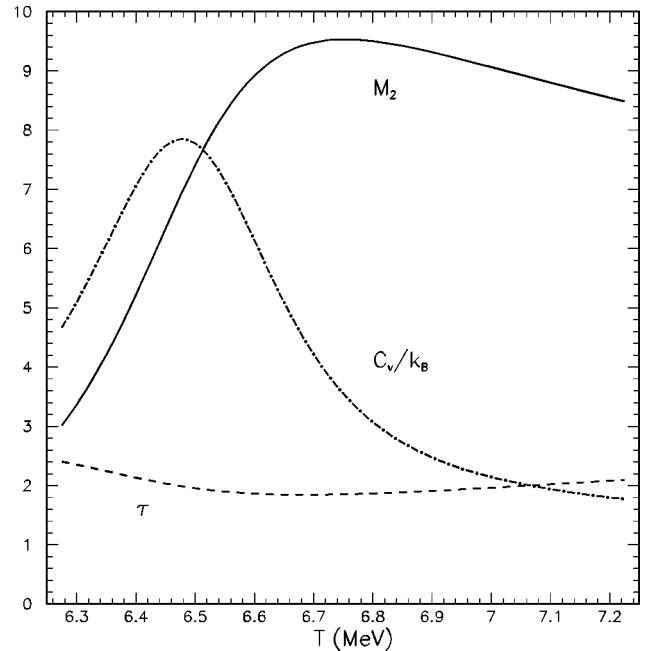

FIG. 5. For a system of 200 particles curves for effective τ, specific heat, and the second moment as a function of temperature. Notice that the minimum of τ and the maximum of M_2 are close to the maximum of C_v.

these figures to determine the value of the boiling point in the infinite matter limit. This limit is more easily obtained from the grand canonical ensemble and using the knowledge gained from Fig. 3 that as one crosses the "boiling point" a large blob of the size $\approx A/2$ suddenly disappears. Equations (2.1), (2.2), and (2.3) are combined to give

$$\langle n_k \rangle = \frac{V_f}{h^3}(2\pi m T)^{3/2} k^{3/2} e^{\beta(\mu k + W_0 k + T^2 k/\epsilon_0 - \sigma(T)k^{2/3})}$$

(5.1)

for $k > 1$ and $\langle n_1 \rangle = e^{\beta\mu}(V_f/h^3)(2\pi m T)^{3/2}$. In the infinite limit the term proportional to k in the exponent must disappear at the "boiling point." Hence we should have

$$1 = \frac{1}{\tilde{\rho}h^3}(2\pi m T)^{3/2}\left[e^{\beta\mu} + \sum_{2}^{\infty} k^{5/2} e^{-\beta\sigma(T)k^{2/3}}\right] \quad (5.2)$$

where $\mu = -W_0 - T^2/\epsilon_0$. This gives for $\tilde{\rho} = 0.07273$ the boiling temperature is 8.187 MeV. The boiling temperature increases with increasing freeze-out density in this model.

There is at least one [15] published work on experimental extraction of the caloric curve. This curve suggests that a peak in C_v is seen around 5 MeV for some finite nuclei. On the theory side the percolation model has often been applied but there is no C_v in percolation model since there is no Hamiltonian. The phase transition in that model is a continuous transition and rather different from the first order transition considered here. However Ref. [8] shows that the percolation model is one limit of the lattice gas model which does have a Hamiltonian and which has several features which can be compared with the model investigated here. More of this comparison appears in our next section, however, in the lattice gas model also one predicts that the one

will likely see a first order transition [16] and in that respect it is similar to the prediction here.

VI. SUMMARY AND DISCUSSION

We have taken a basic statistical model for nuclear multifragmentation and have searched and found a first-order phase transition in the model. This phase transition is quite distinct. Here the C_v goes to infinity at the ''boiling point'' and the second moment M_2 reaches a maximum which is finite in the thermodynamic limit. This is to be contrasted with first order transition in the lattice gas model. In that model the second moment goes to infinity but C_v merely goes through a discontinuous jump. Insofar as the lattice gas model (which can be mapped onto an Ising model) is a more standard description of liquid-gas phase transition, this particular model considered here is quite distinct. One hallmark of this distinctiveness comes from the sudden disappearance of $\langle k_{max}\rangle/A$ which jumps from about 0.5 to nearly, if not exactly, zero as the boiling temperature is traversed. If we identify the large cluster as a liquid then we have to say, looking at Fig. 3, that we can have a mixed phase in which half or more of the total number of particles are in a liquid phase and the rest in gaseous phase; or, we can have all the particles in a gas phase but we cannot, for example, have one-third of the particles in the liquid phase and the rest in the gaseous phase. One has to remind oneself that interactions in the model are treated in a rather undemocratic fashion. Interactions within particles in a composite are treated (witness the appearance of binding energy, surface terms, and excited states of the composite) but interactions between composites are treated less stringently. This would make the model quite unrealistic for high values of freeze-out density but of course the model is designed for low freeze-out densities.

We find it satisfying that the maximum of M_2 and the minimum of τ_{eff} appear at a temperature close to that of the maximum of C_v. Since the measurement of C_v is hard this means one may still locate approximately the ''boiling temperature'' by indirect means. This remains true in the lattice gas model in spite of rather different character of the phase transition there. Thus this seems to be a characteristic shared by many models.

ACKNOWLEDGMENTS

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